



## Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 06:33 PM EDT

PDB ID : 5IYC  
EMDB ID : EMD-8137  
Title : Human core-PIC in the initial transcribing state  
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.  
Deposited on : 2016-03-24  
Resolution : 3.90 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

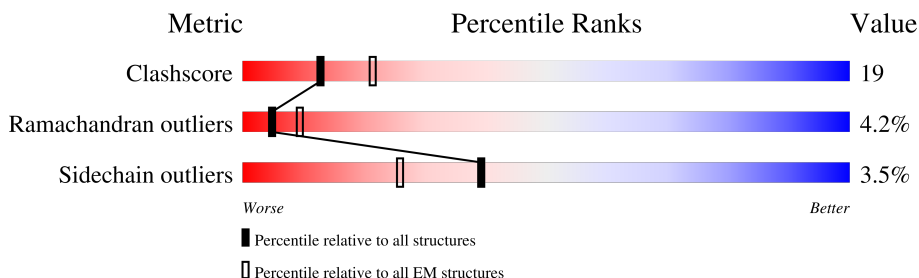
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	80	
23	Y	80	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 47927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1454	Total	C	N	O	S	0	0
			11515	7234	2058	2150	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1165	Total	C	N	O	S	0	0
			9317	5878	1637	1738	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2213	1386	380	440	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			689	437	120	127	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	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	80	Total	C	N	O	P	0	0
			1645	785	292	489	79		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	80	Total	C	N	O	P	0	0
			1624	771	291	483	79		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Mg	0
			2	2	

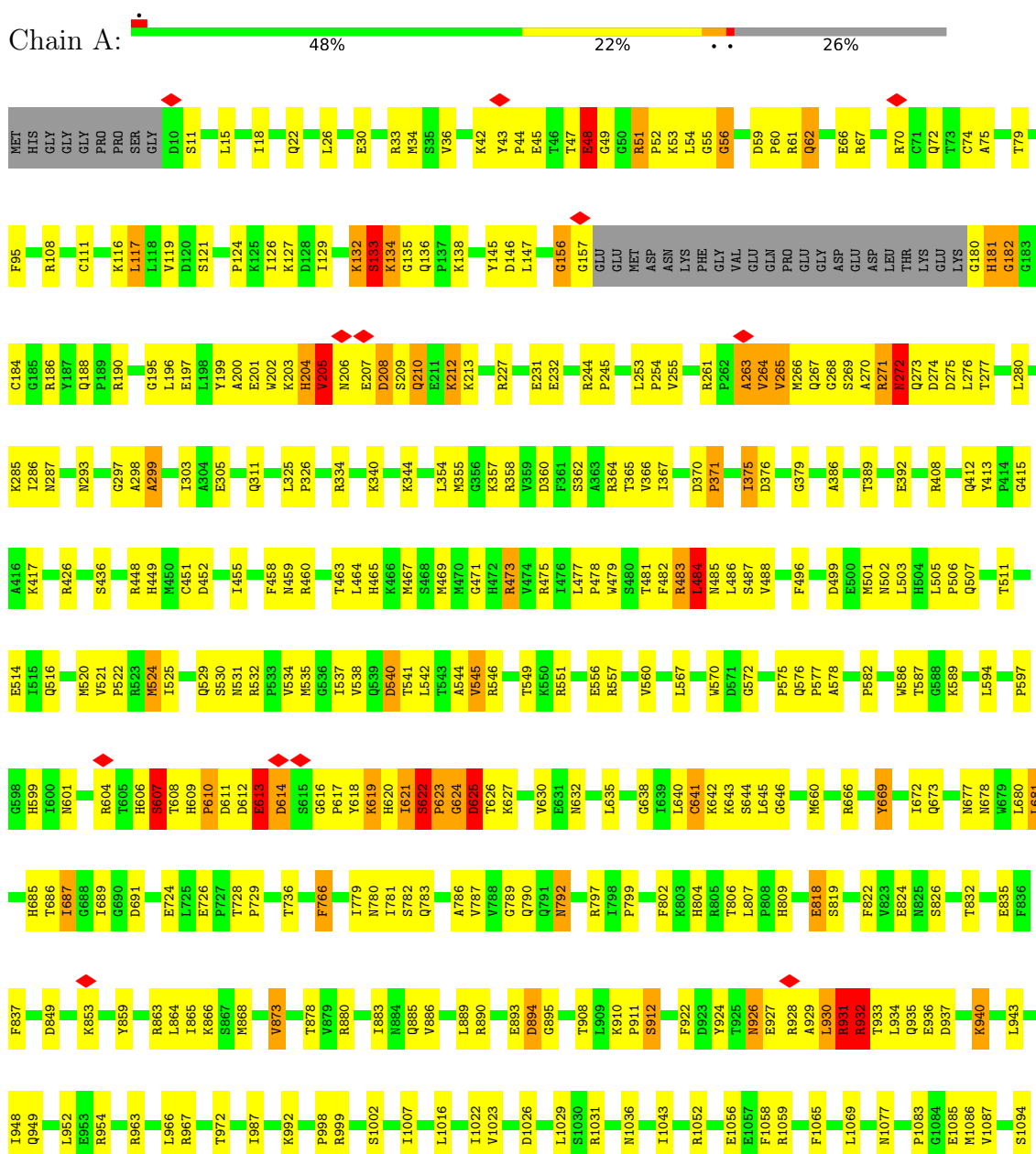
- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

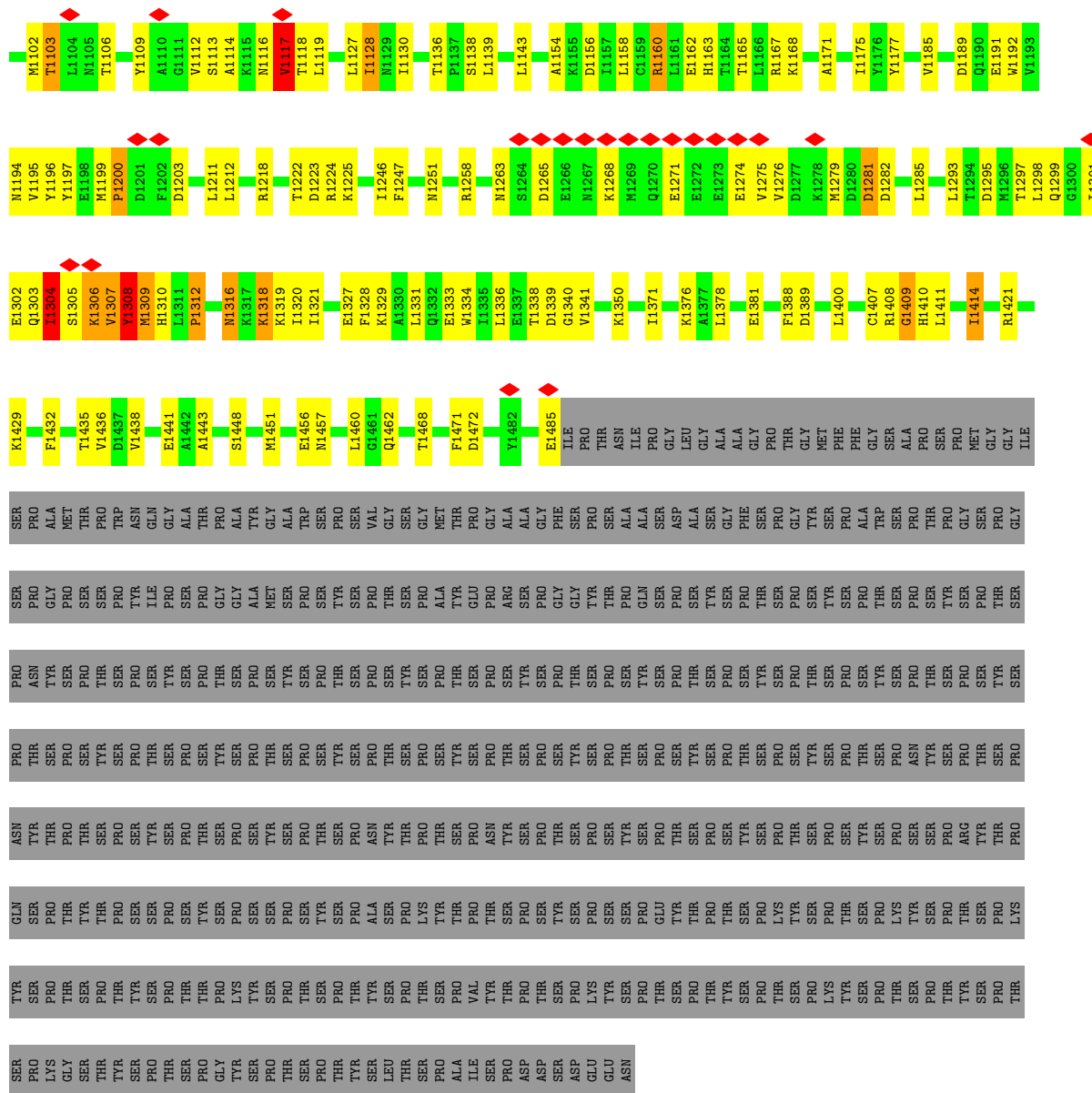
Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	M	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	
25	U	1	Total	Zn	0
			1	1	

