



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 08:58 PM UTC

PDB ID : 8A3Y / pdb_00008a3y
EMDB ID : EMD-15127
Title : Structure of mammalian Pol II-DSIF-SPT6-PAF1-TFIIS-hexasome elongation complex
Authors : Farnung, L.; Ochmann, M.; Garg, G.; Vos, S.M.; Cramer, P.
Deposited on : 2022-06-09
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

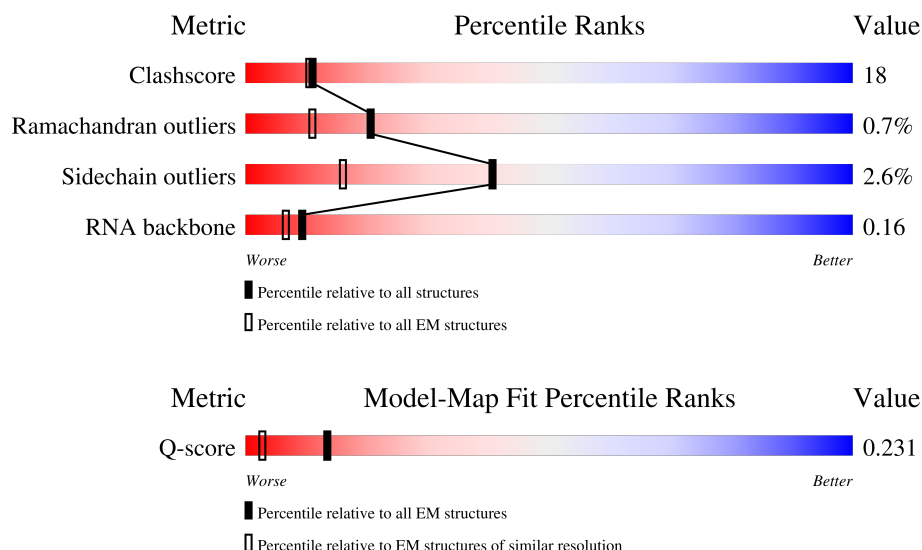
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	270	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1002	
14	N	127	
15	P	28	
16	Q	1845	
16	U	1845	
17	R	248	
18	T	138	
19	V	311	
20	W	305	
21	X	531	
22	Y	121	
23	Z	1087	
24	a	136	
24	e	136	
25	b	103	
25	f	103	

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Mol	Chain	Length	Quality of chain
26	c	103	65% 27% 8%
27	d	95	58% 35% 6%

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 125225 atoms, of which 59820 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms							AltConf	Trace
1	A	1426	Total	C	H	N	O	P	S	0	0
			22642	7074	11387	2014	2095	2	70		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1122	Total	C	H	N	O	S	0	0
			18007	5684	9027	1576	1656	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	258	Total	C	H	N	O	S	0	0
			4097	1300	2025	356	410	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			1985	630	981	170	200	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3458	1089	1738	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	78	Total	C	H	N	O	S	0	0
			1284	401	658	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2654	866	1321	214	245	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	149	Total	C	H	N	O	S	0	0
			2354	759	1157	195	238	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	116	Total	C	H	N	O	S	0	0
			1822	582	880	168	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O	S	0	0
			1068	339	544	88	91	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	47	Total	C	H	N	O	S	0	0
			786	240	396	77	67	6		

- Molecule 13 is a protein called SPT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	1002	Total	C	H	N	O	S	0	0
			7015	2583	2278	1071	1076	7		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	127	Total	C	H	N	O	P	0	0
			4051	1239	1420	507	758	127		

- Molecule 15 is a RNA chain called RNA, Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	28	Total	C	H	N	O	P	0	0
			911	271	307	120	185	28		

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog, RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	890	Total	C	H	N	O	S	0	0
			14396	4579	7170	1264	1352	31		
16	U	125	Total	C	H	N	O	S	0	0
			1524	534	672	151	166	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	linker	UNP Q6PD62
Q	1175	ASN	-	linker	UNP Q6PD62
Q	1176	LEU	-	linker	UNP Q6PD62
Q	1177	TYR	-	linker	UNP Q6PD62
Q	1178	PHE	-	linker	UNP Q6PD62
Q	1179	GLN	-	linker	UNP Q6PD62
U	-5	GLU	-	linker	UNP Q6PD62
U	-4	ASN	-	linker	UNP Q6PD62
U	-3	LEU	-	linker	UNP Q6PD62
U	-2	TYR	-	linker	UNP Q6PD62
U	-1	PHE	-	linker	UNP Q6PD62
U	0	GLN	-	linker	UNP Q6PD62

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	244	Total	C	H	N	O	S	0	0
			3523	1148	1691	340	337	7		

- Molecule 18 is a DNA chain called RNA, Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	138	Total	C	H	N	O	P	0	0
			4353	1331	1550	502	833	137		

- Molecule 19 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	244	Total	C	H	N	O	S	0	0
			3136	1061	1433	305	333	4		

- Molecule 20 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	W	300	Total	C	H	N	O	S	0	0
			4581	1483	2248	392	454	4		

- Molecule 21 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	43	Total	C	H	N	O	0	0
			725	220	372	69	64		

- Molecule 22 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Y	116	Total	C	H	N	O	S	0	0
			1819	570	908	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP Q4R941
Y	-2	PRO	-	expression tag	UNP Q4R941
Y	-1	GLY	-	expression tag	UNP Q4R941
Y	0	SER	-	expression tag	UNP Q4R941

- Molecule 23 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
23	Z	510	Total	C	H	N	O	P	S	0	0
			8063	2550	4040	709	745	1	18		

- Molecule 24 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	97	Total	C	H	N	O	S	0	0
			1643	506	841	155	138	3		
24	e	97	Total	C	H	N	O	S	0	0
			1640	504	839	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	engineered mutation	UNP P84233
e	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 25 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	b	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
25	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

- Molecule 26 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	c	103	Total	C	H	N	O		0	0
			1644	501	849	155	139			

- Molecule 27 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d	95	Total	C	H	N	O	S	0	0
			1521	469	776	134	140	2		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total	Zn	0
			2	2	
28	B	1	Total	Zn	0
			1	1	
28	C	1	Total	Zn	0
			1	1	
28	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
28	J	1	Total 1	Zn 1	0
28	L	1	Total 1	Zn 1	0
28	Y	1	Total 1	Zn 1	0

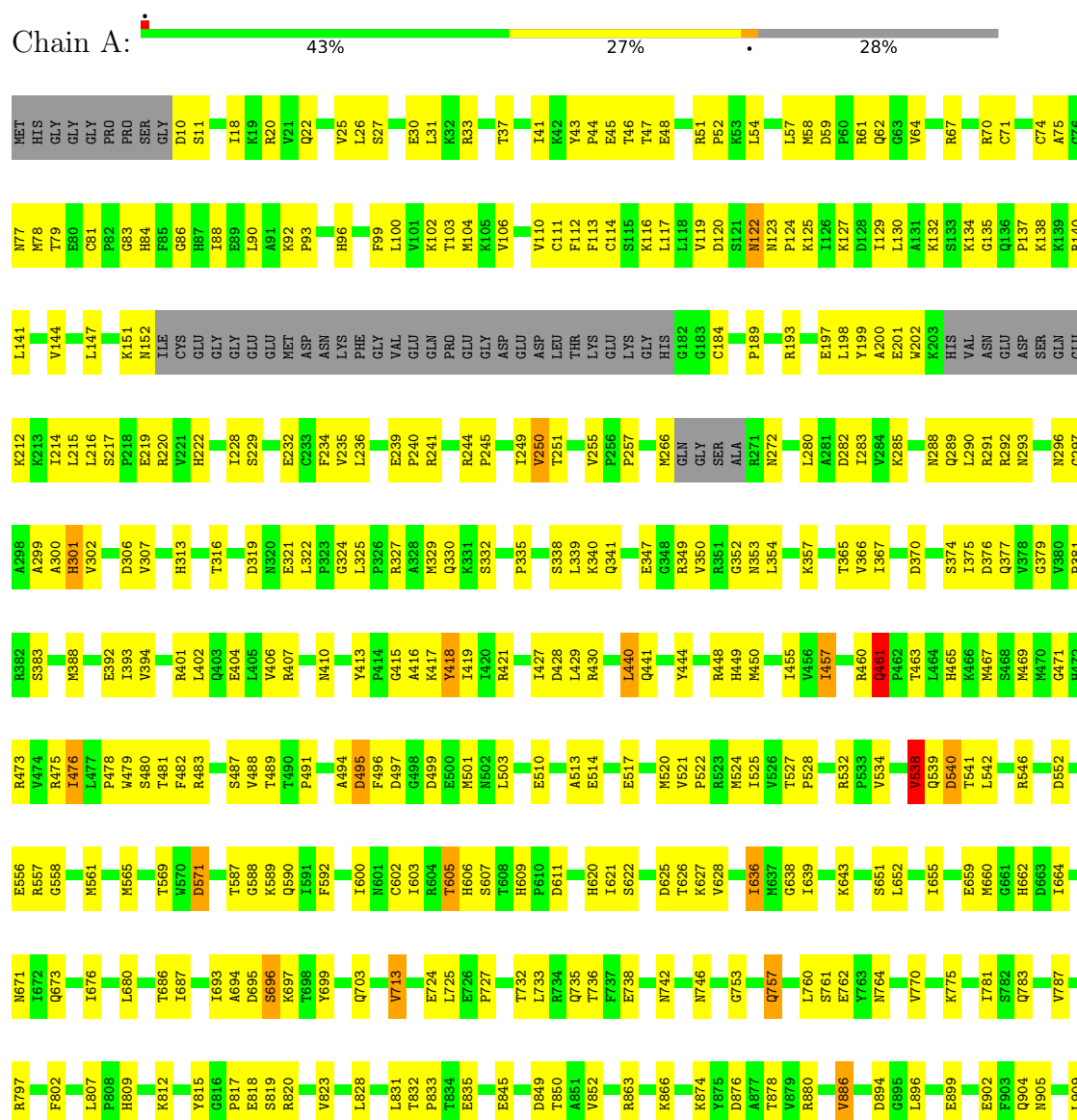
- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
29	P	1	Total 1	Mg 1	0

3 Residue-property plots

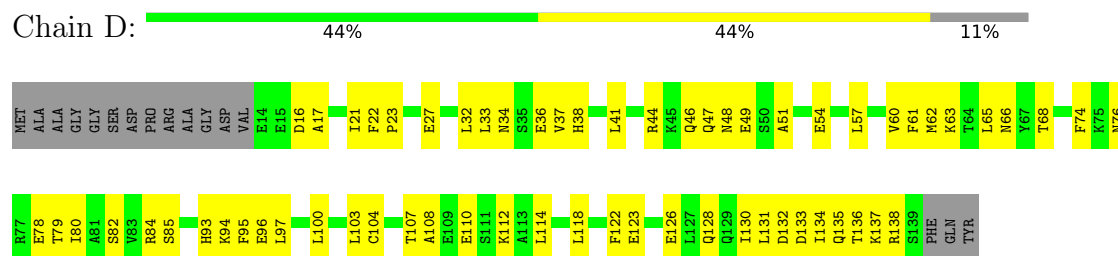
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase subunit

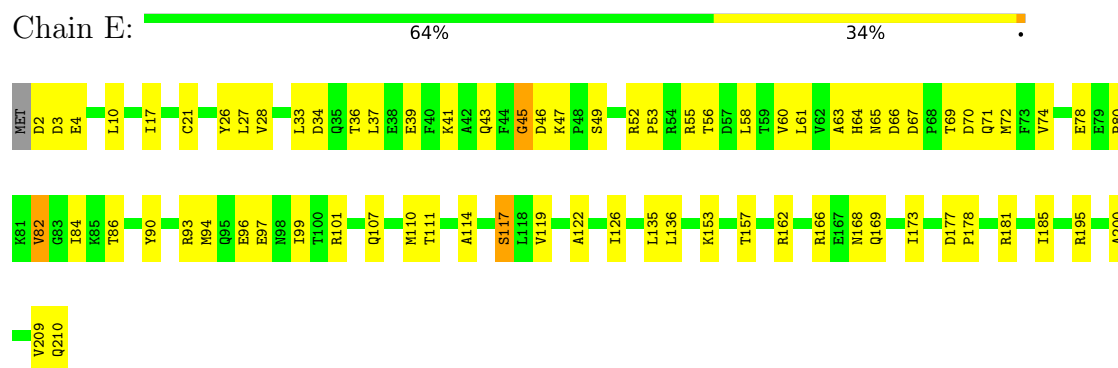




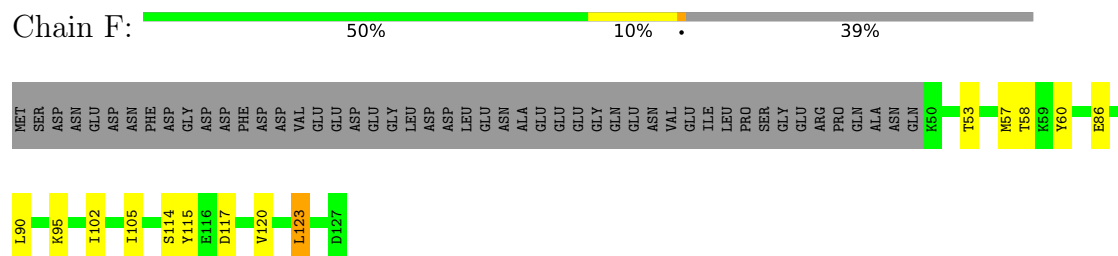
- Molecule 4: RNA polymerase II subunit D



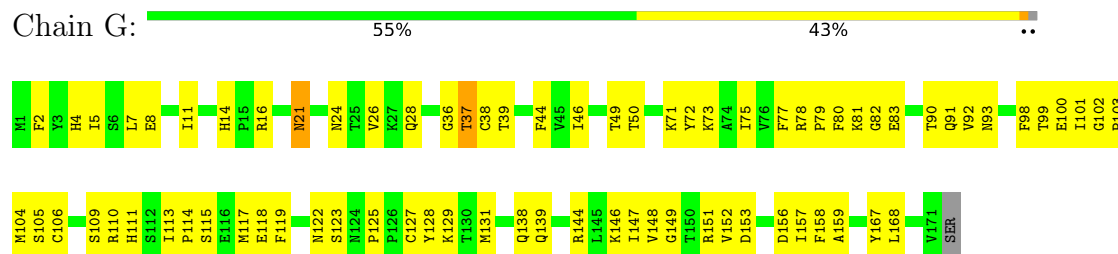
- Molecule 5: DNA-directed RNA polymerase II subunit E



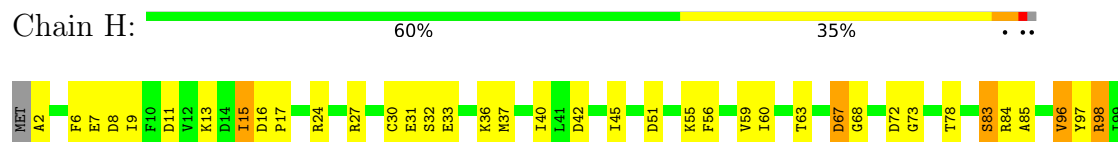
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

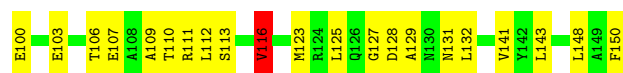


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



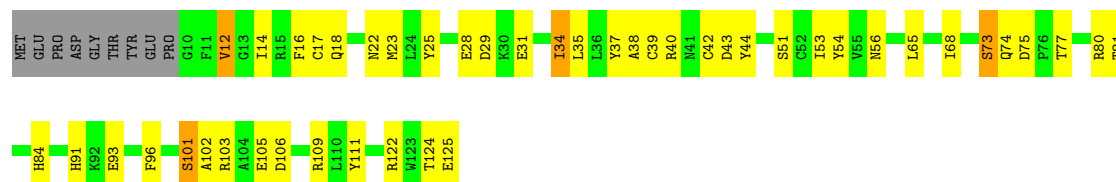
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3





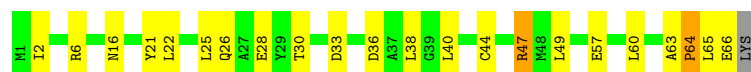
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 56% 34% 7%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 66% 30% 2%



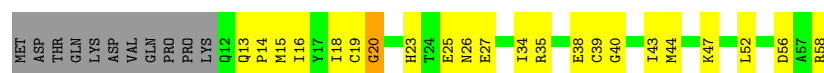
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 74% 23% 3%



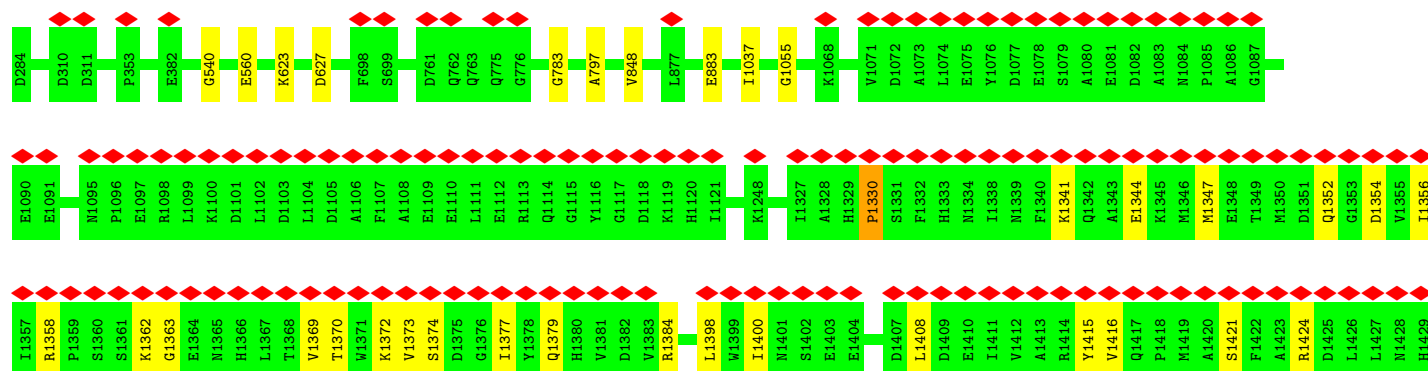
- Molecule 12: RNA polymerase II subunit K

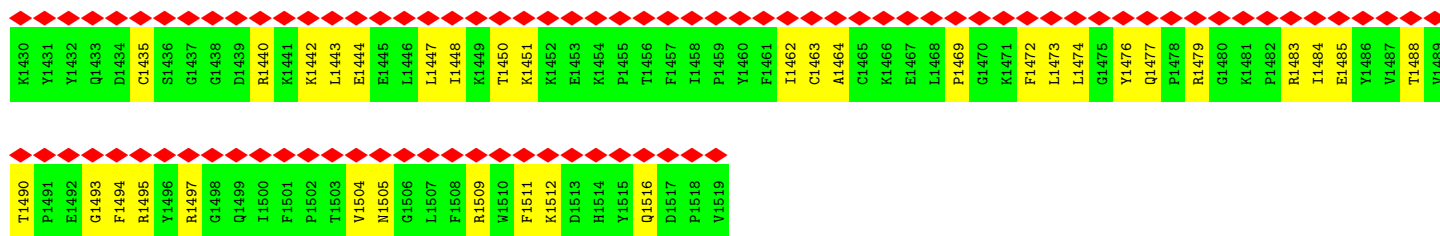
Chain L: 43% 36% 19%



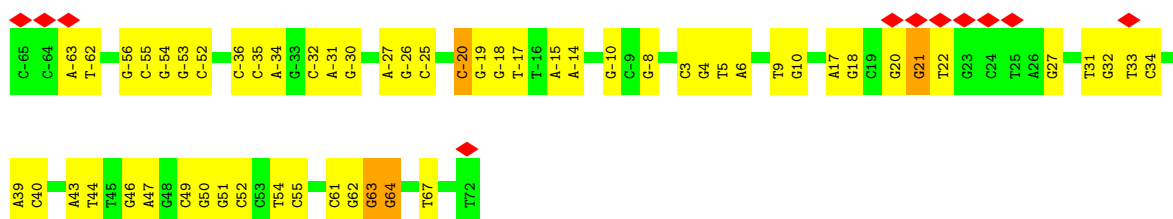
- Molecule 13: SPT6

Chain M: 23% 93% 7%

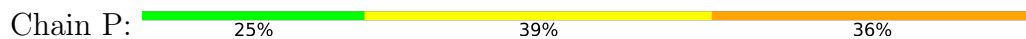




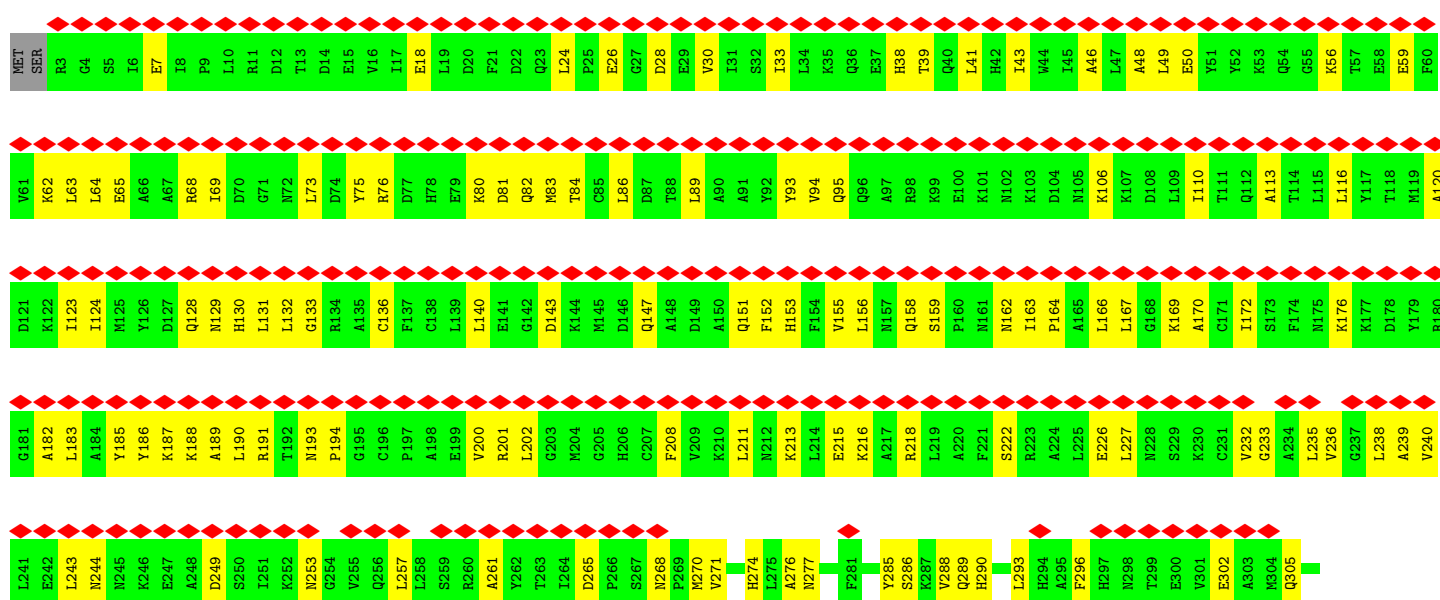
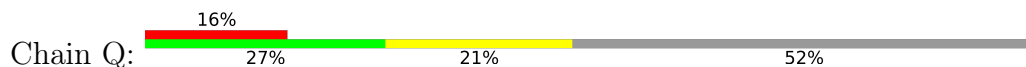
• Molecule 14: Non-template DNA

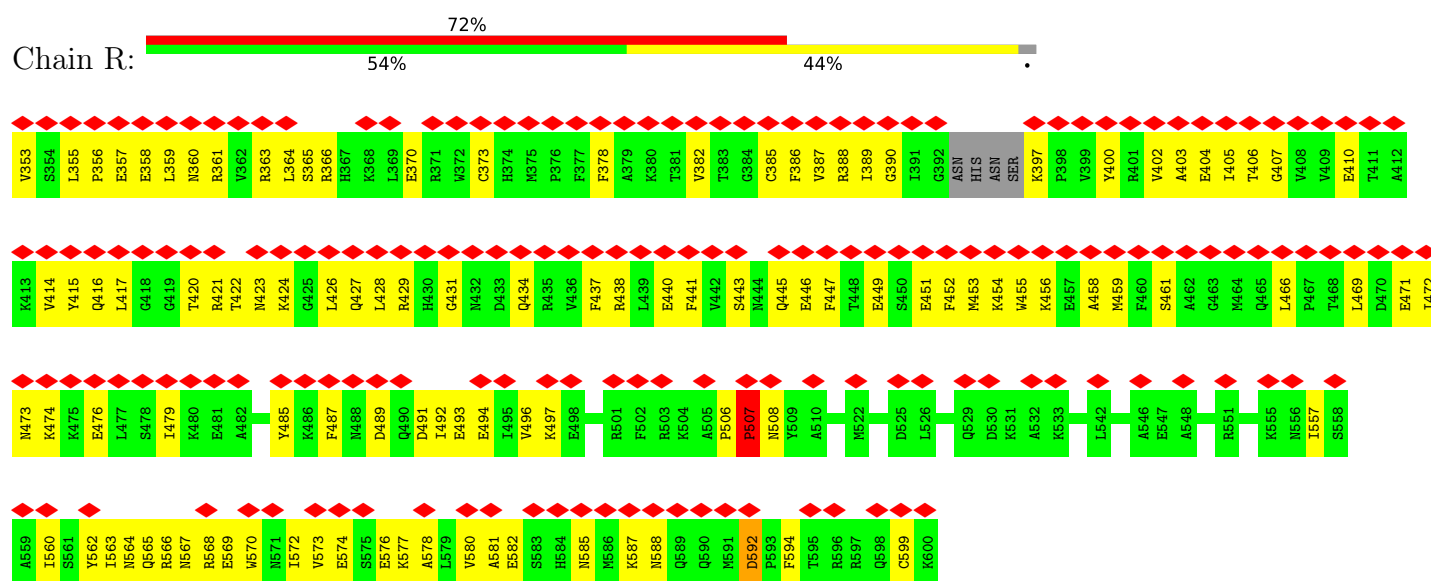


• Molecule 15: RNA, Template DNA

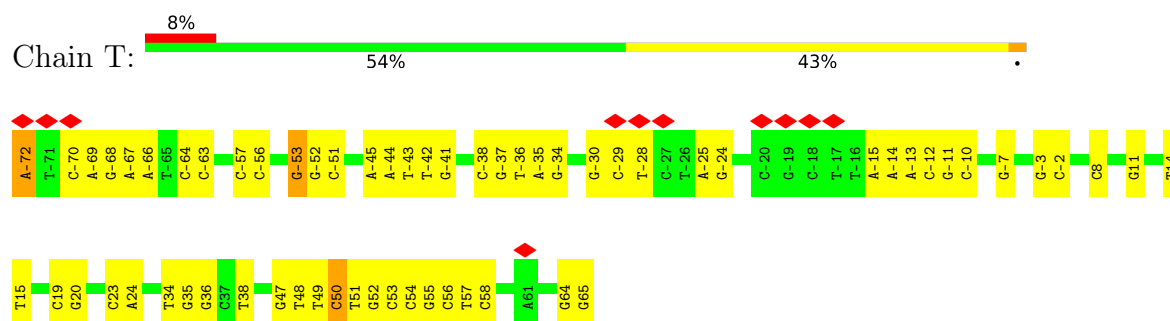


• Molecule 16: RNA polymerase-associated protein CTR9 homolog, RNA polymerase-associated protein LEO1

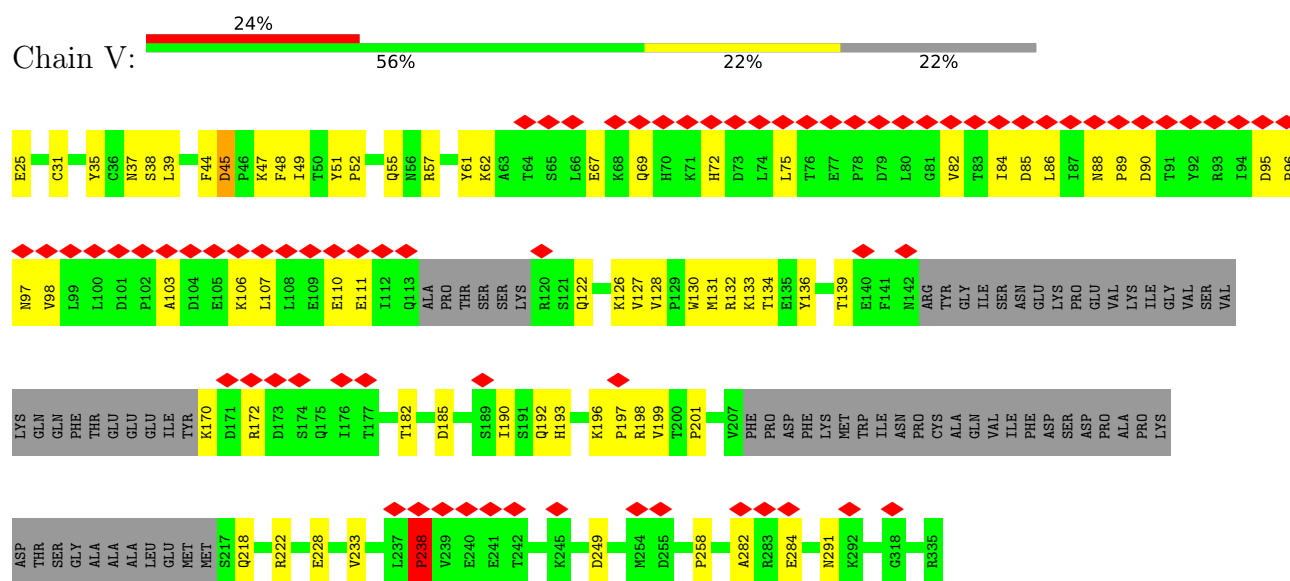




• Molecule 18: RNA, Template DNA



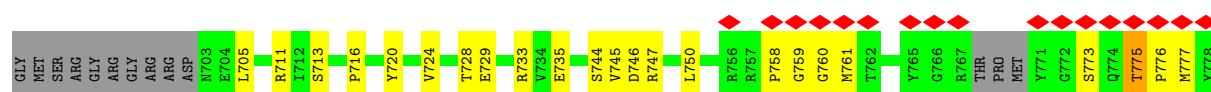
• Molecule 19: RNA polymerase II-associated factor 1 homolog



• Molecule 20: WD repeat-containing protein 61

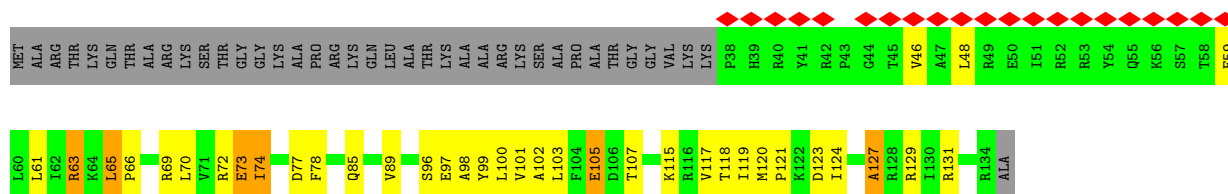
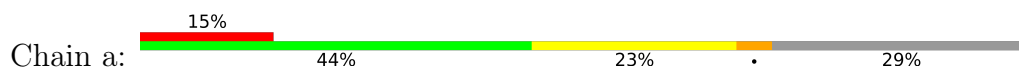




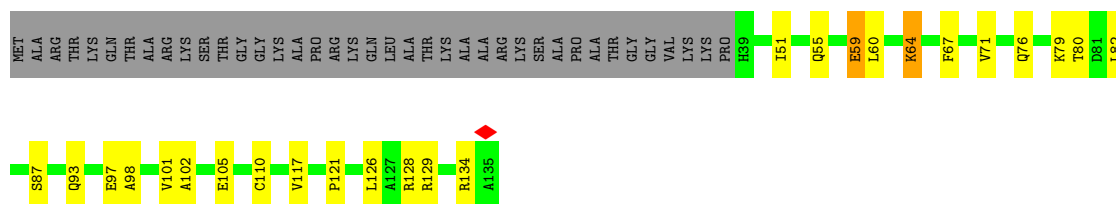




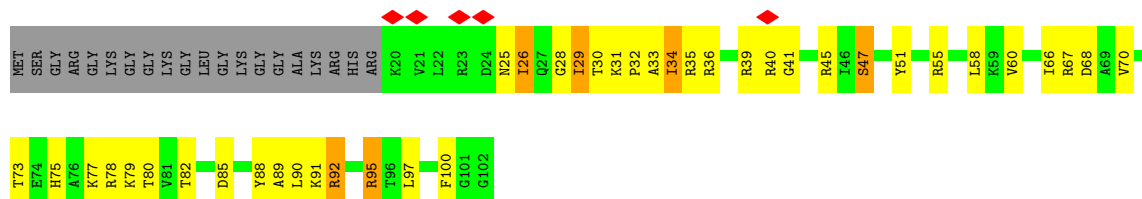
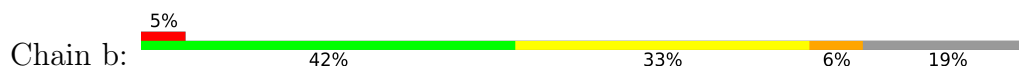
• Molecule 24: Histone H3.2



• Molecule 24: Histone H3.2

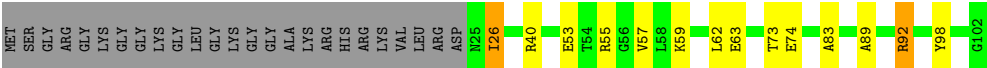


• Molecule 25: Histone H4

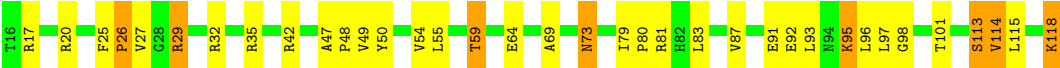


• Molecule 25: Histone H4

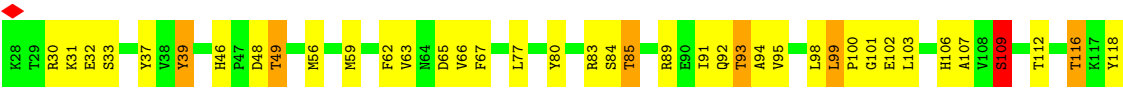




● Molecule 26: Histone H2A



● Molecule 27: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.036	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.41	9/11437 (0.1%)	0.97	12/15433 (0.1%)
2	B	1.57	8/9158 (0.1%)	1.07	20/12360 (0.2%)
3	C	1.69	3/2115 (0.1%)	1.06	5/2873 (0.2%)
4	D	0.40	0/1017	0.51	0/1368
5	E	1.23	0/1751	0.87	0/2366
6	F	1.62	1/636 (0.2%)	0.97	0/859
7	G	0.68	0/1364	0.66	0/1853
8	H	1.59	2/1219 (0.2%)	0.98	0/1644
9	I	1.13	0/964	0.88	0/1305
10	J	1.75	1/533 (0.2%)	1.00	0/719
11	K	1.69	1/939 (0.1%)	0.94	0/1271
12	L	1.40	0/395	1.11	1/525 (0.2%)
13	M	0.20	0/4763	0.43	1/6084 (0.0%)
14	N	0.44	0/2957	1.02	11/4566 (0.2%)
15	P	0.58	0/678	0.76	1/1055 (0.1%)
16	Q	0.31	0/7365	0.50	0/9927
16	U	0.36	0/864	0.75	3/1173 (0.3%)
17	R	0.36	0/1860	0.60	2/2509 (0.1%)
18	T	0.60	1/3137 (0.0%)	0.97	5/4835 (0.1%)
19	V	0.31	0/1728	0.65	2/2357 (0.1%)
20	W	0.32	0/2392	0.50	0/3257
21	X	0.33	0/356	0.54	0/478
22	Y	0.17	0/927	0.40	0/1250
23	Z	0.41	0/4081	0.52	1/5493 (0.0%)
24	a	0.83	1/814 (0.1%)	1.04	3/1092 (0.3%)
24	e	0.65	0/812	1.05	2/1088 (0.2%)
25	b	0.81	0/669	1.16	2/894 (0.2%)
25	f	0.68	0/626	1.01	0/837
26	c	0.58	0/805	0.97	1/1088 (0.1%)
27	d	0.60	0/756	1.02	2/1015 (0.2%)
All	All	1.04	27/67118 (0.0%)	0.85	74/91574 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
14	N	0	9
17	R	0	1
18	T	0	6
All	All	0	21

