



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 02:58 PM EDT

PDB ID : 8UOT / pdb_00008uot
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:

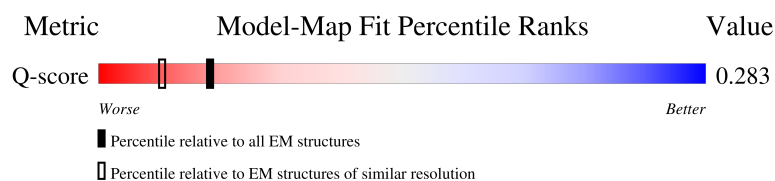
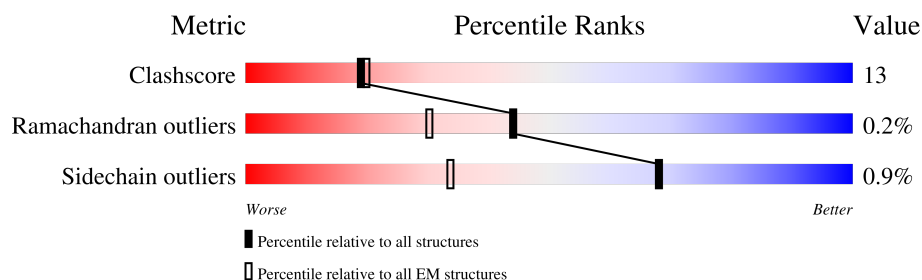
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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.



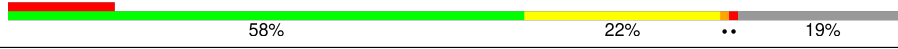
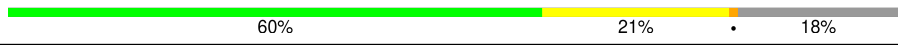
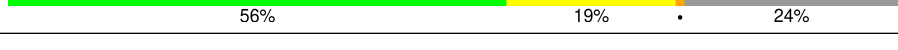
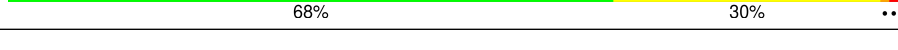
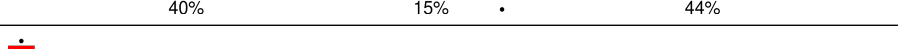
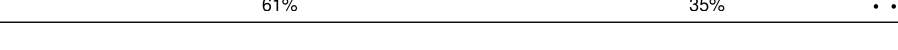
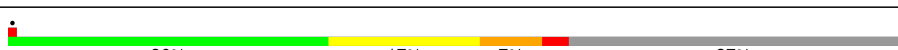
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	0	778	 62% 34% .
2	1	642	 51% 14% 35%
3	2	513	 8% 59% 27% . 13%
4	4	338	 65% 22% 14%

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Mol	Chain	Length	Quality of chain
5	6	461	
6	7	843	
7	M	345	
8	A	1733	
9	B	1224	
10	C	318	
11	D	221	
12	E	215	
13	F	155	
14	G	171	
15	H	146	
16	I	122	
17	J	70	
18	K	120	
19	L	70	
20	Q	735	
21	P	400	
22	S	309	
23	O	240	
24	U	286	
25	V	122	
26	W	482	
27	X	328	
28	5	72	
29	N	64	

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Mol	Chain	Length	Quality of chain
30	T	64	 62% 36%

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 IIIH 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 IIIH 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 IIIH 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 IIIH 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 IIIH 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 IIIH 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		

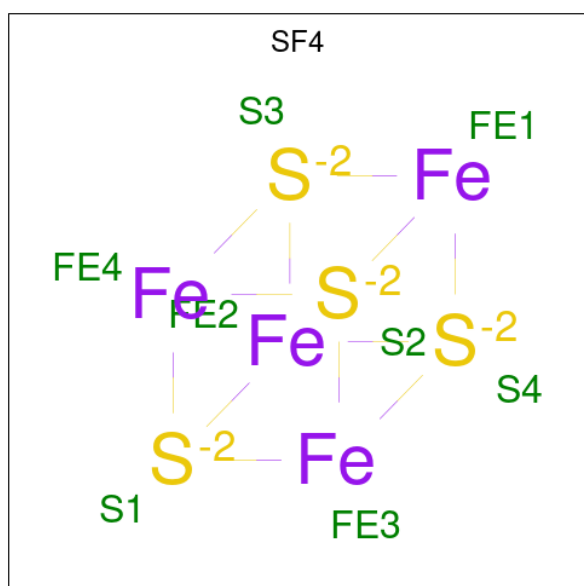
- Molecule 29 is a DNA chain called non-template DNA strand.

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 (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

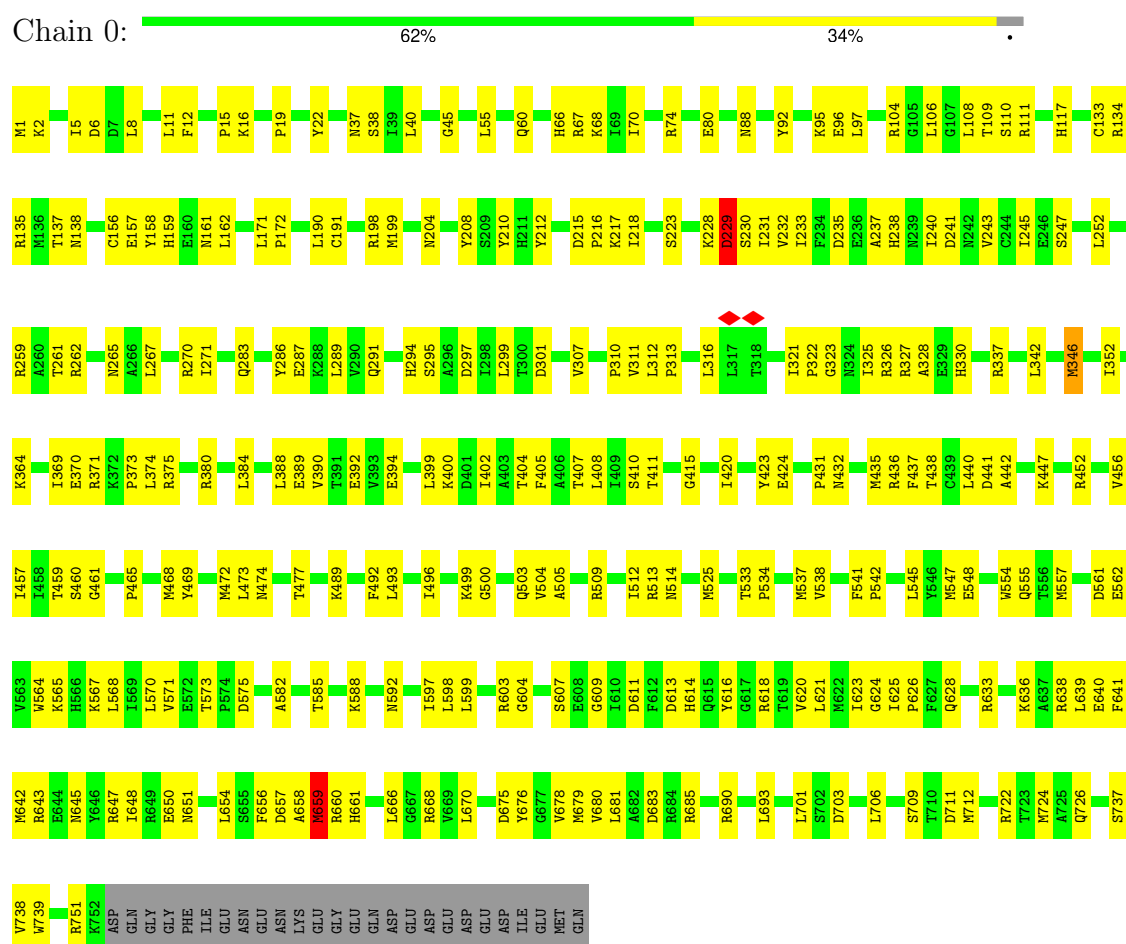
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

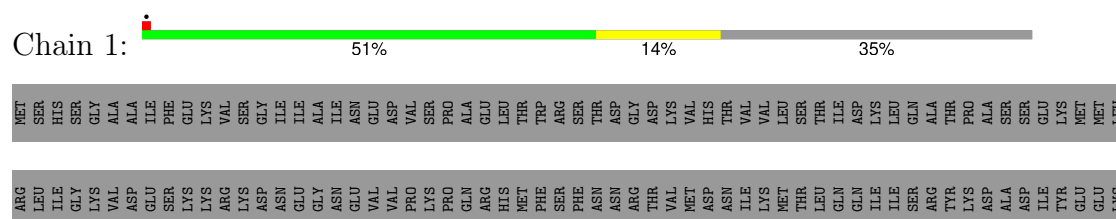
3 Residue-property plots

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.

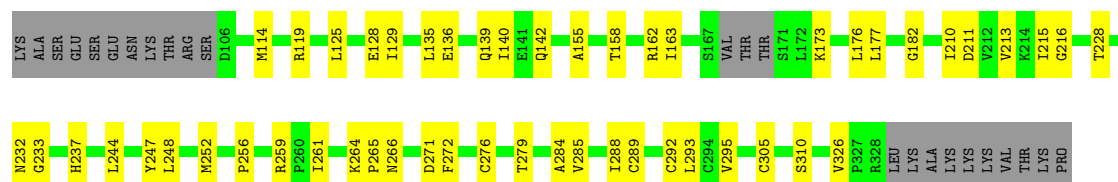
- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3



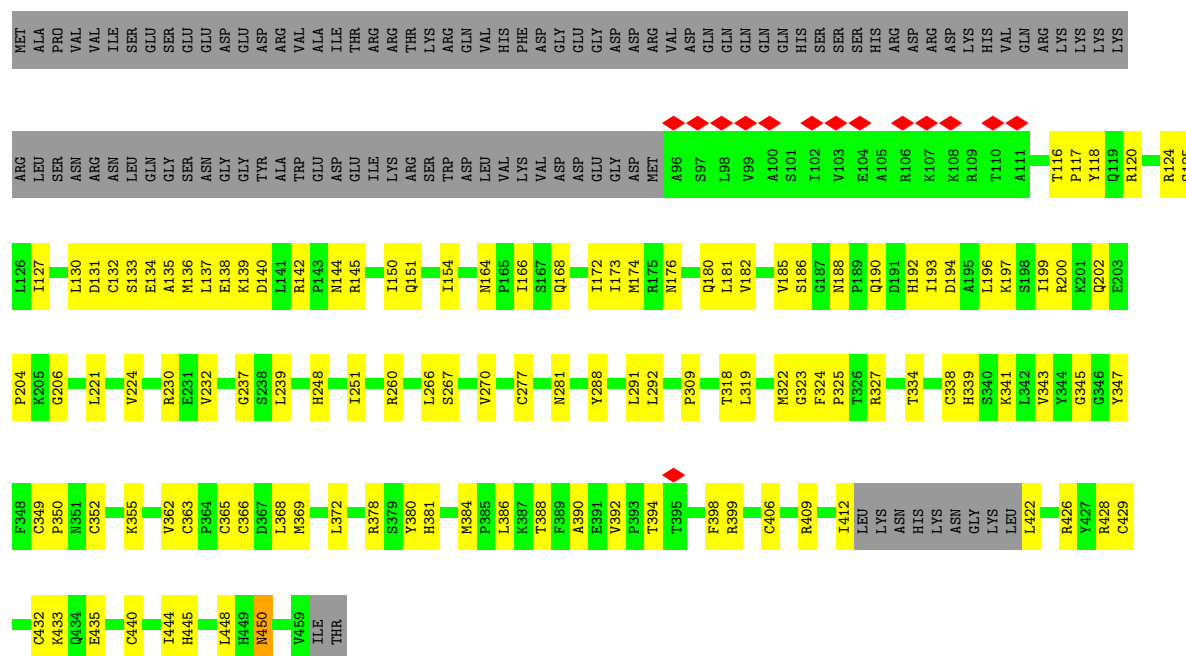
- Molecule 2: General transcription and DNA repair factor IIH subunit TFB1



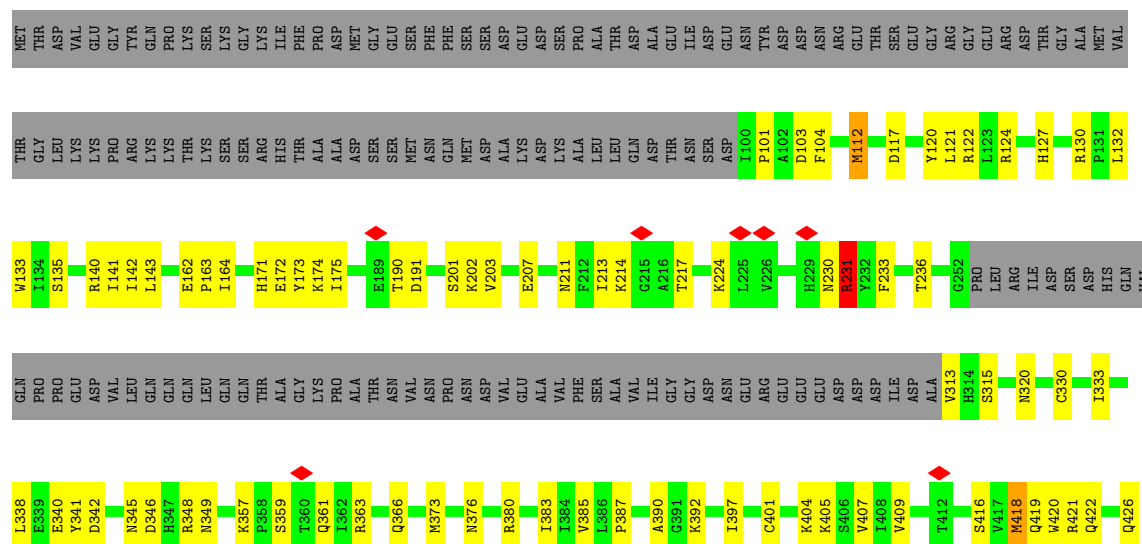


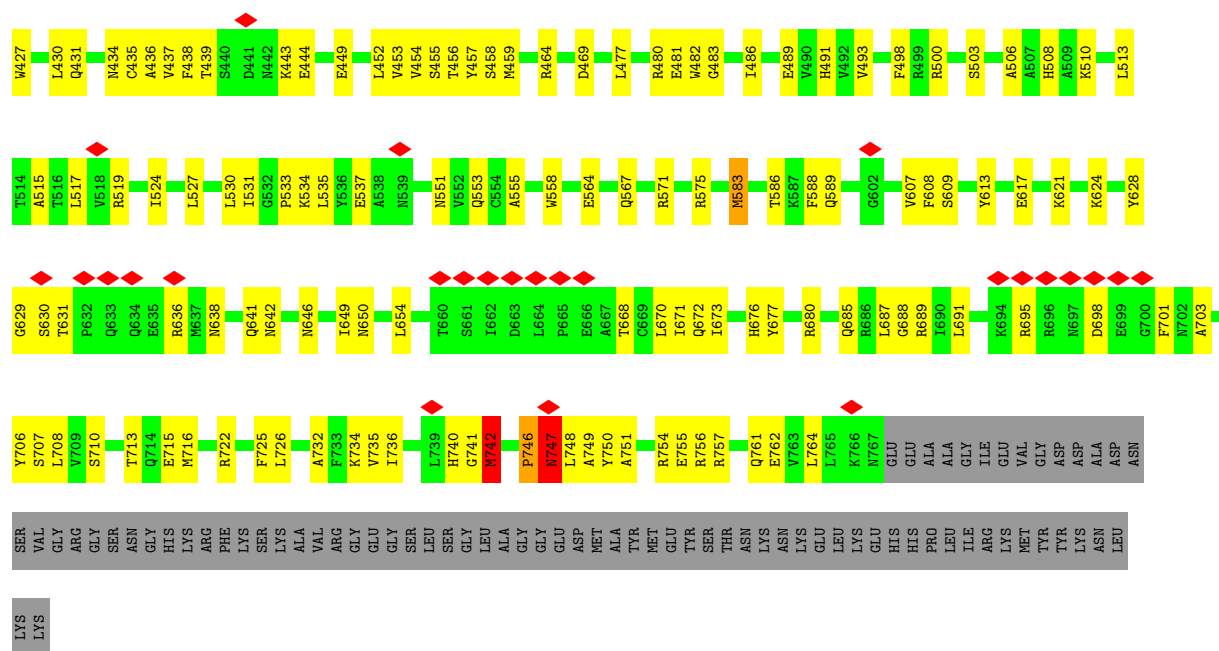


- Molecule 5: General transcription and DNA repair factor IIH subunit SSL1

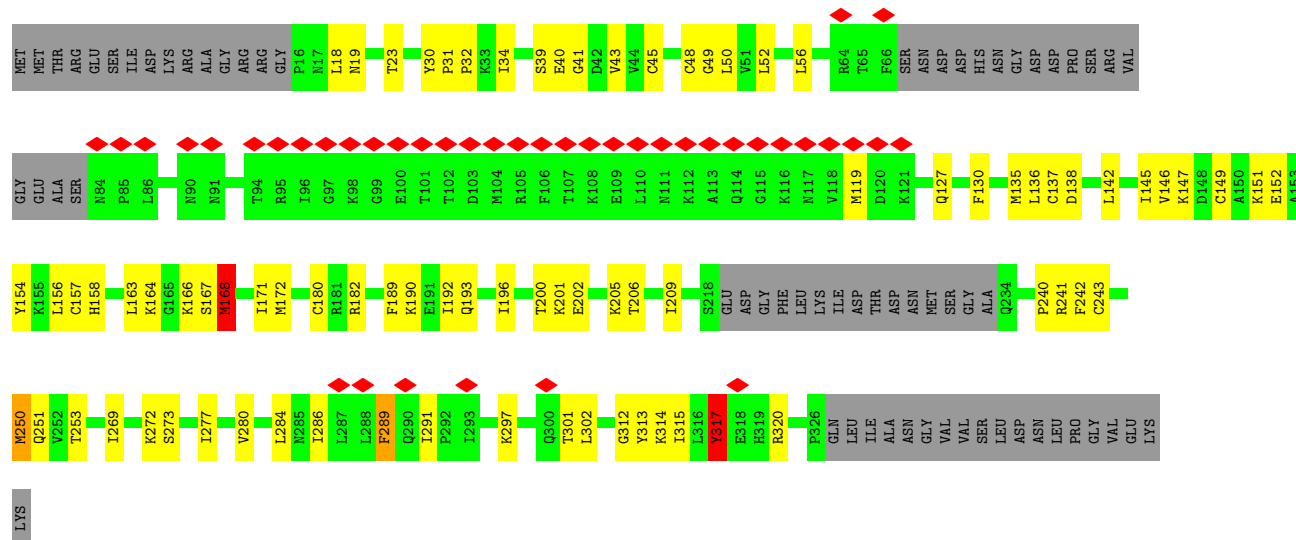


- Molecule 6: General transcription and DNA repair factor IIH helicase subunit XPB