### 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.

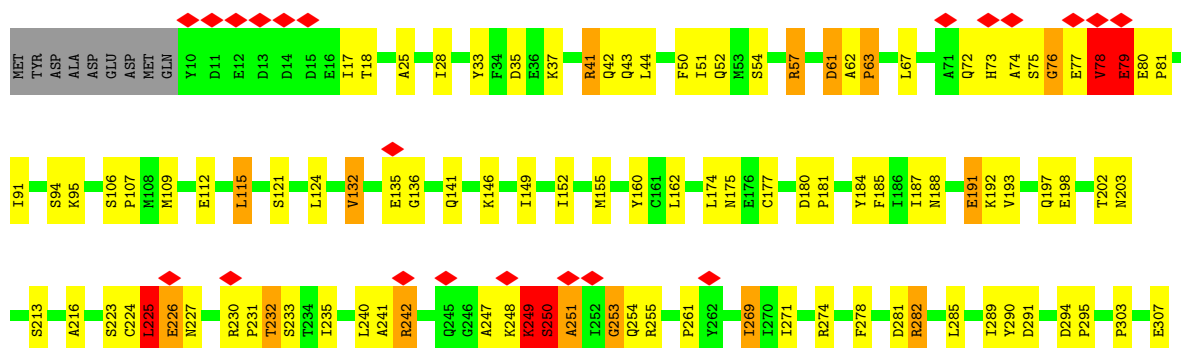
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



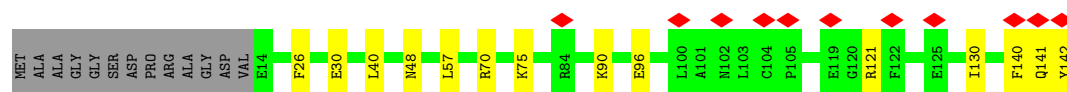


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

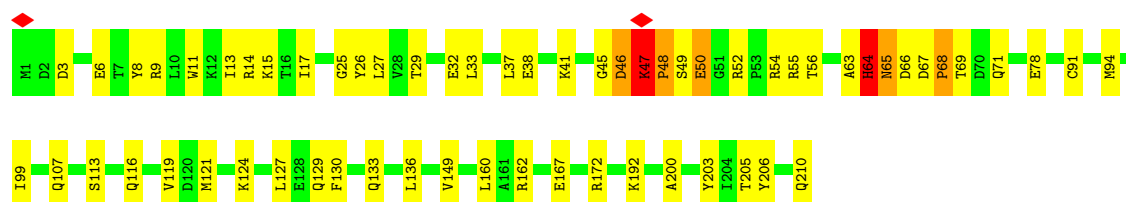
Chain B: 63% 30% 5% ..



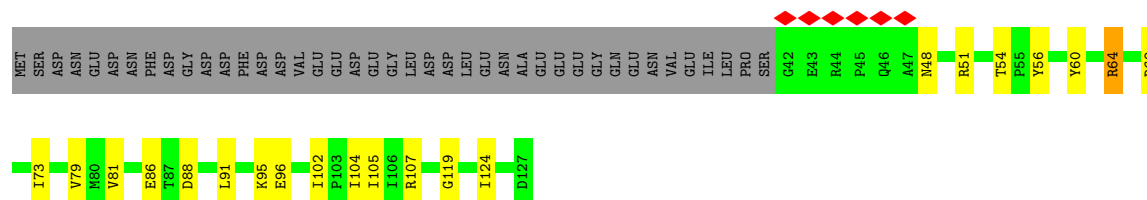




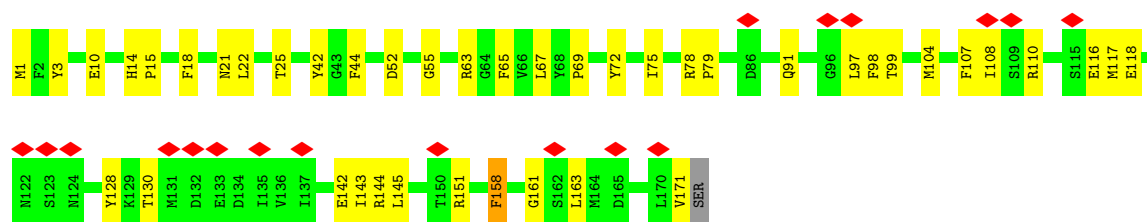
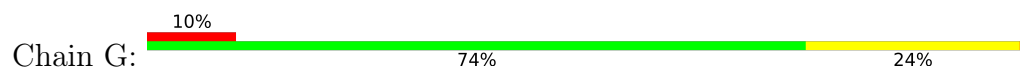
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



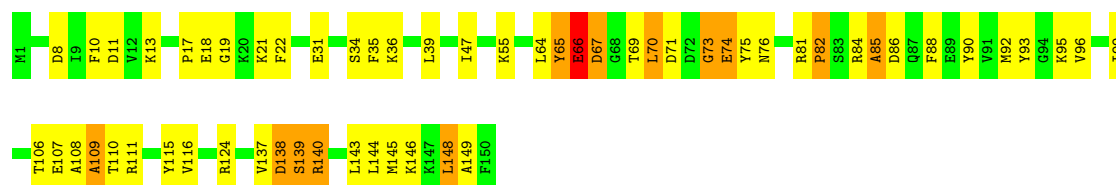
- Molecule 6: DNA-directed RNA polymerase II subunit RPB6



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

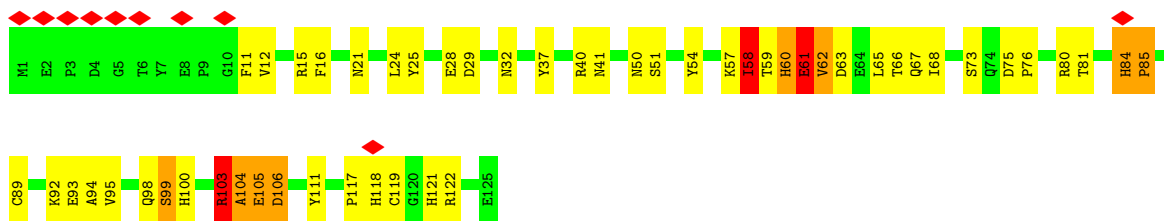


- Molecule 8: DNA-directed RNA polymerase II subunit RPB8



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

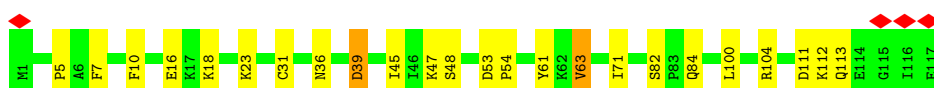
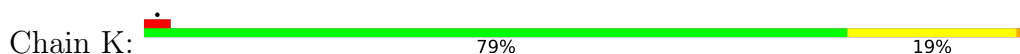




- Molecule 10: DNA-directed RNA polymerase II subunit RPB10



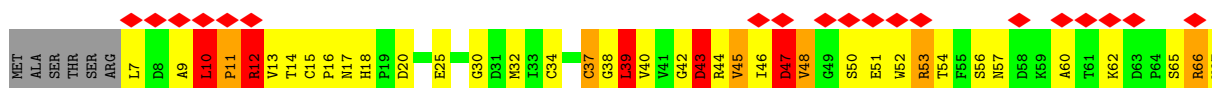
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 12: DNA-directed RNA polymerase II subunit RPB12



- Molecule 13: Transcription initiation factor IIB



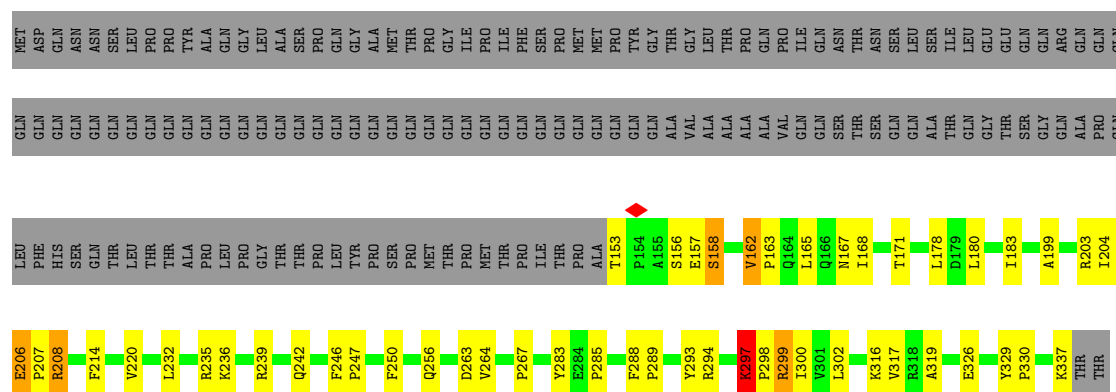
- Molecule 14: Transcription initiation factor IIA subunit 1