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	791	GLU	CA-CB	-13.39	1.20	1.53
2	B	94	SER	C-N	-8.44	1.07	1.33
3	C	104	ASP	CA-CB	-8.21	1.40	1.53
18	T	-72	DA	O5'-C5'	7.53	1.65	1.42
1	A	418	TYR	CA-CB	-6.89	1.43	1.53
2	B	504	THR	CB-CG2	-6.75	1.30	1.52
1	A	1396	ARG	CB-CG	-6.43	1.33	1.52
1	A	999	ARG	C-N	-6.31	1.15	1.33
1	A	590	GLN	CG-CD	-6.11	1.36	1.52
8	H	116	VAL	CB-CG1	-5.97	1.32	1.52
6	F	53	THR	C-N	-5.94	1.23	1.33
2	B	922	ARG	CB-CG	-5.65	1.35	1.52
1	A	26	LEU	C-N	-5.65	1.21	1.33
8	H	98	ARG	CB-CG	-5.49	1.35	1.52
2	B	755	GLN	C-N	-5.43	1.18	1.33
1	A	590	GLN	CB-CG	-5.41	1.36	1.52
2	B	924	ARG	CB-CG	-5.41	1.36	1.52
2	B	663	GLU	CA-CB	-5.39	1.44	1.53
24	a	127	ALA	CA-CB	-5.31	1.45	1.53
10	J	6	ARG	CB-CG	-5.25	1.36	1.52
3	C	44	ILE	CA-CB	-5.24	1.51	1.55
1	A	377	GLN	CB-CG	-5.24	1.36	1.52
3	C	45	ILE	CB-CG2	-5.12	1.35	1.52
11	K	43	GLY	CA-C	-5.11	1.44	1.51
1	A	1140	THR	CA-CB	-5.08	1.36	1.53
1	A	886	VAL	CB-CG1	-5.05	1.35	1.52
2	B	29	VAL	CB-CG2	-5.03	1.35	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	20	DG	O3'-P-O5'	-15.18	81.22	104.00
14	N	20	DG	OP2-P-O3'	-8.28	83.17	108.00
3	C	224	GLY	CA-C-N	8.13	147.27	121.98
3	C	224	GLY	C-N-CA	8.13	147.27	121.98
19	V	258	PRO	N-CA-CB	7.97	110.87	103.46
17	R	507	PRO	N-CA-CB	7.88	111.53	103.25
17	R	506	PRO	N-CA-CB	7.85	110.70	103.08
1	A	636	ILE	N-CA-C	-6.95	105.06	111.67
13	M	1330	PRO	N-CA-CB	6.86	110.45	103.25
19	V	238	PRO	N-CA-CB	6.76	110.35	103.25
1	A	538	VAL	N-CA-C	6.71	123.29	109.34
16	U	463	PRO	N-CA-CB	6.66	110.24	103.25
2	B	575	GLY	N-CA-C	6.58	118.72	112.08
1	A	122	ASN	N-CA-C	-6.52	104.72	114.64
1	A	1368	VAL	N-CA-C	-6.43	105.44	111.48
16	U	493	PRO	N-CA-CB	6.35	109.92	103.25
1	A	1396	ARG	CG-CD-NE	-6.34	98.06	112.00
1	A	457	ILE	CG1-CB-CG2	-6.32	91.75	110.70
2	B	629	GLU	CA-C-N	-6.30	113.11	122.56
2	B	629	GLU	C-N-CA	-6.30	113.11	122.56
18	T	19	DC	C5'-C4'-C3'	-6.29	105.47	114.90
2	B	594	MET	CA-C-N	-6.24	114.04	121.90
2	B	594	MET	C-N-CA	-6.24	114.04	121.90
23	Z	758	PRO	N-CA-CB	6.23	109.80	103.25
2	B	236	TRP	CA-C-N	-6.23	115.74	122.59
2	B	236	TRP	C-N-CA	-6.23	115.74	122.59
2	B	1122	CYS	N-CA-C	-6.22	99.94	109.65
24	a	89	VAL	N-CA-C	-6.15	104.33	110.30
2	B	790	GLN	CA-C-N	-6.13	113.78	123.23
2	B	790	GLN	C-N-CA	-6.13	113.78	123.23
14	N	34	DC	P-O3'-C3'	6.07	129.30	120.20
14	N	64	DG	P-O3'-C3'	5.97	129.16	120.20
2	B	371	ARG	CA-CB-CG	-5.82	102.46	114.10
18	T	20	DG	C5'-C4'-C3'	-5.77	106.24	114.90
3	C	113	ARG	CA-C-N	-5.77	113.93	122.41
3	C	113	ARG	C-N-CA	-5.77	113.93	122.41
25	b	25	ASN	N-CA-C	5.73	118.30	111.71
18	T	-53	DG	P-O3'-C3'	5.70	128.75	120.20
2	B	629	GLU	N-CA-C	5.64	118.51	111.24
14	N	-20	DC	C5'-C4'-C3'	-5.63	106.45	114.90
1	A	524	MET	CG-SD-CE	-5.48	88.85	100.90
24	a	107	THR	N-CA-C	-5.44	105.04	110.97
27	d	99	LEU	CA-C-N	5.40	126.87	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	99	LEU	C-N-CA	5.40	126.87	120.23
2	B	146	LYS	CB-CA-C	-5.39	104.23	111.89
1	A	461	GLN	N-CA-C	5.38	121.70	109.81
14	N	-14	DA	O5'-C5'-C4'	5.38	118.87	110.80
14	N	-8	DG	O5'-C5'-C4'	5.38	118.86	110.80
14	N	63	DG	P-O3'-C3'	5.33	128.20	120.20
12	L	20	GLY	N-CA-C	-5.33	100.56	113.18
14	N	20	DG	OP1-P-O3'	-5.32	92.06	108.00
2	B	146	LYS	CA-CB-CG	5.27	124.64	114.10
15	P	36	A	C4'-C3'-O3'	5.23	117.25	109.40
2	B	839	GLY	N-CA-C	-5.23	105.24	111.36
14	N	54	DT	P-O3'-C3'	5.20	128.00	120.20
1	A	1072	ILE	CA-C-N	-5.18	112.93	120.29
1	A	1072	ILE	C-N-CA	-5.18	112.93	120.29
24	a	103	LEU	N-CA-C	5.18	116.62	110.97
2	B	567	ILE	CG1-CB-CG2	-5.14	95.27	110.70
18	T	-51	DC	P-O3'-C3'	5.11	127.86	120.20
18	T	50	DC	OP1-P-O3'	5.11	123.33	108.00
2	B	959	GLU	CA-C-N	-5.10	111.41	121.41
2	B	959	GLU	C-N-CA	-5.10	111.41	121.41
26	c	95	LYS	N-CA-C	-5.09	105.42	110.97
14	N	21	DG	P-O3'-C3'	5.09	127.84	120.20
2	B	648	TYR	CA-C-N	-5.08	111.84	121.54
2	B	648	TYR	C-N-CA	-5.08	111.84	121.54
16	U	516	ALA	N-CA-C	5.06	121.57	110.80
24	e	64	LYS	CA-C-N	5.04	125.42	119.83
24	e	64	LYS	C-N-CA	5.04	125.42	119.83
25	b	60	VAL	CB-CA-C	-5.02	105.36	112.14
3	C	60	HIS	CB-CA-C	-5.02	100.43	110.42
1	A	1176	TYR	CA-C-N	-5.00	115.10	122.06
1	A	1176	TYR	C-N-CA	-5.00	115.10	122.06

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1434	GLU	Peptide
1	A	910	LYS	Peptide
2	B	20	ASP	Peptide
2	B	547	GLU	Peptide
2	B	686	GLU	Peptide
14	N	-10	DG	Sidechain

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Mol	Chain	Res	Type	Group
14	N	-15	DA	Sidechain
14	N	-17	DT	Sidechain
14	N	-18	DG	Sidechain
14	N	-19	DG	Sidechain
14	N	-20	DC	Sidechain
14	N	-25	DC	Sidechain
14	N	-26	DG	Sidechain
14	N	-27	DA	Sidechain
17	R	592	ASP	Peptide
18	T	11	DG	Sidechain
18	T	14	DT	Sidechain
18	T	15	DT	Sidechain
18	T	23	DC	Sidechain
18	T	24	DA	Sidechain
18	T	8	DC	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	11387	11374	462	0
2	B	8980	9027	9019	320	0
3	C	2072	2025	2019	43	0
4	D	1004	981	980	53	0
5	E	1720	1738	1737	77	0
6	F	626	658	657	11	0
7	G	1333	1321	1321	83	0
8	H	1197	1157	1156	45	0
9	I	942	880	873	41	0
10	J	524	544	541	19	0
11	K	920	942	942	26	0
12	L	390	396	397	13	0
13	M	4737	2278	2262	49	0
14	N	2631	1420	1421	48	0
15	P	604	307	307	30	0
16	Q	7226	7170	7169	367	0
16	U	852	672	668	31	0
17	R	1832	1691	1687	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	T	2803	1550	1550	55	0
19	V	1703	1433	1426	88	0
20	W	2333	2248	2246	154	0
21	X	353	372	371	30	0
22	Y	911	908	908	27	0
23	Z	4023	4040	4035	184	0
24	a	802	841	841	21	0
24	e	801	839	838	16	0
25	b	662	710	709	37	0
25	f	619	660	659	10	0
26	c	795	849	846	26	0
27	d	745	776	773	39	0
28	A	2	0	0	0	0
28	B	1	0	0	0	0
28	C	1	0	0	0	0
28	I	2	0	0	0	0
28	J	1	0	0	0	0
28	L	1	0	0	0	0
28	Y	1	0	0	0	0
29	P	1	0	0	0	0
All	All	65405	59820	59732	2267	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 18.