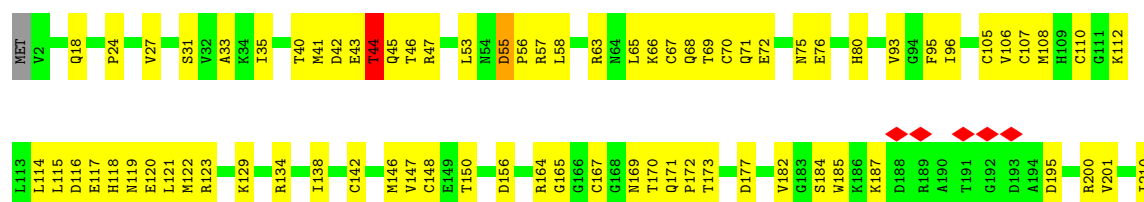


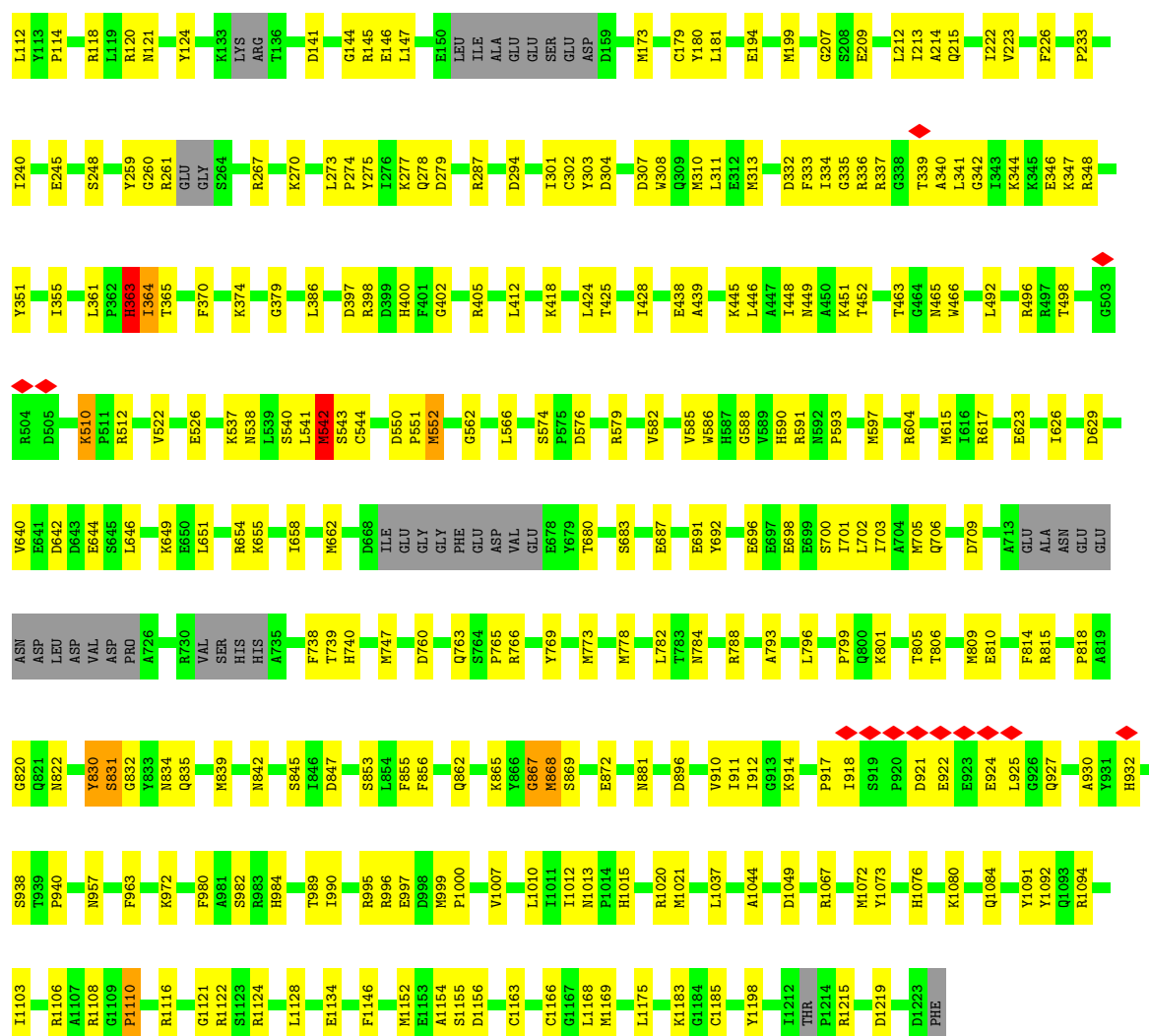


• Molecule 7: Transcription initiation factor IIB

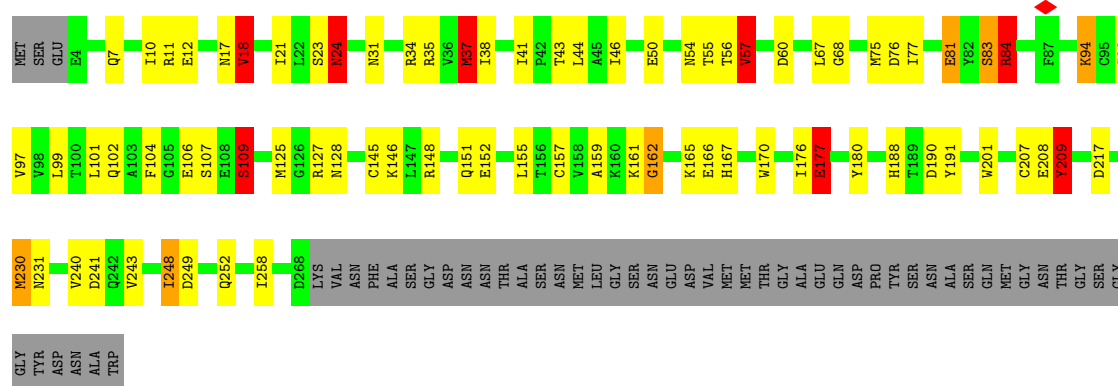


• Molecule 8: DNA-directed RNA polymerase II subunit RPB1





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

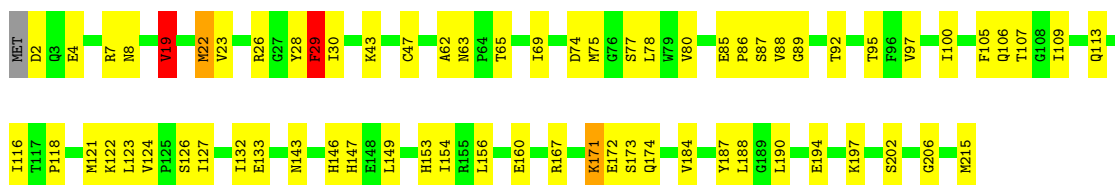


- Molecule 11: DNA-directed RNA polymerase II subunit RPB4

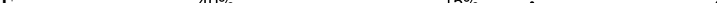


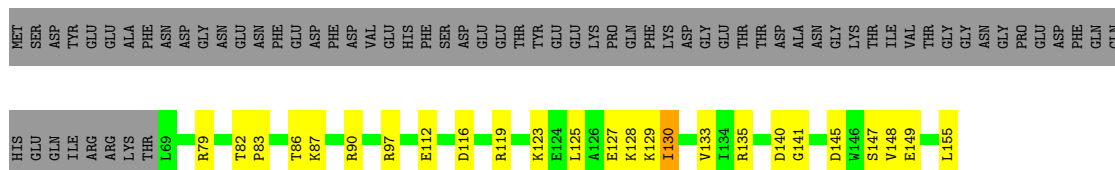
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 68% 30%

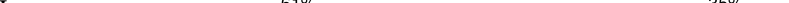


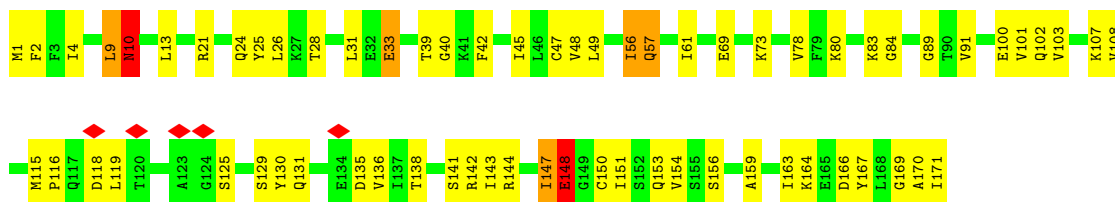
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  40% 15% • 44%



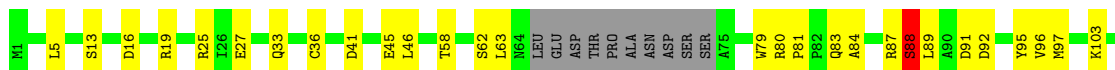
- Molecule 14: DNA-directed RNA polymerase II subunit RPB7

Chain G:  61% 35%



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

Chain H: 63% 28% 8%





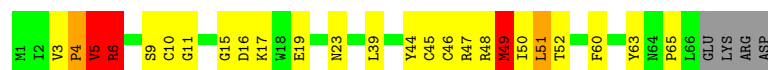
- Molecule 16: DNA-directed RNA polymerase II subunit RPB9

Chain I:



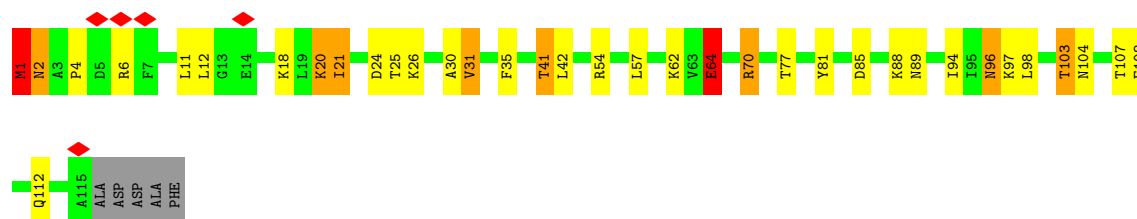
- Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



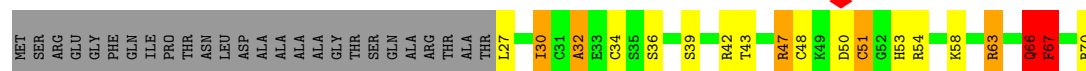
- Molecule 18: DNA-directed RNA polymerase II subunit RPB11

Chain K:



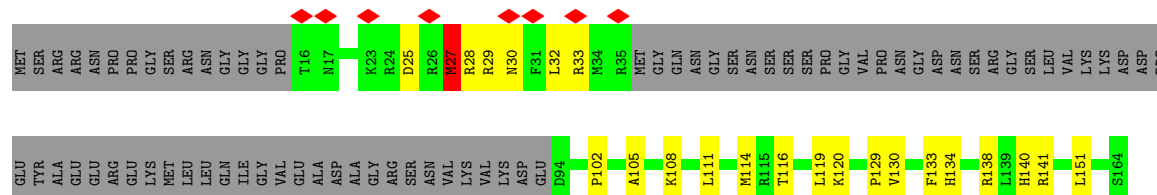
- Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC4

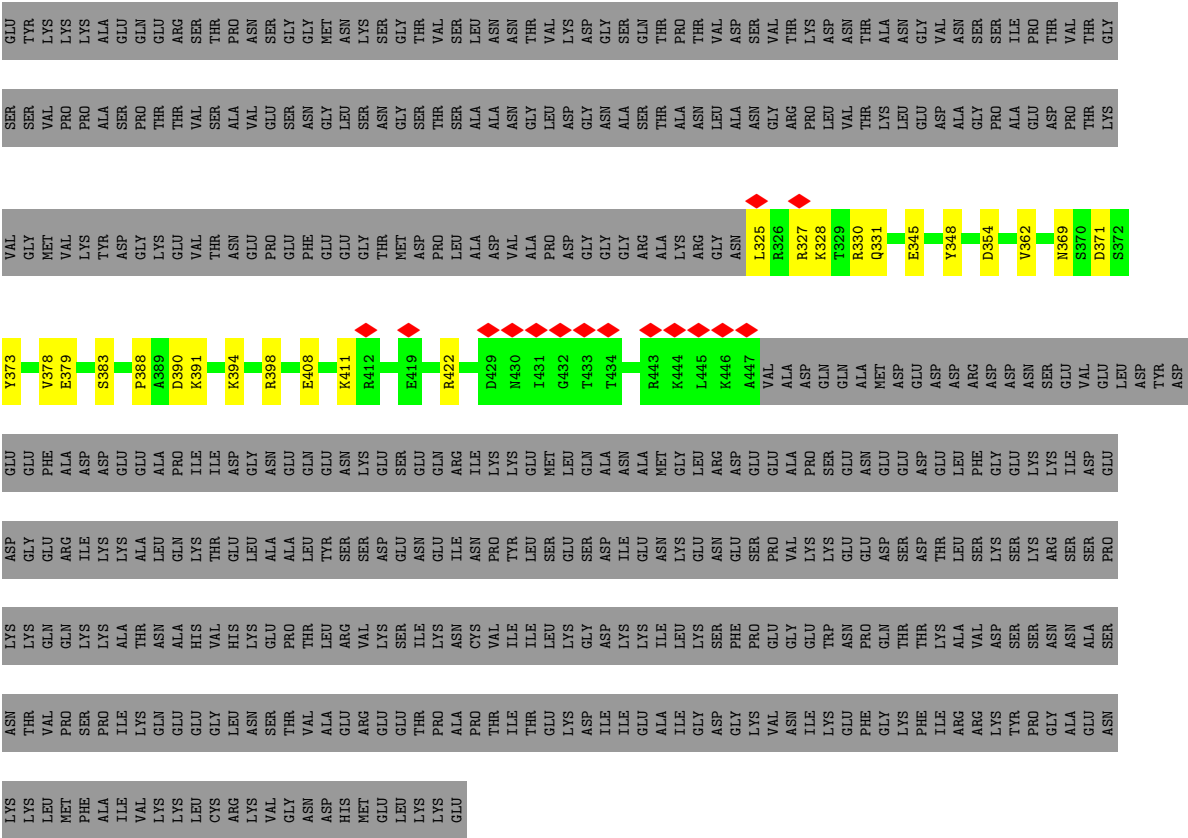
Chain L:



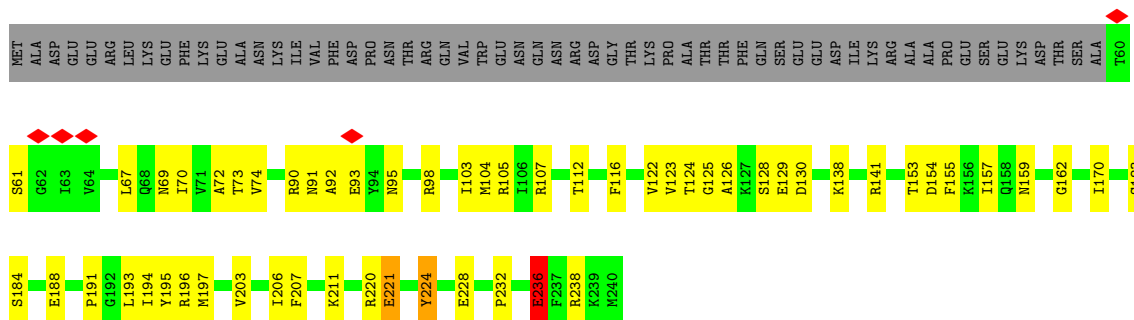
- Molecule 20: Transcription initiation factor IIF subunit alpha

Chain Q:

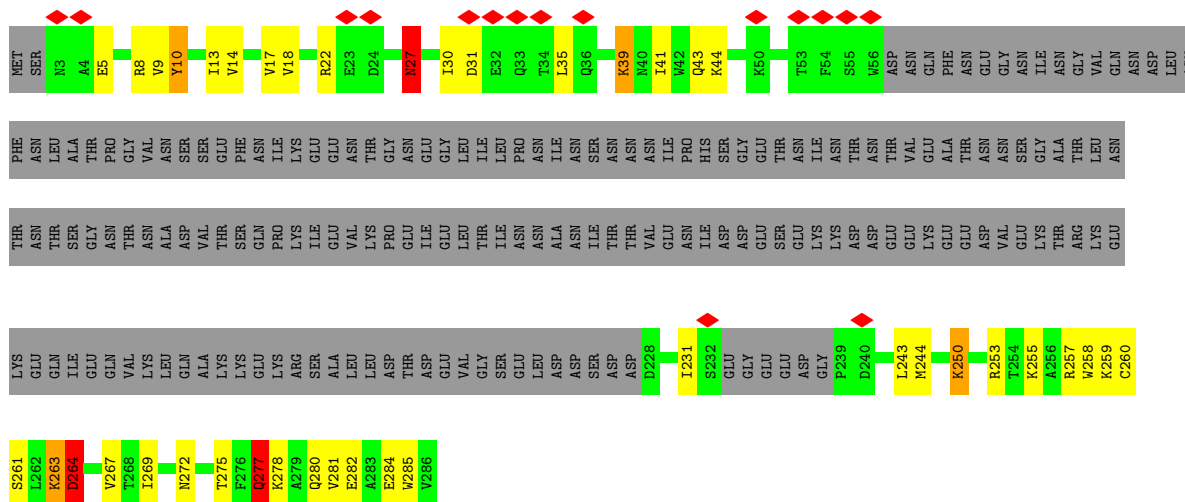




- Molecule 23: TATA-box-binding protein



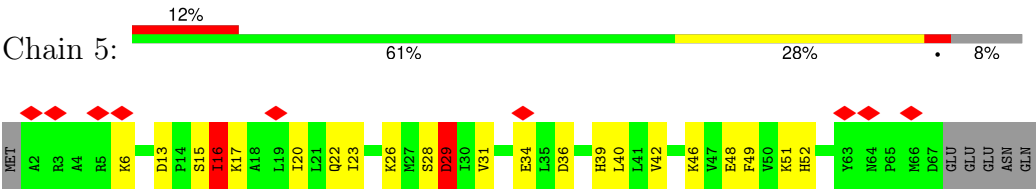
- Molecule 24: Transcription initiation factor IIA large subunit



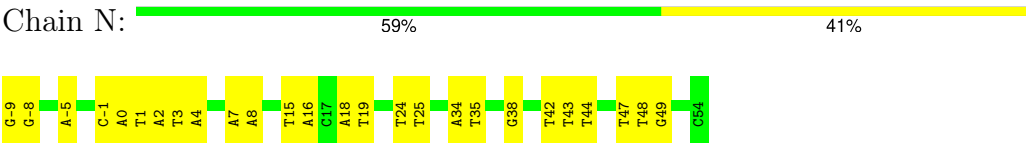
- Molecule 25: Transcription initiation factor IIA subunit 2