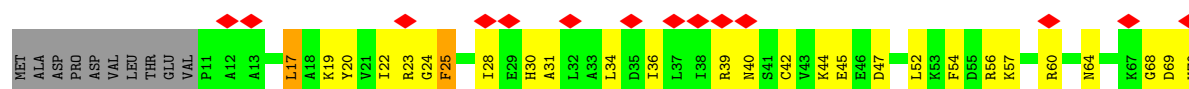
- Molecule 15: Transcription initiation factor IIA subunit 2

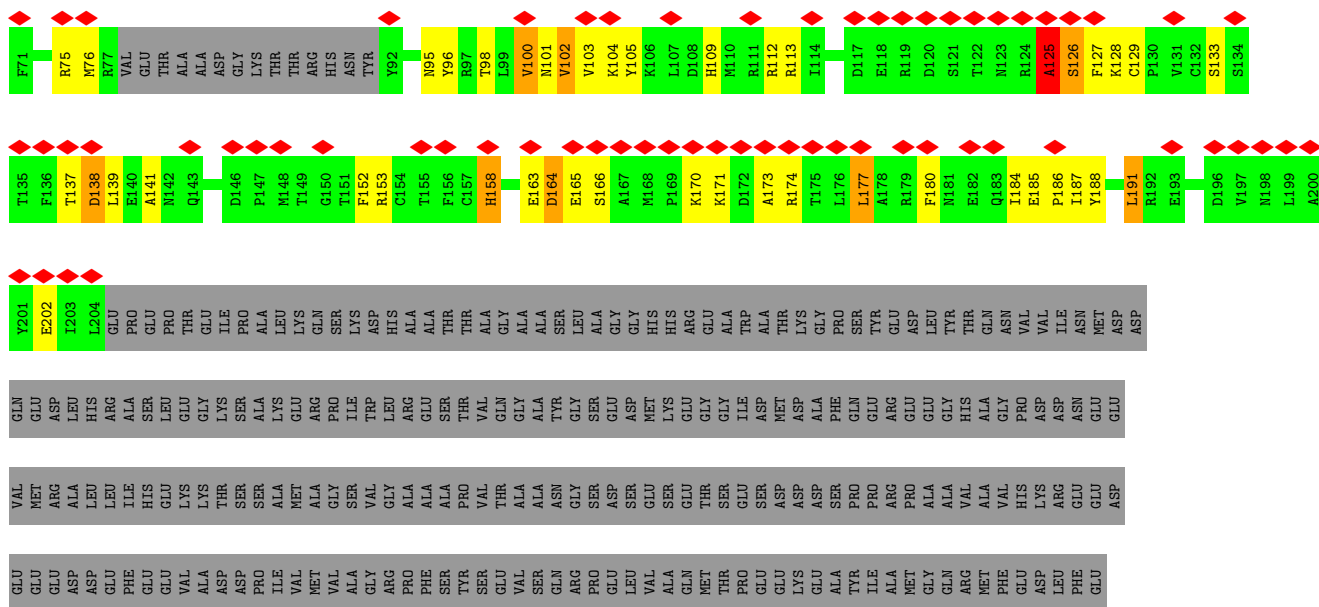


- Molecule 16: TATA-box-binding protein

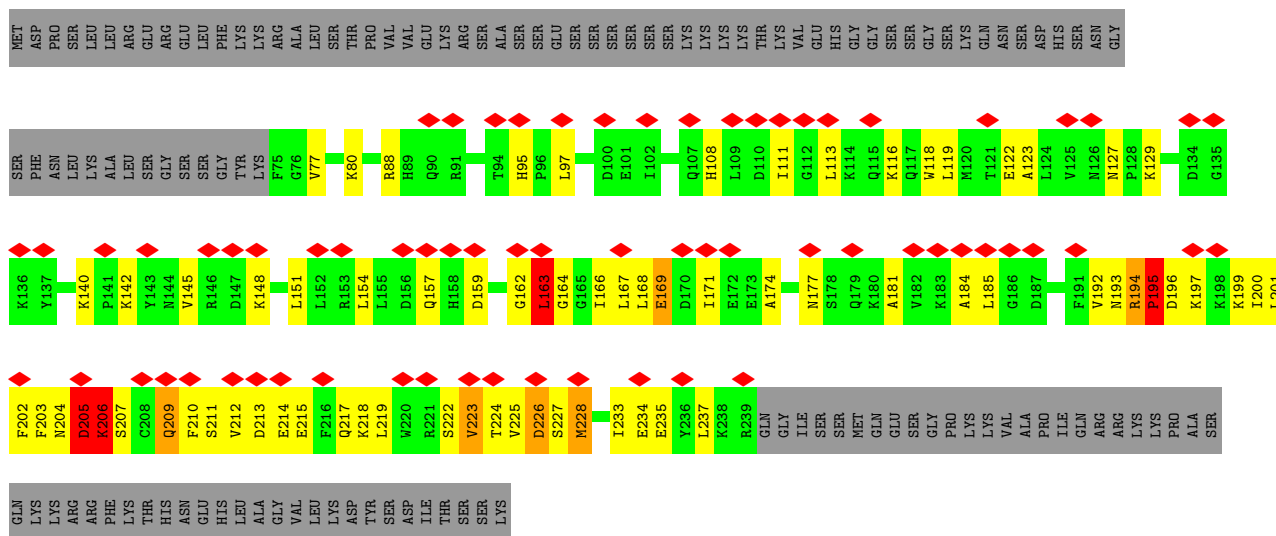
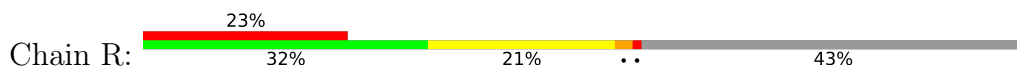