All (2267) 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)
18:T:-72:DA:C5'	18:T:-72:DA:O5'	1.65	1.42
25:b:75:HIS:CD2	27:d:93:THR:HG21	1.58	1.38
25:b:75:HIS:HD2	27:d:93:THR:CG2	1.55	1.19
2:B:953:ASP:OD1	3:C:36:ARG:NH1	1.96	0.98
8:H:37:MET:HE2	8:H:127:GLY:HA3	1.43	0.96
1:A:904:GLN:NE2	1:A:981:CYS:O	2.01	0.93
14:N:-36:DC:H42	18:T:36:DG:H1	1.18	0.92
20:W:278:TRP:HB2	20:W:293:GLY:HA2	1.51	0.91
2:B:105:PRO:HG2	16:U:512:THR:HA	1.51	0.91
16:Q:505:ARG:HH11	19:V:44:PHE:HB2	1.32	0.91
26:c:55:LEU:O	26:c:59:THR:HG22	1.70	0.91
20:W:40:LEU:HD12	20:W:66:GLY:HA3	1.53	0.90
1:A:1227:THR:H	1:A:1230:GLN:HE21	1.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:7:PRO:HG3	22:Y:23:LYS:HA	1.53	0.89
1:A:609:HIS:HD1	1:A:626:THR:HG1	1.09	0.89
16:Q:830:ARG:HA	16:Q:833:LYS:HE2	1.54	0.88
16:Q:768:VAL:HG21	16:Q:778:GLU:HG3	1.55	0.88
2:B:332:LYS:NZ	2:B:333:GLU:OE1	2.07	0.88
16:Q:727:LEU:HB3	16:Q:732:LYS:HB3	1.57	0.87
9:I:103:ARG:NH1	9:I:105:GLU:OE2	2.09	0.86
3:C:193:ARG:NH1	3:C:218:ALA:O	2.09	0.86
8:H:98:ARG:NH1	8:H:100:GLU:OE1	2.09	0.85
17:R:388:ARG:NH2	17:R:446:GLU:O	2.08	0.85
17:R:387:VAL:HG13	17:R:405:ILE:HD11	1.58	0.85
25:b:75:HIS:HD2	27:d:93:THR:HG21	0.71	0.85
23:Z:478:VAL:HB	23:Z:518:LEU:HD11	1.58	0.85
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.40	0.84
4:D:107:THR:HG23	4:D:110:GLU:H	1.43	0.84
22:Y:75:GLN:O	22:Y:111:ARG:NH2	2.09	0.84
1:A:197:GLU:HB2	1:A:215:LEU:HD11	1.60	0.84
16:Q:682:ASP:O	16:Q:686:ASN:ND2	2.09	0.84
18:T:58:DC:H4'	23:Z:283:ARG:HE	1.41	0.84
16:Q:643:ASP:OD2	21:X:239:GLN:NE2	2.11	0.83
2:B:85:LEU:HB2	2:B:131:THR:HB	1.59	0.83
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.10	0.83
20:W:172:ILE:HB	20:W:186:LEU:HB2	1.61	0.83
5:E:166:ARG:HH12	5:E:168:ASN:HD22	1.26	0.83
17:R:570:TRP:HB3	19:V:133:LYS:HE2	1.61	0.83
20:W:35:VAL:HB	20:W:47:TRP:HB2	1.59	0.83
1:A:404:GLU:OE2	1:A:407:ARG:NH2	2.12	0.82
2:B:613:ARG:NH2	2:B:615:TYR:OH	2.12	0.82
1:A:392:GLU:OE2	1:A:401:ARG:NH1	2.11	0.82
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.12	0.82
10:J:25:LEU:HB3	17:R:563:ILE:HD11	1.61	0.82
22:Y:3:LEU:O	22:Y:8:LYS:NZ	2.12	0.82
16:Q:276:ALA:HB1	16:Q:288:VAL:HG23	1.62	0.82
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.62	0.81
20:W:95:ASN:O	20:W:97:LYS:NZ	2.12	0.81
1:A:349:ARG:HE	2:B:1157:LEU:HD22	1.45	0.81
16:Q:268:ASN:HD22	16:Q:271:VAL:H	1.29	0.80
16:Q:387:ALA:N	16:Q:390:ASP:OD2	2.13	0.80
4:D:76:ASN:HD22	4:D:79:THR:HG23	1.45	0.80
19:V:47:LYS:HB3	21:X:228:GLU:HB2	1.63	0.79
2:B:756:LYS:NZ	19:V:134:THR:OG1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:737:LYS:HZ2	16:Q:764:LEU:HD13	1.46	0.79
1:A:571:ASP:OD1	1:A:571:ASP:N	2.13	0.79
16:Q:624:LYS:HG3	16:Q:627:ARG:HH11	1.47	0.79
20:W:237:ASN:HD22	20:W:279:GLY:HA2	1.45	0.79
1:A:1525:TPO:O3P	13:M:1358:ARG:NH1	2.15	0.79
16:Q:41:LEU:HD23	16:Q:81:ASP:HB3	1.65	0.79
20:W:237:ASN:HB3	20:W:280:VAL:HG22	1.65	0.79
1:A:1536:GLY:O	13:M:1483:ARG:NH1	2.16	0.78
15:P:24:A:H3'	15:P:25:A:H8	1.47	0.78
27:d:95:VAL:HG13	27:d:99:LEU:HD12	1.66	0.78
1:A:1182:GLN:O	1:A:1192:TRP:NE1	2.14	0.78
1:A:539:GLN:O	1:A:541:THR:N	2.16	0.78
1:A:1189:ASP:HA	1:A:1192:TRP:HE3	1.48	0.78
2:B:297:MET:HG2	2:B:377:LEU:HD11	1.65	0.78
15:P:25:A:H2'	15:P:26:C:C6	2.19	0.78
16:U:394:TYR:O	19:V:172:ARG:NH1	2.16	0.78
20:W:35:VAL:N	20:W:47:TRP:O	2.12	0.78
7:G:111:HIS:HB3	23:Z:494:ARG:HB2	1.64	0.78
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.66	0.78
14:N:52:DC:N4	18:T:52:DG:O6	2.16	0.78
24:e:121:PRO:HB3	25:f:53:GLU:HG3	1.66	0.78
3:C:154:ARG:NH2	10:J:63:ALA:HB2	1.98	0.78
24:e:60:LEU:HD13	24:e:93:GLN:HG2	1.66	0.78
16:Q:568:TRP:HE1	16:Q:591:ILE:HD12	1.49	0.77
18:T:53:DG:OP2	27:d:39:TYR:OH	2.02	0.77
25:b:75:HIS:CD2	27:d:93:THR:CG2	2.44	0.77
1:A:713:VAL:HG21	1:A:817:PRO:HD3	1.67	0.77
1:A:1180:ASN:O	1:A:1183:SER:OG	2.00	0.77
23:Z:216:VAL:HB	23:Z:226:TYR:HB2	1.65	0.76
15:P:23:G:H2'	15:P:24:A:H8	1.49	0.76
1:A:413:TYR:O	1:A:415:GLY:N	2.17	0.76
1:A:1189:ASP:HA	1:A:1192:TRP:CE3	2.20	0.76
17:R:562:TYR:O	17:R:566:ARG:NE	2.18	0.76
20:W:14:ALA:N	20:W:296:GLN:O	2.13	0.76
16:Q:268:ASN:HD21	16:Q:270:MET:HB3	1.49	0.76
23:Z:257:ILE:HA	23:Z:260:MET:HE2	1.68	0.76
19:V:47:LYS:HE3	21:X:230:VAL:HG22	1.67	0.76
9:I:101:SER:OG	9:I:102:ALA:O	2.03	0.75
23:Z:728:THR:O	23:Z:747:ARG:NH2	2.18	0.75
1:A:272:ASN:ND2	18:T:51:DT:O2	2.19	0.75
16:Q:353:TYR:OH	19:V:57:ARG:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:-53:DG:H2''	18:T:-52:DG:OP2	1.87	0.75
1:A:659:GLU:OE2	1:A:985:ARG:NH2	2.19	0.75
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.52	0.75
11:K:77:THR:OG1	11:K:81:TYR:O	2.04	0.75
1:A:296:ASN:OD1	1:A:297:GLY:N	2.20	0.75
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.68	0.75
1:A:1467:GLY:O	1:A:1469:GLY:N	2.20	0.74
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.66	0.74
16:Q:314:ARG:HH22	16:Q:349:GLN:HE22	1.33	0.74
23:Z:353:ALA:HB3	23:Z:360:ILE:HB	1.69	0.74
1:A:863:ARG:NH1	1:A:1129:ASN:OD1	2.21	0.74
23:Z:295:TYR:N	23:Z:304:SER:OG	2.17	0.74
2:B:834:ARG:NH1	2:B:841:ARG:O	2.20	0.74
16:Q:803:MET:HE1	16:Q:807:LEU:HD11	1.70	0.74
23:Z:492:ILE:HG22	23:Z:502:LEU:HB3	1.70	0.74
23:Z:554:GLU:OE2	23:Z:559:GLN:NE2	2.21	0.74
2:B:388:TYR:H	2:B:504:THR:HG21	1.51	0.74
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.68	0.74
23:Z:438:GLY:HA3	23:Z:452:PRO:HB2	1.68	0.74
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.70	0.73
1:A:1434:GLU:O	1:A:1436:VAL:N	2.19	0.73
15:P:24:A:C3'	15:P:25:A:H8	2.01	0.73
17:R:564:ASN:HD21	19:V:136:TYR:C	1.96	0.73
20:W:251:SER:OG	20:W:253:ASP:OD1	2.05	0.73
2:B:595:ASP:OD1	2:B:596:ILE:N	2.20	0.73
2:B:650:ASN:N	16:U:460:TYR:OH	2.17	0.73
1:A:1184:THR:O	1:A:1186:VAL:N	2.22	0.73
1:A:299:ALA:HB3	1:A:302:VAL:HG12	1.69	0.73
19:V:193:HIS:HB2	19:V:199:VAL:HG12	1.70	0.73
1:A:239:GLU:OE2	1:A:241:ARG:NH2	2.21	0.73
1:A:539:GLN:O	1:A:542:LEU:N	2.21	0.73
2:B:677:MET:H	2:B:682:LEU:HD22	1.52	0.73
2:B:898:THR:O	2:B:899:SER:OG	2.05	0.73
16:U:438:ALA:O	16:U:439:ARG:NH2	2.20	0.73
19:V:110:GLU:HG3	19:V:111:GLU:H	1.53	0.73
2:B:309:PHE:O	9:I:40:ARG:NH2	2.22	0.72
16:Q:534:TYR:HH	16:Q:553:TRP:HD1	1.37	0.72
1:A:289:GLN:O	1:A:293:ASN:HB2	1.89	0.72
2:B:84:TYR:HB3	2:B:132:VAL:HG23	1.70	0.72
14:N:46:DG:H4'	14:N:47:DA:OP1	1.87	0.72
8:H:32:SER:HB3	8:H:37:MET:H	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.72
2:B:348:LEU:O	2:B:361:LYS:NZ	2.22	0.72
16:Q:424:GLN:HB2	21:X:231:TRP:CE3	2.24	0.72
20:W:214:ILE:N	20:W:228:LEU:O	2.21	0.72
22:Y:93:LEU:HD22	22:Y:97:ILE:HD11	1.70	0.72
16:Q:302:GLU:HG3	16:Q:305:GLN:HE21	1.55	0.71
20:W:272:ASP:O	20:W:274:GLN:NE2	2.22	0.71
4:D:131:LEU:HA	4:D:134:ILE:HD12	1.71	0.71
23:Z:470:LYS:HB2	23:Z:516:ARG:HA	1.72	0.71
20:W:81:SER:HB3	20:W:91:TRP:HE1	1.55	0.71
8:H:128:ASP:OD1	8:H:131:ASN:ND2	2.24	0.71
16:Q:799:VAL:O	16:Q:802:LYS:NZ	2.23	0.71
2:B:1125:MET:HE1	2:B:1156:LYS:HG2	1.73	0.71
16:Q:384:LEU:HD13	16:Q:397:ALA:HB2	1.73	0.71
20:W:169:ASP:N	20:W:169:ASP:OD1	2.22	0.71
7:G:110:ARG:HH11	7:G:118:GLU:HA	1.56	0.71
8:H:103:GLU:HG3	8:H:109:ALA:HB2	1.71	0.71
16:U:450:LEU:HD21	16:U:452:LEU:HD23	1.73	0.71
16:U:507:THR:O	16:U:509:ARG:N	2.24	0.71
23:Z:504:SER:OG	23:Z:507:THR:O	2.08	0.71
23:Z:188:GLU:O	23:Z:192:THR:OG1	2.05	0.70
23:Z:759:GLY:O	23:Z:761:MET:N	2.24	0.70
23:Z:563:MET:HA	23:Z:637:VAL:HG11	1.73	0.70
1:A:77:ASN:OD1	1:A:78:MET:N	2.25	0.70
5:E:36:THR:N	5:E:39:GLU:OE2	2.16	0.70
16:Q:163:ILE:HB	16:Q:194:PRO:HG3	1.72	0.70
17:R:405:ILE:HG23	17:R:426:LEU:HD11	1.72	0.70
23:Z:450:ILE:HG23	23:Z:452:PRO:HD3	1.73	0.70
26:c:29:ARG:NH1	27:d:33:SER:O	2.20	0.70
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.72	0.70
20:W:256:VAL:HB	20:W:270:PHE:HB2	1.72	0.70
1:A:1372:GLU:OE2	5:E:195:ARG:NH2	2.25	0.70
4:D:34:ASN:O	4:D:68:THR:OG1	2.09	0.70
1:A:1184:THR:C	1:A:1186:VAL:H	2.00	0.70
10:J:64:PRO:O	12:L:23:HIS:NE2	2.23	0.70
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.72	0.70
16:Q:729:LYS:HE2	16:Q:732:LYS:HD2	1.72	0.70
19:V:192:GLN:HB2	19:V:197:PRO:HB3	1.74	0.70
23:Z:478:VAL:HG21	23:Z:502:LEU:HD22	1.74	0.70
7:G:152:VAL:HG22	7:G:157:ILE:HG22	1.74	0.70
13:M:1462:ILE:HD11	13:M:1472:PHE:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:39:DA:OP2	26:c:35:ARG:NH1	2.24	0.70
16:Q:401:LEU:HD22	16:Q:418:LEU:HG	1.72	0.70
24:e:67:PHE:O	24:e:71:VAL:HG23	1.91	0.70
1:A:917:GLU:OE2	1:A:921:ARG:NH2	2.25	0.69
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.25	0.69
9:I:42:CYS:SG	9:I:43:ASP:N	2.65	0.69
1:A:244:ARG:HE	1:A:245:PRO:HD2	1.57	0.69
7:G:21:ASN:OD1	7:G:21:ASN:N	2.23	0.69
8:H:36:LYS:HG3	16:Q:709:ARG:HH12	1.57	0.69
17:R:410:GLU:OE2	17:R:423:ASN:ND2	2.25	0.69
1:A:140:ARG:HH12	1:A:234:PHE:HD1	1.41	0.69
17:R:405:ILE:HG12	17:R:426:LEU:HD21	1.72	0.69
17:R:428:LEU:HB2	17:R:437:PHE:CD2	2.27	0.69
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.27	0.69
23:Z:307:MET:HE3	23:Z:308:ILE:H	1.57	0.69
1:A:999:ARG:NH1	8:H:103:GLU:OE2	2.24	0.69
4:D:23:PRO:HG2	7:G:78:ARG:HH22	1.58	0.69
5:E:2:ASP:OD1	5:E:4:GLU:N	2.25	0.69
20:W:289:ILE:HB	20:W:301:TYR:HB2	1.74	0.69
23:Z:525:ALA:HB1	23:Z:552:ARG:HH12	1.58	0.69
2:B:85:LEU:N	2:B:131:THR:O	2.25	0.69
7:G:91:GLN:HG2	7:G:93:ASN:HD21	1.58	0.69
8:H:8:ASP:OD2	8:H:32:SER:OG	2.05	0.69
1:A:357:LYS:NZ	2:B:1112:ASP:OD1	2.26	0.69
5:E:97:GLU:HB2	5:E:99:ILE:HG12	1.74	0.69
20:W:113:ALA:HB3	20:W:122:ALA:HB3	1.74	0.69
1:A:100:LEU:HD23	1:A:193:ARG:HE	1.57	0.69
1:A:611:ASP:N	1:A:611:ASP:OD1	2.25	0.69
13:M:1488:THR:HB	13:M:1495:ARG:HB3	1.75	0.69
23:Z:502:LEU:HG	23:Z:511:LEU:HB3	1.75	0.69
26:c:50:TYR:O	26:c:54:VAL:HG23	1.93	0.69
1:A:487:SER:OG	1:A:673:GLN:NE2	2.26	0.68
16:Q:86:LEU:HD11	16:Q:116:LEU:HB3	1.76	0.68
17:R:366:ARG:NH2	23:Z:775:TPO:OG1	2.26	0.68
20:W:236:LEU:N	20:W:250:SER:O	2.27	0.68
2:B:649:ASN:HB2	16:U:460:TYR:OH	1.93	0.68
16:Q:624:LYS:HG3	16:Q:627:ARG:NH1	2.07	0.68
1:A:1212:LEU:HD21	1:A:1289:GLU:HB3	1.75	0.68
13:M:1379:GLN:HG2	13:M:1469:PRO:HB2	1.73	0.68
14:N:-36:DC:N3	18:T:36:DG:N2	2.37	0.68
1:A:116:LYS:NZ	1:A:184:CYS:SG	2.67	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:570:TRP:HD1	19:V:133:LYS:HD2	1.57	0.68
1:A:686:THR:OG1	1:A:687:ILE:N	2.25	0.68
23:Z:433:LEU:HB3	23:Z:436:LEU:HD12	1.75	0.68
13:M:1512:LYS:O	13:M:1516:GLN:NE2	2.24	0.68
1:A:376:ASP:CG	1:A:473:ARG:HH11	2.01	0.68
14:N:-63:DA:H2''	14:N:-62:DT:H72	1.75	0.68
16:Q:534:TYR:OH	16:Q:556:GLU:OE1	2.12	0.68
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.13	0.67
7:G:123:SER:OG	7:G:125:PRO:O	2.11	0.67
1:A:1212:LEU:HD12	1:A:1285:LEU:HD13	1.77	0.67
2:B:1157:LEU:O	2:B:1161:GLU:HG3	1.95	0.67
5:E:82:VAL:HG22	5:E:86:THR:OG1	1.93	0.67
23:Z:419:ASN:OD1	23:Z:516:ARG:NH2	2.28	0.67
8:H:2:ALA:C	8:H:84:ARG:HH12	2.02	0.67
16:Q:886:LYS:O	16:Q:890:MET:HG2	1.94	0.67
20:W:46:VAL:HB	20:W:58:TRP:HB2	1.77	0.67
2:B:633:LEU:HD11	2:B:679:PRO:HB2	1.76	0.67
2:B:1136:GLU:HB2	2:B:1143:LYS:HG2	1.77	0.67
14:N:-32:DC:H2''	14:N:-31:DA:C8	2.30	0.67
1:A:112:PHE:O	1:A:113:PHE:HB2	1.93	0.67
1:A:1024:ASN:O	5:E:162:ARG:NH1	2.28	0.67
3:C:74:THR:OG1	3:C:74:THR:O	2.09	0.67
15:P:24:A:H3'	15:P:25:A:C8	2.29	0.67
16:Q:394:ARG:HB3	16:Q:398:LYS:HE3	1.76	0.67
1:A:539:GLN:NE2	2:B:790:GLN:O	2.28	0.67
16:Q:420:GLN:O	21:X:229:ARG:NH2	2.28	0.67
23:Z:613:GLU:O	23:Z:625:HIS:N	2.28	0.67
11:K:13:PHE:HB2	11:K:16:GLU:HG3	1.77	0.67
2:B:223:SER:OG	2:B:350:HIS:ND1	2.26	0.67
7:G:151:ARG:O	7:G:158:PHE:N	2.22	0.67
13:M:1373:VAL:HG21	13:M:1379:GLN:HG3	1.76	0.67
14:N:-36:DC:N4	18:T:36:DG:H1	1.93	0.67
17:R:406:THR:OG1	17:R:427:GLN:O	2.11	0.67
16:U:474:ARG:H	19:V:218:GLN:HA	1.60	0.67
20:W:13:GLN:NE2	20:W:15:HIS:O	2.27	0.67
23:Z:295:TYR:H	23:Z:304:SER:HG	1.43	0.67
2:B:715:ASP:OD1	2:B:715:ASP:N	2.19	0.66
16:Q:590:ARG:HA	16:Q:593:LYS:HG3	1.76	0.66
23:Z:184:CYS:SG	23:Z:185:LYS:N	2.68	0.66
1:A:413:TYR:O	1:A:449:HIS:HD2	1.77	0.66
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:268:ASN:ND2	16:Q:271:VAL:H	1.93	0.66
16:Q:484:GLU:HB3	16:Q:487:HIS:HB2	1.76	0.66
2:B:22:TRP:CE2	2:B:679:PRO:HG3	2.30	0.66
16:Q:86:LEU:HG	16:Q:120:ALA:HB2	1.76	0.66
20:W:292:VAL:HG12	20:W:298:ILE:HG12	1.76	0.66
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.77	0.66
23:Z:282:LYS:O	23:Z:287:LYS:NZ	2.28	0.66
1:A:819:SER:O	1:A:819:SER:OG	2.05	0.66
10:J:44:CYS:O	10:J:47:ARG:NH2	2.25	0.66
18:T:56:DC:H2''	18:T:57:DT:H71	1.78	0.66
20:W:48:LYS:N	20:W:55:ASP:O	2.27	0.66
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.11	0.66
8:H:72:ASP:OD1	8:H:73:GLY:N	2.29	0.66
17:R:455:TRP:CD1	17:R:459:MET:HE3	2.31	0.66
16:Q:342:LEU:HD11	19:V:67:GLU:HG2	1.78	0.66
2:B:354:SER:OG	2:B:355:ASP:N	2.26	0.66
24:a:119:ILE:O	25:b:47:SER:HB3	1.95	0.66
5:E:27:LEU:O	16:Q:877:GLN:NE2	2.29	0.65
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.79	0.65
14:N:-56:DG:H2''	14:N:-55:DC:C5	2.30	0.65
22:Y:4:GLU:O	22:Y:27:GLN:NE2	2.29	0.65
22:Y:14:ARG:HH11	22:Y:54:SER:HA	1.61	0.65
23:Z:366:TYR:O	23:Z:373:PHE:N	2.28	0.65
7:G:109:SER:HB3	23:Z:493:VAL:HG21	1.77	0.65
16:Q:494:ALA:HB1	21:X:224:ILE:HG12	1.78	0.65
16:Q:856:LEU:HD23	16:Q:857:LEU:HD22	1.78	0.65
1:A:200:ALA:HB3	1:A:214:ILE:HG12	1.78	0.65
2:B:100:GLU:OE1	2:B:100:GLU:N	2.24	0.65
19:V:48:PHE:HB2	21:X:229:ARG:HB2	1.78	0.65
2:B:1003:ASN:O	2:B:1005:ALA:N	2.27	0.65
2:B:1071:ASN:O	2:B:1073:GLN:N	2.29	0.65
17:R:569:GLU:O	17:R:573:VAL:HG23	1.97	0.65
20:W:130:VAL:HB	20:W:144:LEU:HD12	1.78	0.65
5:E:93:ARG:HA	5:E:96:GLU:OE1	1.97	0.65
20:W:218:ASP:N	20:W:223:ASN:O	2.29	0.65
4:D:76:ASN:HD21	4:D:78:GLU:HB2	1.61	0.65
14:N:-35:DC:H2''	14:N:-34:DA:C8	2.32	0.65
17:R:494:GLU:HA	17:R:497:LYS:HD2	1.79	0.65
19:V:45:ASP:N	19:V:45:ASP:OD1	2.30	0.65
16:Q:605:LEU:O	16:Q:609:ASN:ND2	2.30	0.65
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:568:TRP:CZ3	16:Q:592:LEU:HB2	2.32	0.64
17:R:355:LEU:HG	17:R:357:GLU:H	1.62	0.64
23:Z:539:LEU:HD22	23:Z:616:HIS:HB3	1.79	0.64
1:A:1118:THR:O	1:A:1123:ARG:HB2	1.96	0.64
4:D:128:GLN:NE2	4:D:132:ASP:OD1	2.27	0.64
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.79	0.64
14:N:49:DC:H4'	27:d:30:ARG:HG2	1.79	0.64
16:Q:710:LYS:HB2	16:Q:712:TYR:CD1	2.32	0.64
1:A:1099:ALA:HA	1:A:1102:MET:HE3	1.79	0.64
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.78	0.64
16:Q:83:MET:HE3	16:Q:124:ILE:HB	1.80	0.64
20:W:214:ILE:HB	20:W:228:LEU:HB3	1.78	0.64
23:Z:474:MET:HE2	23:Z:494:ARG:HA	1.80	0.64
17:R:564:ASN:OD1	19:V:136:TYR:N	2.29	0.64
16:Q:123:ILE:HG13	16:Q:124:ILE:HG12	1.80	0.64
20:W:26:THR:HG23	20:W:284:GLY:HA2	1.80	0.64
25:b:89:ALA:O	25:b:92:ARG:HB2	1.97	0.64
1:A:329:MET:HA	1:A:335:PRO:HA	1.80	0.63
1:A:1540:THR:HG23	13:M:1479:ARG:HE	1.62	0.63
18:T:55:DG:H2''	18:T:56:DC:C5	2.33	0.63
23:Z:733:ARG:NH2	23:Z:744:SER:OG	2.31	0.63
26:c:92:GLU:OE1	27:d:102:GLU:HB3	1.98	0.63
1:A:30:GLU:HA	1:A:33:ARG:HE	1.63	0.63
20:W:92:ASP:HB3	20:W:95:ASN:OD1	1.98	0.63
4:D:114:LEU:HD21	7:G:167:TYR:HB2	1.80	0.63
20:W:206:VAL:HG11	20:W:238:VAL:HG21	1.81	0.63
16:Q:239:ALA:HB2	16:Q:257:LEU:HB3	1.81	0.63
2:B:93:LEU:O	16:U:507:THR:HA	1.99	0.63
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.81	0.63
16:Q:286:SER:O	16:Q:290:HIS:ND1	2.32	0.63
23:Z:519:GLN:NE2	23:Z:521:CYS:SG	2.71	0.63
11:K:5:PRO:HG2	11:K:8:GLU:HG3	1.81	0.63
23:Z:558:PHE:N	23:Z:570:VAL:O	2.30	0.63
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.33	0.63
16:Q:398:LYS:O	16:Q:402:LYS:HD3	1.99	0.63
16:Q:576:LEU:HD21	16:Q:585:GLN:HE22	1.64	0.63
23:Z:470:LYS:NZ	23:Z:518:LEU:O	2.31	0.63
1:A:1244:ASN:HB2	1:A:1262:MET:HE2	1.80	0.62
2:B:497:LYS:HG3	2:B:498:PRO:HD3	1.80	0.62
4:D:46:GLN:HA	4:D:49:GLU:CD	2.24	0.62
23:Z:506:LEU:HD11	23:Z:552:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:404:GLU:OE2	17:R:455:TRP:NE1	2.32	0.62
2:B:577:HIS:NE2	2:B:583:LEU:HD11	2.13	0.62
16:Q:835:ASP:OD1	16:Q:839:ARG:NE	2.32	0.62
17:R:355:LEU:HD12	17:R:356:PRO:HD2	1.81	0.62
26:c:118:LYS:HA	26:c:118:LYS:HE3	1.81	0.62
16:Q:394:ARG:HD2	16:Q:421:ILE:HG23	1.82	0.62
20:W:206:VAL:HG22	20:W:216:ILE:HG12	1.81	0.62
1:A:694:ALA:HB3	1:A:699:TYR:CE1	2.34	0.62
2:B:787:GLY:O	2:B:790:GLN:HG3	1.98	0.62
5:E:166:ARG:NH1	5:E:168:ASN:HD22	1.95	0.62
9:I:17:CYS:N	9:I:22:ASN:O	2.27	0.62
16:Q:849:LYS:O	16:Q:852:LEU:HG	2.00	0.62
17:R:493:GLU:OE1	17:R:493:GLU:N	2.22	0.62
1:A:481:THR:O	1:A:483:ARG:NH2	2.32	0.62
1:A:1301:ILE:HG22	1:A:1345:ARG:HH11	1.65	0.62
2:B:184:TYR:CE1	2:B:191:GLU:HG2	2.33	0.62
4:D:135:GLN:OE1	4:D:138:ARG:NH2	2.32	0.62
12:L:56:ASP:O	12:L:58:ARG:N	2.33	0.62
1:A:962:ASP:CG	1:A:1046:ARG:HH11	2.08	0.62
2:B:67:LEU:H	2:B:83:ARG:HB2	1.64	0.62
5:E:39:GLU:OE1	5:E:39:GLU:N	2.24	0.62
16:Q:611:TRP:HE1	16:Q:628:HIS:HA	1.64	0.62
17:R:364:LEU:HB2	17:R:387:VAL:HG12	1.81	0.62
20:W:195:SER:OG	20:W:236:LEU:O	2.15	0.62
1:A:565:MET:HE1	11:K:58:PHE:HE2	1.64	0.62
1:A:1140:THR:OG1	1:A:1140:THR:O	2.12	0.62
2:B:646:ARG:C	2:B:648:TYR:H	2.07	0.62
16:Q:86:LEU:HD12	16:Q:89:LEU:HB2	1.80	0.62
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.82	0.62
16:Q:128:GLN:HE22	19:V:86:LEU:HD13	1.64	0.62
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.81	0.62
16:Q:249:ASP:O	16:Q:253:ASN:ND2	2.33	0.62
1:A:797:ARG:NH1	1:A:815:TYR:O	2.32	0.61
2:B:67:LEU:HG	2:B:84:TYR:OH	2.00	0.61
9:I:12:VAL:HG21	9:I:53:ILE:O	2.00	0.61
1:A:88:ILE:O	1:A:90:LEU:N	2.33	0.61
5:E:55:ARG:HB2	5:E:78:GLU:HG3	1.82	0.61
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.81	0.61
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.82	0.61
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.82	0.61
1:A:922:PHE:H	1:A:1052:ARG:HH21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:729:LYS:HB2	16:Q:732:LYS:HD2	1.82	0.61
2:B:19:PRO:O	2:B:21:LEU:N	2.32	0.61
3:C:91:GLU:OE1	23:Z:713:SER:HB2	2.01	0.61
23:Z:390:LEU:HD12	23:Z:393:LEU:HD12	1.82	0.61
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.34	0.61
5:E:45:GLY:HA3	5:E:53:PRO:HD3	1.82	0.61
5:E:64:HIS:N	5:E:70:ASP:O	2.31	0.61
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.66	0.61
19:V:110:GLU:HG3	19:V:111:GLU:N	2.14	0.61
1:A:556:GLU:OE1	1:A:556:GLU:N	2.33	0.61
2:B:228:SER:O	2:B:405:ARG:NH2	2.34	0.61
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.17	0.61
7:G:151:ARG:HB3	7:G:158:PHE:O	2.01	0.61
14:N:50:DG:H2"	14:N:51:DG:OP2	2.01	0.61
22:Y:66:PRO:HB2	22:Y:78:SER:HA	1.82	0.61
16:Q:68:ARG:HE	16:Q:89:LEU:HD12	1.65	0.61
1:A:1468:THR:H	6:F:60:TYR:HB3	1.66	0.61
16:Q:65:GLU:HA	16:Q:89:LEU:HD11	1.82	0.61
23:Z:554:GLU:OE1	23:Z:557:THR:OG1	2.18	0.61
2:B:100:GLU:HA	2:B:105:PRO:HG3	1.82	0.61
20:W:176:ASP:HB2	20:W:183:LEU:HD11	1.83	0.61
27:d:92:GLN:O	27:d:95:VAL:HB	2.01	0.61
2:B:177:CYS:SG	2:B:180:ASP:N	2.74	0.60
4:D:60:VAL:HA	4:D:63:LYS:HG2	1.82	0.60
16:Q:862:GLU:HA	16:Q:865:LEU:HG	1.82	0.60
1:A:381:PRO:HB3	1:A:480:SER:HA	1.81	0.60
1:A:620:HIS:O	8:H:97:TYR:OH	2.15	0.60
11:K:49:GLN:NE2	11:K:93:ASP:OD2	2.34	0.60
16:Q:80:LYS:O	16:Q:83:MET:HG3	2.01	0.60
16:Q:774:SER:H	16:Q:830:ARG:NH1	1.99	0.60
20:W:125:THR:OG1	20:W:131:ASN:ND2	2.34	0.60
3:C:154:ARG:HH21	10:J:63:ALA:HB2	1.61	0.60
6:F:114:SER:OG	6:F:115:TYR:N	2.33	0.60
16:Q:38:HIS:HE1	16:Q:73:LEU:HD13	1.66	0.60
16:Q:222:SER:O	16:Q:226:GLU:HG2	2.02	0.60
16:Q:715:GLN:HB2	16:Q:746:VAL:HG11	1.83	0.60
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.01	0.60
16:Q:48:ALA:HB2	16:Q:63:LEU:HD11	1.84	0.60
19:V:196:LYS:O	19:V:198:ARG:HG3	2.01	0.60
20:W:53:ARG:NH2	20:W:54:LEU:O	2.35	0.60
25:b:32:PRO:O	25:b:35:ARG:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:26:THR:HA	20:W:284:GLY:HA2	1.83	0.60
3:C:190:ASN:ND2	3:C:195:THR:O	2.20	0.60
16:Q:620:ARG:HG3	16:Q:625:GLU:HB2	1.84	0.60
26:c:25:PHE:CZ	26:c:59:THR:HG21	2.37	0.60
1:A:123:ASN:O	1:A:127:LYS:HG2	2.02	0.60
1:A:1481:LYS:O	13:M:1384:ARG:NH2	2.34	0.60
3:C:60:HIS:HB2	3:C:63:PHE:HB2	1.83	0.60
16:Q:163:ILE:HG21	16:Q:189:ALA:HA	1.83	0.60
16:Q:534:TYR:HH	16:Q:553:TRP:CD1	2.18	0.60
16:Q:646:ASN:HA	21:X:239:GLN:HA	1.82	0.60
20:W:27:ASN:O	20:W:32:SER:OG	2.19	0.60
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.84	0.60
16:Q:581:TRP:O	16:Q:585:GLN:HB2	2.02	0.60
1:A:47:THR:HA	1:A:52:PRO:HA	1.81	0.60
2:B:144:HIS:CD2	2:B:431:LEU:HD21	2.36	0.60
16:Q:313:ALA:HB2	16:Q:328:TYR:HB2	1.83	0.60
19:V:233:VAL:O	19:V:238:PRO:N	2.35	0.60
20:W:8:LEU:N	20:W:300:ILE:O	2.30	0.60
23:Z:499:PHE:HD1	23:Z:512:LYS:HB3	1.67	0.60
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.16	0.60
18:T:-72:DA:C5'	18:T:-72:DA:HO5'	2.09	0.60
22:Y:19:CYS:SG	22:Y:21:LEU:HB2	2.42	0.60
23:Z:562:ASN:HD21	23:Z:566:LYS:HG3	1.67	0.60
3:C:55:ASN:ND2	3:C:60:HIS:O	2.34	0.59
3:C:189:ASP:O	3:C:191:ALA:N	2.34	0.59
8:H:32:SER:OG	8:H:33:GLU:N	2.33	0.59
23:Z:365:ARG:HD3	23:Z:374:LYS:HD2	1.84	0.59
23:Z:629:LEU:HB2	23:Z:634:GLY:HA2	1.83	0.59
16:Q:708:LEU:HD21	16:Q:719:VAL:HG21	1.82	0.59
1:A:1210:TRP:CZ2	1:A:1281:ASP:HB3	2.37	0.59
16:Q:158:GLN:HG3	16:Q:159:SER:H	1.66	0.59
1:A:64:VAL:HG11	1:A:78:MET:HA	1.84	0.59
1:A:1005:HIS:HD2	1:A:1007:ILE:H	1.49	0.59
1:A:217:SER:OG	1:A:220:ARG:N	2.35	0.59
1:A:894:ASP:OD2	1:A:1396:ARG:NH1	2.35	0.59
2:B:912:ASN:OD1	2:B:912:ASN:N	2.26	0.59
16:U:445:ASP:OD1	16:U:447:SER:OG	2.19	0.59
14:N:-55:DC:H2''	14:N:-54:DG:C8	2.38	0.59
15:P:24:A:C2	15:P:25:A:C5	2.91	0.59
2:B:743:ARG:NH2	2:B:745:ASP:OD1	2.35	0.59
4:D:103:LEU:O	7:G:144:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:63:DG:H2''	14:N:64:DG:OP2	2.01	0.59
17:R:574:GLU:HA	17:R:577:LYS:HG2	1.84	0.59
1:A:379:GLY:HA2	1:A:475:ARG:O	2.02	0.59
2:B:721:ARG:NH2	2:B:940:GLY:O	2.36	0.59
7:G:109:SER:HB2	23:Z:503:PHE:CZ	2.37	0.59
17:R:363:ARG:NH1	17:R:365:SER:OG	2.36	0.59
2:B:690:CYS:O	2:B:691:SER:OG	2.21	0.59
5:E:93:ARG:HB2	16:Q:891:PHE:CE1	2.38	0.59
7:G:153:ASP:N	7:G:156:ASP:O	2.23	0.59
2:B:784:SER:O	2:B:784:SER:OG	2.14	0.58
5:E:45:GLY:CA	5:E:53:PRO:HD3	2.32	0.58
13:M:1356:ILE:HG22	13:M:1370:THR:HB	1.85	0.58
16:Q:351:TYR:HB2	16:Q:360:ALA:HB2	1.83	0.58
2:B:650:ASN:N	2:B:650:ASN:OD1	2.36	0.58
11:K:39:ASP:OD1	11:K:39:ASP:N	2.35	0.58
13:M:1352:GLN:HE22	13:M:1373:VAL:C	2.11	0.58
16:Q:884:LYS:O	16:Q:887:ASN:N	2.34	0.58
27:d:65:ASP:OD2	25:f:98:TYR:OH	2.20	0.58
1:A:552:ASP:OD2	8:H:24:ARG:NH2	2.37	0.58
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.85	0.58
1:A:1244:ASN:HB2	1:A:1262:MET:CE	2.34	0.58
8:H:63:THR:HG21	8:H:68:GLY:HA2	1.85	0.58
20:W:66:GLY:O	20:W:83:SER:OG	2.11	0.58
2:B:235:ILE:HG13	2:B:348:LEU:HD13	1.85	0.58
2:B:577:HIS:CD2	2:B:583:LEU:HD11	2.38	0.58
16:Q:201:ARG:HH22	16:Q:227:LEU:HD13	1.68	0.58
25:b:77:LYS:HG3	27:d:89:ARG:HH12	1.68	0.58
1:A:117:LEU:C	1:A:119:VAL:H	2.11	0.58
1:A:367:ILE:HA	1:A:482:PHE:O	2.04	0.58
1:A:1231:ILE:O	1:A:1235:ILE:HB	2.03	0.58
16:Q:95:GLN:NE2	19:V:84:ILE:O	2.37	0.58
16:Q:419:ALA:HB2	16:Q:433:ALA:HB3	1.83	0.58
16:Q:624:LYS:HA	16:Q:627:ARG:HH11	1.67	0.58
23:Z:424:ASP:HB2	23:Z:440:ILE:HD12	1.84	0.58
16:Q:776:LEU:O	16:Q:779:VAL:HG22	2.03	0.58
1:A:1177:TYR:OH	1:A:1282:ASP:HA	2.04	0.58
1:A:1222:THR:O	1:A:1225:LYS:N	2.34	0.58
16:Q:505:ARG:NH1	19:V:44:PHE:HB2	2.12	0.58
1:A:1052:ARG:NE	1:A:1056:GLU:OE2	2.36	0.58
2:B:756:LYS:NZ	19:V:134:THR:HG1	2.02	0.58
18:T:45:DA:H5'	27:d:30:ARG:HH22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:192:THR:HG23	23:Z:245:LEU:HD21	1.85	0.58
26:c:20:ARG:O	27:d:118:TYR:HA	2.03	0.58
2:B:83:ARG:O	2:B:83:ARG:NH2	2.37	0.58
5:E:67:ASP:OD1	5:E:69:THR:OG1	2.22	0.58
14:N:51:DG:H2''	14:N:52:DC:OP2	2.04	0.58
16:Q:384:LEU:HG	16:Q:386:ALA:H	1.69	0.58
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.36	0.58
8:H:2:ALA:O	8:H:84:ARG:NH1	2.30	0.58
8:H:116:VAL:CG1	8:H:123:MET:HE2	2.33	0.58
17:R:353:VAL:HG12	17:R:469:LEU:HD13	1.86	0.58
23:Z:280:ARG:HH11	23:Z:288:ASP:HB3	1.69	0.58
24:e:110:CYS:SG	24:e:126:LEU:HD23	2.44	0.58
1:A:394:VAL:HG23	1:A:444:TYR:O	2.04	0.57
1:A:589:LYS:NZ	1:A:625:ASP:OD2	2.36	0.57
2:B:565:THR:HA	2:B:610:ARG:HB3	1.86	0.57
15:P:22:G:O2'	15:P:23:G:H8	1.86	0.57
16:Q:474:PHE:HB2	16:Q:503:LEU:HD13	1.85	0.57
8:H:78:THR:O	8:H:78:THR:OG1	2.21	0.57
8:H:83:SER:OG	8:H:84:ARG:N	2.33	0.57
16:Q:371:TYR:HE2	16:Q:373:ASN:HD21	1.51	0.57
18:T:50:DC:H2''	18:T:51:DT:OP1	2.04	0.57
20:W:48:LYS:HB2	20:W:57:GLN:HB2	1.85	0.57
4:D:133:ASP:O	4:D:136:THR:OG1	2.22	0.57
7:G:37:THR:HA	23:Z:628:LYS:NZ	2.20	0.57
17:R:407:GLY:H	17:R:427:GLN:HB3	1.69	0.57
1:A:92:LYS:HD2	1:A:307:VAL:HG11	1.87	0.57
20:W:152:LEU:HD12	20:W:168:ILE:HA	1.85	0.57
25:f:59:LYS:HE3	25:f:63:GLU:OE2	2.05	0.57
1:A:202:TRP:CE3	1:A:212:LYS:HB2	2.38	0.57
7:G:122:ASN:OD1	7:G:123:SER:N	2.38	0.57
23:Z:450:ILE:HG21	23:Z:468:LEU:HD11	1.87	0.57
24:a:101:VAL:HG11	25:b:40:ARG:HG2	1.87	0.57
1:A:392:GLU:HG2	1:A:402:LEU:HD11	1.86	0.57
1:A:1146:GLN:OE1	1:A:1153:ARG:HD3	2.05	0.57
1:A:282:ASP:HB3	1:A:313:HIS:CE1	2.39	0.57
5:E:90:TYR:HA	16:Q:891:PHE:HZ	1.69	0.57
16:Q:156:LEU:HD11	16:Q:169:LYS:HE2	1.86	0.57
20:W:112:LEU:HD22	20:W:121:LEU:HD21	1.87	0.57
23:Z:501:ILE:HD11	23:Z:510:GLU:HB3	1.87	0.57
1:A:699:TYR:O	1:A:703:GLN:HG2	2.05	0.57
24:a:65:LEU:HB3	24:a:66:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HG	1:A:232:GLU:OE2	2.05	0.57
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.85	0.57
2:B:298:MET:HE3	9:I:14:ILE:HD12	1.85	0.57
2:B:743:ARG:HH21	2:B:743:ARG:HB3	1.69	0.57
3:C:4:ALA:HB2	11:K:93:ASP:HB2	1.86	0.57
4:D:104:CYS:HB3	4:D:135:GLN:HE22	1.70	0.57
1:A:11:SER:O	2:B:1135:TYR:OH	2.14	0.57
16:Q:678:ALA:O	16:Q:684:TRP:NE1	2.38	0.57
16:Q:802:LYS:HE2	16:Q:807:LEU:HB2	1.87	0.57
19:V:88:ASN:OD1	19:V:89:PRO:HD3	2.04	0.57
26:c:26:PRO:HD3	27:d:37:TYR:CD1	2.40	0.57
1:A:140:ARG:NH1	1:A:234:PHE:HD1	2.03	0.56
1:A:565:MET:HE3	11:K:60:GLY:HA3	1.85	0.56
5:E:66:ASP:OD1	5:E:67:ASP:N	2.36	0.56
14:N:-54:DG:H2''	14:N:-53:DG:H8	1.70	0.56
16:Q:211:LEU:HD12	16:Q:213:LYS:HZ1	1.70	0.56
25:b:26:ILE:HG13	25:b:55:ARG:HD3	1.87	0.56
1:A:1190:GLN:O	1:A:1193:VAL:HG12	2.04	0.56
2:B:285:LEU:HD23	9:I:16:PHE:HZ	1.70	0.56
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.85	0.56
13:M:1505:ASN:O	13:M:1509:ARG:HG2	2.05	0.56
18:T:-64:DC:H2''	18:T:-63:DC:OP2	2.05	0.56
1:A:96:HIS:HD2	1:A:99:PHE:CD2	2.23	0.56
1:A:546:ARG:HG2	1:A:546:ARG:O	2.04	0.56
15:P:32:C:H5''	15:P:33:A:C2	2.39	0.56
16:Q:188:LYS:HB3	16:Q:191:ARG:HH21	1.70	0.56
16:Q:504:ALA:HB2	16:Q:519:LEU:HB3	1.86	0.56
16:Q:772:GLU:HA	16:Q:773:LYS:HB2	1.87	0.56
17:R:560:ILE:HA	17:R:563:ILE:HG22	1.87	0.56
23:Z:416:ARG:HE	23:Z:466:GLN:HE21	1.52	0.56
24:e:60:LEU:HD12	24:e:64:LYS:HE2	1.87	0.56
1:A:1005:HIS:CD2	1:A:1007:ILE:H	2.23	0.56
2:B:1129:ASN:HB3	2:B:1134:THR:HG22	1.87	0.56
25:b:33:ALA:C	25:b:35:ARG:N	2.60	0.56
1:A:299:ALA:O	1:A:301:HIS:N	2.39	0.56
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.06	0.56
9:I:25:TYR:O	9:I:37:TYR:HA	2.04	0.56
1:A:538:VAL:O	1:A:538:VAL:HG12	2.06	0.56
1:A:809:HIS:HE1	2:B:506:TRP:CZ2	2.23	0.56
1:A:1484:MET:HB2	13:M:1362:LYS:HE3	1.86	0.56
10:J:16:ASN:OD1	10:J:16:ASN:N	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:VAL:HG12	5:E:169:GLN:O	2.06	0.56
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.39	0.56
2:B:177:CYS:HB2	2:B:738:THR:OG1	2.06	0.56
2:B:833:THR:C	2:B:835:GLU:H	2.12	0.56
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.87	0.56
7:G:110:ARG:HH22	7:G:115:SER:HA	1.69	0.56
20:W:9:PHE:HB3	20:W:300:ILE:CG1	2.35	0.56
23:Z:420:PHE:HB3	23:Z:440:ILE:HD13	1.88	0.56
23:Z:478:VAL:HG11	23:Z:492:ILE:HG23	1.87	0.56
1:A:528:PRO:HB3	1:A:899:GLU:HG3	1.87	0.56
16:Q:777:LYS:HE3	16:Q:781:ASN:HD21	1.71	0.56
17:R:415:TYR:CZ	17:R:438:ARG:HB3	2.41	0.56
19:V:61:TYR:N	19:V:62:LYS:HA	2.21	0.56
23:Z:542:LEU:HD22	23:Z:570:VAL:HG11	1.87	0.56
1:A:476:ILE:O	1:A:476:ILE:HG13	2.00	0.56
1:A:1211:LEU:HD12	1:A:1213:ARG:N	2.21	0.56
2:B:1115:GLN:HG2	2:B:1150:ARG:HG2	1.86	0.56
10:J:57:GLU:OE1	17:R:557:ILE:HG12	2.06	0.56
1:A:62:GLN:HE22	1:A:255:VAL:HG13	1.71	0.56
1:A:1180:ASN:CG	1:A:1182:GLN:HE21	2.14	0.56
8:H:110:THR:O	8:H:129:ALA:N	2.32	0.56
16:Q:211:LEU:HB2	16:Q:213:LYS:HZ2	1.71	0.56
17:R:473:ASN:HA	17:R:476:GLU:CD	2.30	0.56
20:W:19:ILE:HG12	20:W:39:SER:OG	2.06	0.56
26:c:32:ARG:NH1	27:d:32:GLU:OE1	2.35	0.56
1:A:469:MET:HG3	2:B:1093:CYS:SG	2.46	0.55
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.88	0.55
16:Q:208:PHE:HD1	16:Q:213:LYS:HD2	1.70	0.55
20:W:68:VAL:HG13	20:W:83:SER:HA	1.87	0.55
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.87	0.55
2:B:588:ARG:O	2:B:592:ARG:HD3	2.07	0.55
5:E:114:ALA:O	5:E:117:SER:OG	2.23	0.55
7:G:118:GLU:O	7:G:128:TYR:HA	2.06	0.55
16:Q:302:GLU:HG3	16:Q:305:GLN:NE2	2.20	0.55
16:U:395:GLU:HA	19:V:172:ARG:HH11	1.71	0.55
22:Y:14:ARG:NH2	22:Y:55:SER:OG	2.39	0.55
23:Z:546:THR:HG23	23:Z:563:MET:HE2	1.88	0.55
2:B:279:VAL:HG23	2:B:312:GLN:O	2.06	0.55
2:B:639:HIS:O	2:B:643:LEU:HB2	2.06	0.55
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.88	0.55
2:B:933:ASP:OD2	2:B:1050:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:PHE:HE2	4:D:80:ILE:HG12	1.72	0.55
15:P:23:G:H2'	15:P:24:A:C8	2.35	0.55
17:R:360:ASN:HA	17:R:363:ARG:HB2	1.89	0.55
23:Z:472:PHE:HB3	23:Z:476:ASP:OD2	2.06	0.55
27:d:59:MET:O	27:d:63:VAL:HG23	2.07	0.55
1:A:229:SER:OG	1:A:232:GLU:HB2	2.07	0.55
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.35	0.55
1:A:1234:LYS:HE2	1:A:1298:LEU:HA	1.87	0.55
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.40	0.55
2:B:859:ARG:HH22	2:B:901:THR:HG22	1.72	0.55
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.06	0.55
16:Q:451:PRO:HD3	16:Q:480:ARG:HG3	1.88	0.55
17:R:363:ARG:NE	17:R:446:GLU:HA	2.21	0.55
17:R:569:GLU:O	17:R:572:ILE:HG22	2.07	0.55
16:U:384:VAL:HA	16:U:418:ASN:HB3	1.86	0.55
1:A:365:THR:HG22	1:A:366:VAL:H	1.70	0.55
1:A:522:PRO:O	1:A:662:HIS:HB2	2.07	0.55
2:B:995:GLU:OE1	19:V:131:MET:HB3	2.05	0.55
20:W:108:ASP:HA	20:W:126:HIS:CE1	2.41	0.55
1:A:727:PRO:HA	1:A:736:THR:HG21	1.89	0.55
13:M:1369:VAL:HG11	13:M:1416:VAL:HG21	1.88	0.55
14:N:31:DT:H2''	14:N:32:DG:C8	2.41	0.55
16:Q:697:TYR:OH	16:Q:726:ALA:O	2.21	0.55
20:W:27:ASN:HB2	20:W:31:ASN:HD21	1.70	0.55
21:X:233:THR:O	21:X:236:THR:OG1	2.22	0.55
1:A:760:LEU:HD13	1:A:764:ASN:HD22	1.71	0.55
1:A:1302:GLU:C	1:A:1304:ILE:H	2.15	0.55
2:B:218:THR:HG23	2:B:238:SER:HB3	1.88	0.55
3:C:60:HIS:HB2	3:C:63:PHE:H	1.71	0.55
5:E:55:ARG:O	5:E:56:THR:OG1	2.23	0.55
13:M:1344:GLU:HA	13:M:1347:MET:HE2	1.87	0.55
16:U:379:PRO:HD2	16:U:382:LEU:HD12	1.89	0.55
23:Z:416:ARG:NE	23:Z:466:GLN:HE21	2.04	0.55
24:e:102:ALA:O	24:e:105:GLU:HB2	2.06	0.55
1:A:353:ASN:OD1	2:B:1071:ASN:ND2	2.39	0.55
23:Z:610:ARG:HD2	23:Z:629:LEU:HD21	1.89	0.55
1:A:1208:SER:O	1:A:1260:ARG:HD3	2.07	0.55
18:T:48:DT:H2''	18:T:49:DT:H5'	1.89	0.55
26:c:54:VAL:HG13	27:d:107:ALA:HB1	1.88	0.55
27:d:106:HIS:O	27:d:109:SER:HB2	2.06	0.55
1:A:874:LYS:HG3	1:A:880:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:THR:HA	2:B:164:ASN:ND2	2.22	0.55
7:G:117:MET:N	7:G:117:MET:SD	2.80	0.55
9:I:17:CYS:HB3	9:I:22:ASN:H	1.72	0.55
10:J:36:ASP:OD1	10:J:36:ASP:N	2.28	0.55
16:Q:772:GLU:HB3	16:Q:774:SER:CB	2.37	0.55
20:W:236:LEU:HD13	20:W:278:TRP:CE3	2.42	0.55
20:W:256:VAL:O	20:W:269:THR:HA	2.07	0.55
16:Q:525:ARG:HG3	16:Q:526:GLU:HG3	1.88	0.54
1:A:290:LEU:HD13	1:A:306:ASP:CG	2.33	0.54
2:B:649:ASN:ND2	16:U:460:TYR:OH	2.40	0.54
13:M:1476:TYR:OH	13:M:1483:ARG:NH2	2.40	0.54
16:Q:94:VAL:HG23	16:Q:140:LEU:HD11	1.89	0.54
16:Q:568:TRP:CD2	16:Q:592:LEU:HD13	2.42	0.54
17:R:471:GLU:HG2	17:R:474:LYS:HE3	1.88	0.54
19:V:127:VAL:HG23	19:V:128:VAL:H	1.71	0.54
20:W:76:LEU:HD12	20:W:77:PRO:HD2	1.90	0.54
8:H:37:MET:HE3	8:H:131:ASN:HD22	1.71	0.54
17:R:492:ILE:O	17:R:496:VAL:HG13	2.06	0.54
19:V:95:ASP:OD1	19:V:95:ASP:N	2.39	0.54
20:W:81:SER:HB3	20:W:91:TRP:NE1	2.20	0.54
21:X:250:PHE:CE1	21:X:253:LEU:HD22	2.42	0.54
1:A:141:LEU:HA	1:A:144:VAL:HG22	1.89	0.54
1:A:695:ASP:O	1:A:697:LYS:N	2.39	0.54
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.90	0.54
14:N:43:DA:H2"	14:N:44:DT:OP2	2.08	0.54
15:P:24:A:C2	18:T:50:DC:O2	2.61	0.54
16:Q:313:ALA:HB2	16:Q:328:TYR:CB	2.37	0.54
16:Q:511:CYS:O	20:W:229:SER:OG	2.24	0.54
20:W:33:GLU:O	20:W:49:TRP:N	2.41	0.54
16:Q:147:GLN:O	16:Q:151:GLN:HG2	2.08	0.54
16:Q:309:CYS:HB3	16:Q:328:TYR:HD1	1.73	0.54
16:Q:316:PHE:HB2	16:Q:325:ALA:HB2	1.90	0.54
26:c:55:LEU:HD22	27:d:63:VAL:HG13	1.88	0.54
1:A:606:HIS:HB3	1:A:626:THR:HB	1.89	0.54
16:Q:46:ALA:O	16:Q:50:GLU:HG2	2.08	0.54
20:W:29:LYS:O	20:W:77:PRO:HB3	2.08	0.54
23:Z:235:VAL:O	23:Z:239:ILE:HG12	2.07	0.54
1:A:48:GLU:OE2	1:A:51:ARG:HB2	2.08	0.54
2:B:309:PHE:HD2	9:I:40:ARG:NE	2.04	0.54
2:B:714:PRO:HD2	2:B:1001:PRO:HG3	1.88	0.54
2:B:1010:LYS:HE3	19:V:130:TRP:CZ3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:364:PHE:HB3	16:Q:380:ILE:HD11	1.90	0.54
16:Q:546:ASN:HD22	16:Q:577:ALA:HB2	1.73	0.54
20:W:31:ASN:HB2	20:W:72:ILE:HG21	1.90	0.54
23:Z:244:ASN:HB3	23:Z:245:LEU:HD22	1.90	0.54
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.38	0.54
2:B:169:ARG:NH1	19:V:139:THR:OG1	2.40	0.54
2:B:792:ASP:CG	2:B:975:ARG:HH12	2.16	0.54
9:I:39:CYS:SG	9:I:40:ARG:N	2.81	0.54
16:Q:274:HIS:HA	16:Q:277:ASN:ND2	2.23	0.54
16:Q:505:ARG:HE	19:V:44:PHE:HB3	1.73	0.54
16:Q:776:LEU:HD22	16:Q:831:ALA:HA	1.88	0.54
23:Z:364:ASN:O	23:Z:374:LYS:NZ	2.39	0.54
2:B:957:THR:HG22	2:B:1028:LEU:HD22	1.90	0.54
7:G:36:GLY:O	23:Z:628:LYS:NZ	2.23	0.54
7:G:46:ILE:HB	7:G:75:ILE:HG13	1.89	0.54
17:R:564:ASN:ND2	19:V:136:TYR:C	2.64	0.54
19:V:55:GLN:OE1	19:V:57:ARG:NE	2.35	0.54
20:W:41:ASP:OD1	20:W:41:ASP:N	2.40	0.54
20:W:108:ASP:HA	20:W:126:HIS:ND1	2.23	0.54
25:b:33:ALA:C	25:b:35:ARG:H	2.16	0.54
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.89	0.54
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.90	0.54
20:W:248:VAL:HG12	20:W:258:VAL:HG22	1.90	0.54
22:Y:40:LEU:HD22	22:Y:42:MET:HB3	1.89	0.54
1:A:350:VAL:HA	1:A:354:LEU:HB2	1.89	0.53
9:I:29:ASP:HB3	9:I:34:ILE:HG13	1.89	0.53
18:T:-29:DC:H2"	18:T:-28:DT:OP2	2.08	0.53
20:W:163:LEU:O	20:W:175:PHE:N	2.34	0.53
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.89	0.53
2:B:959:GLU:OE1	2:B:959:GLU:N	2.41	0.53
7:G:117:MET:HB3	7:G:128:TYR:HB3	1.89	0.53
16:Q:553:TRP:HD1	16:Q:556:GLU:OE1	1.91	0.53
16:Q:761:LEU:HD22	16:Q:785:GLU:HB3	1.90	0.53
16:Q:774:SER:O	16:Q:830:ARG:NH2	2.41	0.53
17:R:560:ILE:O	17:R:563:ILE:HG22	2.08	0.53
1:A:606:HIS:CG	1:A:607:SER:H	2.26	0.53
2:B:22:TRP:CH2	2:B:679:PRO:HD3	2.43	0.53
2:B:395:LEU:HD11	2:B:532:ILE:HD12	1.91	0.53
9:I:68:ILE:HB	9:I:122:ARG:HD3	1.91	0.53
16:Q:392:GLU:HG2	16:Q:393:LYS:HG2	1.90	0.53
16:Q:772:GLU:HB3	16:Q:774:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.90	0.53
2:B:388:TYR:CE1	2:B:505:LEU:HD21	2.43	0.53
4:D:61:PHE:CE2	4:D:65:LEU:HD21	2.44	0.53
7:G:7:LEU:N	7:G:72:TYR:O	2.40	0.53
7:G:93:ASN:O	7:G:128:TYR:OH	2.27	0.53
16:Q:867:GLU:O	16:Q:871:GLN:HG3	2.08	0.53
1:A:64:VAL:HG12	1:A:81:CYS:SG	2.48	0.53
5:E:45:GLY:HA3	5:E:52:ARG:HB2	1.91	0.53
5:E:119:VAL:HA	5:E:122:ALA:HB2	1.90	0.53
10:J:65:LEU:HD12	10:J:66:GLU:OE1	2.09	0.53
13:M:1440:ARG:O	13:M:1444:GLU:HG2	2.08	0.53
16:Q:190:LEU:O	16:Q:193:ASN:ND2	2.41	0.53
16:Q:776:LEU:O	16:Q:780:LEU:HD12	2.08	0.53
17:R:355:LEU:HD11	17:R:357:GLU:HG2	1.90	0.53
17:R:356:PRO:HB3	17:R:452:PHE:HB2	1.90	0.53
7:G:8:GLU:HA	7:G:71:LYS:HA	1.91	0.53
7:G:100:GLU:OE1	7:G:105:SER:HB3	2.08	0.53
16:Q:454:LEU:HA	16:Q:457:VAL:HG12	1.91	0.53
17:R:385:CYS:O	17:R:405:ILE:HD12	2.08	0.53
17:R:449:GLU:O	17:R:453:MET:HG2	2.07	0.53
17:R:577:LYS:O	17:R:580:VAL:HG22	2.09	0.53
18:T:-45:DA:H5'	27:d:30:ARG:NH2	2.24	0.53
18:T:-11:DG:H2''	18:T:-10:DC:OP2	2.09	0.53
2:B:108:MET:HE2	2:B:113:ALA:HB2	1.90	0.53
2:B:141:GLN:O	2:B:143:GLN:N	2.42	0.53
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.89	0.53
16:Q:384:LEU:HD21	16:Q:386:ALA:HB3	1.91	0.53
17:R:452:PHE:CZ	17:R:456:LYS:HE2	2.43	0.53
23:Z:279:VAL:HA	23:Z:386:VAL:HG21	1.90	0.53
1:A:802:PHE:HD2	2:B:671:GLU:HG2	1.74	0.53
1:A:845:GLU:OE2	2:B:500:GLN:NE2	2.42	0.53
1:A:1180:ASN:ND2	1:A:1182:GLN:HE21	2.07	0.53
2:B:741:HIS:CD2	2:B:742:VAL:HG23	2.43	0.53
7:G:109:SER:HB3	23:Z:493:VAL:HG11	1.91	0.53
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.91	0.53
18:T:34:DT:H2''	18:T:35:DG:C8	2.44	0.53
20:W:217:TYR:HA	20:W:224:LEU:HA	1.91	0.53
20:W:228:LEU:HD13	20:W:264:ARG:HB3	1.90	0.53
1:A:86:GLY:C	1:A:255:VAL:HG12	2.34	0.53
1:A:525:ILE:O	1:A:534:VAL:HG22	2.09	0.53
8:H:15:ILE:O	8:H:16:ASP:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:450:LEU:CD2	16:U:452:LEU:HD23	2.37	0.53
19:V:45:ASP:HB3	21:X:232:ARG:HE	1.73	0.53
25:b:31:LYS:N	25:b:32:PRO:HD2	2.23	0.53
2:B:651:TYR:HB2	16:U:460:TYR:CZ	2.44	0.53
2:B:851:ASP:HB2	12:L:15:MET:HG2	1.91	0.53
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.39	0.53
12:L:35:ARG:HH11	12:L:40:GLY:CA	2.20	0.53
16:Q:631:ARG:O	16:Q:635:ILE:HG12	2.09	0.53
1:A:102:LYS:HE2	1:A:138:LYS:HZ3	1.75	0.52
16:Q:763:ARG:HG2	19:V:25:GLU:HG3	1.91	0.52
23:Z:422:PRO:HG3	23:Z:443:VAL:HG21	1.91	0.52
25:b:33:ALA:O	25:b:35:ARG:N	2.42	0.52
1:A:241:ARG:HB2	1:A:241:ARG:CZ	2.39	0.52
2:B:342:VAL:HG23	2:B:346:GLU:HB2	1.89	0.52
2:B:1136:GLU:HA	2:B:1143:LYS:HA	1.90	0.52
20:W:9:PHE:H	20:W:300:ILE:HB	1.73	0.52
1:A:129:ILE:HD13	1:A:132:LYS:NZ	2.24	0.52
4:D:82:SER:O	4:D:85:SER:OG	2.25	0.52
4:D:130:ILE:HA	4:D:133:ASP:OD2	2.09	0.52
5:E:36:THR:HG1	5:E:39:GLU:CD	2.15	0.52
13:M:1447:LEU:HB3	13:M:1477:GLN:HG3	1.91	0.52
15:P:24:A:C3'	15:P:25:A:C8	2.87	0.52
16:Q:623:GLU:O	16:Q:627:ARG:NE	2.42	0.52
17:R:458:ALA:HB3	17:R:459:MET:HE2	1.91	0.52
22:Y:45:ASN:HD21	22:Y:48:MET:HB2	1.75	0.52
27:d:67:PHE:CD1	27:d:67:PHE:C	2.88	0.52
2:B:420:GLN:C	2:B:422:PHE:H	2.17	0.52
4:D:63:LYS:HA	4:D:66:ASN:HD21	1.75	0.52
8:H:9:ILE:HD12	8:H:148:LEU:HD11	1.90	0.52
19:V:193:HIS:H	19:V:197:PRO:HA	1.73	0.52
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.90	0.52
2:B:789:ASN:O	2:B:968:ASN:HB2	2.09	0.52
3:C:212:ASP:OD1	3:C:212:ASP:N	2.28	0.52
1:A:1359:SER:O	1:A:1359:SER:OG	2.16	0.52
5:E:111:THR:HG23	5:E:114:ALA:H	1.73	0.52
13:M:1473:LEU:HD11	13:M:1484:ILE:HD12	1.92	0.52
16:Q:380:ILE:HD12	16:Q:400:HIS:HE1	1.75	0.52
20:W:39:SER:HB2	20:W:41:ASP:OD1	2.10	0.52
23:Z:193:ALA:O	23:Z:197:MET:HG3	2.10	0.52
25:f:26:ILE:HD12	25:f:55:ARG:HB3	1.92	0.52
16:Q:239:ALA:HA	16:Q:257:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:244:ASN:ND2	19:V:69:GLN:HA	2.24	0.52
20:W:176:ASP:HB2	20:W:183:LEU:HD21	1.92	0.52
2:B:624:PRO:HA	2:B:663:GLU:O	2.09	0.52
7:G:37:THR:OG1	7:G:38:CYS:N	2.43	0.52
8:H:83:SER:HG	8:H:85:ALA:H	1.57	0.52
13:M:1443:LEU:HD13	13:M:1473:LEU:HD22	1.92	0.52
1:A:927:GLU:HG3	1:A:943:LEU:HD11	1.92	0.52
2:B:609:GLU:O	2:B:609:GLU:HG2	2.09	0.52
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.92	0.52
4:D:63:LYS:HE2	7:G:102:GLY:O	2.10	0.52
9:I:81:THR:HG23	9:I:96:PHE:CE1	2.45	0.52
16:Q:172:ILE:HG22	16:Q:176:LYS:HZ1	1.75	0.52
16:Q:240:VAL:HG21	16:Q:270:MET:HE3	1.90	0.52
16:Q:682:ASP:OD1	16:Q:683:VAL:N	2.43	0.52
18:T:52:DG:C2	18:T:53:DC:C2	2.97	0.52
5:E:84:ILE:HG12	5:E:114:ALA:HA	1.91	0.52
7:G:4:HIS:C	7:G:73:LYS:HZ1	2.17	0.52
13:M:1494:PHE:HE2	13:M:1504:VAL:HG12	1.74	0.52
16:Q:513:PHE:HB2	20:W:213:TYR:HE1	1.75	0.52
16:Q:768:VAL:HG13	16:Q:769:LEU:HG	1.91	0.52
16:Q:777:LYS:HA	16:Q:780:LEU:HD13	1.91	0.52
17:R:403:ALA:HB1	17:R:428:LEU:HB3	1.91	0.52
3:C:36:ARG:NH2	11:K:41:THR:OG1	2.40	0.51
5:E:166:ARG:HH12	5:E:168:ASN:ND2	1.99	0.51
1:A:123:ASN:HD22	1:A:125:LYS:HD3	1.75	0.51
2:B:177:CYS:SG	2:B:737:ILE:HD11	2.50	0.51
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.92	0.51
14:N:3:DC:H2"	14:N:4:DG:C8	2.45	0.51
16:Q:26:GLU:HG3	16:Q:28:ASP:H	1.74	0.51
23:Z:568:VAL:HG13	23:Z:570:VAL:HG13	1.91	0.51
1:A:410:ASN:HD22	1:A:430:ARG:HD2	1.76	0.51
1:A:428:ASP:OD1	1:A:430:ARG:NH2	2.43	0.51
2:B:56:GLN:HG2	2:B:91:ILE:HG22	1.92	0.51
2:B:997:GLY:HA2	19:V:131:MET:HG2	1.91	0.51
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.91	0.51
20:W:116:PRO:HD3	20:W:156:TYR:HB3	1.92	0.51
4:D:51:ALA:O	4:D:54:GLU:HB2	2.10	0.51
4:D:61:PHE:O	4:D:65:LEU:HG	2.11	0.51
16:Q:143:ASP:N	16:Q:143:ASP:OD1	2.44	0.51
17:R:493:GLU:H	17:R:493:GLU:CD	2.16	0.51
23:Z:745:VAL:HG11	23:Z:750:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:993:LYS:HG2	2:B:1018:TYR:OH	2.11	0.51
5:E:209:VAL:O	5:E:210:GLN:HB2	2.10	0.51
11:K:80:ASP:OD1	11:K:80:ASP:N	2.32	0.51
14:N:-32:DC:H2''	14:N:-31:DA:H8	1.76	0.51
17:R:581:ALA:O	17:R:585:ASN:ND2	2.43	0.51
16:U:394:TYR:C	19:V:172:ARG:HH11	2.18	0.51
23:Z:454:HIS:HE2	23:Z:463:PHE:HE2	1.58	0.51
23:Z:588:ASP:HA	23:Z:640:THR:O	2.10	0.51
1:A:43:TYR:HB3	1:A:45:GLU:OE1	2.11	0.51
1:A:44:PRO:HG2	1:A:285:LYS:HD3	1.93	0.51
2:B:1142:ASN:O	2:B:1144:THR:HG22	2.10	0.51
4:D:63:LYS:HD3	7:G:103:PRO:HA	1.92	0.51
7:G:46:ILE:HD11	7:G:77:PHE:CB	2.40	0.51
18:T:53:DC:C2	18:T:54:DC:C5	2.99	0.51
23:Z:206:THR:OG1	23:Z:207:ASP:N	2.43	0.51
23:Z:232:GLN:HE21	23:Z:252:GLN:HB2	1.75	0.51
23:Z:478:VAL:HG22	23:Z:490:GLY:O	2.11	0.51
1:A:651:SER:O	1:A:655:ILE:HG12	2.11	0.51
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.93	0.51
4:D:123:GLU:OE1	4:D:123:GLU:N	2.44	0.51
14:N:6:DA:N6	18:T:-7:DG:C6	2.78	0.51
16:Q:93:TYR:HB3	16:Q:113:ALA:HB2	1.93	0.51
16:Q:164:PRO:HA	16:Q:167:LEU:HB2	1.93	0.51
16:Q:420:GLN:HA	21:X:229:ARG:HH12	1.75	0.51
16:Q:790:HIS:HA	16:Q:793:PHE:CD2	2.45	0.51
20:W:22:VAL:HG23	20:W:37:THR:HG22	1.92	0.51
20:W:44:VAL:HB	20:W:60:LEU:HB2	1.93	0.51
20:W:231:HIS:ND1	20:W:235:VAL:HG22	2.26	0.51
21:X:248:ASN:OD1	21:X:249:ILE:HG13	2.10	0.51
1:A:1546:PHE:HD2	13:M:1516:GLN:HG3	1.75	0.51
2:B:169:ARG:NH1	19:V:139:THR:O	2.43	0.51
4:D:37:VAL:HG21	7:G:2:PHE:HD2	1.75	0.51
13:M:1476:TYR:OH	13:M:1485:GLU:OE1	2.20	0.51
16:Q:744:ARG:HG2	16:Q:748:PRO:HA	1.93	0.51
16:Q:769:LEU:HD13	16:Q:824:ALA:HB2	1.91	0.51
17:R:493:GLU:O	17:R:496:VAL:HG22	2.11	0.51
16:U:373:LEU:HD23	16:U:375:PHE:H	1.76	0.51
20:W:295:ASP:OD2	20:W:297:GLU:HB2	2.11	0.51
1:A:140:ARG:O	1:A:144:VAL:HG13	2.11	0.51
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.93	0.51
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:417:LEU:N	17:R:420:THR:O	2.40	0.51
22:Y:40:LEU:HD21	22:Y:52:CYS:SG	2.51	0.51
23:Z:436:LEU:HB3	23:Z:454:HIS:CE1	2.45	0.51
1:A:316:THR:HA	1:A:319:ASP:O	2.11	0.51
1:A:1177:TYR:CE1	1:A:1210:TRP:HB3	2.46	0.51
1:A:1229:GLU:O	1:A:1233:GLU:HG3	2.10	0.51
7:G:91:GLN:HA	7:G:139:GLN:NE2	2.26	0.51
17:R:452:PHE:HB3	17:R:453:MET:HE2	1.93	0.51
17:R:454:LYS:NZ	17:R:458:ALA:HB2	2.26	0.51
23:Z:199:LYS:HG2	23:Z:210:LEU:HD21	1.93	0.51
23:Z:312:ASP:O	23:Z:315:ARG:HG2	2.11	0.51
1:A:120:ASP:O	1:A:122:ASN:ND2	2.44	0.50
2:B:44:LEU:HD23	2:B:155:MET:HE3	1.92	0.50
2:B:848:LEU:HD23	2:B:865:VAL:HG13	1.93	0.50
7:G:118:GLU:HG2	7:G:129:LYS:O	2.11	0.50
18:T:54:DC:H2"	18:T:55:DG:C8	2.46	0.50
20:W:108:ASP:HA	20:W:126:HIS:HD1	1.76	0.50
23:Z:440:ILE:HA	23:Z:450:ILE:HD11	1.93	0.50
1:A:725:LEU:HD23	1:A:733:LEU:HD11	1.93	0.50
1:A:922:PHE:N	1:A:1052:ARG:HH21	2.09	0.50
5:E:47:LYS:O	5:E:53:PRO:HD2	2.11	0.50
16:Q:166:LEU:HA	16:Q:169:LYS:NZ	2.26	0.50
16:Q:244:ASN:HD22	19:V:69:GLN:HA	1.76	0.50
17:R:410:GLU:HA	17:R:424:LYS:HA	1.93	0.50
21:X:252:ILE:HG13	21:X:253:LEU:N	2.26	0.50
23:Z:478:VAL:O	23:Z:489:THR:HG23	2.11	0.50
1:A:383:SER:HB3	11:K:2:ASN:HD21	1.76	0.50
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.29	0.50
16:Q:750:ASP:HB3	16:Q:753:LEU:HG	1.93	0.50
16:Q:837:GLU:O	16:Q:840:GLU:HG3	2.11	0.50
17:R:404:GLU:O	17:R:428:LEU:HA	2.11	0.50
23:Z:470:LYS:HD2	23:Z:472:PHE:CZ	2.46	0.50
1:A:324:GLY:O	1:A:325:LEU:HD22	2.12	0.50
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.93	0.50
1:A:1176:TYR:C	1:A:1177:TYR:HD1	2.19	0.50
2:B:388:TYR:OH	2:B:524:LYS:HE3	2.10	0.50
2:B:1142:ASN:ND2	2:B:1145:GLN:O	2.45	0.50
5:E:21:CYS:O	5:E:26:TYR:HB2	2.12	0.50
7:G:151:ARG:HG3	23:Z:477:HIS:NE2	2.27	0.50
18:T:-12:DC:H2"	18:T:-11:DG:C8	2.47	0.50
20:W:159:ASP:OD2	20:W:161:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:63:MET:SD	22:Y:72:SER:HB2	2.51	0.50
1:A:419:ILE:HD12	1:A:440:LEU:HD23	1.92	0.50
1:A:1227:THR:N	1:A:1230:GLN:HE21	1.98	0.50
1:A:1467:GLY:C	1:A:1469:GLY:N	2.70	0.50
5:E:177:ASP:O	5:E:181:ARG:HG3	2.11	0.50
7:G:101:ILE:N	7:G:104:MET:O	2.43	0.50
13:M:1347:MET:HB2	13:M:1372:LYS:HE3	1.94	0.50
16:Q:163:ILE:HB	16:Q:164:PRO:HD3	1.94	0.50
20:W:110:TRP:H	20:W:123:THR:HG23	1.76	0.50
20:W:172:ILE:N	20:W:186:LEU:O	2.42	0.50
20:W:258:VAL:O	20:W:267:VAL:HG22	2.11	0.50
26:c:95:LYS:O	26:c:98:GLY:N	2.45	0.50
1:A:299:ALA:C	1:A:301:HIS:H	2.20	0.50
1:A:587:THR:HG22	1:A:588:GLY:N	2.27	0.50
1:A:1474:LEU:HB2	6:F:105:ILE:HG12	1.93	0.50
16:Q:530:TYR:HD2	16:Q:533:CYS:HB2	1.76	0.50
26:c:17:ARG:HG2	27:d:118:TYR:HE1	1.76	0.50
15:P:23:G:N3	15:P:24:A:C8	2.80	0.50
16:Q:829:ALA:HA	16:Q:832:ARG:HD2	1.94	0.50
16:Q:880:GLN:HB2	16:Q:884:LYS:HZ3	1.75	0.50
19:V:126:LYS:HE3	19:V:126:LYS:HA	1.94	0.50
1:A:330:GLN:C	1:A:332:SER:H	2.17	0.50
2:B:130:LYS:HB3	2:B:142:THR:HG23	1.94	0.50
16:Q:129:ASN:OD1	16:Q:132:LEU:HD13	2.12	0.50
16:Q:635:ILE:O	16:Q:639:VAL:HG22	2.11	0.50
17:R:414:VAL:HG22	17:R:423:ASN:HB3	1.94	0.50
1:A:738:GLU:OE2	1:A:797:ARG:NH2	2.45	0.50
2:B:170:ASP:N	2:B:170:ASP:OD1	2.43	0.50
13:M:1374:SER:HB2	13:M:1377:ILE:HD13	1.93	0.50
14:N:31:DT:H2''	14:N:32:DG:H8	1.74	0.50
16:Q:128:GLN:HA	16:Q:158:GLN:NE2	2.26	0.50
16:Q:128:GLN:NE2	19:V:86:LEU:HD13	2.26	0.50
17:R:592:ASP:O	17:R:594:PHE:N	2.38	0.50
20:W:231:HIS:ND1	20:W:251:SER:HB3	2.26	0.50
1:A:428:ASP:OD1	1:A:430:ARG:HG3	2.11	0.49
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.47	0.49
14:N:-31:DA:H2''	14:N:-30:DG:H8	1.75	0.49
14:N:17:DA:H2''	14:N:18:DG:C8	2.46	0.49
15:P:24:A:H2'	15:P:25:A:C8	2.47	0.49
16:Q:841:LEU:HD23	16:Q:844:LYS:HD3	1.93	0.49
16:U:448:MET:HE2	16:U:461:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:289:ILE:N	20:W:301:TYR:O	2.41	0.49
23:Z:215:VAL:HG12	23:Z:227:VAL:HG23	1.94	0.49
24:a:70:LEU:O	24:a:74:ILE:HD12	2.12	0.49
27:d:62:PHE:O	27:d:66:VAL:HG23	2.11	0.49
1:A:1288:ILE:HA	1:A:1291:ASN:ND2	2.26	0.49
2:B:237:VAL:HG11	2:B:369:VAL:HG22	1.94	0.49
2:B:679:PRO:HG2	2:B:680:ASP:H	1.78	0.49
4:D:133:ASP:O	4:D:137:LYS:HG2	2.12	0.49
10:J:22:LEU:HD22	17:R:563:ILE:HG21	1.94	0.49
16:Q:68:ARG:NE	16:Q:89:LEU:HD12	2.27	0.49
16:Q:106:LYS:O	16:Q:110:ILE:HG12	2.12	0.49
16:Q:310:TYR:CE2	16:Q:342:LEU:HD13	2.46	0.49
17:R:403:ALA:HB3	17:R:428:LEU:HD13	1.93	0.49
17:R:441:PHE:HA	23:Z:776:PRO:O	2.11	0.49
20:W:17:ASP:HB2	20:W:41:ASP:HB3	1.92	0.49
21:X:233:THR:HG22	21:X:236:THR:HG23	1.94	0.49
2:B:1007:ASN:N	2:B:1007:ASN:OD1	2.42	0.49
3:C:86:ARG:NH2	23:Z:716:PRO:O	2.45	0.49
4:D:33:LEU:HB2	4:D:36:GLU:HB2	1.93	0.49
7:G:7:LEU:O	7:G:72:TYR:N	2.27	0.49
16:Q:38:HIS:CE1	16:Q:73:LEU:HD22	2.47	0.49
17:R:358:GLU:HA	17:R:361:ARG:NE	2.27	0.49
17:R:363:ARG:HE	17:R:446:GLU:HG2	1.78	0.49
18:T:-67:DA:H2''	18:T:-66:DA:O4'	2.13	0.49
16:U:453:GLY:HA2	19:V:185:ASP:OD2	2.12	0.49
25:b:28:GLY:O	25:b:30:THR:HG23	2.12	0.49
1:A:471:GLY:O	1:A:521:VAL:HG23	2.12	0.49
1:A:1173:THR:HG23	1:A:1214:VAL:HG22	1.94	0.49
1:A:1218:ARG:HH22	1:A:1253:GLU:HA	1.77	0.49
7:G:46:ILE:HD11	7:G:77:PHE:HB3	1.94	0.49
7:G:110:ARG:HD2	7:G:113:ILE:HB	1.95	0.49
9:I:96:PHE:HA	9:I:111:TYR:O	2.13	0.49
13:M:783:GLY:N	13:M:797:ALA:O	2.46	0.49
14:N:51:DG:OP2	14:N:51:DG:H2'	2.12	0.49
20:W:228:LEU:HD11	20:W:259:TRP:CZ3	2.48	0.49
1:A:496:PHE:HB2	2:B:791:GLU:O	2.12	0.49
1:A:742:ASN:O	1:A:746:ASN:ND2	2.45	0.49
1:A:833:PRO:HB2	2:B:677:MET:SD	2.52	0.49
2:B:431:LEU:HD23	2:B:431:LEU:H	1.77	0.49
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.76	0.49
4:D:108:ALA:N	4:D:128:GLN:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:HIS:HB2	5:E:70:ASP:OD2	2.12	0.49
13:M:1398:LEU:HD23	13:M:1400:ILE:HG23	1.93	0.49
16:Q:288:VAL:HG13	16:Q:289:GLN:HG3	1.93	0.49
17:R:431:GLY:N	17:R:459:MET:HE1	2.27	0.49
22:Y:33:CYS:SG	22:Y:36:CYS:N	2.85	0.49
23:Z:426:VAL:HG13	23:Z:440:ILE:HD11	1.95	0.49
1:A:926:ASN:O	1:A:930:LEU:HG	2.13	0.49
1:A:1000:LEU:O	1:A:1059:ARG:NH2	2.45	0.49
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.29	0.49
1:A:1182:GLN:C	1:A:1192:TRP:HE1	2.18	0.49
2:B:1120:ASN:HD22	2:B:1145:GLN:HB3	1.77	0.49
14:N:9:DT:H2"	14:N:10:DG:C8	2.48	0.49
16:Q:163:ILE:O	16:Q:166:LEU:HG	2.12	0.49
16:Q:524:LEU:HD11	16:Q:537:LEU:HD12	1.94	0.49
16:Q:743:ALA:O	16:Q:746:VAL:HG22	2.12	0.49
17:R:570:TRP:CD1	19:V:133:LYS:HD2	2.43	0.49
1:A:202:TRP:HE3	1:A:212:LYS:HB2	1.76	0.49
4:D:76:ASN:O	4:D:79:THR:OG1	2.31	0.49
12:L:16:ILE:HG13	12:L:26:ASN:O	2.13	0.49
16:Q:24:LEU:HD11	16:Q:56:LYS:HZ3	1.77	0.49
16:Q:183:LEU:O	16:Q:187:LYS:HG2	2.13	0.49
16:Q:268:ASN:HB3	16:Q:271:VAL:HG12	1.95	0.49
17:R:359:LEU:HD22	17:R:452:PHE:CE1	2.47	0.49
19:V:97:ASN:ND2	19:V:98:VAL:O	2.46	0.49
23:Z:342:ALA:HB1	23:Z:346:ARG:NH1	2.28	0.49
23:Z:366:TYR:HB2	23:Z:374:LYS:HA	1.95	0.49
23:Z:735:GLU:HG3	23:Z:735:GLU:O	2.13	0.49
25:b:29:ILE:O	25:b:34:ILE:HD11	2.13	0.49
27:d:46:HIS:HB3	27:d:49:THR:OG1	2.12	0.49
1:A:54:LEU:O	1:A:61:ARG:NH1	2.45	0.49
1:A:963:ARG:O	1:A:967:ARG:HG3	2.13	0.49
1:A:1311:LEU:HD22	1:A:1332:GLN:HG2	1.95	0.49
2:B:650:ASN:C	16:U:460:TYR:CE2	2.91	0.49
2:B:728:MET:SD	2:B:942:LYS:HB3	2.52	0.49
8:H:60:ILE:HD11	8:H:123:MET:HE1	1.93	0.49
16:Q:379:LYS:HZ1	19:V:61:TYR:HE2	1.59	0.49
16:Q:578:LYS:HB2	16:Q:580:GLU:HG3	1.94	0.49
16:Q:764:LEU:HD22	16:Q:785:GLU:OE1	2.12	0.49
16:U:443:TRP:HA	19:V:201:PRO:HA	1.95	0.49
23:Z:529:ASP:HB3	23:Z:553:LEU:HD23	1.94	0.49
2:B:537:GLN:HG3	2:B:538:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ASP:O	2:B:872:THR:HG23	2.13	0.49
20:W:65:LEU:HD12	20:W:84:LEU:C	2.38	0.49
23:Z:470:LYS:HB3	23:Z:472:PHE:HE2	1.78	0.49
23:Z:588:ASP:HB3	23:Z:594:ILE:HG13	1.95	0.49
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.95	0.49
2:B:332:LYS:HB3	2:B:332:LYS:HE3	1.57	0.49
7:G:90:THR:HG23	7:G:99:THR:HA	1.95	0.49
13:M:1463:CYS:O	13:M:1473:LEU:N	2.30	0.49
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.14	0.48
3:C:92:GLU:HG2	23:Z:711:ARG:CZ	2.43	0.48
8:H:11:ASP:OD1	8:H:11:ASP:N	2.46	0.48
14:N:9:DT:H2"	14:N:10:DG:H8	1.77	0.48
16:Q:80:LYS:O	16:Q:84:THR:HG23	2.13	0.48
16:Q:232:VAL:O	16:Q:236:VAL:HG22	2.13	0.48
17:R:389:ILE:O	17:R:400:TYR:HD1	1.95	0.48
17:R:416:GLN:HA	17:R:421:ARG:HA	1.94	0.48
20:W:65:LEU:HG	20:W:85:ASP:HB3	1.94	0.48
21:X:242:GLY:O	21:X:243:LYS:HE2	2.13	0.48
23:Z:626:CYS:HB3	23:Z:629:LEU:HD12	1.95	0.48
26:c:42:ARG:HG3	27:d:85:THR:HG23	1.95	0.48
16:Q:855:LYS:O	16:Q:858:LYS:HG3	2.13	0.48
17:R:471:GLU:O	17:R:474:LYS:HG3	2.13	0.48
18:T:-3:DG:C5	18:T:-2:DC:C4	3.01	0.48
23:Z:444:ASP:HB3	23:Z:448:ILE:HA	1.93	0.48
1:A:1087:VAL:HG23	1:A:1400:LEU:HD21	1.95	0.48
1:A:1245:CYS:O	1:A:1246:ILE:HD13	2.13	0.48
2:B:130:LYS:NZ	2:B:429:PHE:O	2.46	0.48
2:B:357:CYS:SG	2:B:360:LYS:NZ	2.85	0.48
4:D:60:VAL:HG11	7:G:44:PHE:CZ	2.48	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:HE3	1.94	0.48
16:Q:663:PHE:HB3	16:Q:690:ILE:HG23	1.95	0.48
17:R:416:GLN:HE21	17:R:421:ARG:CZ	2.26	0.48
23:Z:746:ASP:OD1	23:Z:747:ARG:N	2.46	0.48
1:A:922:PHE:N	1:A:1052:ARG:HD2	2.19	0.48
1:A:1049:LEU:HG	1:A:1054:MET:HE3	1.96	0.48
1:A:1128:ILE:CG2	1:A:1414:ILE:HB	2.43	0.48
1:A:1162:GLU:HG2	1:A:1163:HIS:N	2.29	0.48
1:A:1263:ASN:N	1:A:1263:ASN:OD1	2.47	0.48
2:B:626:LEU:HD13	2:B:698:ILE:HG12	1.94	0.48
8:H:36:LYS:CE	16:Q:709:ARG:HH22	2.26	0.48
16:Q:166:LEU:HA	16:Q:169:LYS:HZ3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:390:ASP:HB2	16:Q:392:GLU:OE2	2.14	0.48
16:Q:835:ASP:O	16:Q:839:ARG:HG3	2.14	0.48
16:U:522:THR:O	16:U:524:LYS:N	2.46	0.48
20:W:35:VAL:O	20:W:47:TRP:N	2.44	0.48
20:W:89:ARG:HA	20:W:101:SER:HA	1.94	0.48
20:W:108:ASP:HB3	20:W:125:THR:HG23	1.95	0.48
23:Z:206:THR:HG23	23:Z:208:THR:H	1.79	0.48
1:A:104:MET:CE	1:A:193:ARG:HD2	2.44	0.48
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.79	0.48
1:A:488:VAL:O	1:A:491:PRO:HD2	2.14	0.48
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.48
2:B:816:GLU:OE2	2:B:869:LYS:HE3	2.13	0.48
4:D:44:ARG:HA	4:D:47:GLN:OE1	2.12	0.48
11:K:93:ASP:OD1	11:K:93:ASP:N	2.41	0.48
15:P:24:A:H2'	15:P:24:A:N3	2.29	0.48
16:Q:568:TRP:CZ2	16:Q:591:ILE:HB	2.48	0.48
16:Q:735:GLU:OE2	16:Q:738:GLN:HB2	2.13	0.48
17:R:363:ARG:HA	17:R:386:PHE:O	2.14	0.48
22:Y:19:CYS:SG	22:Y:35:ASN:ND2	2.84	0.48
23:Z:436:LEU:HD13	23:Z:454:HIS:CD2	2.49	0.48
23:Z:615:ARG:HB2	23:Z:616:HIS:CD2	2.49	0.48
1:A:1073:GLU:HG3	1:A:1074:SER:N	2.28	0.48
2:B:22:TRP:CZ2	2:B:679:PRO:HG3	2.48	0.48
2:B:92:TYR:HD2	16:U:506:ALA:HB3	1.78	0.48