LEU
LYS
ASP
TYR
SER
HIS
ARG
VAL

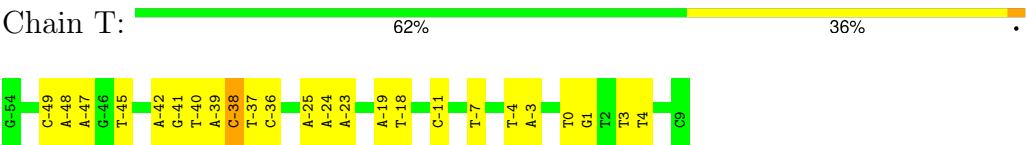
- Molecule 28: General transcription and DNA repair factor IIH subunit TFB5



- Molecule 29: non-template DNA strand



- Molecule 30: template DNA strand



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.66	19/6209 (0.3%)	0.92	18/8384 (0.2%)
2	1	0.55	6/3434 (0.2%)	0.72	9/4624 (0.2%)
3	2	0.85	21/3611 (0.6%)	1.10	26/4881 (0.5%)
4	4	0.28	0/2305	0.47	0/3117
5	6	0.65	4/2843 (0.1%)	1.28	8/3845 (0.2%)
6	7	0.68	18/4992 (0.4%)	0.86	25/6754 (0.4%)
7	M	0.86	8/2204 (0.4%)	1.29	13/2963 (0.4%)
8	A	0.79	32/11368 (0.3%)	1.00	62/15383 (0.4%)
9	B	0.77	15/9402 (0.2%)	0.95	35/12680 (0.3%)
10	C	1.43	35/2124 (1.6%)	1.83	60/2879 (2.1%)
11	D	0.33	0/1339	0.71	5/1793 (0.3%)
12	E	1.25	16/1788 (0.9%)	1.81	22/2406 (0.9%)
13	F	0.63	0/717	0.83	1/967 (0.1%)
14	G	0.72	6/1363 (0.4%)	1.24	17/1840 (0.9%)
15	H	0.92	6/1097 (0.5%)	1.28	11/1484 (0.7%)
16	I	0.96	9/945 (1.0%)	1.44	22/1273 (1.7%)
17	J	1.77	16/549 (2.9%)	1.97	24/738 (3.3%)
18	K	2.06	32/942 (3.4%)	2.56	49/1272 (3.9%)
19	L	2.73	15/354 (4.2%)	3.56	24/468 (5.1%)
20	Q	0.34	1/1648 (0.1%)	0.62	3/2226 (0.1%)
21	P	0.29	0/1511	0.52	0/2035
22	S	0.78	5/1317 (0.4%)	1.05	7/1778 (0.4%)
23	O	1.06	14/1449 (1.0%)	1.84	20/1952 (1.0%)
24	U	1.07	12/898 (1.3%)	1.94	25/1212 (2.1%)
25	V	1.15	6/822 (0.7%)	1.85	16/1109 (1.4%)
26	W	0.71	9/2045 (0.4%)	1.24	14/2757 (0.5%)
27	X	0.68	4/1312 (0.3%)	1.20	7/1767 (0.4%)
28	5	1.27	6/502 (1.2%)	1.66	12/677 (1.8%)
29	N	0.53	0/1464	0.71	0/2258
30	T	0.56	1/1475 (0.1%)	0.62	0/2274
All	All	0.84	316/72029 (0.4%)	1.16	535/97796 (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 (316) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	317	TYR	CG-CD2	24.83	1.91	1.39
18	K	64	GLU	CD-OE2	23.99	1.71	1.25
23	O	224	TYR	CG-CD2	22.33	1.86	1.39
12	E	29	PHE	CA-C	22.31	1.82	1.52
19	L	67	PHE	CB-CG	-20.25	1.04	1.50
19	L	67	PHE	CG-CD2	20.15	1.81	1.38
19	L	47	ARG	CD-NE	-20.01	1.18	1.46
6	7	747	ASN	CA-C	19.91	1.76	1.52
25	V	82	ASN	CG-ND2	19.49	1.74	1.33
18	K	1	MET	C-N	19.03	1.60	1.33
10	C	84	ARG	NE-CZ	-18.55	1.12	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	659	MET	SD-CE	-18.53	1.33	1.79
26	W	34	PHE	CG-CD2	18.20	1.77	1.38
19	L	47	ARG	CB-CG	-17.59	0.99	1.52
5	6	450	ASN	CG-ND2	16.70	1.68	1.33
9	B	194	GLU	CD-OE2	16.38	1.56	1.25
27	X	216	GLN	CD-NE2	16.37	1.67	1.33
22	S	232	ASP	CA-C	16.26	1.77	1.52
7	M	317	TYR	CG-CD1	-16.06	1.05	1.39
2	1	608	MET	CA-C	16.05	1.70	1.52
1	0	659	MET	CG-SD	-16.05	1.40	1.80
18	K	1	MET	CA-C	15.85	1.86	1.52
18	K	2	ASN	CA-C	15.85	1.74	1.52
12	E	22	MET	SD-CE	-15.75	1.40	1.79
19	L	63	ARG	CD-NE	-15.75	1.24	1.46
10	C	37	MET	CA-C	15.62	1.74	1.52
3	2	150	MET	CG-SD	-15.57	1.41	1.80
25	V	38	MET	CA-CB	-15.48	1.29	1.53
5	6	202	GLN	CD-NE2	15.35	1.65	1.33
9	B	662	MET	CB-CG	-15.32	1.06	1.52
6	7	418	MET	CA-C	15.13	1.72	1.53
2	1	358	MET	CA-C	15.09	1.72	1.52
8	A	1188	GLN	CD-NE2	15.08	1.65	1.33
10	C	24	ASN	CA-C	15.05	1.73	1.52
8	A	1188	GLN	CD-OE1	-15.05	0.94	1.23
1	0	547	MET	CB-CG	-15.03	1.07	1.52
9	B	542	MET	SD-CE	-14.90	1.42	1.79
8	A	1267	MET	CG-SD	-14.84	1.43	1.80
12	E	29	PHE	CG-CD2	14.59	1.69	1.38
3	2	487	LYS	CA-C	14.05	1.72	1.52
3	2	463	GLU	C-N	13.57	1.53	1.33
6	7	231	ARG	CG-CD	-13.43	1.12	1.52
18	K	1	MET	N-CA	-13.39	1.20	1.46
10	C	209	TYR	CG-CD2	13.35	1.67	1.39
18	K	64	GLU	CD-OE1	-13.32	1.00	1.25
8	A	1202	MET	CB-CG	-13.25	1.12	1.52
8	A	837	ILE	CA-C	13.13	1.70	1.53
28	5	16	ILE	CA-C	13.10	1.72	1.52
12	E	29	PHE	N-CA	-13.05	1.29	1.46
5	6	202	GLN	CD-OE1	-13.03	0.98	1.23
15	H	146	ARG	CG-CD	-13.01	1.13	1.52
18	K	21	ILE	CA-C	12.86	1.64	1.53
22	S	231	CYS	C-N	12.81	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	97	MET	SD-CE	-12.68	1.47	1.79
9	B	552	MET	CA-C	12.66	1.68	1.52
3	2	81	MET	CA-CB	12.44	1.72	1.53
17	J	6	ARG	CB-CG	-12.44	1.15	1.52
26	W	356	THR	CA-C	12.42	1.69	1.52
7	M	168	MET	CA-CB	12.26	1.69	1.54
5	6	450	ASN	CG-OD1	-12.24	1.00	1.23
10	C	177	GLU	CG-CD	-12.18	1.21	1.52
10	C	209	TYR	CG-CD1	-12.03	1.14	1.39
3	2	150	MET	CA-CB	11.94	1.72	1.53
17	J	6	ARG	NE-CZ	-11.85	1.20	1.33
19	L	63	ARG	CB-CG	-11.74	1.17	1.52
1	0	659	MET	CB-CG	11.66	1.87	1.52
23	O	104	MET	CA-CB	-11.64	1.31	1.53
17	J	49	MET	SD-CE	-11.63	1.50	1.79
9	B	199	MET	CG-SD	-11.57	1.51	1.80
12	E	75	MET	CG-SD	-11.36	1.52	1.80
28	5	16	ILE	CB-CG2	11.36	1.90	1.52
17	J	49	MET	CG-SD	-11.33	1.52	1.80
6	7	112	MET	CA-C	11.22	1.68	1.52
8	A	837	ILE	CB-CG1	-11.22	1.31	1.53
23	O	236	GLU	CA-C	11.22	1.67	1.52
9	B	597	MET	CA-CB	11.21	1.70	1.53
18	K	31	VAL	CA-C	11.12	1.66	1.52
8	A	217	LYS	CD-CE	-11.01	1.19	1.52
3	2	97	MET	CG-SD	-10.98	1.53	1.80
1	0	659	MET	N-CA	-10.93	1.32	1.46
12	E	29	PHE	CA-CB	-10.93	1.34	1.53
6	7	742	MET	N-CA	-10.91	1.32	1.46
28	5	28	SER	C-N	10.76	1.48	1.33
28	5	16	ILE	CB-CG1	-10.73	1.31	1.53
16	I	93	LYS	C-N	-10.67	1.18	1.33
25	V	38	MET	SD-CE	-10.52	1.53	1.79
9	B	194	GLU	CD-OE1	-10.50	1.05	1.25
3	2	97	MET	CB-CG	-10.48	1.21	1.52
14	G	10	ASN	CA-CB	-10.44	1.35	1.52
8	A	837	ILE	CB-CG2	10.33	1.86	1.52
26	W	356	THR	CB-CG2	10.31	1.86	1.52
12	E	19	VAL	CB-CG2	10.30	1.86	1.52
8	A	1267	MET	SD-CE	-10.29	1.53	1.79
17	J	49	MET	CB-CG	-10.25	1.21	1.52
1	0	659	MET	CA-CB	-10.25	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	49	MET	CA-CB	-10.15	1.37	1.53
7	M	168	MET	CB-CG	-10.11	1.22	1.52
19	L	63	ARG	NE-CZ	-9.98	1.22	1.33
18	K	30	ALA	C-N	9.96	1.47	1.33
10	C	248	ILE	CG1-CD1	-9.94	1.12	1.51
10	C	84	ARG	CB-CG	9.88	1.82	1.52
12	E	28	TYR	C-N	-9.81	1.20	1.33
18	K	103	THR	CB-OG1	-9.74	1.28	1.43
24	U	250	LYS	CB-CG	-9.74	1.23	1.52
6	7	418	MET	N-CA	-9.67	1.33	1.46
15	H	88	SER	CB-OG	-9.49	1.23	1.42
8	A	415	LEU	CG-CD2	9.48	1.83	1.52
10	C	37	MET	N-CA	-9.45	1.33	1.46
3	2	150	MET	CA-C	9.42	1.65	1.52
12	E	75	MET	CB-CG	-9.41	1.24	1.52
3	2	457	SER	C-O	-9.25	1.11	1.23
28	5	16	ILE	N-CA	-9.25	1.34	1.46
1	0	659	MET	CA-C	9.24	1.65	1.52
19	L	30	ILE	CG1-CD1	-9.17	1.16	1.51
10	C	24	ASN	N-CA	-9.16	1.34	1.46
3	2	373	MET	CA-C	9.15	1.64	1.53
23	O	224	TYR	CA-CB	9.15	1.67	1.53
14	G	10	ASN	N-CA	-9.14	1.34	1.47
18	K	21	ILE	CB-CG1	-9.12	1.35	1.53
1	0	346	MET	CB-CG	-9.09	1.25	1.52
7	M	250	MET	SD-CE	-9.08	1.56	1.79
15	H	145	ARG	C-N	9.05	1.46	1.33
18	K	70	ARG	CG-CD	-9.01	1.25	1.52
3	2	373	MET	CB-CG	-8.98	1.25	1.52
6	7	112	MET	CA-CB	8.94	1.69	1.53
8	A	217	LYS	N-CA	-8.93	1.34	1.46
10	C	248	ILE	CA-CB	-8.93	1.43	1.54
8	A	904	THR	CB-OG1	-8.92	1.29	1.43
19	L	47	ARG	CA-CB	8.87	1.68	1.53
9	B	542	MET	CA-CB	-8.86	1.40	1.53
1	0	346	MET	CA-C	8.83	1.64	1.52
3	2	150	MET	CB-CG	-8.81	1.26	1.52
8	A	217	LYS	CG-CD	-8.80	1.26	1.52
14	G	10	ASN	CA-C	8.72	1.63	1.53
10	C	84	ARG	CZ-NH1	8.71	1.45	1.32
12	E	29	PHE	CG-CD1	-8.69	1.20	1.38
22	S	282	TYR	CG-CD2	8.55	1.57	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	277	GLN	CA-CB	-8.52	1.41	1.53
8	A	837	ILE	N-CA	-8.51	1.35	1.46
17	J	4	PRO	C-N	-8.49	1.23	1.33
23	O	104	MET	N-CA	-8.48	1.35	1.46
10	C	18	VAL	CB-CG2	8.44	1.80	1.52
18	K	31	VAL	CB-CG2	-8.43	1.24	1.52
16	I	26	LEU	CG-CD2	8.43	1.80	1.52
1	0	346	MET	CG-SD	8.40	2.01	1.80
19	L	30	ILE	CA-CB	8.34	1.64	1.55
10	C	18	VAL	CB-CG1	-8.32	1.25	1.52
8	A	437	MET	CG-SD	-8.31	1.59	1.80
8	A	455	MET	C-N	-8.23	1.21	1.33
8	A	415	LEU	CA-CB	-8.23	1.38	1.53
1	0	229	ASP	CA-C	8.23	1.65	1.52
16	I	94	ASP	N-CA	-8.19	1.35	1.46
27	X	153	MET	SD-CE	-8.17	1.59	1.79
6	7	418	MET	CG-SD	-8.12	1.60	1.80
10	C	230	MET	CG-SD	-8.12	1.60	1.80
24	U	27	ASN	CA-CB	-8.09	1.40	1.53
12	E	19	VAL	CB-CG1	-8.08	1.25	1.52
24	U	39	LYS	CE-NZ	-8.05	1.25	1.49
8	A	761	MET	CG-SD	-8.05	1.60	1.80
24	U	27	ASN	CG-ND2	8.02	1.50	1.33
24	U	263	LYS	C-N	8.00	1.44	1.33
24	U	250	LYS	CA-CB	7.96	1.66	1.53
18	K	21	ILE	CG1-CD1	-7.92	1.20	1.51
24	U	250	LYS	CG-CD	-7.91	1.28	1.52
17	J	51	LEU	CA-C	7.91	1.63	1.52
23	O	224	TYR	CG-CD1	-7.89	1.22	1.39
26	W	34	PHE	CG-CD1	-7.89	1.22	1.38
25	V	82	ASN	CA-C	7.88	1.62	1.53
9	B	1021	MET	SD-CE	-7.87	1.59	1.79
23	O	104	MET	SD-CE	-7.79	1.60	1.79
17	J	5	VAL	CA-C	-7.74	1.43	1.52
10	C	177	GLU	CB-CG	-7.73	1.29	1.52
27	X	216	GLN	CD-OE1	-7.73	1.08	1.23
18	K	64	GLU	N-CA	-7.70	1.37	1.46
8	A	437	MET	CA-CB	7.68	1.64	1.53
17	J	5	VAL	CB-CG2	7.68	1.77	1.52
1	0	346	MET	N-CA	-7.67	1.36	1.46
8	A	415	LEU	CG-CD1	-7.67	1.27	1.52
6	7	231	ARG	CD-NE	-7.61	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	20	LYS	CA-C	7.61	1.63	1.52
10	C	177	GLU	CA-CB	-7.58	1.39	1.54
10	C	94	LYS	CE-NZ	-7.57	1.26	1.49
1	0	346	MET	CA-CB	-7.55	1.41	1.53
8	A	456	MET	CG-SD	-7.50	1.61	1.80
3	2	373	MET	SD-CE	-7.49	1.60	1.79
12	E	22	MET	CB-CG	-7.46	1.30	1.52
7	M	168	MET	CA-C	7.44	1.64	1.52
3	2	373	MET	CG-SD	-7.43	1.62	1.80
3	2	464	THR	N-CA	-7.42	1.36	1.46
23	O	104	MET	CA-C	7.40	1.61	1.52
22	S	282	TYR	CG-CD1	-7.37	1.23	1.39
18	K	31	VAL	N-CA	-7.36	1.37	1.46
2	1	385	MET	CA-C	-7.35	1.42	1.52
24	U	277	GLN	CB-CG	-7.35	1.30	1.52
17	J	5	VAL	CB-CG1	-7.35	1.28	1.52
27	X	153	MET	CA-CB	-7.35	1.40	1.53
18	K	21	ILE	N-CA	-7.32	1.38	1.46
15	H	88	SER	CA-CB	-7.26	1.41	1.53
15	H	146	ARG	CD-NE	-7.20	1.36	1.46
10	C	230	MET	SD-CE	-7.17	1.61	1.79
6	7	112	MET	CB-CG	-7.17	1.30	1.52
10	C	18	VAL	CA-C	-7.16	1.43	1.52
12	E	22	MET	CG-SD	-7.15	1.62	1.80
23	O	236	GLU	CB-CG	-7.14	1.31	1.52
8	A	1454	MET	CB-CG	-7.14	1.31	1.52
23	O	224	TYR	CB-CG	-7.13	1.35	1.51
18	K	20	LYS	CA-C	-7.12	1.44	1.52
17	J	6	ARG	CG-CD	-7.05	1.31	1.52
10	C	24	ASN	CG-OD1	-7.01	1.10	1.23
10	C	81	GLU	N-CA	7.00	1.55	1.45
8	A	1454	MET	CA-CB	-6.97	1.39	1.53
1	0	693	LEU	CA-C	6.88	1.60	1.53
6	7	747	ASN	N-CA	-6.87	1.37	1.46
10	C	57	VAL	CB-CG2	6.87	1.75	1.52
6	7	742	MET	CA-CB	-6.85	1.41	1.53
30	T	-38	DC	C2-O2	-6.84	1.10	1.24
14	G	33	GLU	CB-CG	-6.82	1.31	1.52
18	K	42	LEU	CA-C	-6.75	1.44	1.53
6	7	742	MET	SD-CE	6.74	1.96	1.79
26	W	34	PHE	CB-CG	-6.72	1.35	1.50
3	2	487	LYS	N-CA	-6.70	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	29	ASP	N-CA	-6.70	1.38	1.46
8	A	456	MET	SD-CE	-6.67	1.62	1.79
9	B	194	GLU	CG-CD	-6.65	1.35	1.52
22	S	232	ASP	N-CA	-6.64	1.36	1.46
6	7	418	MET	SD-CE	-6.64	1.62	1.79
10	C	17	ASN	C-N	-6.62	1.24	1.33
18	K	20	LYS	N-CA	6.62	1.53	1.45
1	0	658	ALA	C-N	-6.60	1.24	1.33
26	W	356	THR	CA-CB	-6.55	1.42	1.53
19	L	66	GLN	C-N	6.50	1.41	1.33
18	K	64	GLU	CG-CD	6.47	1.68	1.52
23	O	221	GLU	CB-CG	-6.45	1.33	1.52
6	7	746	PRO	C-N	6.40	1.42	1.33
8	A	415	LEU	N-CA	6.36	1.54	1.46
3	2	483	TRP	CA-CB	-6.36	1.43	1.53
1	0	547	MET	CG-SD	-6.29	1.65	1.80
2	1	607	SER	C-N	6.29	1.46	1.34
10	C	230	MET	CB-CG	-6.29	1.33	1.52
18	K	103	THR	CA-C	-6.29	1.44	1.52
10	C	57	VAL	CA-C	-6.26	1.44	1.52
8	A	456	MET	CA-CB	-6.23	1.39	1.53
24	U	277	GLN	CA-C	6.22	1.60	1.52
12	E	22	MET	CA-C	-6.20	1.44	1.52
9	B	552	MET	CG-SD	-6.19	1.65	1.80
8	A	437	MET	SD-CE	-6.17	1.64	1.79
7	M	168	MET	CG-SD	-6.17	1.65	1.80
6	7	741	GLY	C-N	-6.15	1.25	1.33
17	J	51	LEU	CA-CB	-6.12	1.43	1.53
23	O	221	GLU	CA-CB	-6.09	1.43	1.53
16	I	50	THR	CB-OG1	-6.09	1.34	1.43
10	C	24	ASN	CG-ND2	6.07	1.46	1.33
18	K	20	LYS	CA-CB	-6.07	1.43	1.53
26	W	356	THR	CB-OG1	-6.07	1.34	1.43
2	1	358	MET	CA-CB	-6.06	1.44	1.54
19	L	30	ILE	CB-CG1	-6.04	1.41	1.53
1	0	228	LYS	C-N	6.00	1.42	1.33
18	K	20	LYS	C-N	5.97	1.41	1.33
18	K	70	ARG	CD-NE	-5.97	1.37	1.46
10	C	81	GLU	CA-C	-5.97	1.45	1.52
19	L	66	GLN	CD-NE2	5.93	1.45	1.33
18	K	41	THR	C-N	-5.87	1.25	1.33
12	E	29	PHE	C-N	5.86	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	82	ASN	CA-CB	-5.86	1.45	1.53
17	J	5	VAL	C-N	5.84	1.41	1.33
18	K	2	ASN	N-CA	-5.83	1.38	1.46
17	J	6	ARG	CZ-NH1	5.82	1.40	1.32
1	0	547	MET	CA-C	-5.81	1.45	1.52
24	U	39	LYS	CG-CD	-5.80	1.35	1.52
8	A	1454	MET	CG-SD	5.79	1.95	1.80
9	B	199	MET	CA-CB	-5.78	1.45	1.53
16	I	50	THR	CA-C	-5.78	1.45	1.52
10	C	209	TYR	N-CA	-5.78	1.38	1.46
6	7	231	ARG	CA-CB	-5.72	1.43	1.53
8	A	456	MET	CA-C	-5.72	1.45	1.52
12	E	75	MET	CA-CB	-5.67	1.44	1.53
9	B	199	MET	CB-CG	-5.67	1.35	1.52
17	J	51	LEU	CG-CD1	-5.66	1.33	1.52
1	0	547	MET	CA-CB	-5.63	1.44	1.53
18	K	64	GLU	CA-CB	-5.63	1.44	1.53
18	K	42	LEU	CG-CD1	-5.61	1.34	1.52
20	Q	27	MET	CB-CG	-5.59	1.35	1.52
18	K	103	THR	CA-CB	-5.58	1.44	1.53
24	U	27	ASN	CB-CG	-5.57	1.38	1.52
16	I	26	LEU	N-CA	5.53	1.53	1.46
8	A	904	THR	CA-C	-5.52	1.45	1.53
14	G	9	LEU	C-N	-5.51	1.25	1.33
8	A	903	ASN	C-N	-5.48	1.26	1.33
6	7	430	LEU	C-N	-5.47	1.22	1.33
14	G	148	GLU	CA-CB	-5.47	1.44	1.53
18	K	70	ARG	CB-CG	5.45	1.68	1.52
19	L	66	GLN	CD-OE1	-5.45	1.13	1.23
23	O	221	GLU	N-CA	5.40	1.53	1.46
23	O	103	ILE	C-N	-5.39	1.26	1.33
9	B	597	MET	SD-CE	-5.38	1.66	1.79
7	M	317	TYR	CA-C	-5.38	1.45	1.52
10	C	230	MET	N-CA	5.37	1.52	1.45
3	2	97	MET	N-CA	-5.35	1.39	1.46
10	C	12	GLU	N-CA	-5.33	1.39	1.45
19	L	66	GLN	CA-C	5.31	1.59	1.52
10	C	37	MET	SD-CE	5.25	1.92	1.79
26	W	34	PHE	CA-C	5.23	1.59	1.52
9	B	542	MET	CG-SD	-5.18	1.67	1.80
10	C	109	SER	CA-C	-5.16	1.45	1.52
16	I	20	LYS	CA-CB	5.14	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	81	MET	CB-CG	-5.13	1.37	1.52
16	I	115	LYS	CG-CD	-5.12	1.37	1.52
25	V	38	MET	CG-SD	-5.10	1.68	1.80
2	1	358	MET	CG-SD	5.09	1.93	1.80
18	K	2	ASN	CB-CG	-5.07	1.39	1.52
26	W	34	PHE	CD1-CE1	-5.04	1.23	1.38
10	C	81	GLU	CA-CB	-5.02	1.45	1.54
8	A	217	LYS	CA-C	5.02	1.59	1.52
15	H	88	SER	CA-C	-5.02	1.46	1.52
3	2	463	GLU	C-O	5.02	1.30	1.24
10	C	37	MET	CA-CB	-5.00	1.45	1.53