- Molecule 17: General transcription factor IIE subunit 1

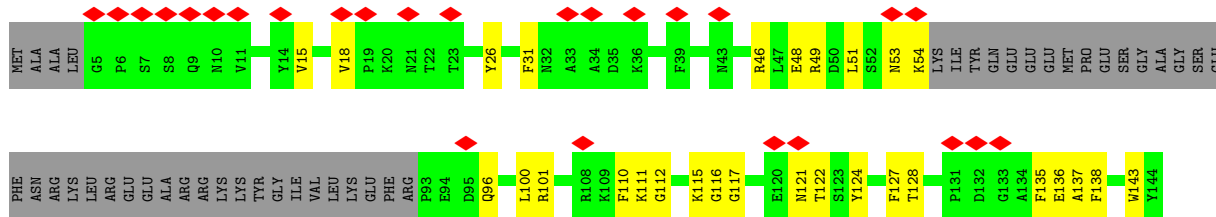


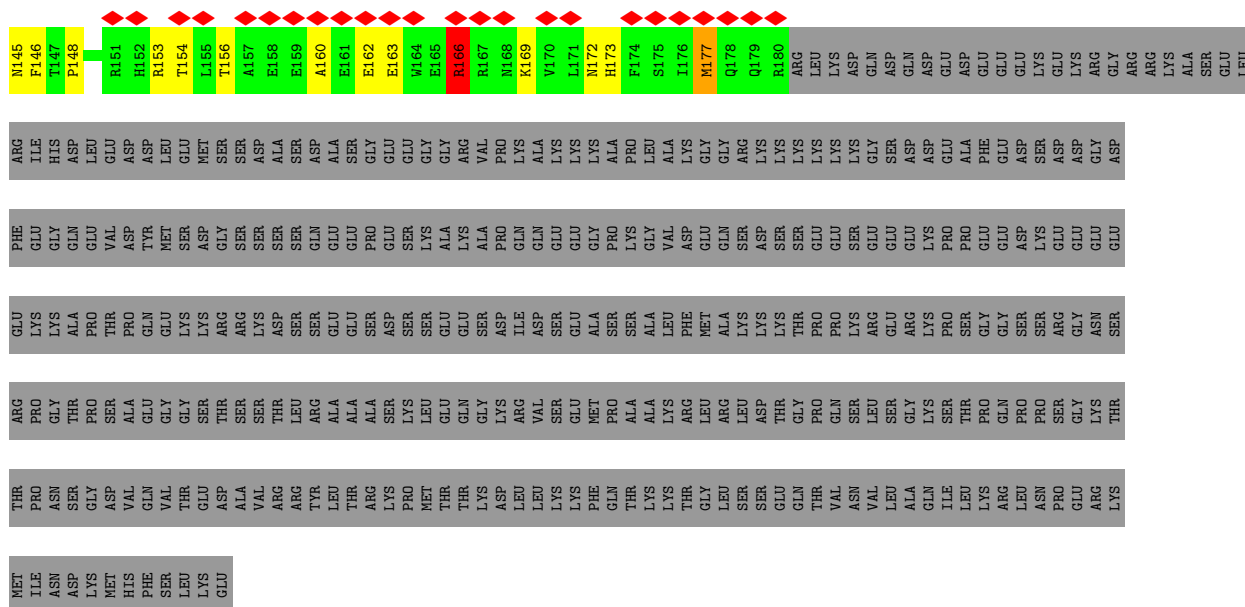


- Molecule 18: Transcription initiation factor IIE subunit beta

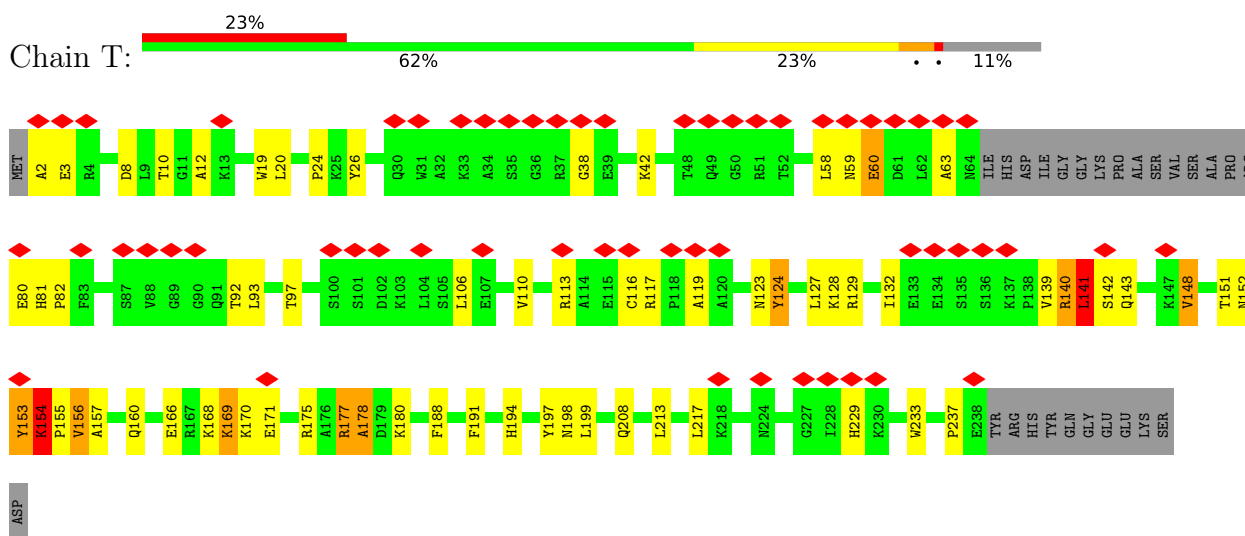


- Molecule 19: General transcription factor IIF subunit 1

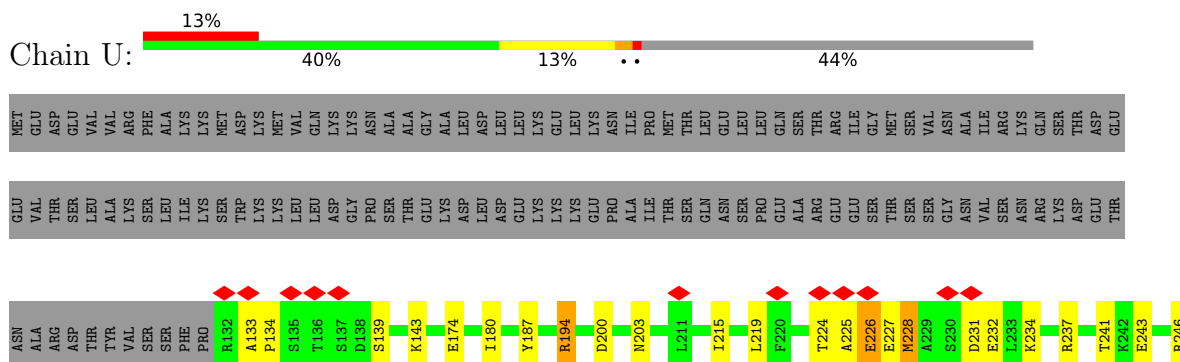


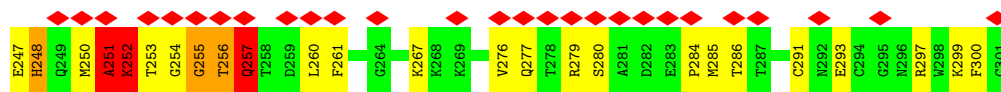


- Molecule 20: General transcription factor IIF subunit 2

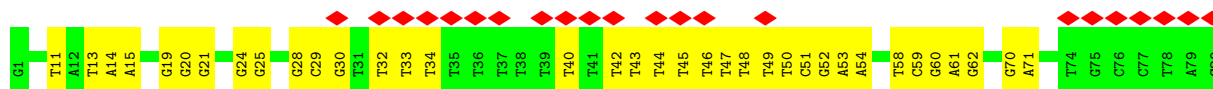


- Molecule 21: Transcription elongation factor A protein 1

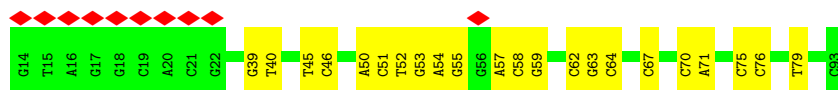
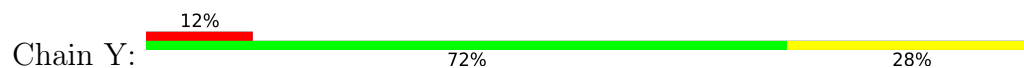




• Molecule 22: SCP-X



• Molecule 23: SCP-Y



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90590	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.62	4/11727 (0.0%)	0.84	24/15833 (0.2%)
2	B	0.75	9/9503 (0.1%)	0.92	27/12831 (0.2%)
3	C	0.60	0/2259	0.85	6/3073 (0.2%)
4	D	0.24	0/1077	0.44	0/1446
5	E	0.46	0/1753	0.71	0/2368
6	F	0.64	0/700	0.78	0/946
7	G	0.29	0/1382	0.53	0/1874
8	H	0.44	0/1227	0.76	3/1654 (0.2%)
9	I	0.37	0/1038	1.08	5/1407 (0.4%)
10	J	0.75	0/542	0.96	2/730 (0.3%)
11	K	0.49	0/956	0.64	0/1294
12	L	0.53	0/394	0.70	0/524
13	M	0.40	0/2429	0.86	11/3281 (0.3%)
14	N	0.26	0/945	0.68	3/1274 (0.2%)
15	O	0.24	0/816	0.49	0/1105
16	P	0.29	0/1489	0.54	1/2005 (0.0%)
17	Q	0.30	0/1507	0.62	1/2023 (0.0%)
18	R	0.51	0/1380	1.04	5/1854 (0.3%)
19	S	0.25	0/1167	0.54	1/1576 (0.1%)
20	T	0.37	2/1817 (0.1%)	0.70	2/2445 (0.1%)
21	U	0.28	0/1358	0.64	3/1820 (0.2%)
22	X	0.66	0/1843	1.01	0/2847
23	Y	0.60	0/1817	0.95	0/2800
All	All	0.56	15/49126 (0.0%)	0.82	94/67010 (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
7	G	0	1
13	M	0	1
14	N	0	2
16	P	0	1
17	Q	0	1
18	R	0	1
19	S	0	1
20	T	0	2
All	All	0	15

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	60	GLU	CD-OE1	7.39	1.33	1.25
2	B	191	GLU	CG-CD	6.38	1.61	1.51
20	T	60	GLU	CD-OE2	5.92	1.32	1.25
2	B	1048	TYR	CD2-CE2	-5.68	1.30	1.39
2	B	1047	TYR	CD1-CE1	-5.66	1.30	1.39
2	B	919	CYS	CB-SG	-5.65	1.72	1.81
2	B	959	GLU	CB-CG	5.43	1.62	1.52
1	A	669	TYR	CE2-CZ	-5.40	1.31	1.38
2	B	924	ARG	CZ-NH1	5.33	1.40	1.33
2	B	927	ARG	CB-CG	-5.24	1.38	1.52
2	B	984	CYS	CB-SG	-5.16	1.73	1.81
2	B	1048	TYR	CD1-CE1	-5.12	1.31	1.39
1	A	556	GLU	CG-CD	5.06	1.59	1.51
1	A	669	TYR	CD2-CE2	-5.04	1.31	1.39
1	A	458	PHE	CB-CG	-5.00	1.42	1.51