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.95	0.48
2:B:425:ARG:HH11	2:B:427:LYS:HD3	1.78	0.48
3:C:74:THR:HG23	3:C:128:ILE:O	2.14	0.48
14:N:61:DC:H2''	14:N:62:DG:N7	2.29	0.48
16:Q:347:LEU:HB2	16:Q:363:CYS:SG	2.54	0.48
16:Q:454:LEU:HB3	16:Q:477:SER:OG	2.13	0.48
20:W:237:ASN:ND2	20:W:279:GLY:HA2	2.21	0.48
1:A:1083:PRO:HD2	6:F:58:THR:HG21	1.96	0.48
1:A:1177:TYR:HD2	9:I:28:GLU:OE1	1.97	0.48
2:B:44:LEU:HD23	2:B:155:MET:CE	2.44	0.48
2:B:719:SER:OG	2:B:720:PRO:HD3	2.14	0.48
15:P:25:A:C2	18:T:49:DT:N3	2.81	0.48
16:Q:153:HIS:HA	16:Q:169:LYS:HE3	1.96	0.48
16:Q:188:LYS:HB3	16:Q:191:ARG:NH2	2.29	0.48
16:Q:844:LYS:O	16:Q:848:GLU:HG3	2.14	0.48
17:R:370:GLU:HA	17:R:373:CYS:SG	2.53	0.48
16:U:459:VAL:HG23	16:U:494:HIS:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:118:THR:HA	25:b:45:ARG:HB3	1.96	0.48
27:d:56:MET:HE3	27:d:56:MET:O	2.13	0.48
1:A:10:ASP:O	2:B:1130:THR:HG21	2.14	0.48
1:A:111:CYS:SG	1:A:114:CYS:HB2	2.54	0.48
2:B:166:LEU:HG	2:B:170:ASP:HB2	1.96	0.48
2:B:320:PHE:O	2:B:323:SER:OG	2.31	0.48
2:B:1007:ASN:O	2:B:1011:ILE:HG13	2.14	0.48
16:Q:7:GLU:OE1	16:Q:18:GLU:HB3	2.14	0.48
16:Q:39:THR:OG1	16:Q:43:ILE:HD13	2.14	0.48
16:Q:542:ARG:NH1	16:Q:574:LEU:HA	2.28	0.48
16:Q:568:TRP:CE2	16:Q:592:LEU:HD13	2.49	0.48
16:Q:815:ARG:O	16:Q:818:SER:OG	2.25	0.48
16:Q:854:GLN:HB2	16:Q:855:LYS:NZ	2.28	0.48
20:W:110:TRP:CD2	20:W:150:PHE:HZ	2.32	0.48
23:Z:257:ILE:O	23:Z:260:MET:HG2	2.13	0.48
24:a:61:LEU:O	25:b:36:ARG:NH1	2.42	0.48
27:d:31:LYS:O	27:d:31:LYS:HD2	2.13	0.48
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.95	0.48
1:A:1467:GLY:C	1:A:1469:GLY:H	2.21	0.48
2:B:680:ASP:O	2:B:684:GLU:HG2	2.14	0.48
2:B:889:LYS:HB2	2:B:889:LYS:HE2	1.46	0.48
7:G:119:PHE:HA	7:G:128:TYR:CD1	2.49	0.48
16:Q:576:LEU:CD2	16:Q:585:GLN:HE22	2.27	0.48
16:Q:645:LYS:HD2	21:X:242:GLY:O	2.14	0.48
17:R:363:ARG:HG3	17:R:447:PHE:CZ	2.49	0.48
17:R:366:ARG:HH12	23:Z:773:SER:H	1.62	0.48
17:R:416:GLN:HG2	17:R:421:ARG:HB3	1.95	0.48
17:R:485:TYR:OH	17:R:489:ASP:OD2	2.32	0.48
17:R:576:GLU:O	17:R:580:VAL:HG13	2.14	0.48
20:W:233:SER:OG	20:W:252:SER:N	2.44	0.48
23:Z:426:VAL:HG21	23:Z:468:LEU:HD13	1.95	0.48
1:A:733:LEU:HB2	9:I:106:ASP:HB2	1.96	0.48
2:B:299:GLU:HA	2:B:302:LYS:HD3	1.95	0.48
2:B:313:GLU:HG2	2:B:316:VAL:HG12	1.96	0.48
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.49	0.48
7:G:49:THR:OG1	7:G:50:THR:N	2.47	0.48
8:H:13:LYS:HG3	8:H:31:GLU:HG2	1.95	0.48
8:H:67:ASP:OD1	8:H:67:ASP:N	2.47	0.48
14:N:-54:DG:C6	14:N:-53:DG:C6	3.02	0.48
16:Q:236:VAL:O	16:Q:240:VAL:HG23	2.13	0.48
16:Q:336:ALA:HB1	16:Q:339:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:359:LEU:HD11	17:R:386:PHE:CE2	2.49	0.48
17:R:563:ILE:O	17:R:566:ARG:HG2	2.13	0.48
18:T:-37:DG:H4'	18:T:-36:DT:OP1	2.14	0.48
16:U:443:TRP:NE1	16:U:449:SER:OG	2.47	0.48
20:W:130:VAL:HG22	20:W:151:ILE:HG13	1.95	0.48
1:A:495:ASP:HB3	1:A:499:ASP:OD2	2.14	0.47
1:A:557:ARG:O	1:A:561:MET:HG3	2.14	0.47
1:A:606:HIS:CG	1:A:607:SER:N	2.82	0.47
1:A:724:GLU:OE1	1:A:724:GLU:N	2.47	0.47
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.14	0.47
2:B:218:THR:HG22	2:B:236:TRP:HD1	1.78	0.47
7:G:109:SER:HB2	23:Z:503:PHE:CE1	2.49	0.47
9:I:84:HIS:CD2	9:I:125:GLU:OE1	2.68	0.47
16:Q:211:LEU:HB2	16:Q:213:LYS:NZ	2.29	0.47
16:Q:753:LEU:O	16:Q:757:VAL:HG13	2.14	0.47
20:W:89:ARG:HG2	20:W:101:SER:OG	2.13	0.47
23:Z:433:LEU:HD13	23:Z:461:LEU:HD13	1.96	0.47
27:d:100:PRO:O	27:d:102:GLU:N	2.47	0.47
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.70	0.47
1:A:357:LYS:HZ3	2:B:1112:ASP:CG	2.21	0.47
1:A:416:ALA:HA	1:A:448:ARG:HA	1.96	0.47
1:A:1003:ASP:OD1	1:A:1003:ASP:N	2.43	0.47
2:B:910:THR:OG1	2:B:911:LEU:N	2.46	0.47
10:J:64:PRO:HG2	10:J:65:LEU:H	1.78	0.47
17:R:507:PRO:HA	17:R:508:ASN:HA	1.49	0.47
20:W:248:VAL:HG13	20:W:282:TYR:OH	2.14	0.47
22:Y:56:SER:HA	23:Z:271:ALA:HA	1.96	0.47
26:c:87:VAL:HG11	26:c:97:LEU:HD12	1.94	0.47
1:A:46:THR:HB	1:A:58:MET:HB2	1.96	0.47
1:A:406:VAL:HG13	1:A:429:LEU:HD11	1.97	0.47
1:A:866:LYS:HG3	1:A:1432:PHE:CD1	2.49	0.47
1:A:1184:THR:O	1:A:1184:THR:OG1	2.28	0.47
2:B:768:ARG:HG3	2:B:771:GLU:OE2	2.15	0.47
16:Q:682:ASP:OD1	16:Q:683:VAL:HG13	2.14	0.47
1:A:621:ILE:HG23	1:A:621:ILE:O	2.14	0.47
1:A:850:THR:HG21	15:P:33:A:C8	2.50	0.47
2:B:255:ARG:CD	2:B:307:GLU:HG3	2.44	0.47
7:G:80:PHE:HB2	7:G:83:GLU:CD	2.39	0.47
7:G:81:LYS:HG3	7:G:148:VAL:C	2.39	0.47
16:Q:68:ARG:HE	16:Q:86:LEU:HD13	1.80	0.47
16:Q:358:GLU:O	16:Q:361:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:689:HIS:HA	16:Q:692:VAL:HG12	1.96	0.47
20:W:254:LYS:HB3	20:W:273:HIS:O	2.14	0.47
23:Z:548:GLY:CA	23:Z:562:ASN:HA	2.44	0.47
25:b:78:ARG:HH12	25:b:85:ASP:CG	2.23	0.47
1:A:527:THR:HG22	1:A:532:ARG:O	2.14	0.47
1:A:539:GLN:O	1:A:540:ASP:C	2.56	0.47
1:A:636:ILE:HD12	1:A:636:ILE:HG23	1.65	0.47
1:A:1129:ASN:O	1:A:1131:SER:N	2.47	0.47
7:G:4:HIS:CG	7:G:73:LYS:HE3	2.50	0.47
14:N:39:DA:H1'	14:N:40:DC:H5'	1.95	0.47
16:Q:373:ASN:HB2	16:Q:376:GLU:HG2	1.96	0.47
16:Q:393:LYS:HE3	16:Q:393:LYS:HB3	1.70	0.47
16:Q:624:LYS:HA	16:Q:627:ARG:HE	1.79	0.47
16:Q:637:LYS:O	16:Q:641:ARG:HD3	2.15	0.47
16:Q:712:TYR:O	16:Q:713:LYS:HG3	2.15	0.47
16:Q:716:ASN:HB3	16:Q:719:VAL:HG22	1.96	0.47
17:R:587:LYS:O	17:R:588:ASN:ND2	2.48	0.47
18:T:-12:DC:H2''	18:T:-11:DG:H8	1.79	0.47
20:W:191:MET:HB2	20:W:209:SER:HB3	1.96	0.47
23:Z:310:ARG:CZ	23:Z:337:GLN:HB2	2.44	0.47
1:A:141:LEU:HB2	1:A:236:LEU:O	2.14	0.47
1:A:239:GLU:HG3	1:A:240:PRO:HD2	1.96	0.47
1:A:1027:ASP:HB3	1:A:1030:SER:HB3	1.96	0.47
1:A:1305:SER:OG	1:A:1306:LYS:N	2.48	0.47
13:M:1447:LEU:HA	13:M:1450:THR:HG22	1.97	0.47
16:Q:786:LEU:HD21	16:Q:820:LEU:HB3	1.96	0.47
17:R:573:VAL:O	17:R:576:GLU:HG3	2.15	0.47
24:a:120:MET:O	24:a:121:PRO:C	2.56	0.47
1:A:71:CYS:HB3	1:A:74:CYS:O	2.15	0.47
1:A:199:TYR:CE1	1:A:215:LEU:HD13	2.49	0.47
1:A:514:GLU:OE1	2:B:1101:GLN:HB2	2.14	0.47
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.97	0.47
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.15	0.47
1:A:1416:ARG:HD2	1:A:1434:GLU:OE2	2.15	0.47
3:C:2:PRO:HB3	11:K:54:PRO:CD	2.44	0.47
5:E:2:ASP:OD1	5:E:3:ASP:N	2.47	0.47
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.96	0.47
16:Q:721:LEU:HD11	19:V:31:CYS:HA	1.97	0.47
17:R:429:ARG:NE	17:R:431:GLY:O	2.42	0.47
20:W:46:VAL:HG11	20:W:58:TRP:HD1	1.78	0.47
23:Z:479:LYS:HD3	23:Z:521:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:521:CYS:HB3	23:Z:523:GLU:OE1	2.15	0.47
24:a:65:LEU:HB3	24:a:66:PRO:CD	2.43	0.47
1:A:465:HIS:HB3	1:A:1097:GLU:HG3	1.97	0.47
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.96	0.47
1:A:951:GLU:HG2	1:A:1007:ILE:HD11	1.97	0.47
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.97	0.47
2:B:646:ARG:C	2:B:648:TYR:N	2.73	0.47
2:B:690:CYS:SG	2:B:693:TYR:CZ	3.08	0.47
14:N:-54:DG:C4	14:N:-53:DG:C8	3.02	0.47
16:Q:30:VAL:HA	16:Q:33:ILE:HG12	1.96	0.47
16:Q:346:GLY:HA2	16:Q:349:GLN:HE21	1.79	0.47
16:Q:750:ASP:OD2	16:Q:753:LEU:N	2.40	0.47
20:W:76:LEU:HG	20:W:78:ILE:HG23	1.95	0.47
20:W:151:ILE:HG23	20:W:165:SER:OG	2.15	0.47
1:A:1177:TYR:CD2	9:I:28:GLU:OE1	2.68	0.47
1:A:1415:THR:O	1:A:1419:VAL:HG22	2.14	0.47
2:B:621:ILE:HG21	2:B:621:ILE:HD13	1.66	0.47
4:D:62:MET:O	4:D:66:ASN:ND2	2.47	0.47
4:D:122:PHE:HD1	4:D:126:GLU:CD	2.23	0.47
17:R:562:TYR:HB3	17:R:566:ARG:HH11	1.80	0.47
20:W:25:GLY:HA3	20:W:31:ASN:C	2.40	0.47
27:d:99:LEU:HA	27:d:100:PRO:HD3	1.75	0.47
24:e:79:LYS:HG3	25:f:74:GLU:OE2	2.14	0.47
1:A:93:PRO:HG2	1:A:219:GLU:OE1	2.15	0.47
1:A:111:CYS:HG	1:A:114:CYS:HB2	1.79	0.47
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.96	0.47
1:A:1474:LEU:HD12	6:F:105:ILE:HD11	1.97	0.47
2:B:329:GLY:HA3	2:B:334:LYS:HB3	1.97	0.47
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.47
2:B:834:ARG:HH12	2:B:842:HIS:HA	1.80	0.47
4:D:48:ASN:HB3	4:D:57:LEU:HD11	1.97	0.47
7:G:38:CYS:SG	7:G:39:THR:N	2.87	0.47
16:Q:833:LYS:O	16:Q:836:GLU:HG3	2.15	0.47
16:Q:834:GLN:O	16:Q:838:GLU:HG2	2.15	0.47
20:W:204:LEU:HD22	20:W:216:ILE:HG22	1.95	0.47
1:A:70:ARG:HD2	2:B:1131:ARG:HH22	1.80	0.46
1:A:775:LYS:HD2	2:B:974:SER:HB3	1.97	0.46
1:A:1177:TYR:CE2	1:A:1210:TRP:HE3	2.34	0.46
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.46	0.46
5:E:78:GLU:OE1	5:E:78:GLU:N	2.48	0.46
8:H:106:THR:OG1	8:H:107:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:28:C:H2'	15:P:29:A:O4'	2.16	0.46
16:Q:380:ILE:HB	16:Q:400:HIS:CE1	2.51	0.46
16:Q:460:LEU:O	16:Q:464:LEU:HG	2.14	0.46
16:Q:563:ASP:O	16:Q:565:PRO:HD3	2.15	0.46
16:Q:830:ARG:HH21	16:Q:834:GLN:HG3	1.80	0.46
18:T:-30:DG:H2''	18:T:-29:DC:OP2	2.15	0.46
20:W:11:GLN:HB3	20:W:298:ILE:HB	1.97	0.46
20:W:112:LEU:HB3	20:W:121:LEU:HD11	1.96	0.46
22:Y:22:VAL:HB	22:Y:84:VAL:HG12	1.97	0.46
23:Z:182:VAL:O	23:Z:224:TYR:HB2	2.14	0.46
1:A:831:LEU:HB3	1:A:835:GLU:HG3	1.97	0.46
2:B:347:MET:O	2:B:347:MET:HG3	2.15	0.46
5:E:63:ALA:HB3	16:Q:880:GLN:HE22	1.80	0.46
7:G:5:ILE:O	7:G:73:LYS:HD2	2.15	0.46
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.50	0.46
16:Q:167:LEU:HD21	16:Q:189:ALA:HB2	1.96	0.46
16:Q:737:LYS:HE3	16:Q:760:VAL:HG22	1.96	0.46
23:Z:705:LEU:HD21	23:Z:747:ARG:HD2	1.96	0.46
1:A:513:ALA:O	1:A:517:GLU:HG2	2.15	0.46
2:B:425:ARG:NH1	2:B:427:LYS:HD3	2.30	0.46
2:B:553:LEU:HD12	2:B:553:LEU:HA	1.73	0.46
7:G:82:GLY:HA2	7:G:146:LYS:HE3	1.96	0.46
7:G:111:HIS:ND1	23:Z:494:ARG:HB3	2.30	0.46
20:W:86:ALA:HB1	20:W:105:GLY:HA2	1.96	0.46
1:A:455:ILE:HD12	1:A:520:MET:HE1	1.98	0.46
9:I:75:ASP:OD1	9:I:77:THR:HG22	2.16	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.16	0.46
16:Q:750:ASP:OD2	16:Q:752:VAL:N	2.48	0.46
25:b:39:ARG:C	25:b:41:GLY:N	2.68	0.46
1:A:413:TYR:OH	1:A:450:MET:O	2.32	0.46
1:A:732:THR:HG23	1:A:735:GLN:OE1	2.14	0.46
2:B:1006:VAL:HG22	19:V:130:TRP:CB	2.45	0.46
4:D:93:HIS:HB3	4:D:96:GLU:OE1	2.14	0.46
8:H:45:ILE:HD12	8:H:45:ILE:HA	1.68	0.46
9:I:17:CYS:SG	9:I:18:GLN:N	2.89	0.46
16:Q:65:GLU:OE2	16:Q:93:TYR:OH	2.15	0.46
16:Q:411:ASP:HB3	16:Q:415:TRP:CZ3	2.50	0.46
17:R:456:LYS:HZ2	17:R:466:LEU:HD13	1.81	0.46
20:W:5:TYR:CE1	20:W:303:CYS:HB3	2.50	0.46
20:W:215:LYS:HG2	20:W:227:THR:HG22	1.97	0.46
24:e:128:ARG:NH1	24:e:134:ARG:HE	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:MET:HB2	1:A:58:MET:HE2	1.66	0.46
1:A:84:HIS:H	1:A:84:HIS:CD2	2.31	0.46
1:A:124:PRO:HA	1:A:127:LYS:CG	2.46	0.46
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.75	0.46
1:A:1150:ASP:OD1	1:A:1150:ASP:N	2.48	0.46
2:B:84:TYR:HA	2:B:132:VAL:HA	1.97	0.46
2:B:395:LEU:HA	2:B:395:LEU:HD23	1.66	0.46
2:B:594:MET:HE3	2:B:594:MET:HB3	1.76	0.46
2:B:646:ARG:O	2:B:647:GLU:HG2	2.16	0.46
2:B:796:MET:HE2	2:B:796:MET:HB3	1.82	0.46
5:E:153:LYS:O	5:E:157:THR:HG23	2.14	0.46
7:G:113:ILE:HG22	7:G:114:PRO:O	2.15	0.46
12:L:16:ILE:HD12	12:L:27:GLU:OE2	2.16	0.46
13:M:848:VAL:O	13:M:883:GLU:N	2.48	0.46
14:N:4:DG:H2''	14:N:5:DT:OP2	2.15	0.46
15:P:37:A:H2'	15:P:38:A:C8	2.51	0.46
16:Q:41:LEU:HD13	16:Q:75:TYR:HE2	1.81	0.46
16:Q:76:ARG:HH21	16:Q:76:ARG:HG3	1.80	0.46
16:Q:452:GLU:OE1	16:Q:490:HIS:NE2	2.46	0.46
23:Z:239:ILE:O	23:Z:242:VAL:HG22	2.15	0.46
23:Z:340:PHE:HD2	23:Z:370:GLY:HA2	1.81	0.46
1:A:112:PHE:CZ	1:A:220:ARG:NH1	2.84	0.46
1:A:347:GLU:HA	1:A:352:GLY:HA3	1.98	0.46
2:B:19:PRO:C	2:B:21:LEU:N	2.74	0.46
2:B:26:CYS:O	2:B:30:ILE:HG12	2.15	0.46
2:B:285:LEU:HD23	9:I:16:PHE:CZ	2.51	0.46
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.78	0.46
8:H:30:CYS:SG	8:H:56:PHE:HZ	2.38	0.46
16:Q:386:ALA:HB1	16:Q:394:ARG:HG3	1.97	0.46
16:Q:527:HIS:CE1	21:X:220:VAL:HB	2.51	0.46
17:R:574:GLU:HA	17:R:577:LYS:NZ	2.30	0.46
18:T:47:DG:H2'	18:T:48:DT:C6	2.50	0.46
23:Z:182:VAL:HG23	23:Z:225:ILE:HG13	1.98	0.46
23:Z:547:VAL:HG12	23:Z:563:MET:SD	2.54	0.46
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.56	0.46
2:B:548:TRP:CZ2	2:B:586:THR:HG21	2.51	0.46
2:B:566:LYS:HA	2:B:576:ILE:HD12	1.98	0.46
15:P:23:G:C2'	15:P:24:A:H8	2.24	0.46
16:Q:386:ALA:HB2	16:Q:393:LYS:CB	2.46	0.46
19:V:88:ASN:O	19:V:90:ASP:N	2.49	0.46
25:b:77:LYS:HE3	27:d:89:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:79:ILE:HB	26:c:80:PRO:HD2	1.97	0.46
1:A:74:CYS:SG	1:A:81:CYS:HB2	2.56	0.46
1:A:557:ARG:HG3	1:A:558:GLY:N	2.27	0.46
1:A:1222:THR:C	1:A:1225:LYS:H	2.23	0.46
1:A:1236:ASN:O	1:A:1240:GLY:N	2.48	0.46
2:B:255:ARG:HD3	2:B:307:GLU:HG3	1.98	0.46
2:B:684:GLU:OE1	2:B:684:GLU:HA	2.16	0.46
16:Q:850:GLU:O	16:Q:854:GLN:NE2	2.44	0.46
20:W:233:SER:HB3	20:W:253:ASP:HB3	1.98	0.46
22:Y:66:PRO:HD3	22:Y:82:PRO:HG3	1.97	0.46
23:Z:571:ARG:H	23:Z:574:ALA:HB3	1.80	0.46
1:A:753:GLY:O	1:A:757:GLN:HG2	2.16	0.46
1:A:971:PRO:O	1:A:972:THR:OG1	2.26	0.46
2:B:332:LYS:C	2:B:332:LYS:HD2	2.41	0.46
4:D:79:THR:O	4:D:82:SER:OG	2.33	0.46
14:N:-54:DG:N1	18:T:55:DG:N2	2.64	0.46
16:Q:289:GLN:O	16:Q:293:LEU:HD23	2.16	0.46
16:Q:386:ALA:HB2	16:Q:393:LYS:HB3	1.98	0.46
16:Q:872:LYS:O	16:Q:875:LEU:HG	2.16	0.46
17:R:566:ARG:HA	17:R:569:GLU:OE1	2.16	0.46
19:V:196:LYS:O	19:V:198:ARG:N	2.49	0.46
23:Z:178:ASN:OD1	23:Z:179:LEU:N	2.47	0.46
23:Z:469:ARG:NH1	23:Z:497:GLU:O	2.49	0.46
1:A:117:LEU:HD21	1:A:232:GLU:HG3	1.98	0.45
1:A:996:ILE:HA	1:A:996:ILE:HD13	1.62	0.45
1:A:1176:TYR:HD1	9:I:51:SER:O	1.99	0.45
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.98	0.45
2:B:317:ALA:O	2:B:321:ILE:HD12	2.15	0.45
5:E:82:VAL:HG12	5:E:110:MET:CB	2.46	0.45
10:J:25:LEU:HD23	17:R:567:ASN:HD21	1.81	0.45
13:M:1362:LYS:HD3	13:M:1363:GLY:N	2.31	0.45
13:M:1485:GLU:OE2	13:M:1497:ARG:NE	2.34	0.45
20:W:13:GLN:H	20:W:297:GLU:HG2	1.80	0.45
23:Z:470:LYS:HB3	23:Z:472:PHE:CE2	2.51	0.45
25:b:68:ASP:OD2	25:b:92:ARG:HD3	2.15	0.45
1:A:469:MET:HB3	1:A:469:MET:HE2	1.68	0.45
1:A:989:ASN:O	1:A:993:ILE:HG13	2.16	0.45
3:C:45:ILE:HG22	3:C:165:ALA:HB1	1.98	0.45
5:E:58:LEU:HD23	5:E:58:LEU:H	1.82	0.45
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.50	0.45
16:Q:366:LYS:HG3	16:Q:369:LYS:HZ3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:54:DC:H6	18:T:54:DC:H5'	1.81	0.45
20:W:252:SER:HA	20:W:276:GLN:HB3	1.98	0.45
20:W:254:LYS:HG2	20:W:275:ASP:C	2.42	0.45
1:A:123:ASN:HB3	1:A:125:LYS:HG2	1.98	0.45
2:B:355:ASP:OD1	2:B:356:PHE:N	2.46	0.45
2:B:757:PRO:HB2	2:B:760:THR:HG22	1.99	0.45
9:I:73:SER:O	9:I:80:ARG:NH1	2.50	0.45
16:Q:131:LEU:HD12	16:Q:155:VAL:HG22	1.98	0.45
19:V:75:LEU:HD12	19:V:75:LEU:HA	1.81	0.45
23:Z:539:LEU:O	23:Z:578:LYS:HB3	2.15	0.45
23:Z:639:LYS:HB2	23:Z:642:HIS:HB2	1.99	0.45
24:e:87:SER:OG	25:f:83:ALA:HB2	2.16	0.45
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.99	0.45
2:B:92:TYR:N	2:B:92:TYR:CD1	2.84	0.45
13:M:1463:CYS:SG	13:M:1464:ALA:N	2.90	0.45
16:Q:265:ASP:OD2	16:Q:268:ASN:HB2	2.16	0.45
16:Q:620:ARG:HH12	16:Q:660:LYS:HA	1.81	0.45
16:Q:855:LYS:HD3	16:Q:855:LYS:HA	1.59	0.45
17:R:565:GLN:HA	17:R:568:ARG:CZ	2.47	0.45
16:U:378:LEU:HD23	16:U:382:LEU:O	2.17	0.45
20:W:7:ILE:HA	20:W:301:TYR:HA	1.98	0.45
23:Z:294:ASP:HB2	23:Z:306:LYS:HE2	1.98	0.45
23:Z:546:THR:HG22	23:Z:547:VAL:N	2.32	0.45
25:f:53:GLU:O	25:f:57:VAL:HG23	2.16	0.45
2:B:1136:GLU:CB	2:B:1143:LYS:HG2	2.44	0.45
3:C:92:GLU:HG2	23:Z:711:ARG:NH2	2.32	0.45
5:E:97:GLU:OE1	5:E:97:GLU:N	2.50	0.45
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.98	0.45
10:J:26:GLN:HA	17:R:566:ARG:HD2	1.98	0.45
16:Q:133:GLY:HA2	16:Q:136:CYS:SG	2.57	0.45
16:Q:200:VAL:HA	19:V:82:VAL:HG22	1.97	0.45
16:Q:450:PRO:HB2	16:Q:452:GLU:HG2	1.98	0.45
16:Q:716:ASN:OD1	16:Q:717:THR:N	2.50	0.45
16:U:469:ASN:HA	19:V:222:ARG:HA	1.98	0.45
21:X:253:LEU:O	21:X:256:VAL:HG12	2.16	0.45
23:Z:480:VAL:HG13	23:Z:487:GLY:H	1.81	0.45
1:A:465:HIS:NE2	1:A:467:MET:HB2	2.31	0.45
1:A:1226:LEU:HA	1:A:1230:GLN:NE2	2.31	0.45
2:B:133:ILE:HD12	2:B:139:GLN:HB3	1.98	0.45
2:B:841:ARG:HA	2:B:841:ARG:HD3	1.77	0.45
9:I:29:ASP:CB	9:I:34:ILE:HG13	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:380:ILE:HG21	16:Q:396:ILE:HD12	1.99	0.45
16:Q:566:ASP:OD1	21:X:234:ARG:HD3	2.16	0.45
16:Q:710:LYS:HB2	16:Q:712:TYR:CE1	2.52	0.45
16:Q:870:GLU:HA	16:Q:873:LYS:NZ	2.32	0.45
20:W:182:LEU:HD21	20:W:185:THR:OG1	2.16	0.45
20:W:281:LYS:HA	20:W:281:LYS:HD2	1.80	0.45
22:Y:35:ASN:ND2	22:Y:85:TYR:OH	2.49	0.45
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.17	0.45
1:A:1117:VAL:HA	1:A:1136:THR:HG21	1.97	0.45
2:B:649:ASN:OD1	2:B:649:ASN:N	2.46	0.45
2:B:681:ASP:OD1	2:B:681:ASP:N	2.50	0.45
4:D:38:HIS:HB2	4:D:68:THR:OG1	2.16	0.45
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.98	0.45
8:H:40:ILE:O	8:H:123:MET:HA	2.17	0.45
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.97	0.45
15:P:22:G:H2'	15:P:23:G:C8	2.52	0.45
16:Q:170:ALA:HB2	16:Q:185:TYR:HB2	1.99	0.45
17:R:388:ARG:HD3	17:R:445:GLN:HB2	1.99	0.45
17:R:402:VAL:HG23	17:R:451:GLU:HG2	1.98	0.45
17:R:428:LEU:HB2	17:R:437:PHE:CE2	2.52	0.45
18:T:-69:DA:H2''	18:T:-68:DG:OP2	2.17	0.45
19:V:282:ALA:C	19:V:284:GLU:H	2.25	0.45
20:W:46:VAL:CB	20:W:58:TRP:HB2	2.45	0.45
23:Z:280:ARG:HG3	23:Z:386:VAL:HG13	1.98	0.45
24:a:97:GLU:O	24:a:98:ALA:C	2.60	0.45
24:a:102:ALA:O	24:a:105:GLU:HB2	2.17	0.45
25:b:39:ARG:C	25:b:41:GLY:H	2.24	0.45
1:A:609:HIS:HA	1:A:626:THR:HG21	1.97	0.45
2:B:139:GLN:OE1	2:B:139:GLN:N	2.49	0.45
2:B:319:ASN:HD21	2:B:332:LYS:HG2	1.82	0.45
2:B:407:MET:HE1	2:B:443:GLY:C	2.42	0.45
5:E:3:ASP:OD1	5:E:47:LYS:HD2	2.15	0.45
16:Q:128:GLN:HA	16:Q:158:GLN:HE22	1.82	0.45
16:Q:474:PHE:CB	16:Q:503:LEU:HD13	2.46	0.45
16:Q:620:ARG:NH2	16:Q:659:HIS:O	2.47	0.45
23:Z:571:ARG:HB2	23:Z:574:ALA:HB2	1.98	0.45
23:Z:729:GLU:O	23:Z:747:ARG:NH1	2.50	0.45
25:b:28:GLY:O	25:b:30:THR:N	2.48	0.45
25:f:89:ALA:O	25:f:92:ARG:HB2	2.16	0.45
1:A:291:ARG:HG3	1:A:292:ARG:N	2.32	0.45
1:A:807:LEU:HA	1:A:807:LEU:HD23	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:714:PRO:CD	2:B:1001:PRO:HG3	2.47	0.45
18:T:-25:DA:H1'	18:T:-24:DG:C8	2.52	0.45
19:V:38:SER:OG	19:V:39:LEU:N	2.49	0.45
23:Z:614:ILE:HA	23:Z:624:LEU:HA	1.98	0.45
2:B:155:MET:HE3	2:B:183:GLY:HA2	1.99	0.45
2:B:545:LEU:HB3	2:B:550:MET:HE3	1.99	0.45
2:B:650:ASN:C	16:U:460:TYR:HE2	2.25	0.45
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.99	0.45
5:E:26:TYR:CZ	5:E:72:MET:HE3	2.52	0.45
5:E:126:ILE:H	5:E:126:ILE:HD12	1.81	0.45
14:N:55:DC:H2'	14:N:55:DC:OP2	2.17	0.45
16:Q:763:ARG:HE	19:V:25:GLU:N	2.14	0.45
20:W:235:VAL:HA	20:W:251:SER:HA	1.98	0.45
23:Z:489:THR:HB	23:Z:505:ASP:OD2	2.17	0.45
1:A:365:THR:HG22	1:A:366:VAL:N	2.31	0.44
1:A:602:CYS:SG	1:A:652:LEU:HD13	2.57	0.44
1:A:902:GLU:O	1:A:978:VAL:HA	2.17	0.44
1:A:1118:THR:HG21	1:A:1135:LYS:HB2	1.99	0.44
2:B:497:LYS:HG3	2:B:498:PRO:CD	2.46	0.44
2:B:995:GLU:CD	19:V:131:MET:HB3	2.42	0.44
2:B:1134:THR:HG23	2:B:1134:THR:O	2.17	0.44
16:Q:538:GLY:HA2	16:Q:553:TRP:HE3	1.82	0.44
17:R:353:VAL:HG23	17:R:456:LYS:NZ	2.33	0.44
18:T:-38:DC:H2''	18:T:-37:DG:OP2	2.16	0.44
19:V:182:THR:HA	19:V:185:ASP:OD2	2.17	0.44
20:W:17:ASP:OD2	20:W:40:LEU:HB3	2.17	0.44
23:Z:243:GLY:O	23:Z:246:ARG:HG2	2.17	0.44
24:a:118:THR:HA	25:b:45:ARG:O	2.17	0.44
25:b:32:PRO:O	25:b:36:ARG:HG3	2.17	0.44
27:d:65:ASP:C	27:d:65:ASP:OD1	2.60	0.44
27:d:83:ARG:NH2	27:d:83:ARG:HB3	2.32	0.44
24:e:79:LYS:HB3	24:e:82:LEU:HD11	1.99	0.44
1:A:189:PRO:HB2	1:A:201:GLU:H	1.81	0.44
2:B:236:TRP:HB2	2:B:259:THR:HB	1.98	0.44
2:B:305:LEU:HA	2:B:305:LEU:HD12	1.74	0.44
2:B:358:GLU:H	2:B:358:GLU:HG3	1.62	0.44
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.16	0.44
4:D:93:HIS:CE1	4:D:94:LYS:HG3	2.52	0.44
14:N:-54:DG:C4	14:N:-53:DG:N7	2.84	0.44
17:R:356:PRO:HB3	17:R:452:PHE:CB	2.47	0.44
20:W:37:THR:HA	20:W:70:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:56:LEU:HD21	20:W:59:SER:OG	2.16	0.44
20:W:203:GLN:OE1	20:W:204:LEU:HG	2.17	0.44
22:Y:8:LYS:HE2	22:Y:27:GLN:NE2	2.32	0.44
23:Z:492:ILE:HA	23:Z:502:LEU:HA	1.99	0.44
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.79	0.44
2:B:651:TYR:N	16:U:460:TYR:OH	2.49	0.44
8:H:111:ARG:HA	8:H:128:ASP:HA	1.99	0.44
8:H:150:PHE:C	21:X:242:GLY:HA3	2.43	0.44
16:Q:527:HIS:HD2	16:Q:530:TYR:HB2	1.82	0.44
16:Q:591:ILE:HG22	16:Q:592:LEU:HD12	1.97	0.44
17:R:456:LYS:NZ	17:R:466:LEU:HD13	2.33	0.44
20:W:29:LYS:HE2	20:W:75:THR:HA	1.99	0.44
21:X:222:ARG:HA	21:X:225:VAL:HG22	1.97	0.44
25:f:62:LEU:O	25:f:63:GLU:C	2.60	0.44
2:B:1084:LEU:HA	2:B:1084:LEU:HD13	1.56	0.44
4:D:33:LEU:HD21	4:D:97:LEU:HD23	2.00	0.44
16:Q:729:LYS:HB2	16:Q:732:LYS:CD	2.46	0.44
17:R:397:LYS:O	23:Z:777:MET:HE3	2.17	0.44
22:Y:18:LEU:HD23	22:Y:18:LEU:HA	1.86	0.44
23:Z:280:ARG:HB2	23:Z:382:ILE:HG23	2.00	0.44
23:Z:464:PRO:HD2	23:Z:467:GLU:HB3	1.99	0.44
2:B:145:GLN:O	2:B:146:LYS:C	2.61	0.44
2:B:388:TYR:HB2	2:B:504:THR:HG23	1.99	0.44
2:B:479:LEU:O	2:B:483:ARG:HG3	2.17	0.44
2:B:577:HIS:CE1	2:B:583:LEU:HD11	2.53	0.44
4:D:93:HIS:HE1	4:D:94:LYS:HE3	1.82	0.44
13:M:1435:CYS:SG	13:M:1442:LYS:HG2	2.58	0.44
14:N:17:DA:H2"	14:N:18:DG:H8	1.82	0.44
16:Q:95:GLN:HG3	19:V:85:ASP:OD2	2.17	0.44
16:Q:120:ALA:HB1	16:Q:130:HIS:HE1	1.83	0.44
16:Q:847:GLN:O	16:Q:851:LEU:HG	2.17	0.44
17:R:353:VAL:HG11	17:R:472:ILE:HD12	1.99	0.44
17:R:455:TRP:O	17:R:459:MET:HG2	2.17	0.44
19:V:190:ILE:HG13	19:V:190:ILE:O	2.17	0.44
19:V:193:HIS:HB3	19:V:196:LYS:O	2.18	0.44
20:W:64:GLN:OE1	20:W:89:ARG:NH1	2.49	0.44
20:W:295:ASP:O	20:W:297:GLU:HG3	2.17	0.44
25:b:31:LYS:HG3	25:b:51:TYR:CE1	2.53	0.44
1:A:738:GLU:CD	1:A:797:ARG:HH21	2.26	0.44
1:A:982:ASN:HD22	1:A:985:ARG:HB2	1.83	0.44
2:B:705:GLY:O	2:B:709:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:VAL:HG11	7:G:44:PHE:HZ	1.83	0.44
7:G:4:HIS:CD2	7:G:73:LYS:HE3	2.52	0.44
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.83	0.44
9:I:91:HIS:CD2	9:I:93:GLU:H	2.35	0.44
16:Q:64:LEU:HD23	16:Q:64:LEU:HA	1.82	0.44
16:Q:415:TRP:HA	16:Q:418:LEU:HD12	2.00	0.44
16:Q:423:GLU:OE1	21:X:231:TRP:NE1	2.43	0.44
16:Q:503:LEU:HG	16:Q:507:TYR:CE2	2.53	0.44
19:V:127:VAL:HG23	19:V:128:VAL:N	2.32	0.44
20:W:152:LEU:N	20:W:166:GLY:O	2.34	0.44
20:W:252:SER:HB3	20:W:276:GLN:OE1	2.18	0.44
23:Z:188:GLU:OE1	23:Z:188:GLU:N	2.51	0.44
1:A:249:ILE:O	1:A:249:ILE:HG13	2.16	0.44
1:A:600:ILE:HG21	1:A:600:ILE:HD13	1.58	0.44
1:A:605:THR:HG21	15:P:38:A:H3'	1.99	0.44
1:A:962:ASP:OD2	1:A:1046:ARG:NH1	2.35	0.44
2:B:573:TRP:CD1	2:B:573:TRP:C	2.96	0.44
2:B:655:ASP:O	2:B:659:SER:HB3	2.17	0.44
9:I:65:LEU:HA	9:I:65:LEU:HD23	1.74	0.44
15:P:25:A:H2'	15:P:26:C:H6	1.77	0.44
16:Q:841:LEU:HA	16:Q:844:LYS:HG2	1.99	0.44
23:Z:272:ASN:ND2	23:Z:384:GLU:HB2	2.32	0.44
23:Z:502:LEU:HD21	23:Z:511:LEU:HD22	2.00	0.44
26:c:95:LYS:O	26:c:96:LEU:C	2.60	0.44
1:A:59:ASP:OD2	1:A:61:ARG:HB2	2.18	0.44
1:A:539:GLN:C	1:A:541:THR:N	2.74	0.44
1:A:1302:GLU:O	1:A:1304:ILE:N	2.51	0.44
2:B:313:GLU:HG3	2:B:315:ASN:H	1.82	0.44
8:H:11:ASP:HB3	8:H:55:LYS:HG2	2.00	0.44
8:H:143:LEU:HD12	8:H:143:LEU:HA	1.62	0.44
20:W:191:MET:HG3	20:W:211:ASP:HB3	1.99	0.44
1:A:417:LYS:HE2	1:A:418:TYR:CE2	2.53	0.44
1:A:1178:ASP:OD1	1:A:1185:VAL:HG13	2.18	0.44
1:A:1484:MET:N	1:A:1484:MET:SD	2.91	0.44
1:A:1547:SEP:HA	1:A:1548:PRO:HD3	1.78	0.44
2:B:897:ARG:CB	2:B:900:GLU:HG3	2.48	0.44
2:B:1038:THR:HA	3:C:195:THR:HA	1.99	0.44
14:N:17:DA:P	24:a:69:ARG:HH11	2.41	0.44
15:P:24:A:N1	15:P:25:A:C6	2.86	0.44
16:Q:208:PHE:CD1	16:Q:213:LYS:HD2	2.51	0.44
16:Q:310:TYR:OH	19:V:67:GLU:OE2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:677:THR:HG22	16:Q:679:ASP:H	1.83	0.44
16:Q:762:GLN:O	16:Q:766:THR:HG22	2.18	0.44
17:R:492:ILE:H	17:R:492:ILE:HD12	1.83	0.44
18:T:-69:DA:H1'	18:T:-68:DG:H5'	2.00	0.44
18:T:52:DG:N2	18:T:53:DC:O2	2.51	0.44
19:V:103:ALA:O	19:V:107:LEU:HG	2.17	0.44
23:Z:242:VAL:HG23	23:Z:245:LEU:HB2	2.00	0.44
24:a:123:ASP:O	24:a:124:ILE:C	2.61	0.44
26:c:93:LEU:HD23	27:d:103:LEU:HD21	1.99	0.44
2:B:67:LEU:HD13	2:B:420:GLN:OE1	2.17	0.43
2:B:544:PHE:O	2:B:547:GLU:N	2.48	0.43
2:B:576:ILE:HD12	2:B:576:ILE:HA	1.79	0.43
2:B:679:PRO:HG2	2:B:680:ASP:N	2.33	0.43
11:K:11:LEU:HA	11:K:11:LEU:HD23	1.74	0.43
16:Q:239:ALA:O	16:Q:243:LEU:HG	2.17	0.43
20:W:171:ILE:HG23	20:W:187:GLU:HG2	2.00	0.43
23:Z:291:ALA:HB2	23:Z:307:MET:HG2	2.00	0.43
23:Z:499:PHE:HB3	23:Z:512:LYS:HD2	2.00	0.43
1:A:117:LEU:C	1:A:119:VAL:N	2.76	0.43
2:B:1116:VAL:HG11	2:B:1125:MET:HE3	2.00	0.43
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.51	0.43
5:E:55:ARG:HA	5:E:58:LEU:CD2	2.48	0.43
16:Q:456:ASN:OD1	19:V:48:PHE:HA	2.18	0.43
16:Q:568:TRP:CE3	16:Q:592:LEU:HB2	2.51	0.43
18:T:-57:DC:H2''	18:T:-56:DC:C5	2.53	0.43
23:Z:602:VAL:HG21	23:Z:636:PHE:HE2	1.83	0.43
1:A:388:MET:HB3	1:A:388:MET:HE2	1.42	0.43
2:B:472:ARG:HH21	2:B:472:ARG:HD3	1.65	0.43
2:B:479:LEU:HD23	2:B:479:LEU:HA	1.79	0.43
2:B:544:PHE:O	2:B:545:LEU:C	2.61	0.43
8:H:15:ILE:HG23	8:H:16:ASP:N	2.33	0.43
16:Q:123:ILE:HG23	16:Q:124:ILE:H	1.82	0.43
16:Q:365:GLU:HG2	16:Q:369:LYS:HZ1	1.83	0.43
16:Q:471:LYS:O	16:Q:475:LEU:HD23	2.18	0.43
16:Q:513:PHE:HB2	20:W:213:TYR:CE1	2.53	0.43
16:Q:736:CYS:O	16:Q:739:THR:HG22	2.17	0.43
16:Q:772:GLU:HB3	16:Q:774:SER:OG	2.18	0.43
17:R:581:ALA:CB	19:V:127:VAL:HG21	2.48	0.43
20:W:17:ASP:CG	20:W:40:LEU:HB3	2.42	0.43
20:W:84:LEU:HD21	20:W:110:TRP:CZ3	2.53	0.43
20:W:253:ASP:OD1	20:W:253:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:593:ASN:HB3	23:Z:595:HIS:CE1	2.54	0.43
26:c:27:VAL:HG11	26:c:49:VAL:HG22	1.99	0.43
1:A:818:GLU:OE2	17:R:599:CYS:HA	2.18	0.43
1:A:933:THR:OG1	1:A:934:LEU:HG	2.19	0.43
2:B:121:SER:HA	2:B:153:PRO:HA	1.98	0.43
15:P:20:A:H5'	15:P:21:G:OP2	2.18	0.43
16:Q:158:GLN:HG3	16:Q:159:SER:N	2.33	0.43
16:Q:527:HIS:CD2	16:Q:530:TYR:HB2	2.53	0.43
16:Q:542:ARG:HD2	16:Q:554:PHE:HE2	1.83	0.43
16:Q:667:ARG:HD3	16:Q:691:TYR:HE1	1.83	0.43
17:R:366:ARG:HH22	23:Z:775:TPO:HA	1.83	0.43
18:T:-42:DT:H2''	18:T:-41:DG:C8	2.54	0.43
23:Z:479:LYS:O	23:Z:519:GLN:HG2	2.17	0.43
1:A:37:THR:O	1:A:37:THR:OG1	2.30	0.43
1:A:106:VAL:O	1:A:110:VAL:HG22	2.19	0.43
1:A:621:ILE:HG21	1:A:621:ILE:HD13	1.78	0.43
1:A:820:ARG:HH21	1:A:820:ARG:HD3	1.66	0.43
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.63	0.43
1:A:1080:ILE:HD12	1:A:1080:ILE:HG23	1.69	0.43
1:A:1177:TYR:CE2	1:A:1210:TRP:CE3	3.06	0.43
1:A:1403:ASP:O	1:A:1407:CYS:HB2	2.18	0.43
2:B:100:GLU:HA	2:B:105:PRO:HB3	1.99	0.43
2:B:501:LEU:HD12	2:B:505:LEU:HD12	2.01	0.43
2:B:866:ILE:HG23	2:B:866:ILE:HD12	1.57	0.43
3:C:107:CYS:HB3	3:C:154:ARG:O	2.17	0.43
6:F:105:ILE:HG21	6:F:105:ILE:HD13	1.62	0.43
7:G:104:MET:HG3	7:G:157:ILE:O	2.19	0.43
13:M:1344:GLU:HG2	13:M:1347:MET:HE2	2.00	0.43
16:Q:162:ASN:CG	16:Q:164:PRO:HD2	2.43	0.43
16:Q:689:HIS:HB2	19:V:35:TYR:HE1	1.84	0.43
18:T:64:DG:H2''	18:T:65:DG:H5'	1.99	0.43
20:W:191:MET:HE2	20:W:210:ASP:O	2.19	0.43
23:Z:200:PHE:HA	23:Z:210:LEU:HD13	2.00	0.43
23:Z:389:THR:O	23:Z:393:LEU:HG	2.18	0.43
1:A:966:LEU:HA	1:A:966:LEU:HD23	1.74	0.43
2:B:83:ARG:HH22	2:B:133:ILE:CG2	2.31	0.43
14:N:-31:DA:H2''	14:N:-30:DG:C8	2.53	0.43
16:Q:56:LYS:HZ1	16:Q:59:GLU:HG3	1.83	0.43
16:Q:653:ILE:O	16:Q:656:VAL:HG22	2.19	0.43
16:Q:691:TYR:HB3	16:Q:699:SER:OG	2.19	0.43
19:V:47:LYS:HD3	19:V:47:LYS:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:61:ILE:HD12	22:Y:63:MET:HE2	2.00	0.43
23:Z:540:VAL:HB	23:Z:575:VAL:CG2	2.49	0.43
1:A:1129:ASN:O	1:A:1130:ILE:C	2.61	0.43
2:B:115:LEU:HG	2:B:908:MET:HE3	1.99	0.43
2:B:544:PHE:CZ	2:B:548:TRP:NE1	2.87	0.43
2:B:568:PHE:CE1	2:B:573:TRP:HB2	2.54	0.43
13:M:540:GLY:HA2	13:M:560:GLU:H	1.83	0.43
16:Q:508:GLU:OE2	16:Q:540:MET:HG3	2.19	0.43
20:W:113:ALA:C	20:W:121:LEU:HD12	2.44	0.43
23:Z:439:LYS:H	23:Z:453:LYS:H	1.66	0.43
24:a:85:GLN:NE2	25:b:82:THR:HG22	2.34	0.43
25:b:66:ILE:HG22	25:b:70:VAL:HG23	2.01	0.43
24:e:59:GLU:H	24:e:59:GLU:HG3	1.58	0.43
1:A:198:LEU:O	1:A:215:LEU:HD12	2.18	0.43
1:A:488:VAL:O	1:A:488:VAL:HG12	2.18	0.43
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.19	0.43
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.52	0.43
1:A:1467:GLY:O	1:A:1468:THR:C	2.62	0.43
2:B:428:ASP:OD1	2:B:429:PHE:N	2.52	0.43
2:B:597:ILE:HG22	2:B:601:VAL:HB	2.01	0.43
2:B:807:ARG:HE	2:B:807:ARG:HB2	1.69	0.43
3:C:75:SER:HB3	3:C:79:VAL:HB	2.01	0.43
5:E:33:LEU:HA	5:E:33:LEU:HD12	1.63	0.43
10:J:60:LEU:HD23	10:J:60:LEU:HA	1.78	0.43
13:M:1398:LEU:HD11	13:M:1415:TYR:CD1	2.53	0.43
16:Q:464:LEU:HB2	16:Q:466:ASN:HD22	1.84	0.43
16:Q:750:ASP:OD2	16:Q:753:LEU:HG	2.18	0.43
20:W:9:PHE:CE2	20:W:54:LEU:HB3	2.54	0.43
20:W:163:LEU:HB2	20:W:177:ILE:HG23	2.00	0.43
20:W:170:GLY:HA2	20:W:193:ILE:HG13	2.01	0.43
20:W:231:HIS:CG	20:W:251:SER:HB3	2.54	0.43
21:X:222:ARG:O	21:X:226:SER:OG	2.31	0.43
22:Y:76:ARG:HH21	22:Y:109:LYS:HD3	1.83	0.43
22:Y:116:LYS:HA	22:Y:116:LYS:HD3	1.74	0.43
25:b:97:LEU:HD21	25:b:100:PHE:CD2	2.54	0.43
1:A:812:LYS:HE2	9:I:77:THR:HG23	1.99	0.43
1:A:1298:LEU:HA	1:A:1298:LEU:HD23	1.77	0.43
1:A:1302:GLU:C	1:A:1304:ILE:N	2.77	0.43
2:B:194:LEU:HD23	2:B:194:LEU:HA	1.80	0.43
2:B:212:ASP:OD1	2:B:212:ASP:N	2.46	0.43
2:B:1151:MET:HE2	2:B:1155:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:246:LEU:HA	3:C:246:LEU:HD23	1.87	0.43
3:C:268:GLN:HG3	3:C:269:SER:N	2.34	0.43
5:E:3:ASP:OD1	5:E:49:SER:OG	2.20	0.43
7:G:131:MET:SD	7:G:131:MET:N	2.92	0.43
7:G:151:ARG:HA	23:Z:477:HIS:CE1	2.54	0.43
15:P:21:G:O2'	15:P:22:G:OP2	2.29	0.43
16:Q:218:ARG:HD3	16:Q:238:LEU:HD11	2.00	0.43
16:Q:484:GLU:HB2	16:Q:492:TYR:HB3	2.00	0.43
17:R:359:LEU:HD22	17:R:452:PHE:HE1	1.84	0.43
18:T:-14:DA:C2	18:T:-13:DA:C4	3.07	0.43
23:Z:548:GLY:HA3	23:Z:562:ASN:HA	2.01	0.43
23:Z:557:THR:O	23:Z:558:PHE:CD1	2.71	0.43
1:A:419:ILE:HD13	1:A:419:ILE:HG21	1.70	0.43
2:B:319:ASN:ND2	2:B:332:LYS:HG2	2.34	0.43
4:D:22:PHE:HB2	4:D:27:GLU:OE1	2.18	0.43
4:D:137:LYS:HA	4:D:137:LYS:HD3	1.83	0.43
5:E:37:LEU:HD21	5:E:41:LYS:HZ3	1.84	0.43
7:G:151:ARG:HH21	23:Z:477:HIS:CD2	2.36	0.43
16:Q:611:TRP:HZ2	16:Q:631:ARG:HH21	1.65	0.43
17:R:378:PHE:CZ	17:R:382:VAL:HG11	2.54	0.43
19:V:49:ILE:HG22	21:X:227:ARG:HG3	2.01	0.43
19:V:96:PRO:HA	19:V:97:ASN:HA	1.57	0.43
20:W:40:LEU:HA	20:W:66:GLY:HA3	2.01	0.43
23:Z:199:LYS:HG3	23:Z:203:TYR:HD2	1.84	0.43
23:Z:261:THR:O	23:Z:264:LEU:HG	2.19	0.43
26:c:113:SER:O	26:c:115:LEU:N	2.52	0.43
24:e:76:GLN:NE2	24:e:80:THR:HG22	2.34	0.43
1:A:189:PRO:HA	1:A:201:GLU:O	2.19	0.42
1:A:393:ILE:H	1:A:393:ILE:HG12	1.72	0.42
1:A:603:ILE:HD13	1:A:603:ILE:HG21	1.78	0.42
2:B:43:GLN:O	2:B:155:MET:HE1	2.19	0.42
2:B:1125:MET:HE1	2:B:1156:LYS:CG	2.47	0.42
3:C:67:ARG:NH2	10:J:2:ILE:HG23	2.33	0.42
3:C:94:CYS:SG	3:C:95:PRO:HD2	2.59	0.42
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.42
5:E:96:GLU:OE1	5:E:96:GLU:N	2.52	0.42
5:E:136:LEU:HD23	5:E:136:LEU:HA	1.87	0.42
7:G:119:PHE:HA	7:G:128:TYR:CE1	2.54	0.42
14:N:-52:DC:OP2	23:Z:186:ILE:HD12	2.19	0.42
16:Q:68:ARG:NH2	16:Q:82:GLN:HE22	2.16	0.42
20:W:25:GLY:N	20:W:72:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:152:LEU:HD12	20:W:167:ALA:O	2.19	0.42
1:A:503:LEU:O	1:A:503:LEU:HD23	2.19	0.42
1:A:770:VAL:HG21	1:A:781:ILE:HD11	2.01	0.42
1:A:1179:PRO:HA	1:A:1209:PRO:CB	2.49	0.42
2:B:952:GLU:H	2:B:952:GLU:HG2	1.50	0.42
2:B:982:ILE:HG21	2:B:982:ILE:HD13	1.74	0.42
10:J:49:LEU:HA	10:J:49:LEU:HD23	1.82	0.42
12:L:35:ARG:HH11	12:L:40:GLY:HA3	1.83	0.42
13:M:1476:TYR:CE2	13:M:1483:ARG:HD3	2.54	0.42
16:Q:182:ALA:O	16:Q:186:TYR:CD2	2.72	0.42
16:Q:380:ILE:HD12	16:Q:400:HIS:CE1	2.53	0.42
16:Q:424:GLN:HB2	21:X:231:TRP:CZ3	2.54	0.42
16:Q:707:CYS:HA	16:Q:710:LYS:HZ3	1.85	0.42
17:R:578:ALA:HA	19:V:127:VAL:HB	2.01	0.42
23:Z:478:VAL:O	23:Z:489:THR:HA	2.19	0.42
26:c:47:ALA:N	26:c:48:PRO:HD2	2.34	0.42
1:A:37:THR:HG21	1:A:41:ILE:HD11	2.01	0.42
1:A:465:HIS:CD2	1:A:467:MET:HE2	2.55	0.42
2:B:388:TYR:H	2:B:504:THR:CG2	2.27	0.42
2:B:520:VAL:HG13	2:B:520:VAL:O	2.19	0.42
2:B:607:ILE:HG23	2:B:607:ILE:HD12	1.72	0.42
5:E:64:HIS:ND1	5:E:65:ASN:N	2.68	0.42
16:Q:651:ASN:HB3	19:V:37:ASN:HD21	1.82	0.42
16:Q:745:HIS:HB2	20:W:20:TRP:CH2	2.53	0.42
16:Q:750:ASP:O	16:Q:754:MET:HE2	2.18	0.42
17:R:397:LYS:HA	17:R:397:LYS:HD2	1.85	0.42
18:T:58:DC:H4'	23:Z:283:ARG:NE	2.21	0.42
20:W:84:LEU:HA	20:W:84:LEU:HD23	1.77	0.42
23:Z:562:ASN:ND2	23:Z:566:LYS:HG3	2.33	0.42
23:Z:593:ASN:HB3	23:Z:595:HIS:HE1	1.84	0.42
1:A:75:ALA:O	2:B:1131:ARG:NH2	2.52	0.42
1:A:77:ASN:CG	1:A:78:MET:H	2.26	0.42
1:A:427:ILE:N	1:A:427:ILE:HD12	2.34	0.42
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.54	0.42
1:A:676:ILE:HG23	1:A:676:ILE:HD12	1.76	0.42
1:A:909:LEU:O	1:A:910:LYS:HG2	2.20	0.42
2:B:376:ALA:C	2:B:378:GLY:N	2.76	0.42
2:B:583:LEU:O	2:B:587:LEU:HD23	2.20	0.42
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.79	0.42
4:D:100:LEU:HD11	4:D:118:LEU:HD21	2.01	0.42
5:E:61:LEU:HD23	16:Q:884:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:HIS:CD2	23:Z:501:ILE:HD13	2.54	0.42
13:M:1408:LEU:HD23	13:M:1408:LEU:H	1.84	0.42
16:Q:530:TYR:CE2	16:Q:532:ASP:HB2	2.53	0.42
16:Q:645:LYS:HE3	21:X:243:LYS:NZ	2.33	0.42
16:Q:651:ASN:ND2	16:Q:682:ASP:OD2	2.52	0.42
16:Q:725:ARG:NE	19:V:31:CYS:SG	2.92	0.42
16:Q:877:GLN:OE1	16:Q:881:TYR:CE1	2.72	0.42
16:Q:880:GLN:HE21	16:Q:884:LYS:CE	2.32	0.42
22:Y:29:GLU:HG3	22:Y:45:ASN:O	2.19	0.42
23:Z:420:PHE:HE1	23:Z:470:LYS:HG2	1.83	0.42
23:Z:439:LYS:O	23:Z:452:PRO:HA	2.19	0.42
24:e:97:GLU:O	24:e:98:ALA:C	2.62	0.42
1:A:54:LEU:HA	1:A:54:LEU:HD12	1.85	0.42
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.55	0.42
1:A:965:VAL:O	1:A:968:VAL:HG22	2.19	0.42
1:A:1401:LEU:O	1:A:1405:MET:HG3	2.19	0.42
2:B:506:TRP:CD1	2:B:506:TRP:C	2.97	0.42
2:B:666:ASP:N	2:B:666:ASP:OD1	2.48	0.42
2:B:835:GLU:OE1	2:B:835:GLU:N	2.53	0.42
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.00	0.42
3:C:172:GLU:HG2	11:K:10:PHE:CE1	2.54	0.42
4:D:17:ALA:HB1	4:D:95:PHE:CZ	2.54	0.42
7:G:127:CYS:SG	7:G:138:GLN:HB3	2.60	0.42
11:K:37:LYS:HD3	11:K:37:LYS:HA	1.81	0.42
16:Q:188:LYS:HA	16:Q:191:ARG:HG2	2.00	0.42
16:Q:211:LEU:HB2	16:Q:213:LYS:CE	2.49	0.42
16:Q:268:ASN:HD22	16:Q:271:VAL:HG12	1.84	0.42
16:Q:285:TYR:HA	16:Q:288:VAL:HG12	2.01	0.42
17:R:414:VAL:HA	17:R:423:ASN:HB3	2.02	0.42
19:V:182:THR:HA	19:V:185:ASP:CG	2.44	0.42
20:W:135:VAL:HG23	20:W:136:GLU:HG2	2.01	0.42
21:X:221:THR:O	21:X:225:VAL:HG22	2.19	0.42
26:c:83:LEU:O	26:c:87:VAL:HG23	2.19	0.42
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.85	0.42
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.85	0.42
1:A:1090:LEU:HA	1:A:1090:LEU:HD23	1.79	0.42
2:B:53:MET:HB3	2:B:57:ARG:HH11	1.84	0.42
4:D:112:LYS:HB2	4:D:112:LYS:HE3	1.74	0.42
5:E:99:ILE:O	5:E:99:ILE:HG13	2.18	0.42
7:G:111:HIS:HB3	23:Z:494:ARG:CB	2.44	0.42
8:H:125:LEU:HD12	8:H:125:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:553:TRP:HA	16:Q:556:GLU:OE1	2.19	0.42
16:Q:772:GLU:HA	16:Q:773:LYS:CB	2.50	0.42
17:R:402:VAL:HB	17:R:455:TRP:HB2	2.02	0.42
17:R:452:PHE:O	17:R:456:LYS:HG2	2.20	0.42
20:W:196:LEU:HD13	20:W:205:LEU:HD11	2.01	0.42
20:W:288:LYS:HA	20:W:288:LYS:HD3	1.77	0.42
23:Z:588:ASP:OD1	23:Z:592:ASN:N	2.44	0.42
1:A:374:SER:OG	1:A:375:ILE:N	2.53	0.42
1:A:501:MET:HE2	1:A:501:MET:HB3	1.86	0.42
1:A:1172:ASN:HB2	1:A:1215:GLU:CD	2.44	0.42
1:A:1463:LEU:HA	1:A:1463:LEU:HD12	1.59	0.42
1:A:1551:ALA:O	13:M:1509:ARG:HD2	2.19	0.42
2:B:649:ASN:HB2	2:B:650:ASN:H	1.62	0.42
2:B:685:LYS:HD2	2:B:685:LYS:HA	1.81	0.42
2:B:839:GLY:O	2:B:891:ASP:HB2	2.20	0.42
3:C:78:ILE:HG23	3:C:78:ILE:HD12	1.78	0.42
7:G:106:CYS:SG	7:G:159:ALA:HB3	2.59	0.42
13:M:1490:THR:OG1	13:M:1493:GLY:N	2.52	0.42
14:N:-56:DG:H2''	14:N:-55:DC:C6	2.54	0.42
16:Q:132:LEU:HD11	19:V:85:ASP:HA	2.01	0.42
16:Q:468:GLY:O	16:Q:472:LYS:HG2	2.20	0.42
18:T:-70:DC:H2'	18:T:-69:DA:C8	2.55	0.42
19:V:132:ARG:HB3	19:V:133:LYS:H	1.70	0.42
25:b:88:TYR:CZ	27:d:80:TYR:CD1	3.07	0.42
1:A:413:TYR:O	1:A:449:HIS:CD2	2.67	0.42
1:A:487:SER:HG	1:A:673:GLN:NE2	2.18	0.42
1:A:592:PHE:CD2	1:A:592:PHE:O	2.71	0.42
1:A:932:ARG:HD3	8:H:106:THR:O	2.19	0.42
1:A:1060:LEU:HD23	1:A:1060:LEU:HA	1.60	0.42
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.42
2:B:376:ALA:C	2:B:378:GLY:H	2.28	0.42
2:B:472:ARG:HA	2:B:472:ARG:HD2	1.92	0.42
3:C:3:TYR:HB3	3:C:4:ALA:H	1.73	0.42
5:E:34:ASP:OD1	5:E:34:ASP:N	2.52	0.42
5:E:37:LEU:O	5:E:41:LYS:HG3	2.20	0.42
5:E:135:LEU:HA	5:E:135:LEU:HD23	1.83	0.42
7:G:82:GLY:N	7:G:147:ILE:O	2.34	0.42
14:N:-35:DC:H2''	14:N:-34:DA:H8	1.80	0.42
15:P:22:G:C2'	15:P:23:G:H8	2.33	0.42
16:Q:116:LEU:HD23	16:Q:116:LEU:HA	1.91	0.42
16:Q:215:GLU:HG2	16:Q:216:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:240:VAL:HG11	19:V:72:HIS:O	2.20	0.42
16:Q:365:GLU:HG2	16:Q:369:LYS:NZ	2.34	0.42
16:Q:719:VAL:HG23	16:Q:720:VAL:N	2.35	0.42
17:R:440:GLU:HG3	17:R:441:PHE:CE1	2.55	0.42
21:X:250:PHE:HA	21:X:253:LEU:HB3	2.02	0.42
23:Z:258:LYS:HB3	23:Z:258:LYS:HE2	1.73	0.42
23:Z:705:LEU:HD12	23:Z:724:VAL:HG11	2.01	0.42
1:A:20:ARG:NH2	1:A:22:GLN:OE1	2.52	0.42
1:A:321:GLU:HG2	1:A:327:ARG:NH2	2.35	0.42
1:A:338:SER:OG	1:A:341:GLN:HG2	2.19	0.42
1:A:643:LYS:HD2	15:P:38:A:OP2	2.19	0.42
1:A:1217:ASP:OD1	1:A:1218:ARG:N	2.53	0.42
2:B:254:GLN:O	2:B:303:PRO:HB2	2.19	0.42
2:B:420:GLN:C	2:B:422:PHE:N	2.78	0.42
3:C:131:THR:HG22	3:C:147:ASP:OD1	2.20	0.42
13:M:1421:SER:OG	13:M:1424:ARG:NH1	2.53	0.42
14:N:-54:DG:C6	18:T:55:DG:N2	2.87	0.42
16:Q:62:LYS:HA	16:Q:62:LYS:HD3	1.74	0.42
16:Q:773:LYS:HE2	16:Q:827:HIS:HE1	1.84	0.42
17:R:429:ARG:NH1	17:R:431:GLY:O	2.51	0.42
17:R:452:PHE:HD2	17:R:453:MET:CE	2.33	0.42
20:W:108:ASP:OD1	20:W:126:HIS:ND1	2.53	0.42
23:Z:450:ILE:O	23:Z:462:GLU:HA	2.20	0.42
23:Z:499:PHE:CD1	23:Z:512:LYS:HB3	2.53	0.42
1:A:130:LEU:HD11	1:A:235:VAL:HG13	2.01	0.42
2:B:422:PHE:HB3	2:B:429:PHE:CB	2.50	0.42
2:B:1173:SER:O	2:B:1173:SER:OG	2.36	0.42
5:E:111:THR:O	5:E:114:ALA:N	2.52	0.42
5:E:166:ARG:NH2	5:E:168:ASN:HB3	2.34	0.42
7:G:11:ILE:HG21	7:G:11:ILE:HD13	1.79	0.42
9:I:74:GLN:H	9:I:74:GLN:HG2	1.51	0.42
12:L:38:GLU:C	12:L:40:GLY:H	2.28	0.42
13:M:1037:ILE:H	13:M:1055:GLY:HA2	1.84	0.42
13:M:1354:ASP:O	13:M:1372:LYS:HG2	2.20	0.42
13:M:1485:GLU:CD	13:M:1497:ARG:HH11	2.28	0.42
14:N:61:DC:H2"	14:N:62:DG:C8	2.55	0.42
15:P:25:A:C2	15:P:26:C:C4	3.08	0.42
16:Q:69:ILE:H	16:Q:69:ILE:HD12	1.84	0.42
16:Q:377:THR:OG1	16:Q:400:HIS:O	2.37	0.42
17:R:479:ILE:H	17:R:479:ILE:HG12	1.61	0.42
17:R:485:TYR:HD2	17:R:487:PHE:CE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:8:LEU:HD13	20:W:288:LYS:HE3	2.01	0.42
20:W:228:LEU:HD11	20:W:259:TRP:CE3	2.54	0.42
23:Z:614:ILE:H	23:Z:614:ILE:HG13	1.73	0.42
1:A:46:THR:OG1	1:A:47:THR:N	2.53	0.41
1:A:479:TRP:CD1	1:A:479:TRP:N	2.87	0.41
1:A:497:ASP:HB3	2:B:792:ASP:HB3	2.01	0.41
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.53	0.41
1:A:639:ILE:HG21	1:A:639:ILE:HD13	1.80	0.41
1:A:693:ILE:HG23	1:A:693:ILE:HD12	1.79	0.41
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.41
1:A:1255:LEU:HD12	1:A:1255:LEU:N	2.34	0.41
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.85	0.41
2:B:847:LYS:HE3	2:B:864:ASP:OD2	2.20	0.41
2:B:848:LEU:C	2:B:848:LEU:HD12	2.44	0.41
3:C:36:ARG:HH21	3:C:36:ARG:HD3	1.70	0.41
4:D:16:ASP:H	4:D:21:ILE:CG2	2.32	0.41
4:D:74:PHE:CE2	4:D:80:ILE:HG12	2.52	0.41
5:E:61:LEU:HD12	5:E:61:LEU:HA	1.77	0.41
7:G:7:LEU:HB2	7:G:72:TYR:CE2	2.55	0.41
16:Q:152:PHE:HD2	16:Q:172:ILE:HD11	1.83	0.41
16:Q:384:LEU:HD11	16:Q:393:LYS:O	2.20	0.41
16:Q:652:GLY:O	16:Q:656:VAL:HG13	2.20	0.41
18:T:-35:DA:H1'	18:T:-34:DG:H5'	2.01	0.41
19:V:51:TYR:CD1	19:V:52:PRO:HD2	2.55	0.41
1:A:1137:PRO:O	1:A:1341:VAL:HG23	2.20	0.41
1:A:1212:LEU:CD1	1:A:1285:LEU:HD13	2.48	0.41
2:B:556:ILE:HD12	2:B:556:ILE:HA	1.59	0.41
2:B:557:SER:O	2:B:559:ALA:N	2.53	0.41
2:B:638:ARG:HH11	2:B:639:HIS:CE1	2.38	0.41
2:B:1062:ARG:CZ	2:B:1065:GLY:H	2.32	0.41
16:Q:314:ARG:HH22	16:Q:349:GLN:NE2	2.08	0.41
16:Q:537:LEU:HB3	16:Q:553:TRP:CZ3	2.55	0.41
16:Q:707:CYS:SG	16:Q:708:LEU:N	2.93	0.41
16:Q:807:LEU:HD23	16:Q:807:LEU:HA	1.80	0.41
17:R:429:ARG:HB2	17:R:434:GLN:HB3	2.02	0.41
17:R:582:GLU:HA	17:R:585:ASN:HD21	1.85	0.41
20:W:11:GLN:HE21	20:W:54:LEU:HD23	1.85	0.41
24:a:72:ARG:HH21	24:a:72:ARG:HG2	1.85	0.41
26:c:69:ALA:O	26:c:73:ASN:ND2	2.53	0.41
24:e:51:ILE:O	24:e:55:GLN:HG3	2.20	0.41
1:A:33:ARG:H	1:A:33:ARG:HG2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:O	1:A:463:THR:N	2.52	0.41
2:B:186:ILE:HG21	2:B:186:ILE:HD13	1.74	0.41
2:B:917:LYS:HE2	2:B:917:LYS:HB3	1.75	0.41
5:E:10:LEU:HD23	5:E:10:LEU:HA	1.79	0.41
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.87	0.41
5:E:27:LEU:HD13	5:E:65:ASN:ND2	2.35	0.41
5:E:60:VAL:HG23	5:E:74:VAL:HB	2.03	0.41
6:F:102:ILE:HD13	6:F:102:ILE:HG21	1.79	0.41
9:I:31:GLU:OE1	9:I:31:GLU:N	2.53	0.41
16:Q:18:GLU:N	16:Q:18:GLU:OE1	2.53	0.41
16:Q:202:LEU:HD21	16:Q:233:GLY:HA3	2.02	0.41
16:Q:345:PHE:O	16:Q:349:GLN:HG2	2.20	0.41
16:Q:744:ARG:HG3	16:Q:753:LEU:HD12	2.02	0.41
16:Q:790:HIS:NE2	16:Q:817:CYS:SG	2.94	0.41
16:Q:858:LYS:HA	16:Q:861:GLU:HG3	2.03	0.41
20:W:5:TYR:CD1	20:W:303:CYS:HB3	2.55	0.41
23:Z:526:SER:OG	23:Z:527:GLY:N	2.53	0.41
27:d:112:THR:O	27:d:116:THR:OG1	2.38	0.41
1:A:57:LEU:HA	1:A:57:LEU:HD23	1.73	0.41
1:A:330:GLN:O	1:A:332:SER:N	2.42	0.41
1:A:725:LEU:HD21	1:A:736:THR:HG23	2.02	0.41
1:A:738:GLU:OE1	1:A:797:ARG:HD3	2.21	0.41
1:A:832:THR:HG23	1:A:833:PRO:HD2	2.02	0.41
1:A:1164:THR:O	1:A:1298:LEU:N	2.53	0.41
2:B:566:LYS:HG2	2:B:576:ILE:HD11	2.02	0.41
2:B:574:VAL:O	2:B:574:VAL:HG22	2.20	0.41
2:B:931:ILE:HG21	2:B:931:ILE:HD13	1.75	0.41
5:E:27:LEU:HD12	5:E:27:LEU:HA	1.77	0.41
5:E:97:GLU:CD	16:Q:887:ASN:HD21	2.28	0.41
13:M:1448:ILE:HA	13:M:1451:LYS:HG2	2.03	0.41
13:M:1474:LEU:HD21	13:M:1511:PHE:CE2	2.55	0.41
14:N:21:DG:H2''	14:N:22:DT:OP2	2.21	0.41
16:Q:720:VAL:HG21	16:Q:743:ALA:HB2	2.01	0.41
17:R:429:ARG:HE	17:R:431:GLY:C	2.28	0.41
23:Z:490:GLY:HA3	23:Z:503:PHE:O	2.20	0.41
23:Z:601:LYS:HG3	23:Z:611:GLU:OE2	2.20	0.41
24:a:96:SER:O	24:a:99:TYR:HB3	2.20	0.41
1:A:130:LEU:O	1:A:134:LYS:NZ	2.47	0.41
1:A:140:ARG:NH1	1:A:234:PHE:O	2.50	0.41
1:A:561:MET:SD	11:K:58:PHE:HA	2.60	0.41
1:A:695:ASP:C	1:A:697:LYS:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:THR:HG22	1:A:1329:LYS:HD2	2.01	0.41
2:B:186:ILE:O	2:B:187:ILE:HD13	2.20	0.41
2:B:312:GLN:OE1	9:I:40:ARG:NH2	2.54	0.41
2:B:993:LYS:HD3	19:V:131:MET:SD	2.60	0.41
4:D:84:ARG:HG3	4:D:97:LEU:HD11	2.02	0.41
11:K:93:ASP:OD1	11:K:94:LEU:N	2.53	0.41
17:R:390:GLY:HA2	17:R:400:TYR:CD1	2.55	0.41
17:R:563:ILE:HD12	17:R:566:ARG:HD2	2.03	0.41
20:W:27:ASN:ND2	20:W:74:HIS:O	2.53	0.41
20:W:222:ALA:O	20:W:223:ASN:ND2	2.54	0.41
22:Y:14:ARG:NH2	23:Z:300:GLN:OE1	2.53	0.41
23:Z:389:THR:HG23	23:Z:391:SER:H	1.85	0.41
1:A:349:ARG:HA	1:A:349:ARG:HD3	1.94	0.41
1:A:461:GLN:O	1:A:461:GLN:NE2	2.53	0.41
1:A:849:ASP:HA	1:A:852:VAL:HG22	2.03	0.41
1:A:1379:GLU:O	1:A:1379:GLU:HG2	2.16	0.41
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.38	0.41
2:B:509:VAL:HG11	2:B:524:LYS:HD2	2.01	0.41
2:B:557:SER:C	2:B:559:ALA:H	2.29	0.41
2:B:603:MET:HE2	2:B:603:MET:HB2	1.85	0.41
5:E:173:ILE:HG21	5:E:173:ILE:HD13	1.79	0.41
5:E:185:ILE:H	5:E:185:ILE:HG12	1.62	0.41
7:G:14:HIS:O	7:G:16:ARG:N	2.54	0.41
8:H:96:VAL:HA	8:H:116:VAL:HA	2.03	0.41
15:P:24:A:C2'	15:P:25:A:C8	3.04	0.41
18:T:54:DC:C4	18:T:55:DG:C6	3.08	0.41
19:V:39:LEU:HA	19:V:39:LEU:HD23	1.77	0.41
20:W:155:ALA:O	20:W:163:LEU:HG	2.20	0.41
23:Z:525:ALA:O	23:Z:552:ARG:NH2	2.49	0.41
24:a:63:ARG:CZ	24:a:63:ARG:HB2	2.51	0.41
1:A:1124:LEU:HD12	1:A:1124:LEU:HA	1.67	0.41
2:B:440:ILE:O	2:B:441:SER:C	2.63	0.41
2:B:679:PRO:CG	2:B:680:ASP:N	2.84	0.41
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.02	0.41
4:D:41:LEU:HB3	4:D:65:LEU:CD2	2.50	0.41
5:E:101:ARG:HA	5:E:126:ILE:O	2.20	0.41
7:G:110:ARG:HG2	7:G:119:PHE:CZ	2.56	0.41
14:N:27:DG:P	25:b:79:LYS:HD3	2.61	0.41
16:Q:639:VAL:HA	16:Q:642:ASN:OD1	2.20	0.41
16:Q:859:GLU:O	16:Q:863:LYS:HG2	2.21	0.41
23:Z:551:VAL:HG21	23:Z:632:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HB2	1:A:250:VAL:CG2	2.51	0.41
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.36	0.41
1:A:680:LEU:HD12	1:A:680:LEU:HA	1.85	0.41
1:A:828:LEU:HA	1:A:828:LEU:HD12	1.85	0.41
2:B:100:GLU:HA	2:B:105:PRO:CG	2.50	0.41
7:G:123:SER:HB2	7:G:125:PRO:HD2	2.03	0.41
9:I:109:ARG:HD3	9:I:124:THR:CG2	2.46	0.41
12:L:13:GLN:HA	12:L:14:PRO:HD3	1.88	0.41
14:N:50:DG:OP1	27:d:31:LYS:HE3	2.20	0.41
16:Q:24:LEU:HD11	16:Q:56:LYS:NZ	2.35	0.41
16:Q:153:HIS:CE1	16:Q:156:LEU:HD12	2.56	0.41
16:Q:819:ASP:O	16:Q:822:SER:OG	2.32	0.41
18:T:-15:DA:C6	18:T:-14:DA:C6	3.09	0.41
20:W:83:SER:HB3	20:W:85:ASP:OD1	2.20	0.41
20:W:172:ILE:O	20:W:186:LEU:N	2.54	0.41
20:W:233:SER:OG	20:W:251:SER:HB2	2.21	0.41
24:a:127:ALA:O	24:a:131:ARG:HG3	2.21	0.41
1:A:83:GLY:O	1:A:257:PRO:HG3	2.21	0.41
1:A:99:PHE:O	1:A:103:THR:HG23	2.21	0.41
1:A:111:CYS:HG	1:A:114:CYS:CB	2.34	0.41
1:A:339:LEU:HA	1:A:339:LEU:HD23	1.77	0.41
1:A:565:MET:HB2	1:A:565:MET:HE2	1.76	0.41
1:A:626:THR:O	1:A:627:LYS:HB3	2.21	0.41
1:A:762:GLU:H	1:A:762:GLU:CD	2.28	0.41
1:A:939:VAL:H	1:A:939:VAL:HG22	1.63	0.41
1:A:1165:THR:HG22	1:A:1297:THR:H	1.85	0.41
1:A:1216:LEU:HA	1:A:1216:LEU:HD23	1.86	0.41
1:A:1417:HIS:HA	1:A:1421:ARG:NH2	2.35	0.41
2:B:157:ARG:NH1	2:B:177:CYS:O	2.54	0.41
2:B:548:TRP:HB3	2:B:549:SER:H	1.57	0.41
2:B:937:SER:OG	2:B:938:ARG:N	2.53	0.41
3:C:109:GLU:O	3:C:155:LYS:HG3	2.21	0.41
4:D:32:LEU:HD23	4:D:32:LEU:HA	1.83	0.41
7:G:7:LEU:HA	7:G:7:LEU:HD23	1.76	0.41
7:G:79:PRO:HG3	7:G:104:MET:HE1	2.02	0.41
7:G:92:VAL:H	7:G:139:GLN:HE21	1.69	0.41
8:H:6:PHE:CZ	8:H:37:MET:SD	3.14	0.41
8:H:42:ASP:OD1	8:H:42:ASP:N	2.54	0.41
11:K:103:GLU:O	11:K:107:VAL:HG13	2.20	0.41
13:M:623:LYS:O	13:M:627:ASP:N	2.51	0.41
13:M:1341:LYS:HD2	13:M:1341:LYS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:67:DT:H3	18:T:-67:DA:H61	1.69	0.41
16:Q:56:LYS:HB3	16:Q:56:LYS:HE2	1.71	0.41
16:Q:218:ARG:HH21	16:Q:238:LEU:CD2	2.33	0.41
16:Q:296:PHE:CE1	16:Q:305:GLN:HB2	2.56	0.41
16:Q:790:HIS:CD2	16:Q:817:CYS:SG	3.14	0.41
16:Q:791:ARG:HH22	20:W:87:HIS:CD2	2.38	0.41
16:Q:858:LYS:O	16:Q:861:GLU:HG3	2.21	0.41
18:T:47:DG:H2''	18:T:48:DT:H5'	2.03	0.41
20:W:214:ILE:HD12	20:W:228:LEU:HD23	2.02	0.41
22:Y:48:MET:HE3	22:Y:48:MET:HA	2.03	0.41
23:Z:571:ARG:HB2	23:Z:574:ALA:CB	2.51	0.41
24:a:73:GLU:O	24:a:74:ILE:C	2.63	0.41
27:d:91:ILE:O	27:d:94:ALA:HB3	2.21	0.41
1:A:27:SER:O	1:A:31:LEU:N	2.40	0.41
1:A:939:VAL:O	1:A:943:LEU:HD12	2.21	0.41
1:A:1166:LEU:HD23	1:A:1166:LEU:HA	1.84	0.41
1:A:1290:SER:O	1:A:1294:THR:HG23	2.21	0.41
2:B:241:ALA:O	2:B:242:ARG:C	2.63	0.41
2:B:242:ARG:HH11	2:B:252:ILE:N	2.19	0.41
2:B:273:PHE:CG	2:B:284:ILE:HG23	2.56	0.41
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.61	0.41
3:C:44:ILE:HD13	3:C:44:ILE:HG21	1.48	0.41
5:E:3:ASP:CG	5:E:47:LYS:HD2	2.45	0.41
7:G:24:ASN:O	7:G:28:GLN:HG2	2.21	0.41
7:G:81:LYS:HE2	7:G:149:GLY:HA2	2.03	0.41
7:G:152:VAL:HA	7:G:157:ILE:HA	2.02	0.41
20:W:46:VAL:CG2	20:W:58:TRP:HB2	2.51	0.41
24:a:78:PHE:CZ	25:b:67:ARG:HB2	2.56	0.41
24:a:100:LEU:HD11	25:b:58:LEU:HD13	2.03	0.41
25:b:75:HIS:C	25:b:77:LYS:H	2.28	0.41
1:A:151:LYS:O	1:A:152:ASN:ND2	2.53	0.40
1:A:266:MET:HE3	1:A:266:MET:HB3	1.84	0.40
1:A:322:LEU:HD13	1:A:322:LEU:HA	1.94	0.40
1:A:660:MET:HB2	1:A:660:MET:HE2	1.86	0.40
1:A:1121:VAL:N	1:A:1122:PRO:CD	2.84	0.40
1:A:1376:LYS:O	1:A:1380:ARG:HG3	2.21	0.40
2:B:791:GLU:O	2:B:792:ASP:HB2	2.20	0.40
2:B:976:MET:HE3	2:B:976:MET:HB2	1.87	0.40
7:G:50:THR:HG22	7:G:73:LYS:HB3	2.03	0.40
9:I:38:ALA:HA	9:I:44:TYR:O	2.21	0.40
15:P:12:A:O2'	15:P:13:A:O5'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:868:LYS:HA	16:Q:868:LYS:HD3	1.79	0.40
18:T:-45:DA:C6	18:T:-44:DA:C6	3.09	0.40
18:T:38:DT:H6	18:T:38:DT:H2'	1.67	0.40
1:A:135:GLY:O	1:A:137:PRO:HD3	2.21	0.40
1:A:288:ASN:HD22	1:A:288:ASN:HA	1.72	0.40
1:A:410:ASN:HD22	1:A:430:ARG:CD	2.34	0.40
1:A:1178:ASP:HA	1:A:1179:PRO:HD3	1.87	0.40
1:A:1321:ILE:O	1:A:1328:PHE:O	2.39	0.40
1:A:1451:MET:HE3	1:A:1451:MET:HB3	1.91	0.40
2:B:322:GLY:CA	2:B:339:ALA:HB2	2.50	0.40
2:B:739:ASN:OD1	2:B:739:ASN:N	2.53	0.40
2:B:1080:ARG:HD3	2:B:1080:ARG:HA	1.96	0.40
2:B:1124:ILE:HG23	2:B:1124:ILE:HD12	1.81	0.40
5:E:39:GLU:O	5:E:43:GLN:HB2	2.20	0.40
12:L:18:ILE:HD11	12:L:47:LYS:HG3	2.02	0.40
16:Q:49:LEU:HD13	16:Q:49:LEU:HA	1.89	0.40
16:Q:235:LEU:HD23	16:Q:261:ALA:HB2	2.02	0.40
16:Q:572:GLY:O	16:Q:576:LEU:HG	2.21	0.40
17:R:562:TYR:O	17:R:565:GLN:HG2	2.21	0.40
18:T:-43:DT:OP2	26:c:17:ARG:NH1	2.51	0.40
19:V:122:GLN:O	19:V:122:GLN:NE2	2.54	0.40
23:Z:192:THR:OG1	23:Z:244:ASN:ND2	2.54	0.40
23:Z:260:MET:N	23:Z:260:MET:SD	2.94	0.40
23:Z:420:PHE:CE1	23:Z:470:LYS:HG2	2.56	0.40
23:Z:457:LEU:HD12	23:Z:457:LEU:HA	1.92	0.40
25:b:30:THR:O	25:b:34:ILE:HG13	2.21	0.40
25:b:90:LEU:HB3	25:b:95:ARG:O	2.21	0.40
1:A:120:ASP:O	1:A:122:ASN:N	2.54	0.40
1:A:513:ALA:HB2	6:F:90:LEU:HD11	2.04	0.40
2:B:545:LEU:HD23	2:B:550:MET:HE3	2.03	0.40
2:B:783:ALA:HB2	2:B:1041:ILE:HG21	2.04	0.40
7:G:168:LEU:HD23	7:G:168:LEU:HA	1.90	0.40
9:I:53:ILE:HA	9:I:53:ILE:HD13	1.70	0.40
10:J:30:THR:HG22	10:J:33:ASP:HB2	2.02	0.40
12:L:52:LEU:HD12	12:L:52:LEU:HA	1.68	0.40
14:N:32:DG:H2''	14:N:33:DT:H71	2.03	0.40
16:Q:333:THR:HG21	16:Q:347:LEU:HD12	2.02	0.40
16:Q:537:LEU:HD23	16:Q:537:LEU:HA	1.92	0.40
16:Q:689:HIS:HB2	19:V:35:TYR:CE1	2.56	0.40
17:R:454:LYS:HA	17:R:454:LYS:HD2	1.77	0.40
20:W:54:LEU:HD12	20:W:54:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:246:SER:HA	21:X:249:ILE:HD12	2.02	0.40
23:Z:200:PHE:HB2	23:Z:210:LEU:HD22	2.02	0.40
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.78	0.40
1:A:1150:ASP:OD2	1:A:1153:ARG:HG3	2.21	0.40
1:A:1218:ARG:O	1:A:1222:THR:HG23	2.22	0.40
1:A:1466:ALA:C	1:A:1467:GLY:O	2.65	0.40
2:B:50:PHE:HA	2:B:54:SER:HB3	2.02	0.40
2:B:309:PHE:CD2	9:I:40:ARG:NE	2.88	0.40
5:E:94:MET:HA	5:E:99:ILE:HD11	2.03	0.40
16:Q:24:LEU:HD12	16:Q:24:LEU:HA	1.95	0.40
16:Q:274:HIS:HA	16:Q:277:ASN:HD21	1.84	0.40
16:Q:333:THR:OG1	16:Q:347:LEU:HD11	2.21	0.40
16:Q:741:LEU:HA	16:Q:741:LEU:HD23	1.77	0.40
17:R:388:ARG:HG2	17:R:443:SER:HB2	2.03	0.40
16:U:399:GLU:HA	19:V:170:LYS:N	2.36	0.40
20:W:16:ASP:N	20:W:41:ASP:OD2	2.55	0.40
26:c:32:ARG:HH12	27:d:32:GLU:CD	2.27	0.40
24:e:101:VAL:HG11	25:f:40:ARG:HG2	2.03	0.40
1:A:350:VAL:HG21	1:A:1435:THR:HG23	2.03	0.40
1:A:538:VAL:O	1:A:539:GLN:HG2	2.22	0.40
1:A:695:ASP:O	1:A:696:SER:OG	2.35	0.40
1:A:912:SER:O	1:A:914:LYS:N	2.54	0.40
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.04	0.40
1:A:1188:GLU:O	1:A:1192:TRP:CZ3	2.74	0.40
1:A:1394:ASN:OD1	1:A:1395:TYR:N	2.54	0.40
1:A:1439:LEU:HD23	1:A:1439:LEU:HA	1.89	0.40
2:B:360:LYS:HE3	2:B:554:GLU:OE2	2.21	0.40
2:B:866:ILE:HD13	2:B:866:ILE:HA	1.60	0.40
2:B:1129:ASN:O	2:B:1133:HIS:N	2.54	0.40
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.81	0.40
9:I:14:ILE:HG23	9:I:23:MET:HG3	2.03	0.40
16:Q:211:LEU:HD12	16:Q:213:LYS:NZ	2.36	0.40
16:Q:841:LEU:CD2	16:Q:844:LYS:HD3	2.51	0.40
16:Q:851:LEU:O	16:Q:855:LYS:HG2	2.21	0.40
17:R:458:ALA:HA	17:R:461:SER:OG	2.21	0.40
17:R:473:ASN:HA	17:R:476:GLU:OE2	2.22	0.40
17:R:487:PHE:HB3	17:R:491:ASP:OD2	2.22	0.40
19:V:106:LYS:HA	19:V:106:LYS:HD2	1.87	0.40
23:Z:480:VAL:HG12	23:Z:488:ASP:O	2.21	0.40
24:e:101:VAL:O	24:e:102:ALA:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1281 (91%)	117 (8%)	10 (1%)	18	49
2	B	1112/1251 (89%)	998 (90%)	105 (9%)	9 (1%)	16	45
3	C	254/270 (94%)	232 (91%)	19 (8%)	3 (1%)	10	37
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	24	55
6	F	76/127 (60%)	70 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
8	H	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	18	49
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	60 (94%)	2 (3%)	2 (3%)	3	20
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
13	M	976/1002 (97%)	903 (92%)	72 (7%)	1 (0%)	48	75
16	Q	888/1845 (48%)	836 (94%)	52 (6%)	0	100	100
16	U	117/1845 (6%)	88 (75%)	21 (18%)	8 (7%)	1	7
17	R	240/248 (97%)	225 (94%)	14 (6%)	1 (0%)	30	60
19	V	234/311 (75%)	197 (84%)	33 (14%)	4 (2%)	7	30
20	W	298/305 (98%)	269 (90%)	29 (10%)	0	100	100
21	X	41/531 (8%)	41 (100%)	0	0	100	100
22	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100	100
23	Z	497/1087 (46%)	460 (93%)	36 (7%)	1 (0%)	43	71
24	a	95/136 (70%)	83 (87%)	9 (10%)	3 (3%)	3	19
24	e	95/136 (70%)	87 (92%)	8 (8%)	0	100	100
25	b	81/103 (79%)	70 (86%)	8 (10%)	3 (4%)	2	17
25	f	76/103 (74%)	67 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	101/103 (98%)	88 (87%)	9 (9%)	4 (4%)	2	15
27	d	93/95 (98%)	82 (88%)	9 (10%)	2 (2%)	5	26
All	All	7779/12644 (62%)	7099 (91%)	627 (8%)	53 (1%)	20	49