All (535) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	V	82	ASN	OD1-CG-ND2	-40.19	82.41	122.60
5	6	450	ASN	OD1-CG-ND2	-39.96	82.64	122.60
12	E	29	PHE	N-CA-CB	36.11	171.52	110.49
26	W	34	PHE	CB-CG-CD1	34.69	179.66	120.70
10	C	177	GLU	CB-CG-CD	34.37	171.02	112.60
1	0	659	MET	CG-SD-CE	32.89	173.27	100.90
27	X	216	GLN	OE1-CD-NE2	-32.13	90.47	122.60
3	2	97	MET	CG-SD-CE	31.80	170.87	100.90
5	6	202	GLN	OE1-CD-NE2	-31.74	90.86	122.60
18	K	21	ILE	CB-CG1-CD1	31.52	179.99	113.80
23	O	224	TYR	CB-CG-CD1	31.45	167.97	120.80
19	L	63	ARG	CD-NE-CZ	31.06	167.88	124.40
18	K	64	GLU	CB-CG-CD	-30.33	61.03	112.60
7	M	317	TYR	CD1-CG-CD2	-29.64	73.63	118.10
5	6	202	GLN	CG-CD-OE1	29.57	179.94	120.80
23	O	104	MET	CA-CB-CG	28.07	170.23	114.10
23	O	224	TYR	CG-CD1-CE1	27.82	162.93	121.20
8	A	1188	GLN	OE1-CD-NE2	-27.82	94.78	122.60
24	U	250	LYS	CB-CG-CD	27.53	174.62	111.30
18	K	1	MET	N-CA-CB	27.48	157.22	110.50
10	C	84	ARG	NE-CZ-NH1	-25.81	95.69	121.50
6	7	231	ARG	CG-CD-NE	25.64	168.41	112.00
5	6	450	ASN	CB-CG-OD1	25.54	171.88	120.80
1	0	346	MET	CA-CB-CG	25.31	164.71	114.10
19	L	63	ARG	CA-CB-CG	24.34	162.77	114.10
12	E	29	PHE	CA-CB-CG	-23.56	90.24	113.80
23	O	224	TYR	CB-CG-CD2	-23.55	85.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	224	TYR	CD1-CG-CD2	-23.22	83.28	118.10
23	O	104	MET	N-CA-CB	22.94	150.48	110.80
25	V	82	ASN	CB-CG-ND2	-22.89	82.06	116.40
19	L	67	PHE	CB-CG-CD2	-22.81	81.93	120.70
9	B	194	GLU	CG-CD-OE1	22.75	170.73	118.40
19	L	63	ARG	NE-CZ-NH1	-22.58	98.92	121.50
7	M	317	TYR	CG-CD1-CE1	22.56	155.04	121.20
19	L	63	ARG	NE-CZ-NH2	22.44	139.40	119.20
27	X	216	GLN	CG-CD-NE2	-22.34	82.89	116.40
26	W	34	PHE	CG-CD1-CE1	22.34	158.68	120.70
12	E	75	MET	CA-CB-CG	21.63	157.35	114.10
12	E	28	TYR	CA-C-N	21.55	162.71	121.54
12	E	28	TYR	C-N-CA	21.55	162.71	121.54
24	U	27	ASN	CA-CB-CG	21.52	134.12	112.60
12	E	75	MET	CB-CG-SD	21.39	176.88	112.70
7	M	168	MET	CB-CG-SD	21.18	176.22	112.70
15	H	146	ARG	CG-CD-NE	21.07	158.34	112.00
17	J	6	ARG	NE-CZ-NH1	-21.03	100.47	121.50
14	G	10	ASN	N-CA-CB	20.95	150.49	111.11
12	E	22	MET	CA-CB-CG	20.93	155.95	114.10
1	0	547	MET	CA-CB-CG	20.84	155.78	114.10
9	B	199	MET	CB-CG-SD	20.48	174.15	112.70
26	W	34	PHE	CD1-CG-CD2	-20.29	88.17	118.60
7	M	317	TYR	CB-CG-CD1	20.15	151.03	120.80
10	C	24	ASN	CA-CB-CG	-19.89	92.71	112.60
10	C	177	GLU	CA-CB-CG	19.81	153.72	114.10
8	A	1454	MET	CA-CB-CG	19.77	153.64	114.10
9	B	199	MET	CA-CB-CG	19.52	153.15	114.10
19	L	67	PHE	CD1-CG-CD2	-19.30	89.64	118.60
22	S	232	ASP	N-CA-C	-19.27	86.52	110.61
12	E	29	PHE	CD1-CG-CD2	-19.26	89.71	118.60
7	M	317	TYR	CB-CG-CD2	-19.25	91.93	120.80
15	H	146	ARG	CB-CG-CD	19.18	155.42	111.30
1	0	659	MET	N-CA-CB	19.17	142.88	110.49
12	E	29	PHE	CB-CG-CD1	19.14	153.23	120.70
24	U	27	ASN	CB-CG-ND2	-18.71	88.34	116.40
8	A	217	LYS	CD-CE-NZ	18.39	170.75	111.90
5	6	450	ASN	CA-CB-CG	18.36	130.96	112.60
18	K	64	GLU	OE1-CD-OE2	-18.30	78.98	122.90
5	6	202	GLN	CG-CD-NE2	-18.21	89.08	116.40
1	0	346	MET	N-CA-CB	18.14	138.24	110.30
5	6	450	ASN	CB-CG-ND2	-18.09	89.26	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	547	MET	CB-CA-C	17.86	139.32	110.92
3	2	463	GLU	CA-C-N	-17.71	95.87	122.09
3	2	463	GLU	C-N-CA	-17.71	95.87	122.09
1	0	547	MET	CB-CG-SD	17.54	165.31	112.70
16	I	94	ASP	CA-CB-CG	-17.49	95.11	112.60
16	I	93	LYS	CA-C-N	17.29	149.28	122.49
16	I	93	LYS	C-N-CA	17.29	149.28	122.49
26	W	34	PHE	CB-CG-CD2	-17.17	91.51	120.70
18	K	64	GLU	CG-CD-OE1	17.16	157.86	118.40
19	L	67	PHE	CB-CG-CD1	17.14	149.85	120.70
10	C	248	ILE	CB-CG1-CD1	17.14	149.79	113.80
24	U	277	GLN	CA-CB-CG	17.04	148.18	114.10
8	A	217	LYS	CB-CG-CD	16.98	150.35	111.30
12	E	29	PHE	CB-CG-CD2	-16.97	91.85	120.70
10	C	209	TYR	CD1-CG-CD2	-16.96	92.67	118.10
6	7	231	ARG	CA-CB-CG	16.84	147.78	114.10
12	E	29	PHE	CG-CD1-CE1	16.83	149.31	120.70
14	G	10	ASN	CA-CB-CG	16.60	129.20	112.60
23	O	221	GLU	CA-CB-CG	16.36	146.82	114.10
19	L	67	PHE	CG-CD1-CE1	16.30	148.41	120.70
6	7	112	MET	CB-CG-SD	16.19	161.27	112.70
9	B	194	GLU	OE1-CD-OE2	-16.12	84.21	122.90
25	V	82	ASN	CA-CB-CG	16.12	128.72	112.60
28	5	16	ILE	N-CA-C	-16.10	93.41	113.22
8	A	1267	MET	CG-SD-CE	16.10	136.32	100.90
23	O	236	GLU	CB-CG-CD	15.94	139.70	112.60
3	2	150	MET	CB-CG-SD	15.91	160.45	112.70
7	M	168	MET	CA-CB-CG	-15.87	82.36	114.10
28	5	16	ILE	CA-CB-CG1	15.85	137.34	110.40
3	2	463	GLU	O-C-N	15.68	143.44	122.59
10	C	84	ARG	CB-CG-CD	-15.56	75.50	111.30
17	J	6	ARG	CB-CG-CD	15.55	147.06	111.30
19	L	30	ILE	CB-CG1-CD1	15.50	146.35	113.80
2	1	358	MET	N-CA-C	-15.35	93.76	113.72
9	B	542	MET	CA-CB-CG	15.29	144.67	114.10
6	7	112	MET	N-CA-C	-15.22	94.71	113.28
8	A	1188	GLN	CG-CD-NE2	-15.04	93.84	116.40
14	G	9	LEU	CA-C-N	15.00	147.22	122.76
14	G	9	LEU	C-N-CA	15.00	147.22	122.76
6	7	747	ASN	N-CA-C	-14.95	83.50	108.76
3	2	373	MET	CB-CG-SD	14.90	157.39	112.70
8	A	217	LYS	CA-CB-CG	-14.80	84.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	88	SER	CA-CB-OG	14.70	140.51	111.10
3	2	97	MET	CA-CB-CG	14.65	143.40	114.10
18	K	64	GLU	CA-CB-CG	14.61	143.32	114.10
3	2	373	MET	CG-SD-CE	14.55	132.91	100.90
14	G	33	GLU	CA-CB-CG	14.53	143.17	114.10
12	E	22	MET	CB-CG-SD	14.53	156.28	112.70
17	J	49	MET	CA-CB-CG	14.47	143.04	114.10
2	1	608	MET	N-CA-C	-14.35	89.82	113.50
1	0	659	MET	CA-CB-CG	-14.28	85.54	114.10
18	K	70	ARG	CD-NE-CZ	-14.25	104.45	124.40
27	X	216	GLN	CB-CG-CD	14.21	136.75	112.60
10	C	37	MET	N-CA-C	-14.05	94.49	112.90
18	K	1	MET	CA-C-N	-14.00	94.80	121.54
18	K	1	MET	C-N-CA	-14.00	94.80	121.54
8	A	217	LYS	CG-CD-CE	13.94	143.36	111.30
3	2	150	MET	CA-CB-CG	-13.86	86.37	114.10
19	L	30	ILE	CA-CB-CG1	-13.81	86.93	110.40
24	U	27	ASN	CB-CG-OD1	13.79	148.39	120.80
10	C	248	ILE	CA-CB-CG1	13.76	133.79	110.40
27	X	216	GLN	CG-CD-OE1	13.71	148.23	120.80
25	V	38	MET	CB-CG-SD	13.62	153.57	112.70
3	2	487	LYS	N-CA-C	-13.56	93.60	112.45
28	5	29	ASP	CA-CB-CG	-13.49	99.11	112.60
26	W	356	THR	CA-CB-CG2	-13.49	87.57	110.50
23	O	236	GLU	N-CA-C	-13.44	96.84	113.38
24	U	39	LYS	CG-CD-CE	13.27	141.81	111.30
9	B	194	GLU	CB-CG-CD	-13.22	90.12	112.60
9	B	662	MET	CA-CB-CG	13.12	140.33	114.10
19	L	66	GLN	OE1-CD-NE2	-13.02	109.58	122.60
26	W	356	THR	N-CA-C	-13.00	95.70	111.69
10	C	18	VAL	CG1-CB-CG2	-12.97	82.26	110.80
8	A	837	ILE	N-CA-C	-12.86	94.49	113.39
8	A	837	ILE	CA-CB-CG1	12.81	132.19	110.40
24	U	264	ASP	CA-CB-CG	12.68	125.28	112.60
1	0	229	ASP	N-CA-C	-12.68	94.65	110.88
23	O	236	GLU	CB-CA-C	-12.66	87.62	109.65
26	W	34	PHE	CA-CB-CG	-12.62	101.19	113.80
24	U	277	GLN	CB-CG-CD	12.60	134.02	112.60
18	K	1	MET	CA-CB-CG	-12.60	88.91	114.10
7	M	168	MET	N-CA-C	-12.57	94.41	113.51
28	5	16	ILE	N-CA-CB	12.54	131.13	112.07
19	L	63	ARG	CB-CG-CD	12.53	140.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	19	VAL	CG1-CB-CG2	-12.52	83.26	110.80
26	W	356	THR	CB-CA-C	-12.52	87.80	110.70
18	K	21	ILE	CA-CB-CG1	-12.47	89.20	110.40
26	W	356	THR	OG1-CB-CG2	-12.33	84.63	109.30
10	C	84	ARG	CG-CD-NE	12.21	138.86	112.00
22	S	231	CYS	CA-C-N	-12.20	100.34	122.54
22	S	231	CYS	C-N-CA	-12.20	100.34	122.54
12	E	29	PHE	CB-CA-C	-12.14	86.25	110.42
2	1	358	MET	CB-CA-C	-12.04	89.32	109.55
10	C	17	ASN	CA-C-N	12.02	138.28	122.90
10	C	17	ASN	C-N-CA	12.02	138.28	122.90
18	K	30	ALA	CA-C-N	-11.99	104.83	122.58
18	K	30	ALA	C-N-CA	-11.99	104.83	122.58
18	K	20	LYS	CA-CB-CG	11.90	137.90	114.10
24	U	277	GLN	N-CA-CB	-11.86	93.14	110.80
22	S	282	TYR	CD1-CG-CD2	-11.83	100.35	118.10
8	A	1202	MET	N-CA-CB	-11.83	91.69	110.14
23	O	221	GLU	CB-CG-CD	11.81	132.68	112.60
14	G	33	GLU	CB-CA-C	11.81	130.03	111.02
10	C	84	ARG	CD-NE-CZ	11.77	140.88	124.40
18	K	31	VAL	CA-CB-CG2	11.76	130.39	110.40
24	U	39	LYS	CD-CE-NZ	11.71	149.36	111.90
9	B	662	MET	CB-CA-C	11.67	133.08	110.67
9	B	662	MET	N-CA-CB	-11.65	92.22	110.28
23	O	221	GLU	N-CA-CB	-11.64	92.38	110.30
9	B	194	GLU	CG-CD-OE2	-11.58	91.76	118.40
9	B	597	MET	CA-CB-CG	-11.55	90.99	114.10
6	7	418	MET	CB-CG-SD	11.52	147.26	112.70
18	K	20	LYS	CG-CD-CE	11.50	137.76	111.30
17	J	49	MET	CG-SD-CE	11.45	126.09	100.90
5	6	202	GLN	CB-CG-CD	11.40	131.97	112.60
6	7	418	MET	N-CA-C	-11.25	95.84	112.04
18	K	20	LYS	CA-C-N	-11.25	112.27	122.96
18	K	20	LYS	C-N-CA	-11.25	112.27	122.96
3	2	373	MET	CB-CA-C	-11.15	92.58	111.31
8	A	437	MET	CA-CB-CG	-11.12	91.86	114.10
23	O	221	GLU	N-CA-C	-11.11	98.23	112.23
24	U	27	ASN	OD1-CG-ND2	-11.06	111.54	122.60
10	C	37	MET	CG-SD-CE	-11.03	76.63	100.90
17	J	6	ARG	CA-CB-CG	11.01	136.12	114.10
1	0	658	ALA	CA-C-N	11.01	142.57	121.54
1	0	658	ALA	C-N-CA	11.01	142.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	742	MET	N-CA-CB	10.91	128.94	110.49
24	U	250	LYS	CA-CB-CG	-10.85	92.40	114.10
18	K	70	ARG	CB-CG-CD	-10.80	86.47	111.30
8	A	1202	MET	CB-CA-C	10.74	131.12	111.03
6	7	112	MET	CG-SD-CE	-10.63	77.51	100.90
17	J	5	VAL	CG1-CB-CG2	-10.58	87.52	110.80
7	M	317	TYR	CA-CB-CG	-10.56	94.89	113.90
8	A	1188	GLN	CG-CD-OE1	10.52	141.85	120.80
18	K	20	LYS	N-CA-CB	-10.48	94.08	110.85
12	E	19	VAL	CA-CB-CG1	10.44	128.14	110.40
10	C	94	LYS	CD-CE-NZ	10.43	145.28	111.90
2	1	607	SER	CA-C-N	-10.42	104.12	120.17
2	1	607	SER	C-N-CA	-10.42	104.12	120.17
18	K	64	GLU	CG-CD-OE2	-10.41	94.45	118.40
17	J	5	VAL	N-CA-CB	10.40	122.45	110.49
25	V	38	MET	CA-CB-CG	10.39	134.89	114.10
8	A	456	MET	CA-CB-CG	10.39	134.88	114.10
18	K	70	ARG	CG-CD-NE	10.39	134.85	112.00
3	2	81	MET	CA-CB-CG	-10.38	93.33	114.10
9	B	542	MET	CB-CA-C	10.38	129.10	110.72
28	5	16	ILE	CG1-CB-CG2	-10.38	79.57	110.70
24	U	277	GLN	CG-CD-NE2	10.35	131.92	116.40
3	2	466	GLN	CB-CG-CD	10.32	130.14	112.60
8	A	415	LEU	CD1-CG-CD2	-10.31	88.13	110.80
16	I	47	GLU	CB-CG-CD	10.30	130.12	112.60
7	M	168	MET	N-CA-CB	-10.23	103.87	114.10
1	0	346	MET	CB-CG-SD	-10.22	82.04	112.70
8	A	837	ILE	CG1-CB-CG2	-10.19	80.12	110.70
24	U	277	GLN	N-CA-C	-10.19	98.32	113.61
17	J	6	ARG	NE-CZ-NH2	10.19	128.37	119.20
6	7	741	GLY	CA-C-N	10.17	140.96	121.54
6	7	741	GLY	C-N-CA	10.17	140.96	121.54
17	J	49	MET	CB-CG-SD	10.15	143.14	112.70
8	A	904	THR	N-CA-CB	-10.09	94.55	110.19
10	C	12	GLU	N-CA-CB	9.99	128.34	111.66
10	C	84	ARG	NH1-CZ-NH2	-9.96	106.35	119.30
8	A	415	LEU	N-CA-CB	-9.96	92.96	110.39
6	7	418	MET	CG-SD-CE	9.92	122.73	100.90
16	I	26	LEU	CD1-CG-CD2	-9.91	88.99	110.80
19	L	66	GLN	CG-CD-NE2	-9.90	101.55	116.40
10	C	18	VAL	N-CA-CB	9.89	122.78	111.21
1	0	346	MET	CB-CA-C	-9.85	90.28	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	18	VAL	CA-CB-CG1	9.81	127.08	110.40
26	W	34	PHE	N-CA-C	-9.77	100.71	111.36
10	C	248	ILE	N-CA-CB	-9.74	97.29	110.54
8	A	217	LYS	N-CA-CB	9.73	126.93	110.49
18	K	21	ILE	N-CA-C	-9.73	91.73	106.42
1	O	547	MET	N-CA-CB	-9.69	95.09	109.82
10	C	24	ASN	N-CA-CB	9.67	126.84	110.49
8	A	837	ILE	N-CA-CB	9.67	128.71	111.98
14	G	148	GLU	CB-CG-CD	9.66	129.02	112.60
17	J	5	VAL	N-CA-C	9.65	121.96	108.93
10	C	18	VAL	N-CA-C	9.56	121.94	107.99
23	O	104	MET	CB-CA-C	-9.54	92.43	109.70
18	K	31	VAL	N-CA-C	-9.49	93.43	108.81
18	K	42	LEU	N-CA-C	9.47	125.67	112.04
10	C	24	ASN	N-CA-C	-9.38	90.82	110.80
16	I	49	ILE	CA-C-N	9.33	135.34	122.19
16	I	49	ILE	C-N-CA	9.33	135.34	122.19
15	H	146	ARG	N-CA-CB	9.31	126.33	110.50
18	K	103	THR	N-CA-CB	-9.27	94.83	110.49
18	K	64	GLU	CB-CA-C	9.21	125.45	110.90
7	M	317	TYR	CD1-CE1-CZ	-9.20	103.05	119.60
3	2	150	MET	N-CA-C	-9.20	100.85	112.90
27	X	216	GLN	CA-CB-CG	9.18	132.45	114.10
10	C	81	GLU	N-CA-CB	-9.18	96.84	111.43
28	5	28	SER	CA-C-N	-9.16	108.70	123.91
28	5	28	SER	C-N-CA	-9.16	108.70	123.91