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-28.89	57.05	120.60
18	R	194	ARG	C-N-CD	-24.66	66.35	120.60
13	M	10	LEU	C-N-CD	-22.77	70.51	120.60
3	C	6	GLN	C-N-CD	-20.32	75.89	120.60
1	A	483	ARG	NE-CZ-NH1	11.54	126.07	120.30
9	I	103	ARG	N-CA-C	-11.08	81.08	111.00
2	B	924	ARG	NE-CZ-NH1	-11.01	114.80	120.30
13	M	42	GLY	N-CA-C	9.63	137.18	113.10
13	M	39	LEU	N-CA-C	9.08	135.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	526	LEU	CB-CG-CD1	-8.86	95.94	111.00
1	A	622	SER	C-N-CD	-8.83	101.17	120.60
8	H	74	GLU	N-CA-C	-8.57	87.87	111.00
1	A	503	LEU	CA-CB-CG	8.56	134.98	115.30
17	Q	102	VAL	N-CA-C	-8.41	88.29	111.00
21	U	255	GLY	N-CA-C	8.17	133.52	113.10
18	R	195	PRO	N-CA-C	-8.07	91.11	112.10
13	M	94	ASP	N-CA-C	-8.03	89.32	111.00
1	A	483	ARG	NH1-CZ-NH2	-7.97	110.63	119.40
13	M	91	ALA	N-CA-C	-7.90	89.66	111.00
10	J	65	LEU	N-CA-C	-7.88	89.71	111.00
2	B	249	LYS	N-CA-C	-7.84	89.82	111.00
2	B	882	SER	N-CA-C	-7.76	90.04	111.00
2	B	945	CYS	CA-CB-SG	7.61	127.69	114.00
9	I	61	GLU	N-CA-C	-7.44	90.91	111.00
1	A	360	ASP	CB-CG-OD1	-7.32	111.71	118.30
2	B	747	LEU	CA-CB-CG	-7.32	98.47	115.30
1	A	681	LEU	CB-CG-CD2	-7.28	98.63	111.00
2	B	927	ARG	NE-CZ-NH1	7.17	123.88	120.30
8	H	73	GLY	N-CA-C	7.14	130.94	113.10
13	M	89	GLY	N-CA-C	-7.14	95.26	113.10
1	A	271	ARG	N-CA-C	-7.06	91.95	111.00
3	C	211	LEU	N-CA-C	-7.04	92.00	111.00
2	B	483	ARG	NE-CZ-NH1	6.90	123.75	120.30
3	C	137	ASN	N-CA-C	-6.84	92.54	111.00
13	M	37	CYS	C-N-CA	-6.83	107.95	122.30
18	R	169	GLU	OE1-CD-OE2	-6.64	115.33	123.30
9	I	58	ILE	N-CA-C	-6.60	93.19	111.00
1	A	483	ARG	N-CA-C	-6.59	93.21	111.00
2	B	79	GLU	C-N-CA	-6.56	105.31	121.70
18	R	163	LEU	N-CA-C	6.51	128.58	111.00
13	M	38	GLY	N-CA-C	-6.50	96.86	113.10
3	C	68	LEU	CB-CG-CD1	-6.39	100.13	111.00
2	B	1043	ILE	CG1-CB-CG2	-6.39	97.34	111.40
2	B	115	LEU	CB-CG-CD2	-6.36	100.20	111.00
20	T	141	LEU	N-CA-C	-6.35	93.85	111.00
1	A	484	LEU	CB-CG-CD1	6.34	121.78	111.00
1	A	205	VAL	N-CA-C	6.32	128.07	111.00
2	B	924	ARG	NH1-CZ-NH2	6.30	126.33	119.40
2	B	922	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	B	730	LYS	CD-CE-NZ	6.20	125.95	111.70
3	C	35	ARG	CG-CD-NE	-6.19	98.79	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	231	ASP	N-CA-C	-6.19	94.28	111.00
14	N	356	GLY	N-CA-C	6.15	128.48	113.10
13	M	43	ASP	N-CA-C	-6.06	94.64	111.00
2	B	880	LEU	N-CA-C	6.05	127.35	111.00
1	A	1160	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	483	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	A	1117	VAL	N-CA-C	-5.88	95.12	111.00
1	A	133	SER	N-CA-C	5.87	126.85	111.00
3	C	49	TRP	CA-CB-CG	5.84	124.79	113.70
2	B	704	LEU	CB-CG-CD1	-5.82	101.11	111.00
2	B	1050	ARG	NE-CZ-NH2	5.81	123.20	120.30
18	R	205	ASP	N-CA-C	5.81	126.68	111.00
1	A	182	GLY	N-CA-C	5.78	127.55	113.10
10	J	46	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	540	ASP	CB-CG-OD2	-5.68	113.18	118.30
2	B	1054	MET	CB-CG-SD	5.65	129.35	112.40
1	A	1378	LEU	CB-CG-CD1	-5.63	101.43	111.00
14	N	325	GLY	N-CA-C	5.55	126.98	113.10
1	A	484	LEU	CB-CG-CD2	-5.48	101.68	111.00
2	B	77	GLU	N-CA-C	5.42	125.63	111.00
21	U	251	ALA	N-CA-C	-5.40	96.42	111.00
2	B	162	LEU	CB-CG-CD1	-5.37	101.87	111.00
2	B	529	MET	CB-CG-SD	5.35	128.46	112.40
13	M	87	GLY	C-N-CA	-5.35	108.33	121.70
2	B	44	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	A	473	ARG	CG-CD-NE	-5.32	100.62	111.80
1	A	546	ARG	NE-CZ-NH2	5.31	122.96	120.30
2	B	964	ASP	CB-CG-OD1	-5.31	113.52	118.30
13	M	87	GLY	N-CA-C	5.25	126.23	113.10
20	T	154	LYS	N-CA-C	5.24	125.14	111.00
2	B	162	LEU	CA-CB-CG	5.20	127.26	115.30
2	B	758	LEU	CA-CB-CG	-5.19	103.37	115.30
16	P	232	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	567	LEU	CA-CB-CG	5.17	127.19	115.30
8	H	85	ALA	N-CA-C	-5.14	97.11	111.00
1	A	502	ASN	N-CA-CB	-5.14	101.35	110.60
14	N	326	GLN	N-CA-C	5.14	124.87	111.00
2	B	974	SER	N-CA-CB	-5.11	102.84	110.50
19	S	166	ARG	NE-CZ-NH1	5.10	122.85	120.30
9	I	84	HIS	N-CA-C	5.06	124.66	111.00
1	A	375	ILE	CG1-CB-CG2	-5.02	100.36	111.40
1	A	641	CYS	CA-CB-SG	-5.02	104.97	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	981	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1086	MET	Peptide
1	A	1308	TYR	Peptide
2	B	416	ARG	Sidechain
2	B	525	ASN	Peptide
2	B	873	LEU	Mainchain
7	G	151	ARG	Sidechain
13	M	45	VAL	Mainchain
14	N	355	ASP	Peptide
14	N	371	ILE	Peptide
16	P	158	SER	Peptide
17	Q	125	ALA	Peptide
18	R	215	GLU	Mainchain
19	S	148	PRO	Peptide
20	T	123	ASN	Peptide
20	T	177	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11607	525	0
2	B	9317	0	9308	354	0
3	C	2213	0	2153	90	0
4	D	1062	0	1042	11	0
5	E	1723	0	1745	60	0
6	F	689	0	715	18	0
7	G	1351	0	1358	26	0
8	H	1205	0	1168	44	0
9	I	1013	0	932	55	0
10	J	533	0	553	35	0
11	K	937	0	959	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	388	0	393	26	0
13	M	2391	0	2410	126	0
14	N	930	0	888	23	0
15	O	806	0	818	16	0
16	P	1462	0	1549	58	0
17	Q	1484	0	1494	147	0
18	R	1357	0	1379	205	0
19	S	1138	0	1103	35	0
20	T	1788	0	1819	97	0
21	U	1343	0	1338	45	0
22	X	1645	0	908	34	0
23	Y	1624	0	899	27	0
24	A	2	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	47927	0	46538	1735	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1735) 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)