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
1	A	1185	VAL
1	A	1468	THR
2	B	19	PRO
3	C	93	PHE
13	M	1330	PRO
17	R	507	PRO
16	U	506	ALA
16	U	508	HIS
19	V	238	PRO
23	Z	760	GLY
24	a	73	GLU
25	b	29	ILE
27	d	101	GLY
1	A	1435	THR
16	U	481	GLY
16	U	521	LYS
24	a	77	ASP
27	d	109	SER
2	B	20	ASP
2	B	142	THR
2	B	1004	ASP
10	J	28	GLU
16	U	463	PRO
16	U	513	LEU
16	U	516	ALA
16	U	523	GLN
19	V	228	GLU
19	V	249	ASP
19	V	291	ASN
25	b	34	ILE
1	A	300	ALA
1	A	696	SER
2	B	950	ARG

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Mol	Chain	Res	Type
26	c	64	GLU
26	c	113	SER
1	A	495	ASP
1	A	1130	ILE
2	B	679	PRO
2	B	834	ARG
3	C	60	HIS
3	C	92	GLU
24	a	74	ILE
25	b	26	ILE
2	B	650	ASN
2	B	1001	PRO
1	A	478	PRO
5	E	45	GLY
8	H	17	PRO
10	J	64	PRO
1	A	980	PRO
26	c	114	VAL
26	c	26	PRO