8	A	455	MET	CA-C-N	9.15	136.67	122.94
8	A	455	MET	C-N-CA	9.15	136.67	122.94
18	K	2	ASN	N-CA-C	-9.12	91.37	110.80
8	A	836	TYR	CA-C-N	-9.06	108.69	121.55
8	A	836	TYR	C-N-CA	-9.06	108.69	121.55
6	7	230	ASN	CA-C-N	9.05	136.79	123.13
6	7	230	ASN	C-N-CA	9.05	136.79	123.13
26	W	356	THR	CA-CB-OG1	9.05	123.17	109.60
23	O	224	TYR	CA-CB-CG	-9.03	97.65	113.90
28	5	29	ASP	N-CA-C	9.01	123.92	113.38
9	B	79	THR	CA-C-N	8.94	137.79	121.70
9	B	79	THR	C-N-CA	8.94	137.79	121.70
18	K	20	LYS	CB-CA-C	8.86	125.58	109.37
18	K	64	GLU	N-CA-C	8.85	120.70	111.14
2	1	385	MET	CB-CA-C	8.85	125.42	110.74
8	A	1454	MET	CB-CG-SD	-8.83	86.22	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	221	GLU	CG-CD-OE2	8.80	138.64	118.40
18	K	1	MET	CA-C-O	-8.76	105.90	120.80
10	C	57	VAL	CG1-CB-CG2	-8.75	91.55	110.80
8	A	1267	MET	CB-CG-SD	8.73	138.90	112.70
17	J	5	VAL	CA-CB-CG1	8.73	125.24	110.40
3	2	97	MET	N-CA-CB	8.72	125.22	110.49
10	C	209	TYR	N-CA-CB	8.68	125.58	110.39
10	C	230	MET	N-CA-CB	-8.64	97.02	110.85
8	A	1454	MET	N-CA-CB	-8.50	96.04	110.50
11	D	70	PHE	CA-CB-CG	-8.47	105.33	113.80
12	E	19	VAL	CA-CB-CG2	-8.47	95.99	110.40
10	C	230	MET	CB-CG-SD	8.46	138.09	112.70
6	7	746	PRO	CA-C-N	-8.45	109.72	122.74
6	7	746	PRO	C-N-CA	-8.45	109.72	122.74
24	U	277	GLN	CG-CD-OE1	-8.44	103.92	120.80
8	A	415	LEU	CB-CG-CD1	8.39	135.88	110.70
8	A	456	MET	CB-CG-SD	8.38	137.85	112.70
10	C	57	VAL	CB-CA-C	8.36	125.01	111.29
18	K	96	ASN	N-CA-C	-8.36	101.40	111.69
19	L	67	PHE	N-CA-CB	-8.36	95.82	110.87
23	O	104	MET	CG-SD-CE	8.36	119.28	100.90
10	C	209	TYR	CA-CB-CG	-8.34	98.88	113.90
24	U	250	LYS	CG-CD-CE	-8.30	92.20	111.30
8	A	904	THR	N-CA-C	8.29	123.98	112.04
3	2	150	MET	CG-SD-CE	8.27	119.09	100.90
25	V	44	PHE	CA-CB-CG	8.26	122.06	113.80
9	B	542	MET	N-CA-CB	-8.26	98.59	110.57
22	S	282	TYR	CB-CA-C	8.25	124.29	110.43
16	I	47	GLU	N-CA-CB	8.24	125.22	111.53
16	I	94	ASP	N-CA-CB	8.23	123.04	110.61
6	7	418	MET	CB-CA-C	-8.14	95.67	110.56
9	B	867	GLY	CA-C-N	8.13	136.34	121.70
9	B	867	GLY	C-N-CA	8.13	136.34	121.70
24	U	27	ASN	CB-CA-C	8.13	123.81	110.81
16	I	20	LYS	N-CA-C	-8.12	103.37	113.28
15	H	146	ARG	CD-NE-CZ	-8.11	113.05	124.40
19	L	67	PHE	CB-CA-C	8.08	132.34	113.19
24	U	264	ASP	N-CA-CB	8.07	124.13	110.49
6	7	231	ARG	CB-CA-C	8.07	124.78	111.23
18	K	21	ILE	CG1-CB-CG2	-8.04	86.58	110.70
23	O	221	GLU	CG-CD-OE1	-8.04	99.92	118.40
12	E	29	PHE	N-CA-C	-8.03	93.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	358	MET	CA-CB-CG	7.96	130.02	114.10
10	C	209	TYR	CB-CG-CD2	-7.96	108.86	120.80
18	K	31	VAL	N-CA-CB	7.90	126.70	111.92
15	H	88	SER	CB-CA-C	7.89	126.11	110.42
16	I	115	LYS	CB-CG-CD	7.88	129.43	111.30
25	V	81	LYS	CA-C-N	7.85	133.93	122.63
25	V	81	LYS	C-N-CA	7.85	133.93	122.63
24	U	263	LYS	CA-C-N	-7.84	106.57	121.54
24	U	263	LYS	C-N-CA	-7.84	106.57	121.54
10	C	23	SER	CA-C-N	7.82	136.48	121.54
10	C	23	SER	C-N-CA	7.82	136.48	121.54
14	G	148	GLU	CA-CB-CG	7.82	129.73	114.10
3	2	487	LYS	CA-CB-CG	-7.81	98.49	114.10
8	A	1107	VAL	CA-C-N	7.79	135.73	121.70
8	A	1107	VAL	C-N-CA	7.79	135.73	121.70
9	B	918	ILE	CA-C-N	7.62	135.42	121.70
9	B	918	ILE	C-N-CA	7.62	135.42	121.70
3	2	373	MET	N-CA-CB	7.60	122.93	110.39
18	K	41	THR	CA-C-N	7.59	138.20	121.80
18	K	41	THR	C-N-CA	7.59	138.20	121.80
8	A	1202	MET	CA-CB-CG	7.58	129.27	114.10
10	C	18	VAL	CA-CB-CG2	-7.58	97.51	110.40
10	C	24	ASN	CB-CA-C	-7.53	95.44	110.42
8	A	437	MET	CB-CG-SD	7.50	135.20	112.70
10	C	37	MET	CB-CA-C	-7.50	94.61	109.67
25	V	37	ALA	CA-C-N	7.49	133.09	121.19
25	V	37	ALA	C-N-CA	7.49	133.09	121.19
12	E	19	VAL	N-CA-CB	7.48	123.57	111.23
28	5	16	ILE	CA-CB-CG2	-7.48	97.79	110.50
3	2	466	GLN	CA-CB-CG	7.45	129.00	114.10
9	B	662	MET	CG-SD-CE	-7.45	84.52	100.90
10	C	209	TYR	CG-CD1-CE1	7.45	132.37	121.20
23	O	236	GLU	N-CA-CB	7.40	121.56	110.53
10	C	81	GLU	CB-CA-C	7.35	124.86	110.30
17	J	51	LEU	CB-CA-C	-7.35	95.38	110.38
9	B	1021	MET	N-CA-CB	-7.34	101.14	112.30
10	C	24	ASN	CB-CG-ND2	-7.25	105.53	116.40
20	Q	27	MET	N-CA-CB	-7.24	98.59	110.40
17	J	5	VAL	CA-CB-CG2	-7.24	98.09	110.40
3	2	487	LYS	CB-CA-C	-7.16	96.57	110.11
27	X	153	MET	CA-CB-CG	7.15	128.40	114.10
3	2	487	LYS	CB-CG-CD	7.15	127.74	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	761	MET	CB-CG-SD	7.15	134.14	112.70
16	I	50	THR	OG1-CB-CG2	7.14	123.58	109.30
16	I	50	THR	CA-CB-CG2	7.11	122.59	110.50
10	C	230	MET	CG-SD-CE	7.09	116.50	100.90
16	I	50	THR	N-CA-CB	-7.08	98.47	110.16
8	A	437	MET	CG-SD-CE	7.08	116.47	100.90
18	K	1	MET	CB-CA-C	-7.04	96.72	110.10
2	1	358	MET	N-CA-CB	7.03	120.99	110.65
9	B	930	ALA	CA-C-N	7.00	134.31	121.70
9	B	930	ALA	C-N-CA	7.00	134.31	121.70
9	B	542	MET	CB-CG-SD	-6.96	91.83	112.70
15	H	146	ARG	NE-CZ-NH1	-6.95	114.55	121.50
19	L	63	ARG	N-CA-CB	6.95	120.55	110.06
25	V	38	MET	CB-CA-C	6.88	122.26	110.84
6	7	747	ASN	N-CA-CB	6.85	122.65	110.80
10	C	57	VAL	N-CA-CB	-6.83	99.97	111.23
16	I	47	GLU	CA-CB-CG	6.75	127.60	114.10
6	7	747	ASN	CA-CB-CG	6.75	119.35	112.60
10	C	230	MET	CA-CB-CG	-6.71	100.68	114.10
8	A	1453	TYR	CA-C-N	6.69	133.75	121.70
8	A	1453	TYR	C-N-CA	6.69	133.75	121.70
23	O	104	MET	CB-CG-SD	-6.67	92.68	112.70
17	J	5	VAL	CA-C-N	-6.66	108.82	121.54
17	J	5	VAL	C-N-CA	-6.66	108.82	121.54
18	K	103	THR	CB-CA-C	6.65	123.65	110.42
9	B	552	MET	CB-CG-SD	6.64	132.63	112.70
18	K	96	ASN	N-CA-CB	-6.63	100.32	110.20
19	L	30	ILE	CA-C-N	6.63	134.21	121.54
19	L	30	ILE	C-N-CA	6.63	134.21	121.54
8	A	761	MET	CA-CB-CG	6.58	127.26	114.10
12	E	19	VAL	N-CA-C	6.57	122.99	109.34
8	A	456	MET	CB-CA-C	6.55	121.88	109.37
16	I	50	THR	N-CA-C	6.54	120.32	109.46
19	L	67	PHE	CA-CB-CG	6.54	120.34	113.80
8	A	216	VAL	CA-C-N	6.52	133.99	121.54
8	A	216	VAL	C-N-CA	6.52	133.99	121.54
8	A	837	ILE	CA-CB-CG2	-6.52	99.42	110.50
6	7	747	ASN	CB-CA-C	-6.50	97.93	109.70
9	B	542	MET	CG-SD-CE	6.48	115.15	100.90
1	0	228	LYS	CA-C-N	-6.46	110.92	123.13
1	0	228	LYS	C-N-CA	-6.46	110.92	123.13
25	V	38	MET	CG-SD-CE	6.42	115.02	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	18	VAL	CB-CA-C	-6.41	102.20	110.98
17	J	49	MET	N-CA-CB	-6.41	100.77	110.07
8	A	903	ASN	CA-C-N	6.40	135.62	121.80
8	A	903	ASN	C-N-CA	6.40	135.62	121.80
10	C	94	LYS	CG-CD-CE	-6.39	96.59	111.30
25	V	82	ASN	CB-CG-OD1	6.39	133.59	120.80
10	C	24	ASN	OD1-CG-ND2	-6.38	116.22	122.60
18	K	96	ASN	CB-CG-ND2	-6.38	106.83	116.40
9	B	831	SER	CA-C-N	-6.37	108.93	121.41
9	B	831	SER	C-N-CA	-6.37	108.93	121.41
15	H	146	ARG	NE-CZ-NH2	6.32	124.89	119.20
19	L	47	ARG	CD-NE-CZ	-6.32	115.56	124.40
8	A	1188	GLN	CB-CG-CD	6.31	123.33	112.60
28	5	15	SER	CA-C-N	-6.27	112.74	121.77
28	5	15	SER	C-N-CA	-6.27	112.74	121.77
10	C	24	ASN	CB-CG-OD1	6.27	133.33	120.80
3	2	373	MET	N-CA-C	-6.24	96.15	107.75
8	A	904	THR	OG1-CB-CG2	6.23	121.76	109.30
3	2	487	LYS	CG-CD-CE	-6.23	96.98	111.30
17	J	5	VAL	CA-C-O	-6.22	113.33	120.98
8	A	415	LEU	CA-CB-CG	6.18	137.94	116.30
10	C	57	VAL	CA-CB-CG2	-6.11	100.01	110.40
24	U	264	ASP	CB-CG-OD2	6.10	132.42	118.40
27	X	153	MET	CB-CG-SD	-6.09	94.43	112.70
28	5	29	ASP	CB-CG-OD1	6.06	132.34	118.40
10	C	209	TYR	CD1-CE1-CZ	-6.05	108.70	119.60
25	V	38	MET	N-CA-CB	6.05	120.00	109.72
25	V	6	TYR	CB-CG-CD2	-6.04	111.73	120.80
8	A	456	MET	N-CA-C	6.04	119.25	109.40
15	H	145	ARG	CA-C-N	-6.04	110.82	121.70
15	H	145	ARG	C-N-CA	-6.04	110.82	121.70
10	C	12	GLU	CB-CA-C	-6.02	97.50	110.45
10	C	84	ARG	NE-CZ-NH2	6.01	124.61	119.20
12	E	29	PHE	CD1-CE1-CZ	-5.98	109.24	120.00
8	A	44	THR	CA-C-N	5.97	132.45	121.70
8	A	44	THR	C-N-CA	5.97	132.45	121.70
16	I	20	LYS	CA-CB-CG	-5.96	102.18	114.10
20	Q	27	MET	CB-CA-C	5.96	122.44	109.99
8	A	904	THR	CA-CB-CG2	5.95	120.62	110.50
3	2	373	MET	CA-CB-CG	-5.94	102.22	114.10
9	B	1021	MET	CB-CA-C	5.92	120.86	111.51
17	J	6	ARG	N-CA-C	5.92	123.40	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	103	THR	OG1-CB-CG2	5.91	121.12	109.30
7	M	317	TYR	CB-CA-C	5.89	120.57	110.79
10	C	37	MET	N-CA-CB	5.87	119.13	110.33
14	G	148	GLU	N-CA-CB	5.84	120.36	110.49
18	K	21	ILE	CB-CA-C	-5.83	105.34	111.23
18	K	103	THR	CA-CB-CG2	5.82	120.39	110.50
25	V	82	ASN	CB-CA-C	-5.79	103.66	112.11
14	G	33	GLU	N-CA-C	5.78	119.64	112.59
16	I	26	LEU	N-CA-CB	-5.77	101.75	110.35
20	Q	27	MET	CG-SD-CE	-5.75	88.24	100.90
13	F	130	ILE	N-CA-CB	-5.73	104.75	110.08
10	C	83	SER	CA-C-N	5.72	132.47	121.54
10	C	83	SER	C-N-CA	5.72	132.47	121.54
17	J	6	ARG	CD-NE-CZ	5.71	132.39	124.40
12	E	215	MET	CB-CA-C	-5.71	99.26	110.10
16	I	50	THR	CB-CA-C	5.71	119.16	109.80
26	W	356	THR	N-CA-CB	5.71	118.70	110.20
14	G	10	ASN	CA-C-O	-5.68	111.67	120.81
7	M	167	SER	CA-C-N	5.66	135.75	126.86
7	M	167	SER	C-N-CA	5.66	135.75	126.86
16	I	94	ASP	N-CA-C	5.63	120.84	113.30
10	C	109	SER	N-CA-CB	-5.62	100.98	110.49
24	U	27	ASN	N-CA-CB	5.62	118.31	109.94
15	H	146	ARG	N-CA-C	5.60	126.68	111.00
9	B	830	TYR	CA-C-N	5.59	132.23	121.54
9	B	830	TYR	C-N-CA	5.59	132.23	121.54
14	G	10	ASN	CB-CA-C	-5.59	104.11	111.82
26	W	34	PHE	CB-CA-C	-5.57	101.39	110.85
9	B	173	MET	CB-CG-SD	-5.56	96.03	112.70
18	K	21	ILE	O-C-N	-5.54	116.76	122.30
8	A	44	THR	N-CA-C	5.53	117.52	110.61
24	U	250	LYS	CB-CA-C	-5.53	99.92	109.86
8	A	904	THR	CB-CA-C	5.50	120.63	110.56
2	1	608	MET	CA-CB-CG	5.50	125.09	114.10
24	U	264	ASP	CB-CG-OD1	-5.48	105.80	118.40
6	7	418	MET	N-CA-CB	5.47	118.67	110.19
17	J	51	LEU	N-CA-C	-5.46	105.34	112.23
18	K	103	THR	CA-CB-OG1	5.46	117.79	109.60
12	E	22	MET	CB-CA-C	-5.46	99.56	110.42
14	G	56	ILE	CA-C-N	5.43	131.92	121.54
14	G	56	ILE	C-N-CA	5.43	131.92	121.54
10	C	177	GLU	CG-CD-OE2	-5.42	105.94	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	112	MET	CA-CB-CG	-5.39	103.33	114.10
8	A	455	MET	CA-CB-CG	5.38	124.86	114.10
10	C	84	ARG	N-CA-CB	5.37	119.57	110.49
14	G	31	LEU	CA-C-N	-5.37	112.66	122.38
14	G	31	LEU	C-N-CA	-5.37	112.66	122.38
24	U	27	ASN	N-CA-C	5.34	117.51	111.11
10	C	81	GLU	CB-CG-CD	5.33	121.67	112.60
17	J	51	LEU	CD1-CG-CD2	5.33	122.53	110.80
8	A	1267	MET	N-CA-C	5.33	117.50	111.11
22	S	232	ASP	CA-CB-CG	5.30	117.90	112.60
19	L	51	CYS	CA-C-N	5.28	131.76	121.41
19	L	51	CYS	C-N-CA	5.28	131.76	121.41
8	A	904	THR	CA-CB-OG1	5.27	117.51	109.60
19	L	32	ALA	N-CA-C	5.26	115.30	107.88
8	A	415	LEU	CB-CA-C	5.26	120.90	110.17
17	J	6	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
1	0	525	MET	N-CA-CB	5.25	118.96	110.40
3	2	372	ASN	N-CA-C	-5.24	106.79	114.39
18	K	31	VAL	CG1-CB-CG2	5.23	122.31	110.80
8	A	415	LEU	CB-CG-CD2	-5.22	95.03	110.70
22	S	232	ASP	N-CA-CB	5.22	118.95	111.65
18	K	97	LYS	CA-C-N	-5.20	112.50	121.66
18	K	97	LYS	C-N-CA	-5.20	112.50	121.66
6	7	742	MET	CG-SD-CE	-5.20	89.46	100.90
17	J	4	PRO	CA-C-N	5.20	128.35	120.77
17	J	4	PRO	C-N-CA	5.20	128.35	120.77
18	K	2	ASN	CA-CB-CG	5.19	117.79	112.60
26	W	142	PHE	CA-CB-CG	5.18	118.98	113.80
16	I	20	LYS	CD-CE-NZ	5.18	128.47	111.90
10	C	67	LEU	N-CA-C	5.17	116.61	111.07
11	D	144	THR	CA-C-N	-5.16	112.11	121.14
11	D	144	THR	C-N-CA	-5.16	112.11	121.14
3	2	464	THR	N-CA-C	-5.15	101.31	109.96
10	C	75	MET	CA-CB-CG	5.14	124.38	114.10
11	D	145	MET	CB-CG-SD	5.13	128.10	112.70
1	0	659	MET	CA-C-O	5.12	127.83	120.51
9	B	245	GLU	CA-C-N	5.12	130.91	121.70
9	B	245	GLU	C-N-CA	5.12	130.91	121.70
8	A	1202	MET	CG-SD-CE	-5.11	89.65	100.90
11	D	145	MET	N-CA-CB	5.11	118.74	110.40
14	G	33	GLU	CB-CG-CD	5.10	121.27	112.60
9	B	552	MET	N-CA-C	-5.06	98.63	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	26	LEU	CB-CG-CD2	-5.06	95.52	110.70
19	L	66	GLN	CG-CD-OE1	5.05	130.90	120.80
8	A	1267	MET	N-CA-CB	5.03	117.44	109.94
6	7	583	MET	CA-CB-CG	5.03	124.15	114.10