1:A:932:ARG:CG	1:A:943:LEU:CD1	1.74	1.56
18:R:195:PRO:CG	18:R:199:LYS:CB	1.86	1.52
5:E:64:HIS:CE1	5:E:68:PRO:HG3	1.44	1.52
13:M:37:CYS:SG	13:M:39:LEU:HD22	1.46	1.52
1:A:932:ARG:CD	1:A:943:LEU:HD21	1.38	1.50
17:Q:54:PHE:CD1	18:R:194:ARG:CD	1.94	1.50
18:R:195:PRO:HG2	18:R:199:LYS:CB	1.01	1.46
17:Q:54:PHE:CD1	18:R:194:ARG:HD2	1.51	1.45
16:P:206:GLU:CG	16:P:236:LYS:NZ	1.77	1.44
1:A:932:ARG:HG3	1:A:943:LEU:CD1	1.33	1.42
17:Q:113:ARG:NH2	18:R:218:LYS:HE3	1.34	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:9:ALA:C	13:M:10:LEU:HD13	1.44	1.38
1:A:932:ARG:CG	1:A:943:LEU:HD11	0.91	1.38
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.33	1.37
17:Q:112:ARG:CD	18:R:237:LEU:HD11	1.54	1.36
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.44	1.36
17:Q:20:TYR:CE2	18:R:210:PHE:CB	1.93	1.36
18:R:154:LEU:HD23	18:R:163:LEU:CD2	1.54	1.35
17:Q:20:TYR:CE2	18:R:210:PHE:HB3	1.08	1.34
3:C:133:ARG:HA	3:C:136:ASP:OD2	1.23	1.34
1:A:133:SER:OG	1:A:136:GLN:HB2	1.21	1.33
17:Q:112:ARG:NE	18:R:237:LEU:HD11	1.45	1.32
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.31	1.30
18:R:195:PRO:CG	18:R:199:LYS:HB3	1.50	1.30
1:A:199:TYR:OH	13:M:93:PHE:CE2	1.80	1.29
17:Q:113:ARG:NH2	18:R:218:LYS:CE	1.93	1.29
1:A:263:ALA:O	1:A:264:VAL:CG1	1.80	1.28
17:Q:54:PHE:CE1	18:R:194:ARG:HD2	1.66	1.27
1:A:1163:HIS:O	1:A:1305:SER:CB	1.82	1.27
16:P:298:PRO:O	16:P:300:ILE:HG12	1.14	1.26
5:E:26:TYR:HA	5:E:64:HIS:O	1.11	1.26
1:A:201:GLU:HA	1:A:212:LYS:O	1.17	1.25
1:A:1163:HIS:H	1:A:1305:SER:C	1.26	1.24
18:R:195:PRO:CG	18:R:199:LYS:HB2	1.54	1.24
3:C:6:GLN:HB2	11:K:100:LEU:CD2	1.67	1.23
17:Q:187:ILE:HD13	18:R:210:PHE:O	1.37	1.23
18:R:151:LEU:HD12	18:R:163:LEU:CD1	1.67	1.22
1:A:932:ARG:HG3	1:A:943:LEU:CG	1.70	1.21
3:C:6:GLN:CB	11:K:100:LEU:HD23	1.70	1.21
13:M:94:ASP:OD2	13:M:97:GLY:O	1.55	1.20
5:E:46:ASP:O	5:E:48:PRO:HD3	1.42	1.19
1:A:199:TYR:OH	13:M:93:PHE:CZ	1.96	1.19
17:Q:180:PHE:CZ	18:R:213:ASP:CA	2.26	1.18
1:A:622:SER:O	1:A:624:GLY:N	1.73	1.18
1:A:932:ARG:HG2	1:A:943:LEU:CD1	1.49	1.18
13:M:15:CYS:SG	13:M:39:LEU:HD21	1.83	1.18
1:A:608:THR:C	1:A:610:PRO:HD2	1.64	1.17
17:Q:180:PHE:CZ	18:R:213:ASP:HA	1.79	1.17
8:H:74:GLU:O	8:H:76:ASN:N	1.75	1.17
3:C:6:GLN:HG3	11:K:100:LEU:HD21	1.23	1.17
5:E:25:GLY:O	5:E:65:ASN:HA	1.44	1.16
12:L:16:ILE:O	12:L:17:TYR:HB2	1.46	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:298:PRO:O	16:P:300:ILE:CG1	1.93	1.16
2:B:52:GLN:HA	20:T:141:LEU:CD1	1.75	1.15
1:A:132:LYS:O	1:A:133:SER:HB2	1.46	1.14
5:E:64:HIS:HE1	5:E:68:PRO:CG	1.60	1.14
18:R:164:GLY:CA	18:R:203:PHE:CZ	2.30	1.14
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.22	1.13
2:B:880:LEU:O	2:B:881:GLU:HB2	1.40	1.13
17:Q:105:TYR:CE1	18:R:234:GLU:CD	2.22	1.13
18:R:164:GLY:HA2	18:R:203:PHE:CZ	1.84	1.12
1:A:932:ARG:CD	1:A:943:LEU:CD2	2.29	1.11
1:A:932:ARG:CB	1:A:943:LEU:HD11	1.80	1.11
17:Q:54:PHE:CD1	18:R:194:ARG:HD3	1.66	1.11
1:A:263:ALA:O	1:A:264:VAL:HG13	0.96	1.11
1:A:1163:HIS:N	1:A:1305:SER:C	1.98	1.11
5:E:63:ALA:O	5:E:64:HIS:HB2	1.32	1.10
21:U:227:GLU:O	21:U:228:MET:HB3	1.50	1.09
16:P:206:GLU:HB3	16:P:207:PRO:CD	1.82	1.09
17:Q:112:ARG:NE	18:R:237:LEU:CD1	2.15	1.08
18:R:225:VAL:HG12	18:R:227:SER:HB2	1.17	1.08
16:P:206:GLU:CB	16:P:207:PRO:CD	2.32	1.08
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.33	1.08
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.34	1.07
2:B:52:GLN:HA	20:T:141:LEU:HD12	1.33	1.07
2:B:225:LEU:C	2:B:227:ASN:H	1.52	1.07
13:M:9:ALA:O	13:M:10:LEU:HD13	1.52	1.07
13:M:46:ILE:O	13:M:47:ASP:HB2	1.42	1.06
17:Q:23:ARG:NH2	18:R:206:LYS:CA	2.18	1.06
18:R:195:PRO:HG2	18:R:199:LYS:CA	1.86	1.06
2:B:132:VAL:HG21	2:B:141:GLN:HG2	1.35	1.06
18:R:162:GLY:O	18:R:163:LEU:CG	2.04	1.06
2:B:132:VAL:HG23	2:B:141:GLN:HB3	1.36	1.05
16:P:206:GLU:CG	16:P:236:LYS:HZ3	1.51	1.05
17:Q:112:ARG:HD3	18:R:237:LEU:HD11	1.35	1.05
17:Q:180:PHE:CE1	18:R:212:VAL:O	2.10	1.05
17:Q:54:PHE:HD1	18:R:194:ARG:HD3	0.95	1.05
17:Q:180:PHE:CZ	18:R:212:VAL:O	2.10	1.05
1:A:1163:HIS:H	1:A:1306:LYS:N	1.53	1.05
16:P:206:GLU:HG2	16:P:236:LYS:HZ3	0.93	1.04
21:U:251:ALA:O	21:U:252:LYS:HB2	1.51	1.04
1:A:1162:GLU:HB3	1:A:1306:LYS:CB	1.87	1.04
1:A:1163:HIS:O	1:A:1305:SER:HB2	0.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:O	20:T:141:LEU:HD12	1.57	1.04
1:A:264:VAL:HG23	1:A:272:ASN:OD1	1.57	1.03
1:A:1116:ASN:ND2	1:A:1339:ASP:OD1	1.91	1.03
13:M:10:LEU:O	13:M:13:VAL:HG22	1.56	1.03
17:Q:23:ARG:NH2	18:R:206:LYS:CB	2.21	1.03
17:Q:54:PHE:HD1	18:R:194:ARG:CD	1.44	1.03
5:E:64:HIS:CE1	5:E:68:PRO:CG	2.39	1.03
5:E:63:ALA:O	5:E:64:HIS:CB	2.06	1.02
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.50	1.02
3:C:6:GLN:HG2	11:K:104:ARG:HH12	1.20	1.02
2:B:51:ILE:HG22	20:T:141:LEU:CD1	1.88	1.02
18:R:162:GLY:O	18:R:163:LEU:CD2	2.09	1.01
1:A:1163:HIS:C	1:A:1305:SER:HB2	1.79	1.01
1:A:1306:LYS:O	1:A:1308:TYR:HD1	1.40	1.01
18:R:154:LEU:HD23	18:R:163:LEU:HD22	1.02	1.01
1:A:522:PRO:HA	1:A:666:ARG:HE	1.25	1.01
1:A:1162:GLU:HB3	1:A:1306:LYS:HB3	1.04	1.01
18:R:164:GLY:HA3	18:R:203:PHE:HZ	1.23	1.01
1:A:932:ARG:HG2	1:A:943:LEU:HD11	1.05	1.01
16:P:297:LYS:CB	16:P:298:PRO:CD	2.35	1.00
1:A:1162:GLU:CB	1:A:1306:LYS:HB3	1.92	1.00
2:B:51:ILE:CG2	20:T:141:LEU:HD11	1.90	1.00