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	A	1245/1761 (71%)	1214 (98%)	31 (2%)	42	64
2	B	986/1084 (91%)	939 (95%)	47 (5%)	23	52
3	C	235/247 (95%)	232 (99%)	3 (1%)	61	74
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	188 (98%)	3 (2%)	55	72
6	F	68/111 (61%)	66 (97%)	2 (3%)	37	62
7	G	146/153 (95%)	144 (99%)	2 (1%)	59	73
8	H	130/131 (99%)	122 (94%)	8 (6%)	16	45
9	I	104/112 (93%)	100 (96%)	4 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	55/56 (98%)	54 (98%)	1 (2%)	51	70
11	K	104/106 (98%)	102 (98%)	2 (2%)	50	68
12	L	43/55 (78%)	39 (91%)	4 (9%)	8	30
13	M	154/894 (17%)	154 (100%)	0	100	100
16	Q	761/1601 (48%)	759 (100%)	2 (0%)	86	86
16	U	63/1601 (4%)	63 (100%)	0	100	100
17	R	168/222 (76%)	167 (99%)	1 (1%)	78	81
19	V	144/285 (50%)	143 (99%)	1 (1%)	76	80
20	W	255/260 (98%)	253 (99%)	2 (1%)	73	79
21	X	40/467 (9%)	40 (100%)	0	100	100
22	Y	102/105 (97%)	101 (99%)	1 (1%)	68	76
23	Z	434/939 (46%)	432 (100%)	2 (0%)	81	83
24	a	85/111 (77%)	76 (89%)	9 (11%)	6	24
24	e	84/111 (76%)	81 (96%)	3 (4%)	31	58
25	b	68/79 (86%)	62 (91%)	6 (9%)	9	32
25	f	63/79 (80%)	60 (95%)	3 (5%)	23	52
26	c	82/82 (100%)	74 (90%)	8 (10%)	7	28
27	d	81/81 (100%)	70 (86%)	11 (14%)	3	16
All	All	6000/11051 (54%)	5844 (97%)	156 (3%)	41	64