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

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Mol	Chain	Res	Type	Group
8	A	1079	MET	Peptide
8	A	1188	GLN	Sidechain
8	A	1404	GLU	Peptide
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

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Mol	Chain	Res	Type	Group
18	K	64	GLU	Sidechain
18	K	70	ARG	Sidechain
18	K	96	ASN	Sidechain
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	191	0
2	1	3382	0	3436	65	0
3	2	3546	0	3593	93	0
4	4	2267	0	2323	56	0
5	6	2786	0	2804	92	0
6	7	4889	0	4877	136	0
7	M	2175	0	2283	57	0
8	A	11167	0	11188	291	0
9	B	9227	0	9201	221	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	2086	0	2045	74	0
11	D	1331	0	1345	35	0
12	E	1752	0	1775	51	0
13	F	705	0	731	17	0
14	G	1335	0	1345	39	0
15	H	1080	0	1049	38	0
16	I	927	0	880	39	0
17	J	540	0	553	25	0
18	K	924	0	934	32	0
19	L	352	0	374	18	0
20	Q	1619	0	1452	40	0
21	P	1484	0	1480	41	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	34	0
26	W	2010	0	2026	56	0
27	X	1288	0	1307	39	0
28	5	498	0	506	23	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	69593	1783	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 13.

All (1783) 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
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
6:7:747:ASN:CA	6:7:747:ASN:C	1.76	1.57
10:C:37:MET:CA	10:C:37:MET:C	1.74	1.56
16:I:26:LEU:CD2	16:I:26:LEU:CG	1.80	1.56
22:S:232:ASP:CA	22:S:232:ASP:C	1.77	1.55
8:A:415:LEU:CD2	8:A:415:LEU:CG	1.83	1.54
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
5:6:450:ASN:CG	5:6:450:ASN:ND2	1.68	1.51
12:E:29:PHE:CA	12:E:29:PHE:C	1.82	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
1:0:346:MET:CG	1:0:346:MET:SD	2.01	1.48
27:X:216:GLN:CD	27:X:216:GLN:NE2	1.67	1.47
1:0:346:MET:SD	1:0:346:MET:HB2	1.54	1.47
18:K:1:MET:CA	18:K:1:MET:C	1.86	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
25:V:82:ASN:ND2	25:V:82:ASN:CG	1.74	1.43
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
10:C:18:VAL:CG2	10:C:18:VAL:CG1	2.05	1.32
18:K:64:GLU:CD	18:K:64:GLU:OE2	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:659:MET:CG	1:0:659:MET:CA	2.22	1.16
12:E:29:PHE:C	12:E:29:PHE:CB	2.19	1.14
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: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
6:7:747:ASN:C	6:7:747:ASN:N	2.11	1.07
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
22:S:232:ASP:C	22:S:232:ASP:N	2.16	1.02
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
10:C:37:MET:C	10:C:37:MET:CB	2.35	0.99
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
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
12:E:29:PHE:C	12:E:29:PHE:HB2	1.89	0.94
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
10:C:37:MET:C	10:C:37:MET:N	2.27	0.91
5:6:450:ASN:ND2	5:6:450:ASN:CB	2.33	0.91
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:29:PHE:C	12:E:29:PHE:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:2:454:TYR:CZ	3:2:483:TRP:HB2	2.11	0.86
6:7:747:ASN:C	6:7:747:ASN:CB	2.48	0.86
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
18:K:1:MET:C	18:K:1:MET:CB	2.49	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
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
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
18:K:1:MET:C	18:K:1:MET:N	2.38	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
22:S:232:ASP:C	22:S:232:ASP:CB	2.59	0.75
21:P:106:LEU:HB3	21:P:120:TYR:HB2	1.68	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
8:A:456:MET:HE3	8:A:507:VAL:HG12	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:50:LEU:HD11	14:G:2:PHE:HB2	1.72	0.71
9:B:277:LYS:HZ2	9:B:336:ARG:H	1.39	0.71
3:2:337:GLY:H	3:2:351:SER:HB3	1.53	0.71
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
6:7:713:THR:H	6:7:716:MET:HE1	1.58	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
25:V:34:ALA:O	25:V:38:MET:HE2	1.94	0.68
27:X:196:LEU:HB3	27:X:246:TYR:HB2	1.75	0.67
3:2:454:TYR:HH	3:2:483:TRP:CD1	2.12	0.67
9:B:267:ARG:HD3	9:B:313:MET:HE1	1.76	0.67
8:A:1059:HIS:ND1	13:F:86:THR:OG1	2.27	0.67
8:A:700:ASN:O	16:I:115:LYS:NZ	2.25	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
18:K:1:MET:C	18:K:1:MET:HG2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:450:ASN:HD22	5:6:450:ASN:CA	2.07	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
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
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
10:C:37:MET:C	10:C:37:MET:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:A:112:LYS:NZ	8:A:148:CYS:SG	2.71	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
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
18:K:1:MET:C	18:K:1:MET:CG	2.72	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
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
3:2:352: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:B:1000:PRO:HB2	9:B:1072:MET:HE2	1.82	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
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
9:B:806:THR:HG22	9:B:809:MET:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1151:GLU:OE2	16:I:45:ARG:NH1	2.34	0.60
3:2:238:LYS:NZ	3:2:239:ILE:O	2.33	0.60
8:A:116:ASP:O	8:A:118:HIS:ND1	2.34	0.60
8:A:173:THR:HG1	8:A:184:SER:HG	1.49	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
25:V:6:TYR:HB2	25:V:46:LYS:HZ3	1.67	0.59
14:G:47:CYS:SG	14:G:48:VAL:N	2.75	0.59
14:G:167:TYR:HA	14:G:170:ALA:HB3	1.85	0.59
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
11:D:192:LYS:HZ2	11:D:204:ASP:HB2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:460:SER:OG	1:O: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:O:156:CYS:HB3	31:O:801:SF4:S1	2.43	0.58
1:O:492:PHE:HB2	1:O:679:MET:HE1	1.85	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
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
11:D:22:GLU:HG2	14:G:83:LYS:HE2	1.86	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:O:636:LYS:HA	1:O: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:O:38:SER:HA	1:O: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:O: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
9:B:342:GLY:H	9:B:344:LYS:HZ2	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:C:241:ASP:N	10:C:241:ASP:OD1	2.32	0.56
14:G:100:GLU:HB3	14:G:107:LYS:HD2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:6:450:ASN:HD22	5:6:450:ASN:C	2.12	0.56
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
9:B:1155:SER:OG	9:B:1156:ASP:N	2.36	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
2:1:469:MET:HE1	4:4:140:ILE:HD11	1.88	0.55
13:F:112:GLU:OE1	13:F:123:LYS:NZ	2.39	0.55
16:I:96:SER:OG	16:I:97:MET:N	2.37	0.55
18:K:12:LEU:HB2	18:K:18:LYS:HD3	1.88	0.55
1:0:573:THR:OG1	1:0:575:ASP:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
23:O:74:VAL:HG22	23:O:155:PHE:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:6:133:SER:H	5:6:136:MET:HE2	1.73	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
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
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
8:A:31:SER:O	9:B:1183:LYS:NZ	2.35	0.54
16:I:61:ASP:OD1	16:I:61:ASP:N	2.39	0.54
16:I:78:CYS:SG	16:I:105:SER:OG	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:184:LYS:NZ	22:S:195:TYR:O	2.41	0.54
1:O:212:TYR:HA	1:O:218:ILE:HG13	1.88	0.54
1:O:656:PHE:O	1:O: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:O:294:HIS:H	1:O: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
29:N:-9:DG:H2'	29:N:-8:DG:C8	2.42	0.54
1:O:162:LEU:HD21	1:O:190:LEU:HB3	1.89	0.54
1:O:643:ARG:O	1:O: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:O:603:ARG:NH2	1:O: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
9:B:739:THR:OG1	9:B:740:HIS:ND1	2.41	0.53
1:O:570:LEU:O	1:O: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:554:TRP:HA	1:0:557:MET:HE2	1.90	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
26:W:123:MET:HE1	26:W:159:ASP:HA	1.90	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
8:A:1255:GLU:HB3	8:A:1259:MET:HE1	1.91	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
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
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:56:PRO:O	8:A:66:LYS:NZ	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
20:Q:108:LYS:NZ	21:P:84:ARG:O	2.39	0.52
2:1:185:LEU:HA	2:1:191:LEU:HD23	1.92	0.52
8:A:889:SER:HG	8:A:892:ALA:H	1.54	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
11:D:139:LYS:HZ2	11:D:142:LYS:HB2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:X:123:HIS:O	27:X:126:SER:OG	2.24	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
12:E:62:ALA:O	12:E:77:SER:OG	2.25	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
1:0:659:MET:CG	1:0:659:MET:C	2.84	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:2:50:MET:HE1	3:2:100:LEU:H	1.76	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
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
8:A:117:GLU:H	8:A:122:MET:HE1	1.75	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:B:862:GLN:O	9:B:914:LYS:NZ	2.36	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
8:A:95:PHE:HB3	8:A:234:MET:HE3	1.94	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
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
26:W:172:LEU:HG	26:W:176:MET:HE2	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
6:7:190:THR:OG1	6:7:217:THR:OG1	2.30	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
6:7:190:THR:OG1	6:7:213:ILE:O	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:A:1256:GLU:HA	8:A:1259:MET:HE2	1.94	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: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
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
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
8:A:483:ASP:OD1	8:A:483:ASP:N	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:1:472:GLN:HG2	4:4:38:THR:HG22	1.95	0.49
3:2:58:PRO:HD3	3:2:97:MET:HE2	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
18:K:1:MET:HA	18:K:1:MET:HE3	1.95	0.49
27:X:188:SER:N	27:X:191:GLU:OE1	2.44	0.49
8:A:549:MET:HE3	8:A:656:TRP:HB2	1.93	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
6:7:747:ASN:C	6:7:747:ASN:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:153:MET:HE1	27:X:157:ASP:HB2	1.94	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:7:439:THR:HA	6:7:459:MET:HE3	1.96	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
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:111:LEU:HA	20:Q:114:MET:HE2	1.95	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
9:B:778:MET:HE2	9:B:1094:ARG:HG2	1.96	0.47
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:M:39:SER:OG	7:M:40:GLU:OE1	2.33	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:332:ASP:N	9:B:332:ASP:OD1	2.44	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
10:C:37:MET:CA	10:C:38:ILE:N	2.65	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
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
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:849:MET:HE3	8:A:1061:GLY:HA2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:A:1433:MET:HE3	8:A:1433:MET:HB2	1.83	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
3:2:335:PRO:O	3:2:338:SER:OG	2.29	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
6:7:583:MET:HE1	6:7:617:GLU:HG3	1.97	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: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
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:87:SER:OG	12:E:88:VAL:N	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:372:LYS:HZ3	18:K:1:MET:C	2.24	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
8:A:1142:THR:O	8:A:1145:SER:OG	2.28	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:14:ARG:HH21	11:D:17:LYS:HZ1	1.62	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
15:H:123:MET:HE3	15:H:123:MET:HB2	1.62	0.46
22:S:280:SER:OG	22:S:300:GLU:OE2	2.32	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:182:MET:HA	22:S:185:VAL:HG22	1.98	0.46
24:U:264:ASP:H	24:U:277:GLN:C	2.24	0.46
29:N:3:DT:H6	29:N:3:DT:H2'	1.54	0.46
3:2:44:LYS:NZ	4:4:67:PHE:O	2.43	0.46
5:6:120:ARG:HA	5:6:309:PRO:HA	1.98	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
1:0:215:ASP:OD1	1:0:217:LYS:NZ	2.39	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
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
27:X:235:THR:OG1	27:X:238:ASP:O	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:LYS:NZ	9:B:336:ARG:H	2.10	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
1:0:380: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
9:B:364:ILE:HG22	9:B:585:VAL:HG23	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:379:ASN:O	2:1:382:SER:OG	2.30	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
7:M:157:CYS:SG	7:M:158:HIS:N	2.82	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:HD3	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
1:0:109:THR:OG1	1:0:110:SER:N	2.42	0.44
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
8:A:1431:GLY:HA3	9:B:1152:MET:HE2	1.98	0.44
19:L:34:CYS:SG	19:L:36:SER:OG	2.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:B:769:TYR:HB3	9:B:773:MET:HE3	1.99	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
17:J:5:VAL:H	17:J:5:VAL:HG23	1.82	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
9:B:586:TRP:CD1	9:B:588:GLY:H	2.36	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:1220:PHE:CE2	8:A:1267:MET:HE1	2.52	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
1:0:533: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
7:M:154:TYR:CD1	7:M:172:MET:HE1	2.53	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
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
1:0:489:LYS:HE2	1:0:724:MET:HE1	2.00	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
9:B:540:SER:O	9:B:543:SER:OG	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:130:ARG:HG2	15:H:134:ASN:HB3	2.01	0.43
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
9:B:542:MET:HE1	9:B:747:MET:HG3	1.99	0.43
12:E:26:ARG:NH2	12:E:187:TYR:O	2.47	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
4:4:288:ILE:HG23	5:6:322:MET:HG2	2.00	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:260:GLY:C	9:B:267:ARG:HH22	2.26	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:250:MET:HE1	19:L:48:CYS:O	2.19	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:O:243:VAL:O	1:O:247:SER:OG	2.28	0.43
1:O:571:VAL:HA	1:O:599:LEU:HB2	2.01	0.43
1:O:737:SER:OG	1:O: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: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:137:ASN:OD1	11:D:137:ASN:N	2.51	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
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
8:A:1444:MET:HE2	13:F:135:ARG:NH2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:780:VAL:HG13	8:A:789:LYS:HZ1	1.85	0.42
8:A:980:ASP:OD1	8:A:980:ASP:N	2.35	0.42
8:A:1111:MET:C	8:A:1113:THR:H	2.26	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
4:4:211:ASP:HB3	4:4:252:MET:HE1	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
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: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
18:K:1:MET:CA	18:K:1:MET:O	2.51	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
6:7:349: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:233:PRO:C	9:B:261:ARG:HH22	2.28	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
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
17:J:48:ARG:HG3	17:J:49:MET:N	2.34	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
6:7:455:SER:HB2	6:7:459:MET:HE2	2.02	0.41
8:A:457:ALA:HB3	8:A:506:ALA:HA	2.02	0.41
9:B:428:ILE:HD13	9:B:445:LYS:HZ2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:156:LEU:HD12	12:E:160:GLU:HG3	2.02	0.41
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:362:ASP:CG	8:A:459:ARG:HE	2.28	0.41
8:A:1025:ARG:HD3	8:A:1025:ARG:HA	1.81	0.41
8:A:1202:MET:HE2	8:A:1209:MET:HB3	2.02	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
1:0:534:PRO:C	1:0:567:LYS:HZ1	2.28	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
6:7:436: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:1128:GLN:HE22	8:A:1304:TRP:CD1	2.39	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
1:0:40:LEU:O	1:0:459:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:6:197:LYS:HA	5:6:200:ARG:HG3	2.03	0.41
8:A:1368:MET:HE2	8:A:1368:MET:HB3	1.82	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:115:MET:HE3	14:G:130:TYR:HD2	1.85	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
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:1063:MET:HE3	8:A:1436:ILE:HG23	2.01	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
16:I:17:ARG:HE	16:I:28:GLU:CD	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:M:297:LYS:O	7:M:301:THR:OG1	2.32	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
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
25:V:34:ALA:C	25:V:38:MET:HE2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
27:X:234:ARG:C	27:X:242:ARG:HH21	2.28	0.41
28:5:16:ILE:CG2	28:5:16:ILE:C	2.93	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:55:LEU:HD12	1:O:55:LEU:HA	1.85	0.40
2:1:586:LEU:HD22	2:1:623:ILE:HG23	2.03	0.40
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
3:2:454:TYR:HH	3:2:483:TRP:CG	2.39	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:42:ASP:OD2	26:W:217:TYR:OH	2.32	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
7:M:250:MET:O	7:M:253:THR:OG1	2.34	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
8:A:837:ILE:CG2	8:A:837:ILE:C	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:498:THR:OG1	9:B:537:LYS:HG3	2.21	0.40
10:C:145:CYS:SG	10:C:146:LYS:N	2.94	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
16:I:83:ASN:OD1	16:I:83:ASN:N	2.53	0.40
19:L:51:CYS:HB3	19:L:53:HIS:ND1	2.36	0.40
1:O:6:ASP:OD1	1:O: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
9:B:999:MET:HE2	9:B:999:MET:HB2	1.80	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
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%)	24	56
4	4	286/338 (85%)	276 (96%)	10 (4%)	0	100	100
5	6	351/461 (76%)	333 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	7	604/843 (72%)	575 (95%)	28 (5%)	1 (0%)	43	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%)	36	65
10	C	263/318 (83%)	225 (86%)	35 (13%)	3 (1%)	11	42
11	D	164/221 (74%)	153 (93%)	11 (7%)	0	100	100
12	E	212/215 (99%)	191 (90%)	20 (9%)	1 (0%)	24	56
13	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
14	G	169/171 (99%)	145 (86%)	23 (14%)	1 (1%)	21	52
15	H	129/146 (88%)	104 (81%)	23 (18%)	2 (2%)	7	35
16	I	112/122 (92%)	97 (87%)	15 (13%)	0	100	100
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%)	44	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