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.40	1.00
18:R:164:GLY:HA3	18:R:203:PHE:CZ	1.95	1.00
1:A:264:VAL:HG23	1:A:272:ASN:CG	1.81	1.00
1:A:1306:LYS:O	1:A:1308:TYR:CD1	2.15	1.00
17:Q:23:ARG:NH2	18:R:206:LYS:HB3	1.76	1.00
20:T:139:VAL:CG1	20:T:142:SER:CB	2.39	1.00
5:E:26:TYR:CA	5:E:64:HIS:O	2.08	0.99
1:A:201:GLU:CA	1:A:212:LYS:O	2.10	0.99
1:A:609:HIS:N	1:A:610:PRO:CD	2.24	0.99
17:Q:23:ARG:HH22	18:R:206:LYS:HB3	1.26	0.99
1:A:932:ARG:HD2	1:A:943:LEU:CD2	1.91	0.99
18:R:162:GLY:O	18:R:163:LEU:HD23	1.61	0.99
16:P:206:GLU:HB2	16:P:207:PRO:HD2	1.44	0.98
17:Q:105:TYR:CD1	18:R:234:GLU:OE1	2.16	0.98
18:R:151:LEU:HD13	18:R:163:LEU:HD22	1.44	0.98
16:P:206:GLU:HG2	16:P:236:LYS:NZ	1.53	0.98
1:A:1307:VAL:O	1:A:1308:TYR:O	1.78	0.98
1:A:932:ARG:HG2	1:A:943:LEU:HD13	1.46	0.97
1:A:132:LYS:O	1:A:133:SER:CB	2.13	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:MET:O	1:A:669:TYR:OH	1.80	0.97
18:R:195:PRO:HG2	18:R:199:LYS:HB3	1.07	0.97
1:A:932:ARG:HD2	1:A:943:LEU:HD21	0.97	0.96
17:Q:105:TYR:CE1	18:R:234:GLU:OE2	2.17	0.96
18:R:154:LEU:CD2	18:R:163:LEU:HD22	1.95	0.96
17:Q:20:TYR:HE2	18:R:210:PHE:CB	1.70	0.96
1:A:133:SER:OG	1:A:136:GLN:CB	2.13	0.96
17:Q:23:ARG:HH22	18:R:206:LYS:CB	1.78	0.96
18:R:162:GLY:O	18:R:163:LEU:HG	1.63	0.96
3:C:6:GLN:HG3	11:K:100:LEU:CD2	1.96	0.96
1:A:45:GLU:OE1	1:A:48:GLU:HG3	1.65	0.96
18:R:195:PRO:CB	18:R:199:LYS:CB	2.42	0.95
2:B:52:GLN:CA	20:T:141:LEU:HD12	1.95	0.95
3:C:6:GLN:CG	11:K:104:ARG:NH1	2.29	0.95
1:A:1224:ARG:NH2	1:A:1306:LYS:HD3	1.82	0.95
2:B:225:LEU:O	2:B:227:ASN:N	2.00	0.95
3:C:6:GLN:CG	11:K:104:ARG:HH12	1.79	0.95
18:R:151:LEU:HD12	18:R:163:LEU:HD13	1.46	0.94
1:A:609:HIS:N	1:A:610:PRO:HD2	1.83	0.94
18:R:151:LEU:CD1	18:R:163:LEU:HD13	1.97	0.94
2:B:645:GLU:OE1	2:B:649:ASN:ND2	2.01	0.94
2:B:958:CYS:SG	2:B:959:GLU:N	2.37	0.94
3:C:6:GLN:HG2	11:K:104:ARG:NH1	1.83	0.94
18:R:195:PRO:CB	18:R:199:LYS:HB3	1.99	0.93
17:Q:23:ARG:HH22	18:R:206:LYS:CA	1.79	0.93
13:M:182:ALA:HB1	20:T:152:ASN:OD1	1.68	0.93
17:Q:105:TYR:HE1	18:R:234:GLU:OE2	1.49	0.93
16:P:206:GLU:CB	16:P:207:PRO:HD2	1.99	0.92
17:Q:113:ARG:HH21	18:R:218:LYS:HE3	1.09	0.92
13:M:94:ASP:O	13:M:96:PHE:N	2.01	0.92
5:E:45:GLY:O	5:E:46:ASP:O	1.85	0.92
3:C:133:ARG:CA	3:C:136:ASP:OD2	2.17	0.92
1:A:1116:ASN:O	1:A:1117:VAL:HG23	1.70	0.92
18:R:151:LEU:HD12	18:R:163:LEU:CD2	2.00	0.92
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.43	0.92
18:R:154:LEU:HD23	18:R:163:LEU:HD23	1.50	0.92
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.02	0.91
18:R:151:LEU:CD1	18:R:163:LEU:HD22	1.99	0.91
1:A:157:GLY:N	1:A:181:HIS:NE2	2.19	0.91
1:A:197:GLU:OE1	13:M:93:PHE:CD2	2.23	0.91
2:B:874:PRO:O	2:B:875:GLU:HB2	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:GLN:CG	11:K:100:LEU:HD21	2.01	0.91
16:P:205:ARG:O	16:P:206:GLU:O	1.87	0.91
5:E:65:ASN:OD1	5:E:66:ASP:N	2.03	0.91
21:U:227:GLU:O	21:U:228:MET:HE2	1.70	0.91
2:B:132:VAL:HG21	2:B:141:GLN:CG	2.00	0.91
17:Q:23:ARG:NH2	18:R:206:LYS:C	2.04	0.90
1:A:544:ALA:HB2	1:A:680:LEU:HD22	1.54	0.90
17:Q:112:ARG:CD	18:R:237:LEU:CD1	2.48	0.90
21:U:227:GLU:O	21:U:228:MET:CE	2.19	0.90
1:A:932:ARG:CG	1:A:943:LEU:HD21	2.01	0.90
13:M:34:CYS:HB3	13:M:39:LEU:CB	2.01	0.90
2:B:224:CYS:O	2:B:226:GLU:N	2.06	0.89
1:A:932:ARG:CG	1:A:943:LEU:CD2	2.50	0.89
1:A:201:GLU:OE2	1:A:203:LYS:NZ	2.04	0.89
17:Q:105:TYR:CD1	18:R:234:GLU:CD	2.45	0.89
21:U:227:GLU:O	21:U:228:MET:CB	2.19	0.89
1:A:199:TYR:HH	13:M:93:PHE:HE2	0.92	0.89
13:M:92:SER:O	13:M:93:PHE:O	1.91	0.89
1:A:263:ALA:C	1:A:264:VAL:HG13	1.93	0.88
17:Q:180:PHE:CE1	18:R:213:ASP:HA	2.07	0.88
1:A:932:ARG:CG	1:A:943:LEU:CG	2.40	0.88
1:A:197:GLU:OE1	13:M:93:PHE:CE2	2.26	0.88
1:A:932:ARG:NE	1:A:943:LEU:HD21	1.88	0.88
2:B:52:GLN:CA	20:T:141:LEU:CD1	2.52	0.88
3:C:275:ASN:ND2	11:K:31:CYS:SG	2.47	0.88
13:M:9:ALA:C	13:M:10:LEU:CD1	2.39	0.88
2:B:52:GLN:HA	20:T:141:LEU:HD13	1.56	0.88
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.25	0.87
20:T:139:VAL:HG13	20:T:142:SER:CB	2.04	0.87
17:Q:113:ARG:HH21	18:R:218:LYS:CE	1.70	0.87
18:R:151:LEU:CD1	18:R:163:LEU:CD2	2.52	0.87
18:R:151:LEU:CD1	18:R:163:LEU:CD1	2.51	0.87
2:B:225:LEU:C	2:B:227:ASN:N	2.27	0.87
18:R:195:PRO:HG2	18:R:199:LYS:HB2	0.88	0.87
18:R:151:LEU:HD12	18:R:163:LEU:HD11	1.55	0.87
1:A:265:VAL:HA	1:A:272:ASN:HB2	1.57	0.87
1:A:264:VAL:CG2	1:A:272:ASN:ND2	2.34	0.86
3:C:6:GLN:CB	11:K:100:LEU:CD2	2.42	0.86
9:I:61:GLU:O	9:I:63:ASP:N	2.07	0.86
18:R:164:GLY:HA2	18:R:203:PHE:CE2	2.10	0.86
18:R:154:LEU:CD2	18:R:163:LEU:CD2	2.49	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.09	0.85
13:M:46:ILE:O	13:M:47:ASP:CB	2.24	0.85
2:B:132:VAL:CG2	2:B:141:GLN:HB3	2.06	0.85
13:M:89:GLY:O	13:M:90:ALA:CB	2.25	0.85
2:B:51:ILE:C	20:T:141:LEU:HD12	1.96	0.85
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.17	0.85
1:A:273:GLN:NE2	13:M:79:ASP:OD2	2.10	0.85
2:B:492:ASP:O	23:Y:45:DT:C2'	2.24	0.85
1:A:1163:HIS:ND1	1:A:1302:GLU:O	2.09	0.85
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.55	0.85
8:H:65:TYR:HE2	8:H:70:LEU:HB2	1.42	0.85
1:A:264:VAL:CG2	1:A:272:ASN:CG	2.44	0.84
5:E:49:SER:O	5:E:50:GLU:O	1.96	0.84
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.13	0.84
3:C:6:GLN:CG	11:K:100:LEU:CD2	2.55	0.84
1:A:133:SER:HG	1:A:136:GLN:HB2	1.41	0.84