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	67	ARG
1	A	79	THR
1	A	147	LEU
1	A	250	VAL
1	A	251	THR
1	A	283	ILE
1	A	301	HIS
1	A	440	LEU
1	A	457	ILE
1	A	461	GLN
1	A	476	ILE
1	A	538	VAL

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Mol	Chain	Res	Type
1	A	571	ASP
1	A	605	THR
1	A	622	SER
1	A	664	ILE
1	A	713	VAL
1	A	757	GLN
1	A	761	SER
1	A	905	ASN
1	A	942	VAL
1	A	1007	ILE
1	A	1074	SER
1	A	1130	ILE
1	A	1175	ILE
1	A	1186	VAL
1	A	1235	ILE
1	A	1282	ASP
1	A	1385	VAL
1	A	1424	THR
2	B	20	ASP
2	B	90	GLN
2	B	92	TYR
2	B	115	LEU
2	B	147	THR
2	B	154	ILE
2	B	163	LEU
2	B	170	ASP
2	B	176	GLU
2	B	180	ASP
2	B	198	GLU
2	B	218	THR
2	B	267	VAL
2	B	291	ASP
2	B	311	ILE
2	B	331	THR
2	B	348	LEU
2	B	351	VAL
2	B	354	SER
2	B	359	THR
2	B	386	ASP
2	B	411	LEU
2	B	440	ILE
2	B	504	THR

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Mol	Chain	Res	Type
2	B	556	ILE
2	B	567	ILE
2	B	574	VAL
2	B	597	ILE
2	B	626	LEU
2	B	649	ASN
2	B	650	ASN
2	B	659	SER
2	B	665	ILE
2	B	715	ASP
2	B	731	GLN
2	B	738	THR
2	B	743	ARG
2	B	750	VAL
2	B	759	VAL
2	B	784	SER
2	B	909	VAL
2	B	931	ILE
2	B	958	CYS
2	B	1118	VAL
2	B	1130	THR
2	B	1148	LEU
2	B	1174	VAL
3	C	74	THR
3	C	75	SER
3	C	151	VAL
5	E	28	VAL
5	E	82	VAL
5	E	117	SER
6	F	120	VAL
6	F	123	LEU
7	G	21	ASN
7	G	37	THR
8	H	15	ILE
8	H	51	ASP
8	H	67	ASP
8	H	83	SER
8	H	96	VAL
8	H	113	SER
8	H	116	VAL
8	H	141	VAL
9	I	12	VAL

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Mol	Chain	Res	Type
9	I	34	ILE
9	I	73	SER
9	I	101	SER
10	J	47	ARG
11	K	99	SER
11	K	107	VAL
12	L	34	ILE
12	L	39	CYS
12	L	43	ILE
12	L	44	MET
16	Q	552	ASP
16	Q	820	LEU
17	R	422	THR
19	V	45	ASP
20	W	43	LEU
20	W	169	ASP
22	Y	115	ILE
23	Z	614	ILE
23	Z	720	TYR
24	a	46	VAL
24	a	48	LEU
24	a	59	GLU
24	a	63	ARG
24	a	65	LEU
24	a	105	GLU
24	a	115	LYS
24	a	117	VAL
24	a	129	ARG
25	b	47	SER
25	b	73	THR
25	b	80	THR
25	b	91	LYS
25	b	92	ARG
25	b	95	ARG
26	c	29	ARG
26	c	59	THR
26	c	73	ASN
26	c	81	ARG
26	c	91	GLU
26	c	101	THR
26	c	114	VAL
26	c	118	LYS

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Mol	Chain	Res	Type
27	d	39	TYR
27	d	48	ASP
27	d	49	THR
27	d	77	LEU
27	d	84	SER
27	d	85	THR
27	d	93	THR
27	d	98	LEU
27	d	109	SER
27	d	116	THR
27	d	119	THR
24	e	59	GLU
24	e	117	VAL
24	e	129	ARG
25	f	26	ILE
25	f	73	THR
25	f	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	122	ASN
1	A	123	ASN
1	A	143	HIS
1	A	152	ASN
1	A	288	ASN
1	A	313	HIS
1	A	423	ASN
1	A	449	HIS
1	A	465	HIS
1	A	678	ASN
1	A	704	ASN
1	A	780	ASN
1	A	792	ASN
1	A	804	HIS
1	A	809	HIS
1	A	935	GLN
1	A	982	ASN
1	A	991	GLN
1	A	1005	HIS
1	A	1032	GLN

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Mol	Chain	Res	Type
1	A	1082	HIS
1	A	1182	GLN
1	A	1190	GLN
1	A	1230	GLN
1	A	1384	HIS
1	A	1420	ASN
2	B	43	GLN
2	B	52	GLN
2	B	111	ASN
2	B	117	ASN
2	B	175	ASN
2	B	197	GLN
2	B	319	ASN
2	B	481	HIS
2	B	500	GLN
2	B	585	ASN
2	B	631	GLN
2	B	649	ASN
2	B	842	HIS
2	B	1040	GLN
2	B	1094	GLN
2	B	1120	ASN
2	B	1142	ASN
3	C	60	HIS
3	C	83	GLN
3	C	111	GLN
3	C	262	GLN
4	D	19	GLN
4	D	34	ASN
4	D	48	ASN
4	D	66	ASN
4	D	76	ASN
4	D	129	GLN
5	E	30	GLN
5	E	65	ASN
5	E	107	GLN
5	E	129	GLN
5	E	168	ASN
7	G	93	ASN
7	G	139	GLN
8	H	131	ASN
8	H	133	HIS

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Mol	Chain	Res	Type
9	I	56	ASN
9	I	84	HIS
9	I	91	HIS
11	K	29	ASN
11	K	49	GLN
13	M	1352	GLN
16	Q	23	GLN
16	Q	38	HIS
16	Q	40	GLN
16	Q	105	ASN
16	Q	128	GLN
16	Q	151	GLN
16	Q	153	HIS
16	Q	161	ASN
16	Q	244	ASN
16	Q	268	ASN
16	Q	278	HIS
16	Q	294	HIS
16	Q	298	ASN
16	Q	305	GLN
16	Q	319	GLN
16	Q	349	GLN
16	Q	373	ASN
16	Q	407	GLN
16	Q	466	ASN
16	Q	527	HIS
16	Q	573	ASN
16	Q	585	GLN
16	Q	609	ASN
16	Q	616	HIS
16	Q	617	GLN
16	Q	706	ASN
16	Q	714	HIS
16	Q	781	ASN
16	Q	860	GLN
16	Q	877	GLN
16	Q	880	GLN
16	Q	887	ASN
17	R	416	GLN
17	R	432	ASN
17	R	484	ASN
17	R	585	ASN

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Mol	Chain	Res	Type
17	R	588	ASN
16	U	451	HIS
19	V	37	ASN
19	V	69	GLN
19	V	72	HIS
19	V	97	ASN
19	V	122	GLN
19	V	193	HIS
20	W	11	GLN
20	W	15	HIS
20	W	27	ASN
20	W	131	ASN
20	W	173	ASN
20	W	246	HIS
20	W	268	HIS
20	W	273	HIS
22	Y	27	GLN
22	Y	35	ASN
23	Z	232	GLN
23	Z	244	ASN
23	Z	272	ASN
23	Z	466	GLN
23	Z	519	GLN
23	Z	534	HIS
23	Z	595	HIS
23	Z	616	HIS
24	a	39	HIS
24	a	108	ASN
25	b	75	HIS
26	c	73	ASN
26	c	110	ASN
27	d	64	ASN
27	d	81	ASN
24	e	68	GLN
24	e	76	GLN
25	f	64	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	27/28 (96%)	14 (51%)	5 (18%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	13	A
15	P	14	C
15	P	15	C
15	P	16	G
15	P	21	G
15	P	22	G
15	P	24	A
15	P	32	C
15	P	33	A
15	P	34	A
15	P	35	A
15	P	36	A
15	P	37	A
15	P	38	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	13	A
15	P	21	G
15	P	23	G
15	P	34	A
15	P	36	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	TPO	Z	775	23	8,10,11	1.60	1 (12%)	10,14,16	2.21	1 (10%)
1	SEP	A	1547	1	8,9,10	1.55	1 (12%)	7,12,14	1.12	1 (14%)
1	TPO	A	1525	1	8,10,11	1.66	1 (12%)	10,14,16	2.02	1 (10%)

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
23	TPO	Z	775	23	-	1/9/11/13	-
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	4/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	P-O1P	3.57	1.61	1.50
23	Z	775	TPO	P-O1P	3.50	1.61	1.50
1	A	1547	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	775	TPO	P-OG1-CB	-6.55	105.53	123.33
1	A	1525	TPO	P-OG1-CB	-5.57	108.20	123.33
1	A	1547	SEP	OG-CB-CA	2.03	110.12	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	12
2	B	3
14	N	1
16	U	1
19	V	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	1287:MET	C	1327:ILE	N	37.43
1	N	-52:DC	O3'	-40:DG	P	31.66
1	M	477:LYS	C	538:LYS	N	28.32
1	U	497:ASP	C	505:SER	N	25.85
1	M	430:ALA	C	440:ILE	N	16.17
1	M	763:GLN	C	775:GLN	N	13.29
1	V	299:GLU	C	310:ASN	N	12.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	1384:ARG	C	1396:ALA	N	11.29
1	M	815:THR	C	824:GLU	N	6.79
1	M	1334:ASN	C	1338:ILE	N	5.28
1	M	332:LEU	C	349:SER	N	4.97
1	M	572:ASP	C	580:THR	N	4.78
1	M	1039:THR	C	1051:GLU	N	4.71
1	M	932:SER	C	935:GLU	N	4.39
1	M	675:GLY	C	684:THR	N	3.73
1	B	755:GLN	C	756:LYS	N	1.18
1	B	108:MET	C	109:MET	N	1.17
1	A	999:ARG	C	1000:LEU	N	1.15
1	B	94:SER	C	95:LYS	N	1.07

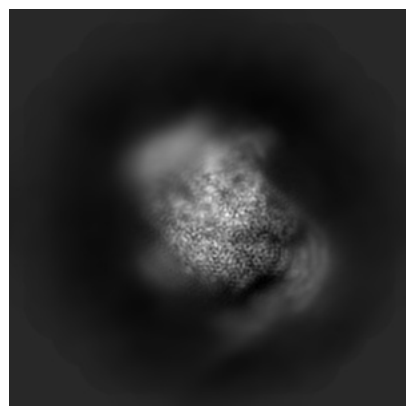
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15127. These allow visual inspection of the internal detail of the map and identification of artifacts.