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Mol	Chain	Res	Type
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 ⓘ

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%)	683 (100%)	1 (0%)	88	88
2	1	389/589 (66%)	386 (99%)	3 (1%)	73	76
3	2	394/468 (84%)	391 (99%)	3 (1%)	73	76
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%)	535 (99%)	5 (1%)	70	75
7	M	245/299 (82%)	243 (99%)	2 (1%)	73	76
8	A	1235/1520 (81%)	1226 (99%)	9 (1%)	76	77
9	B	1000/1061 (94%)	999 (100%)	1 (0%)	88	88
10	C	233/274 (85%)	225 (97%)	8 (3%)	32	55
11	D	146/200 (73%)	146 (100%)	0	100	100
12	E	196/197 (100%)	194 (99%)	2 (1%)	68	74
13	F	77/137 (56%)	77 (100%)	0	100	100
14	G	151/152 (99%)	148 (98%)	3 (2%)	48	64
15	H	118/128 (92%)	116 (98%)	2 (2%)	53	67
16	I	108/116 (93%)	103 (95%)	5 (5%)	24	49
17	J	61/65 (94%)	57 (93%)	4 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	K	99/102 (97%)	94 (95%)	5 (5%)	21	47
19	L	39/57 (68%)	37 (95%)	2 (5%)	21	47
20	Q	147/641 (23%)	146 (99%)	1 (1%)	76	77
21	P	166/363 (46%)	166 (100%)	0	100	100
22	S	141/274 (52%)	140 (99%)	1 (1%)	76	77
23	O	153/205 (75%)	151 (99%)	2 (1%)	61	71
24	U	99/260 (38%)	96 (97%)	3 (3%)	36	57
25	V	94/108 (87%)	92 (98%)	2 (2%)	47	64
26	W	224/429 (52%)	223 (100%)	1 (0%)	84	81
27	X	144/295 (49%)	143 (99%)	1 (1%)	76	77
28	5	53/66 (80%)	51 (96%)	2 (4%)	29	53
All	All	7517/10168 (74%)	7449 (99%)	68 (1%)	68	75

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	659	MET
2	1	358	MET
2	1	385	MET
2	1	608	MET
3	2	97	MET
3	2	150	MET
3	2	466	GLN
6	7	112	MET
6	7	231	ARG
6	7	418	MET
6	7	742	MET
6	7	747	ASN
7	M	168	MET
7	M	317	TYR
8	A	217	LYS
8	A	415	LEU
8	A	437	MET
8	A	456	MET
8	A	761	MET
8	A	837	ILE
8	A	904	THR
8	A	1267	MET

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Mol	Chain	Res	Type
8	A	1454	MET
9	B	542	MET
10	C	18	VAL
10	C	24	ASN
10	C	37	MET
10	C	57	VAL
10	C	109	SER
10	C	209	TYR
10	C	230	MET
10	C	248	ILE
12	E	19	VAL
12	E	22	MET
14	G	10	ASN
14	G	33	GLU
14	G	148	GLU
15	H	88	SER
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	31	VAL
18	K	103	THR
19	L	30	ILE
19	L	63	ARG
20	Q	27	MET
22	S	282	TYR
23	O	221	GLU
23	O	236	GLU
24	U	27	ASN
24	U	264	ASP
24	U	277	GLN
25	V	38	MET
25	V	82	ASN

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Mol	Chain	Res	Type
26	W	356	THR
27	X	153	MET
28	5	16	ILE
28	5	29	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	280	GLN
1	0	521	ASN
1	0	628	GLN
2	1	182	GLN
2	1	262	ASN
2	1	513	GLN
2	1	594	ASN
2	1	598	GLN
3	2	405	HIS
3	2	407	GLN
4	4	139	GLN
4	4	142	GLN
4	4	246	GLN
4	4	315	HIS
5	6	202	GLN
5	6	302	ASN
5	6	351	ASN
5	6	382	HIS
5	6	450	ASN
6	7	169	HIS
6	7	528	ASN
6	7	644	GLN
7	M	158	HIS
7	M	212	ASN
7	M	285	ASN
8	A	4	GLN
8	A	68	GLN
8	A	358	ASN
8	A	425	GLN
8	A	479	ASN
8	A	503	GLN
8	A	626	ASN
8	A	654	ASN
8	A	660	ASN

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Mol	Chain	Res	Type
8	A	935	GLN
8	A	966	ASN
8	A	996	ASN
8	A	1171	GLN
8	A	1270	ASN
8	A	1330	ASN
9	B	278	GLN
9	B	325	GLN
9	B	357	GLN
9	B	395	GLN
9	B	494	HIS
9	B	706	GLN
9	B	770	GLN
9	B	878	GLN
9	B	881	ASN
9	B	1205	GLN
10	C	73	GLN
10	C	102	GLN
10	C	203	GLN
12	E	5	ASN
12	E	113	GLN
12	E	143	ASN
12	E	146	HIS
14	G	153	GLN
16	I	51	ASN
16	I	87	GLN
17	J	23	ASN
18	K	89	ASN
18	K	110	ASN
20	Q	122	GLN
21	P	85	ASN
21	P	234	HIS
21	P	242	ASN
21	P	324	GLN
22	S	205	ASN
23	O	91	ASN
24	U	19	ASN
24	U	33	GLN
24	U	36	GLN
24	U	43	GLN
24	U	280	GLN
25	V	65	ASN

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Mol	Chain	Res	Type
26	W	104	GLN
26	W	165	ASN
27	X	216	GLN
27	X	247	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

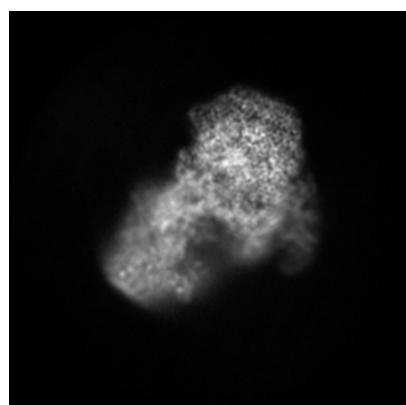
6 Map visualisation [i](#)

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.

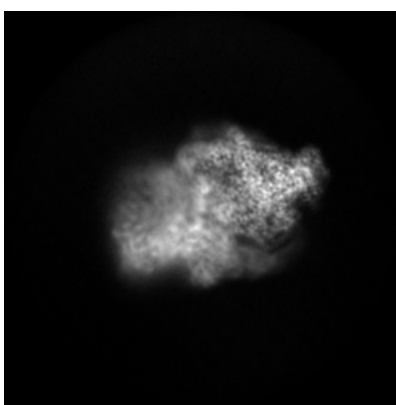
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

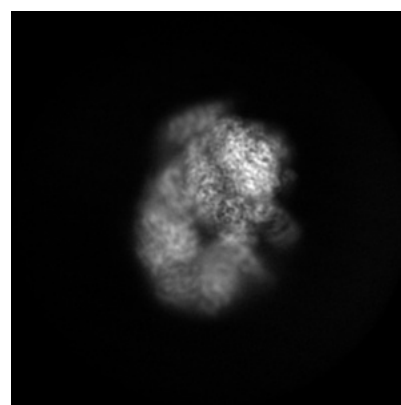
6.1.1 Primary map



X



Y

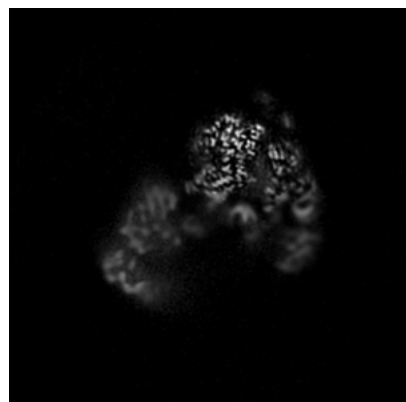


Z

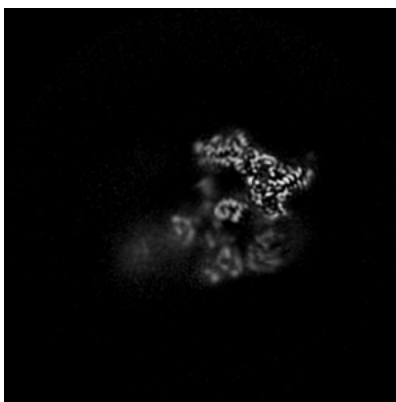
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

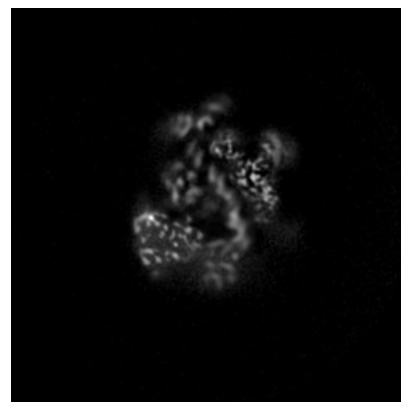
6.2.1 Primary map



X Index: 192



Y Index: 192

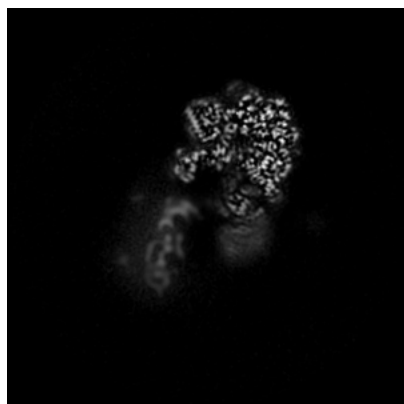


Z Index: 192

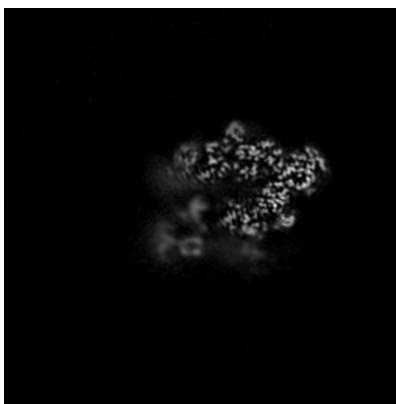
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

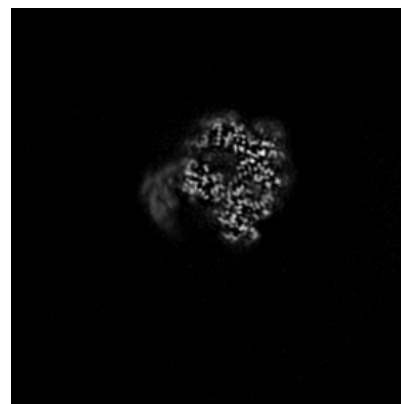
6.3.1 Primary map



X Index: 222



Y Index: 226

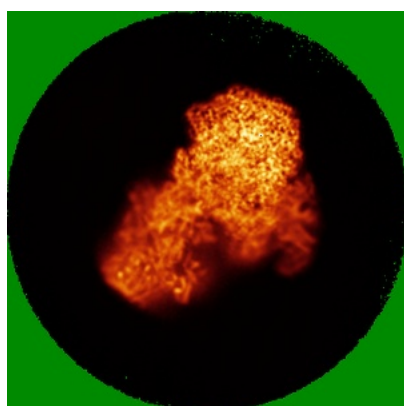


Z Index: 237

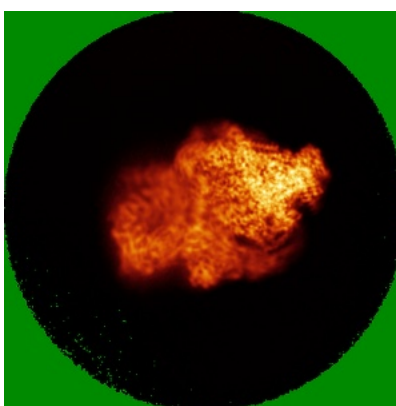
The images above show the largest variance slices of the map in three orthogonal directions.

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

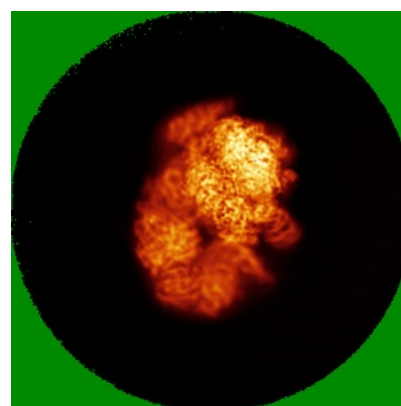
6.4.1 Primary map



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



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.

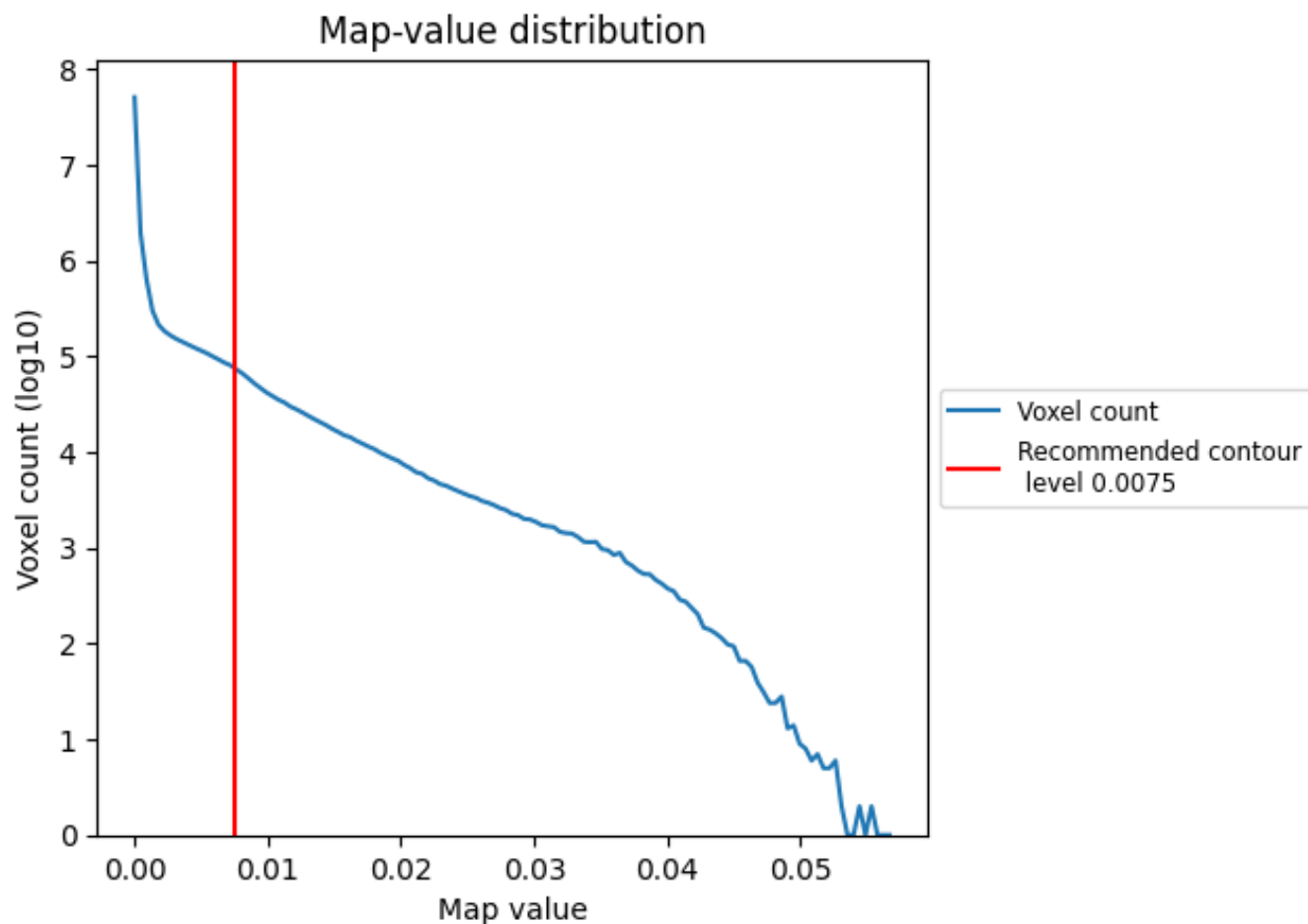
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

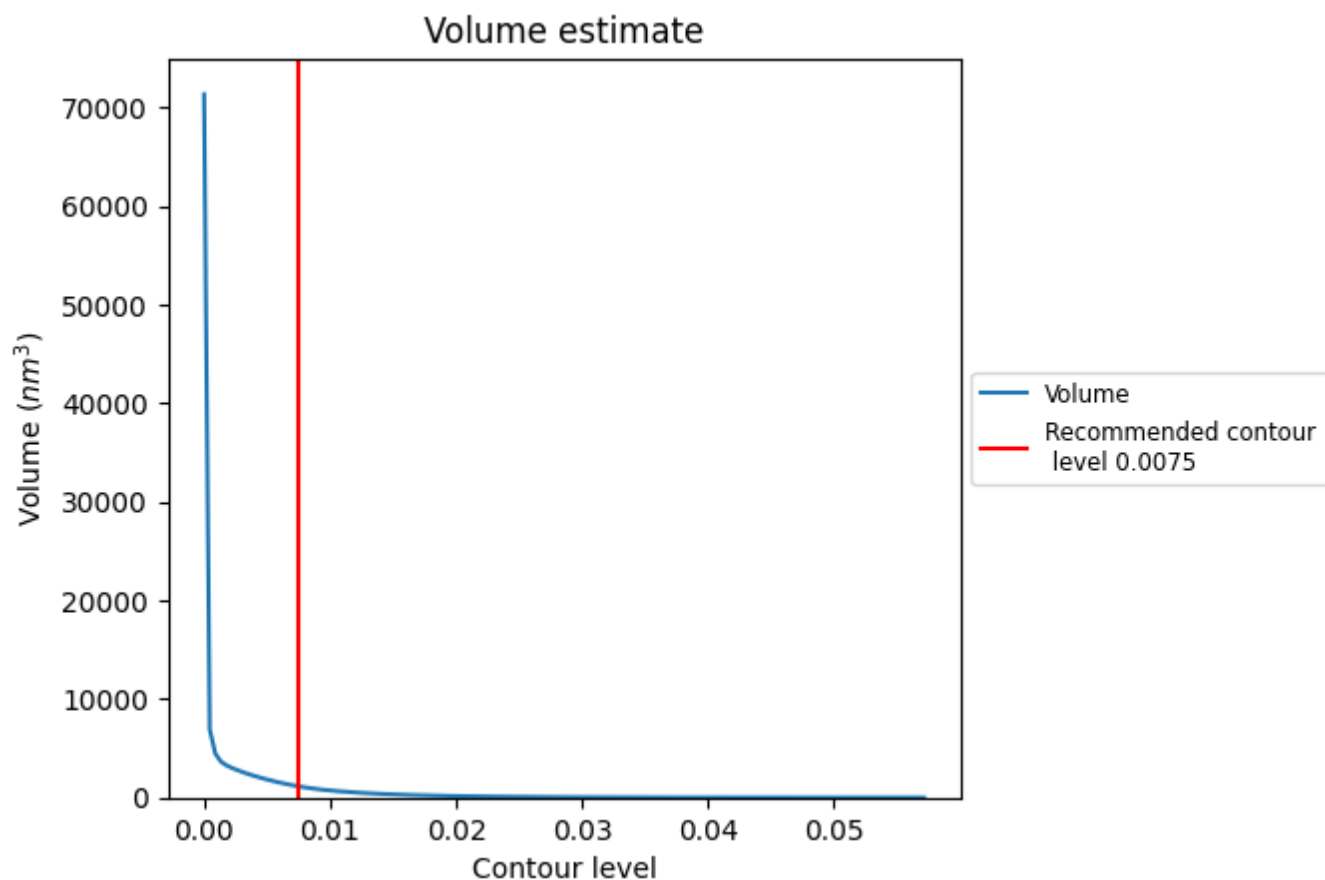
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

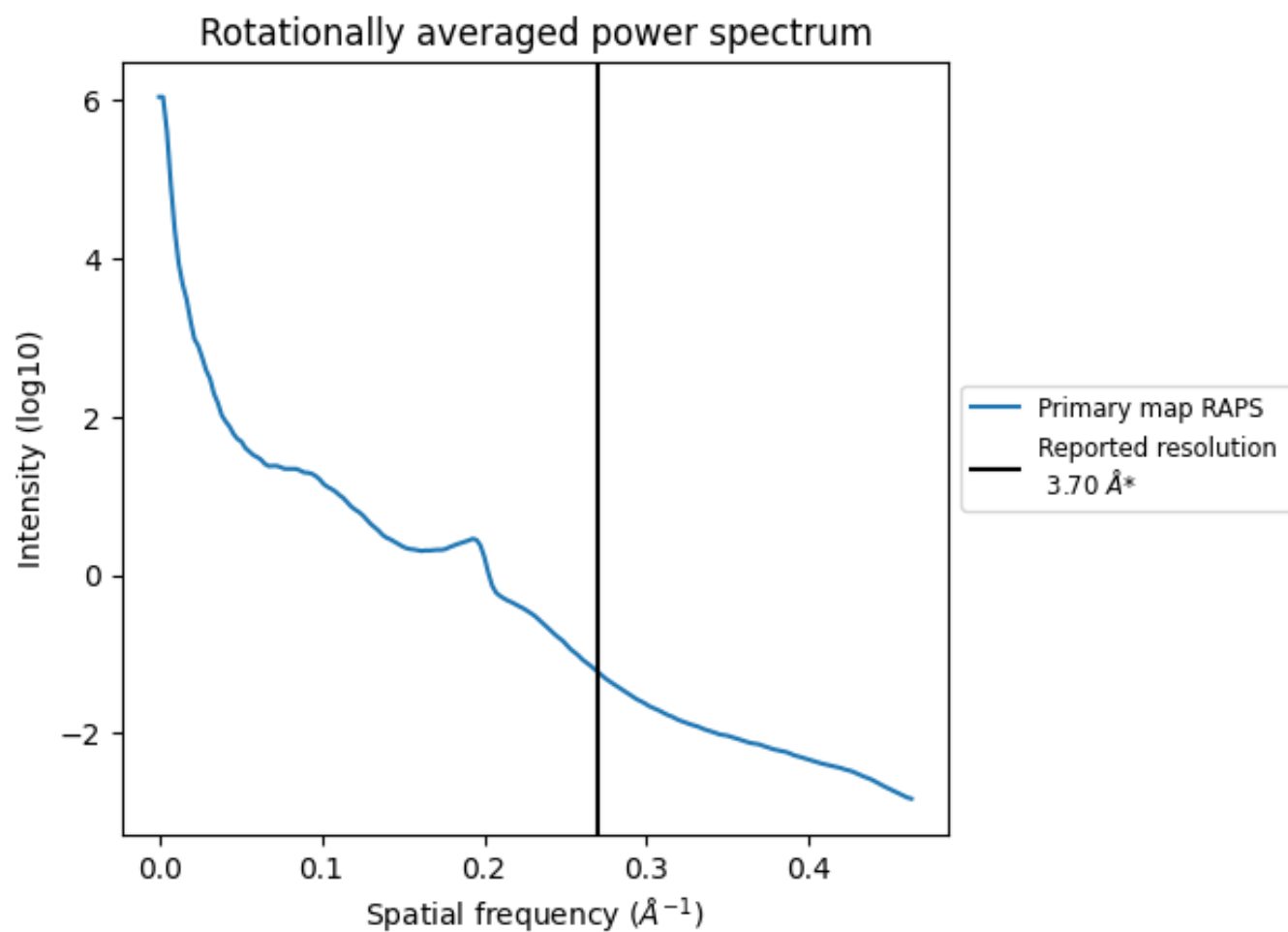
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1139 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

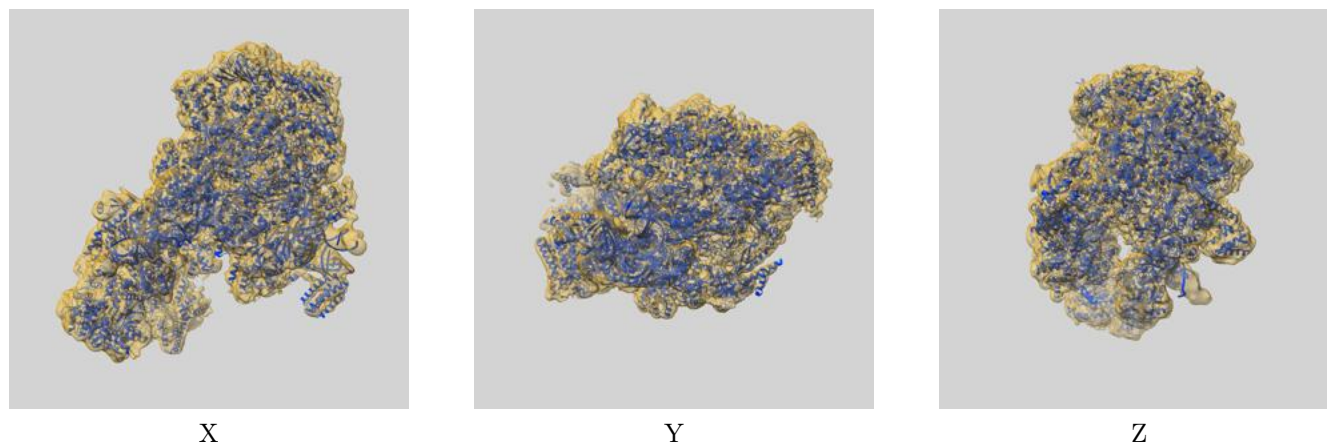
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

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 [i](#)



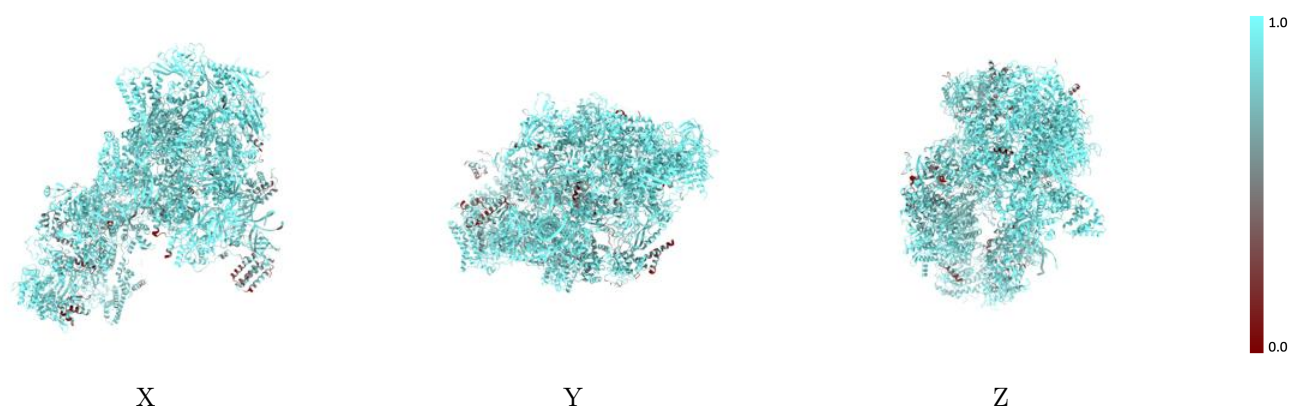
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



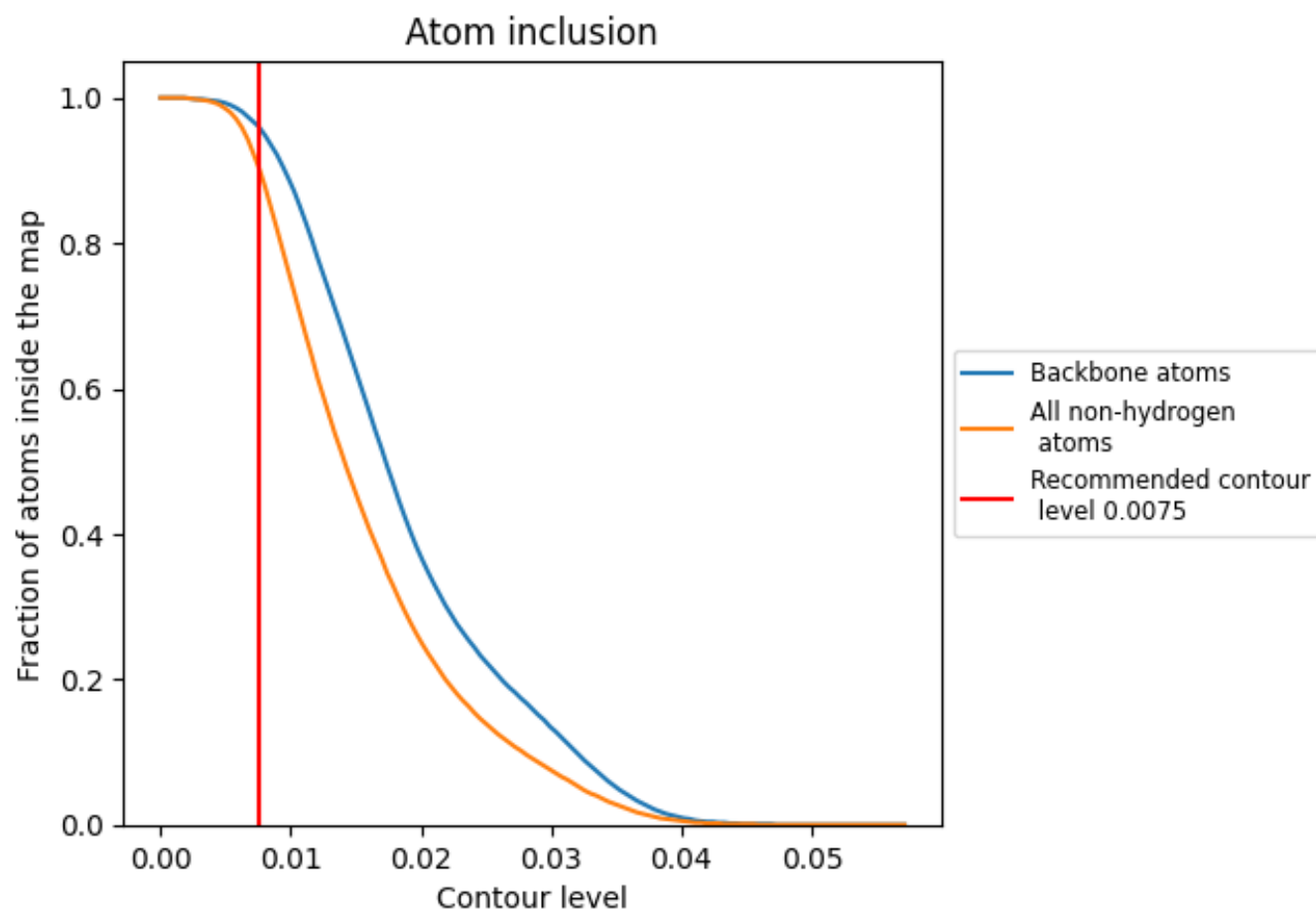
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

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