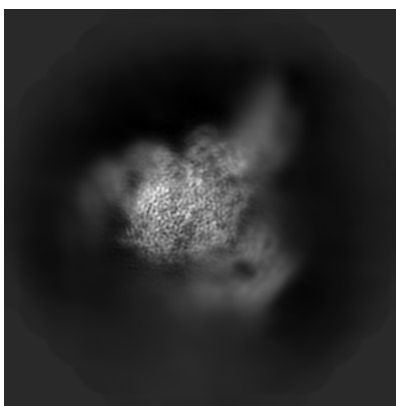
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

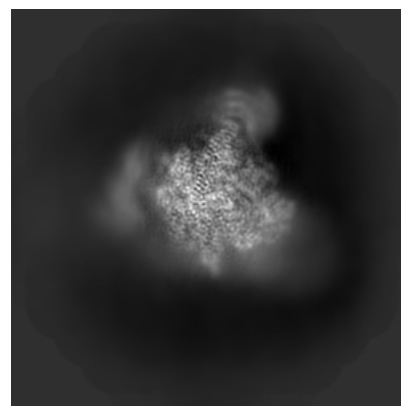
6.1.1 Primary map



X

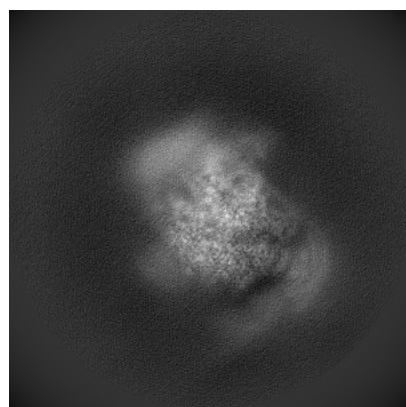


Y

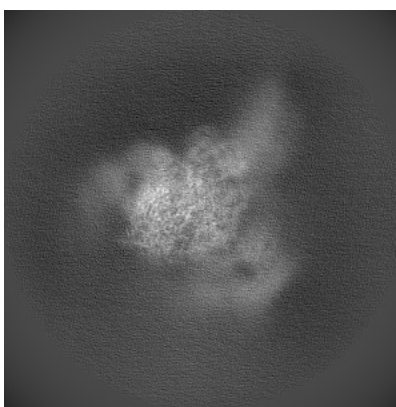


Z

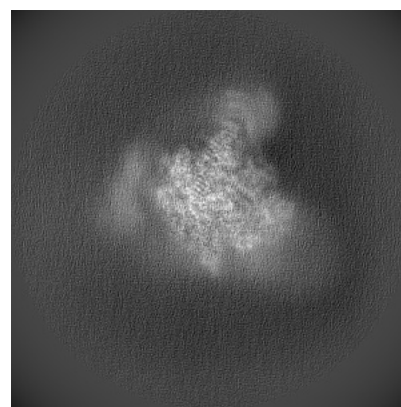
6.1.2 Raw map



X



Y

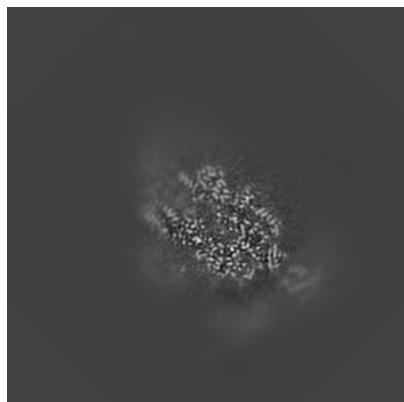


Z

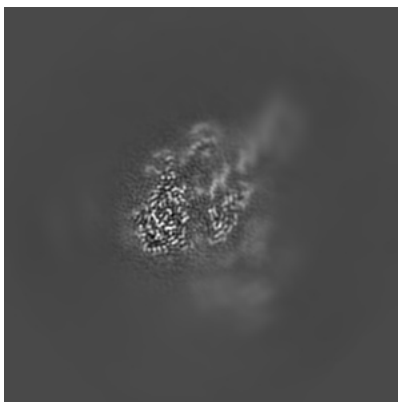
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

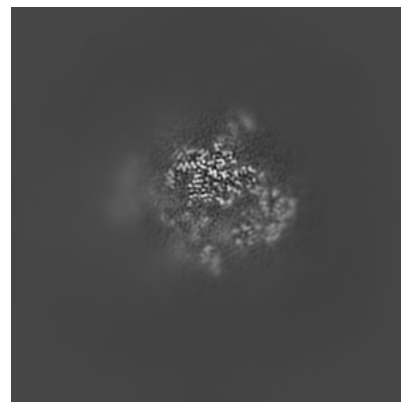
6.2.1 Primary map



X Index: 180

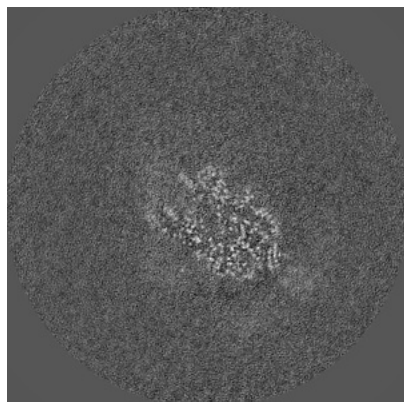


Y Index: 180

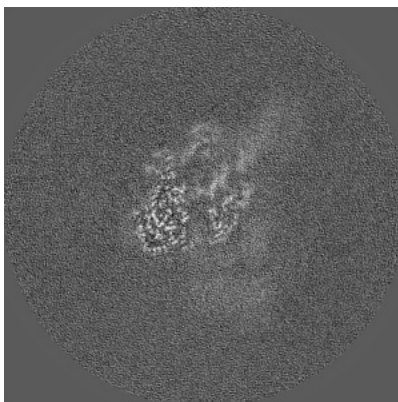


Z Index: 180

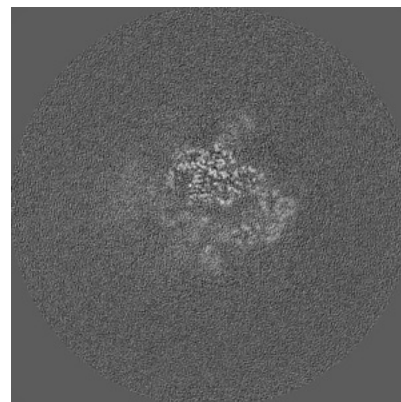
6.2.2 Raw map



X Index: 180



Y Index: 180

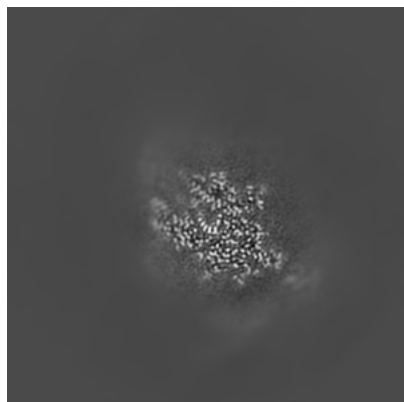


Z Index: 180

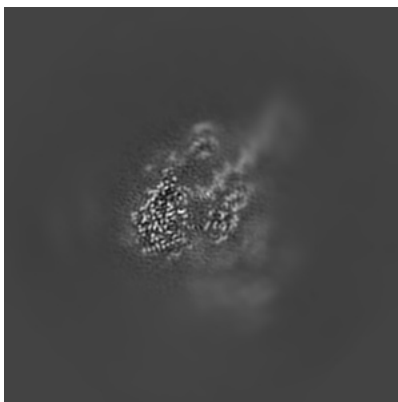
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

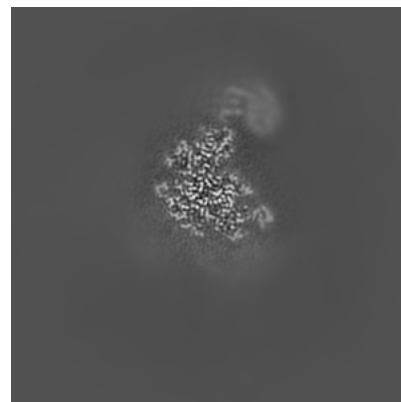
6.3.1 Primary map



X Index: 175

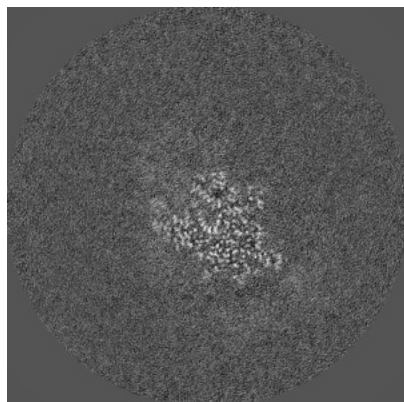


Y Index: 182

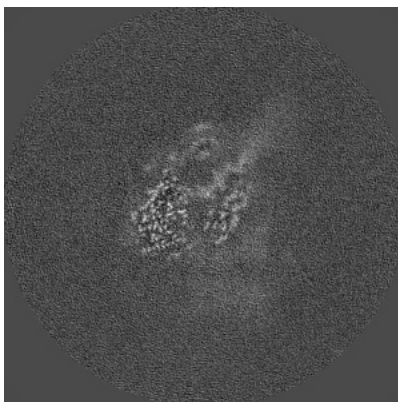


Z Index: 138

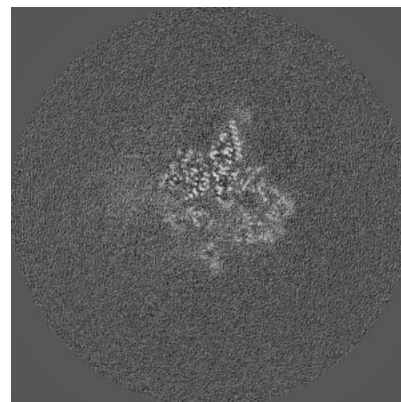
6.3.2 Raw map



X Index: 175



Y Index: 182

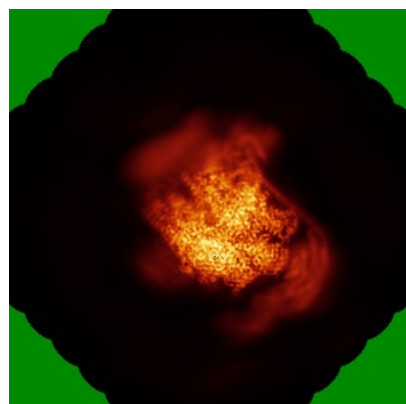


Z Index: 175

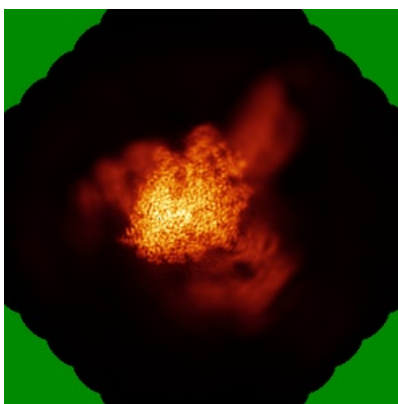
The images above show the largest variance slices of the map in three orthogonal directions.

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

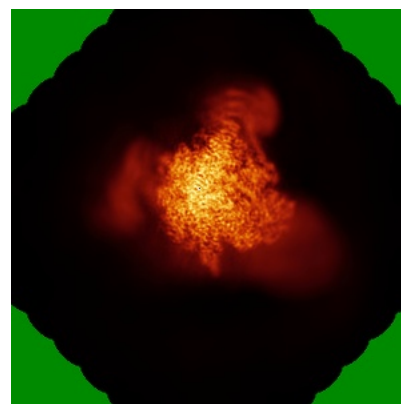
6.4.1 Primary map



X

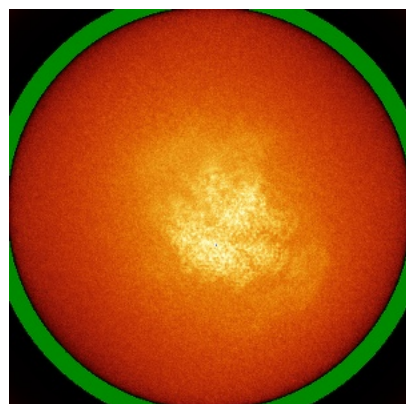


Y

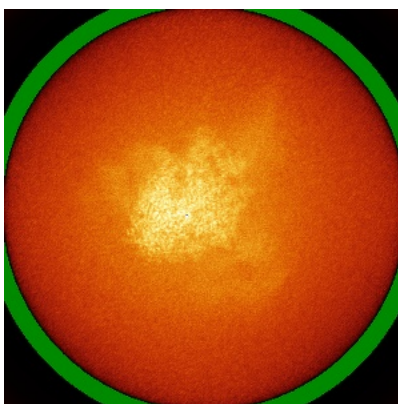


Z

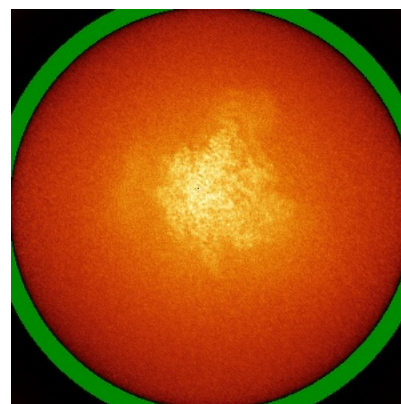
6.4.2 Raw map



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.

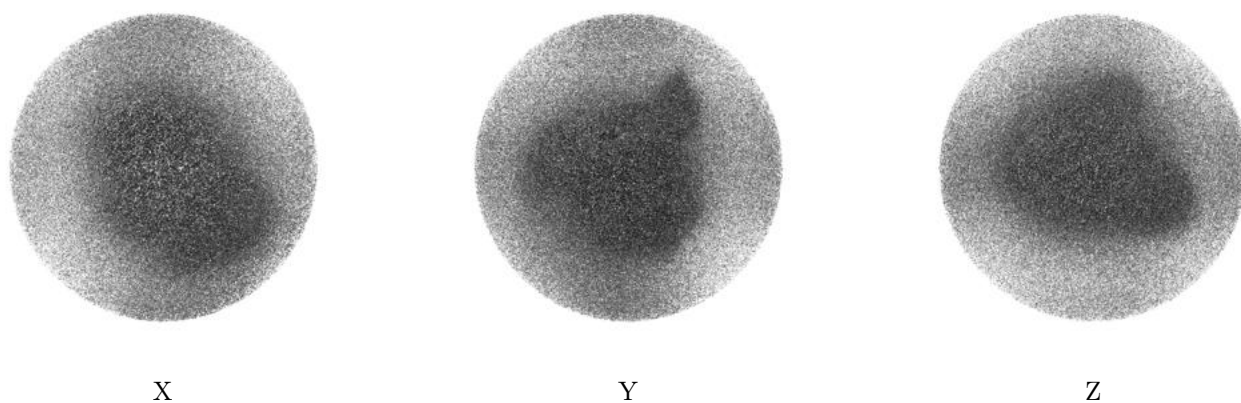
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

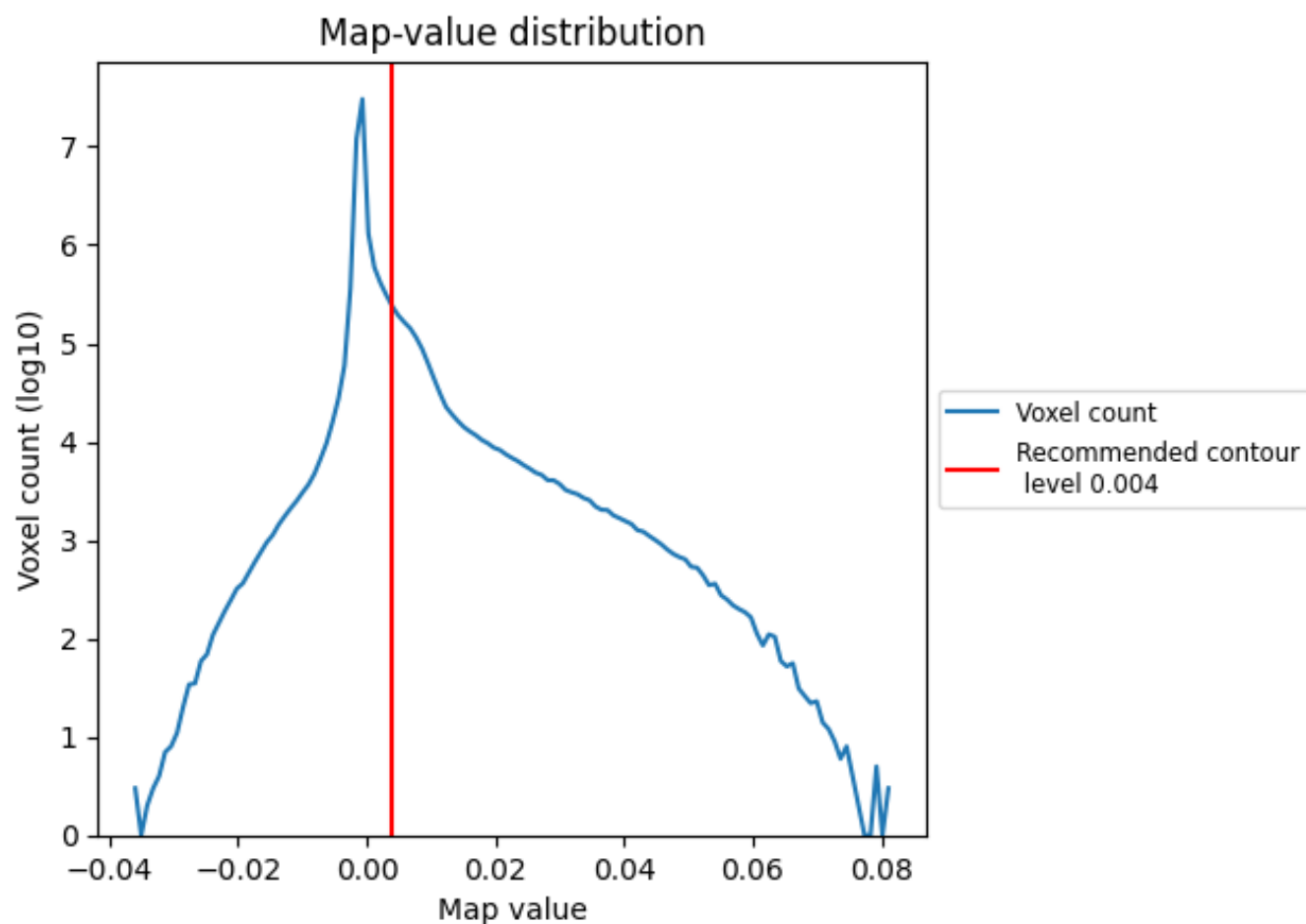
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

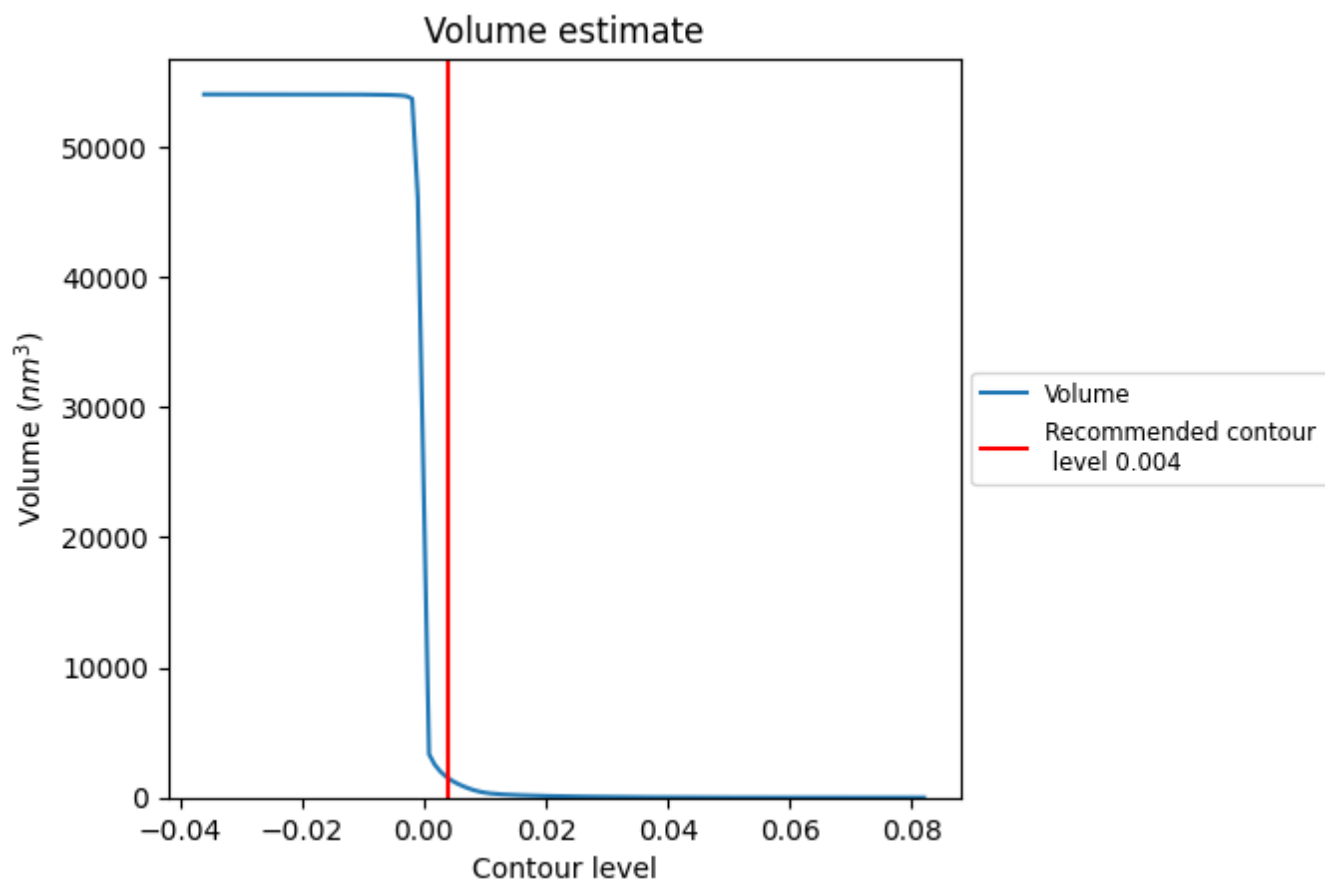
This section contains the results of statistical analysis of the map.

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.

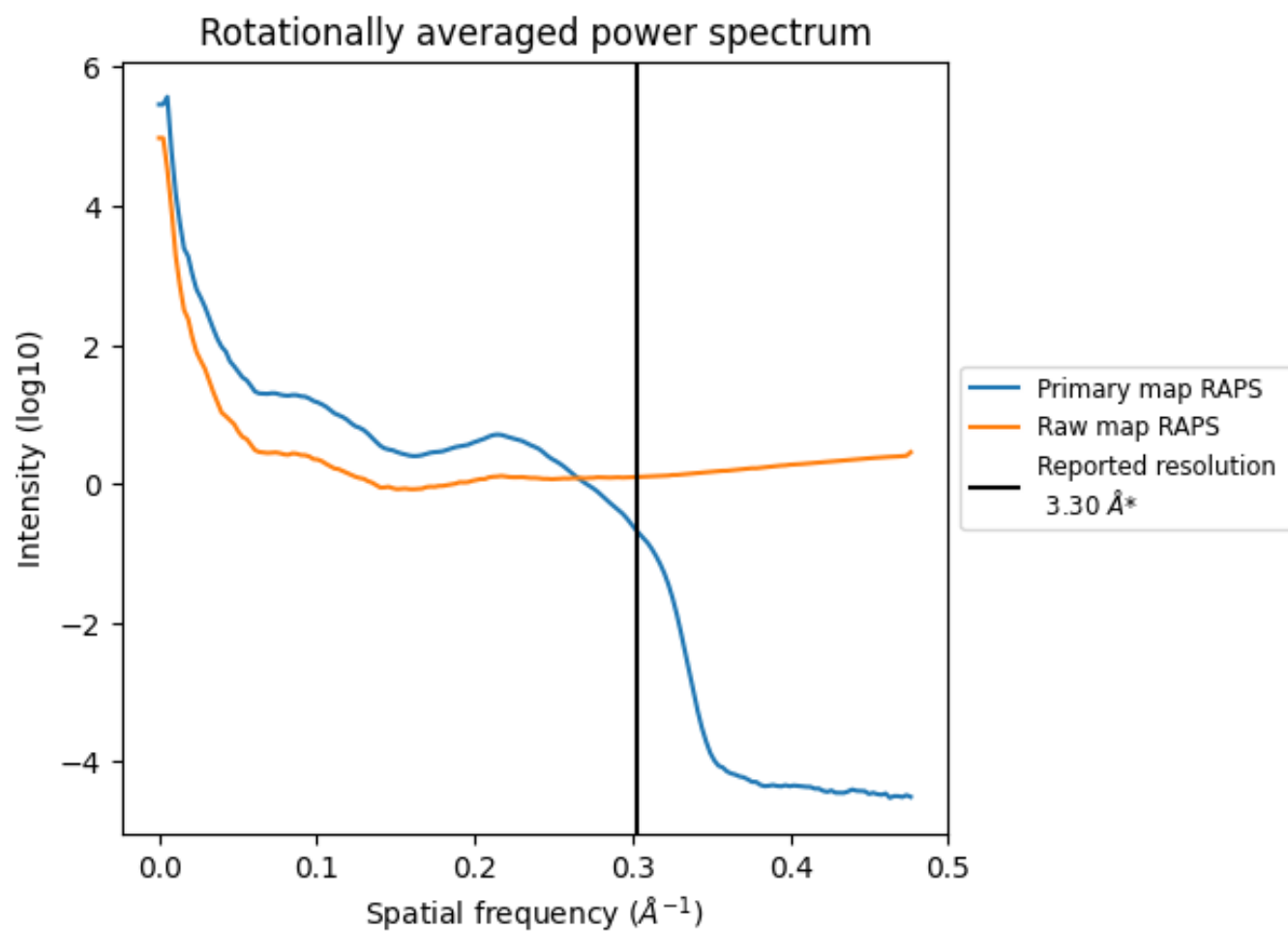
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1502 nm^3 ; this corresponds to an approximate mass of 1357 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

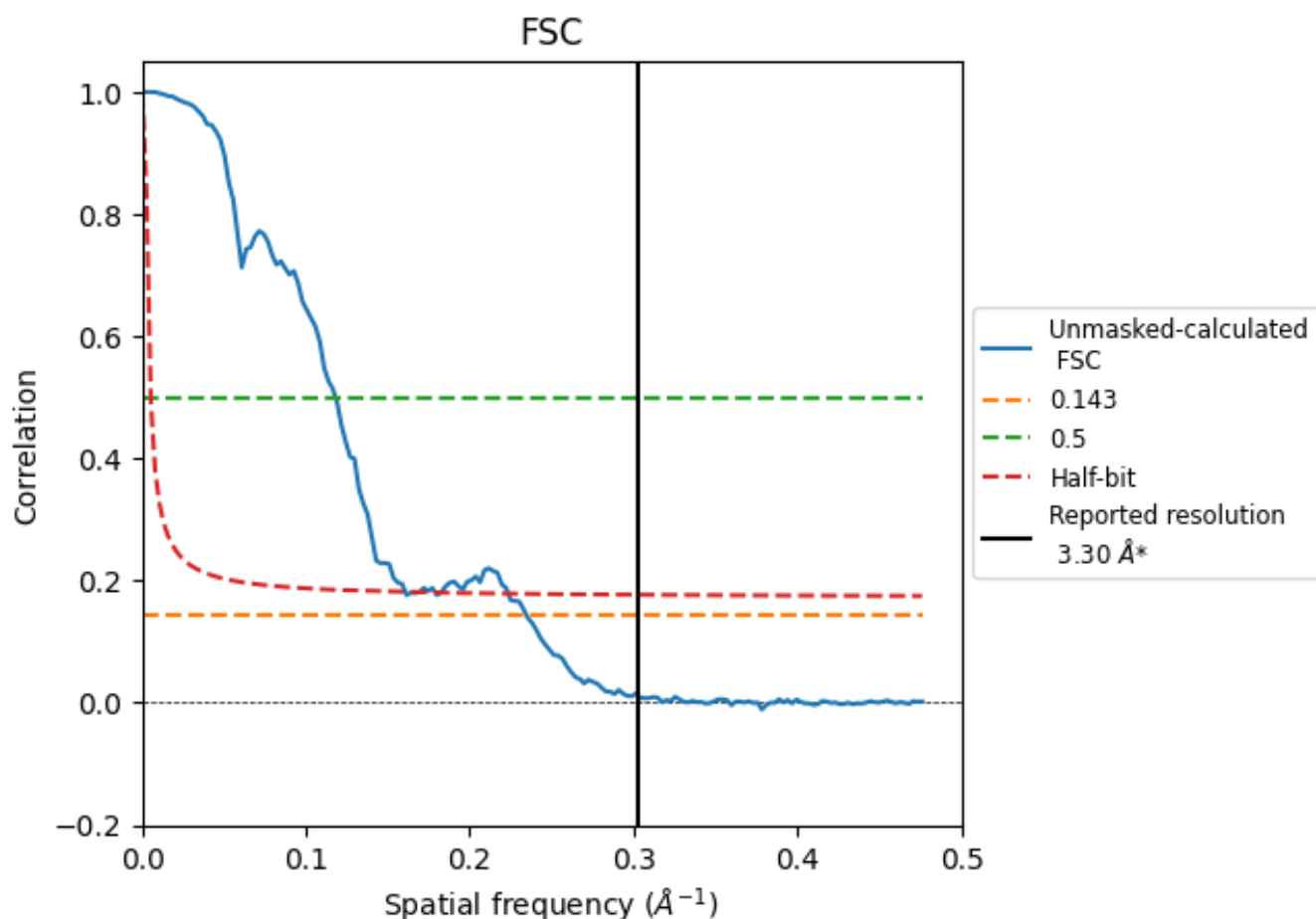


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

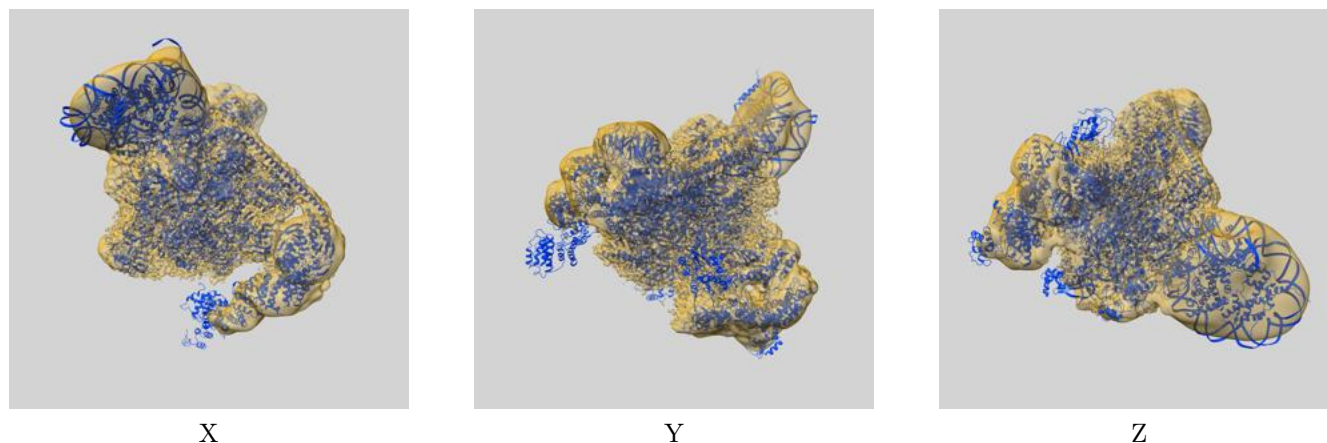
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	8.47	6.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

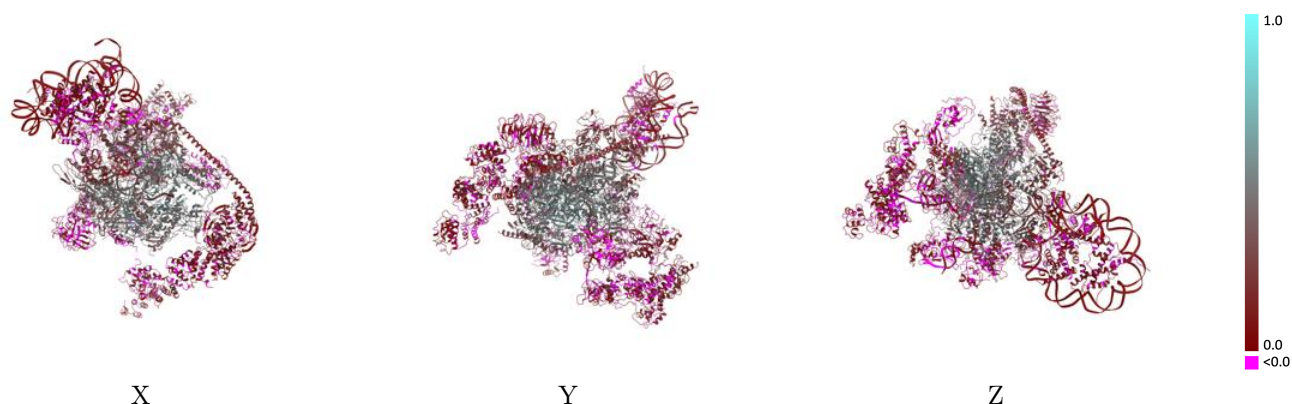
This section contains information regarding the fit between EMDB map EMD-15127 and PDB model 8A3Y. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



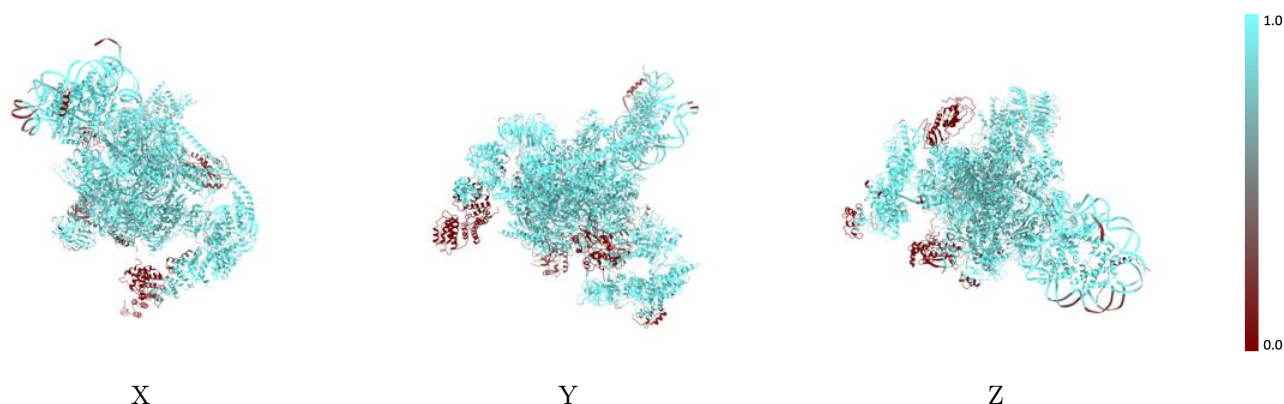
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



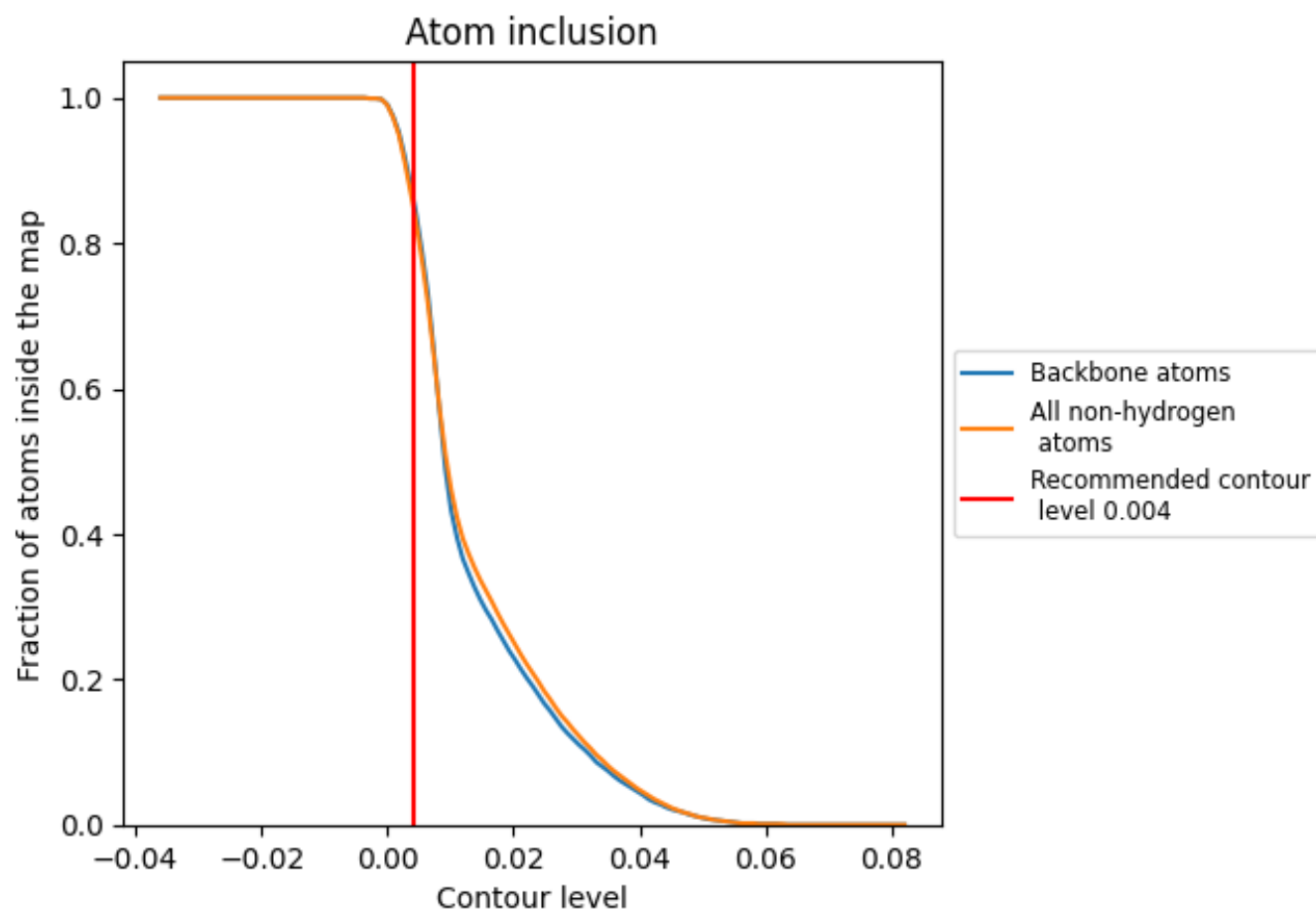
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.2310
A	 0.9610	 0.4150
B	 0.9810	 0.4340
C	 0.9720	 0.4110
D	 0.9750	 0.1460
E	 0.9850	 0.3490
F	 0.9750	 0.4570
G	 0.9780	 0.2040
H	 0.9540	 0.4170
I	 0.9730	 0.2390
J	 0.9790	 0.4590
K	 0.9470	 0.4140
L	 0.9790	 0.3900
M	 0.6510	 0.0520
N	 0.8830	 0.1140
P	 0.9840	 0.2390
Q	 0.6500	 0.1010
R	 0.2380	 0.0400
T	 0.8720	 0.1360
U	 0.8490	 0.0610
V	 0.6360	 0.0580
W	 0.9410	 0.0870
X	 0.9740	 0.1480
Y	 0.8040	 0.0610
Z	 0.7260	 0.0840
a	 0.7730	 0.0370
b	 0.9130	 0.0720
c	 1.0000	 0.0690
d	 0.9900	 0.0620
e	 0.9880	 0.0240
f	 0.9980	 0.0480