1:A:79:THR:HG21	13:M:43:ASP:OD1	1.77	0.83
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.23	0.83
12:L:16:ILE:O	12:L:17:TYR:CB	2.25	0.83
18:R:164:GLY:CA	18:R:203:PHE:CE2	2.61	0.83
1:A:1112:VAL:O	21:U:252:LYS:HB3	1.78	0.83
8:H:65:TYR:CE2	8:H:70:LEU:HB2	2.13	0.83
17:Q:52:LEU:HB3	17:Q:54:PHE:HD2	1.43	0.83
13:M:178:LYS:C	20:T:154:LYS:HE3	1.98	0.82
20:T:139:VAL:CG1	20:T:142:SER:HB3	2.07	0.82
1:A:375:ILE:HG21	1:A:666:ARG:CZ	2.08	0.82
17:Q:184:ILE:HD13	18:R:218:LYS:NZ	1.94	0.82
21:U:256:THR:OG1	21:U:257:GLN:N	2.13	0.82
17:Q:184:ILE:CD1	18:R:218:LYS:HZ2	1.93	0.82
8:H:65:TYR:CD2	8:H:70:LEU:HD22	2.15	0.82
5:E:46:ASP:O	5:E:48:PRO:CD	2.27	0.82
17:Q:20:TYR:CE2	18:R:210:PHE:HB2	2.10	0.81
17:Q:113:ARG:HH22	18:R:218:LYS:CD	1.93	0.81
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.06	0.81
17:Q:113:ARG:NH1	18:R:218:LYS:HG3	1.96	0.81
17:Q:69:ASP:HA	18:R:226:ASP:OD1	1.80	0.81
13:M:9:ALA:O	13:M:10:LEU:CD1	2.27	0.81
17:Q:113:ARG:NH2	18:R:218:LYS:CD	2.43	0.81
2:B:226:GLU:OE2	2:B:617:ASP:HB2	1.81	0.81
21:U:256:THR:O	21:U:257:GLN:HB2	1.81	0.81
3:C:6:GLN:HB2	11:K:100:LEU:HD23	0.85	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:PRO:HB3	1:A:1334:TRP:CZ3	2.16	0.80
3:C:209:SER:O	3:C:212:ASP:OD1	1.97	0.80
5:E:41:LYS:HG3	5:E:46:ASP:OD2	1.82	0.80
16:P:298:PRO:O	16:P:300:ILE:CD1	2.30	0.80
2:B:51:ILE:O	20:T:141:LEU:CD1	2.30	0.80
17:Q:68:GLY:O	18:R:226:ASP:HB3	1.82	0.80
1:A:206:ASN:O	1:A:207:GLU:HB2	1.80	0.80
1:A:932:ARG:HG3	1:A:943:LEU:HD11	0.83	0.79
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	0.67	0.79
18:R:205:ASP:O	18:R:206:LYS:HD2	1.82	0.79
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.48	0.79
1:A:199:TYR:OH	13:M:93:PHE:HE2	1.36	0.78
2:B:566:LYS:HD3	2:B:573:TRP:HE1	1.47	0.78
1:A:264:VAL:HG23	1:A:272:ASN:ND2	1.95	0.78
5:E:55:ARG:NH1	5:E:107:GLN:OE1	2.17	0.78
17:Q:184:ILE:CD1	18:R:218:LYS:NZ	2.47	0.78
1:A:621:ILE:O	1:A:623:PRO:N	2.16	0.78
17:Q:184:ILE:HD11	18:R:218:LYS:HZ2	1.47	0.78
3:C:157:GLN:CG	10:J:65:LEU:HB3	2.13	0.78
2:B:492:ASP:O	23:Y:45:DT:H2'	1.83	0.78
2:B:51:ILE:HG22	20:T:141:LEU:HD11	0.93	0.78
3:C:6:GLN:HG3	11:K:104:ARG:NH1	1.97	0.78
1:A:485:ASN:OD1	1:A:486:LEU:N	2.16	0.77
17:Q:112:ARG:CZ	18:R:237:LEU:HD11	2.14	0.77
2:B:897:ARG:O	2:B:900:GLU:CG	2.32	0.77
2:B:490:GLY:O	2:B:491:ARG:HB2	1.83	0.77
19:S:49:ARG:NH1	19:S:96:GLN:O	2.18	0.77
20:T:155:PRO:O	20:T:157:ALA:N	2.17	0.76
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.18	0.76
1:A:930:LEU:HB3	1:A:934:LEU:HB2	1.67	0.76
17:Q:184:ILE:HD13	18:R:218:LYS:HZ1	1.48	0.76
2:B:132:VAL:HG23	2:B:141:GLN:CB	2.16	0.76
2:B:897:ARG:O	2:B:900:GLU:HG3	1.86	0.76
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.51	0.75
23:Y:63:DG:H3'	23:Y:64:DC:H2'	1.67	0.75
2:B:73:HIS:O	2:B:75:SER:N	2.19	0.75
13:M:34:CYS:HB3	13:M:39:LEU:HB2	1.68	0.75
13:M:178:LYS:HB3	20:T:154:LYS:HD3	1.68	0.75
1:A:133:SER:O	1:A:134:LYS:C	2.22	0.75
20:T:139:VAL:HG13	20:T:142:SER:HB2	1.68	0.75
20:T:139:VAL:HG12	20:T:142:SER:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:C	20:T:141:LEU:CD1	2.55	0.75
1:A:265:VAL:HA	1:A:272:ASN:CB	2.14	0.75
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.68	0.74
1:A:930:LEU:O	1:A:931:ARG:O	2.05	0.74
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.79	0.74
18:R:204:ASN:ND2	18:R:205:ASP:N	2.36	0.74
20:T:152:ASN:O	20:T:154:LYS:N	2.20	0.74
1:A:79:THR:HG21	13:M:43:ASP:CG	2.08	0.74
1:A:199:TYR:OH	13:M:93:PHE:HZ	1.69	0.74
14:N:347:ASN:ND2	14:N:375:GLU:OE2	2.21	0.74
17:Q:188:TYR:HA	17:Q:191:LEU:HD13	1.70	0.74
1:A:263:ALA:O	1:A:264:VAL:CB	2.36	0.74
17:Q:23:ARG:HH22	18:R:206:LYS:C	1.59	0.73
13:M:94:ASP:HB2	13:M:99:SER:H	1.53	0.73
17:Q:112:ARG:CZ	18:R:237:LEU:CD1	2.66	0.73
1:A:1116:ASN:O	1:A:1117:VAL:CG2	2.37	0.73
17:Q:42:CYS:HB3	17:Q:95:ASN:HD21	1.54	0.73
18:R:222:SER:O	18:R:224:THR:N	2.21	0.73
1:A:156:GLY:HA2	1:A:181:HIS:ND1	2.03	0.72
1:A:79:THR:CG2	13:M:43:ASP:OD1	2.38	0.72
2:B:73:HIS:C	2:B:75:SER:H	1.93	0.72
2:B:492:ASP:O	23:Y:45:DT:H2"	1.88	0.72
13:M:182:ALA:HB1	20:T:152:ASN:CG	2.10	0.72
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.70	0.72
1:A:608:THR:CB	1:A:610:PRO:HD2	2.19	0.72
2:B:761:THR:H	2:B:764:MET:HE3	1.54	0.72
2:B:490:GLY:O	2:B:491:ARG:CB	2.36	0.72
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.69	0.72
17:Q:20:TYR:HE2	18:R:210:PHE:HB2	1.50	0.72
1:A:932:ARG:NE	1:A:943:LEU:CD2	2.49	0.72
1:A:1211:LEU:HD11	1:A:1258:ARG:HG3	1.72	0.72
2:B:793:SER:HA	2:B:944:THR:O	1.89	0.72
17:Q:68:GLY:O	18:R:226:ASP:CB	2.38	0.72
2:B:429:PHE:H	20:T:160:GLN:HG2	1.55	0.72
17:Q:54:PHE:CE1	18:R:194:ARG:CD	2.49	0.72
1:A:269:SER:O	1:A:270:ALA:HB3	1.89	0.72
4:D:96:GLU:OE1	4:D:121:ARG:NH1	2.23	0.72
17:Q:180:PHE:CE1	18:R:212:VAL:C	2.62	0.71
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.71
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.72	0.71
2:B:132:VAL:CG2	2:B:141:GLN:CB	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:ASP:HB2	5:E:50:GLU:OE1	1.90	0.71
8:H:66:GLU:O	8:H:67:ASP:HB2	1.90	0.71
17:Q:19:LYS:O	17:Q:22:ILE:HG13	1.88	0.71
1:A:643:LYS:NZ	21:U:299:LYS:O	2.22	0.71
14:N:320:VAL:HB	16:P:236:LYS:HE3	1.71	0.71
2:B:1006:VAL:HG23	2:B:1010:LYS:HB2	1.72	0.71
3:C:136:ASP:N	3:C:136:ASP:OD1	2.22	0.71
1:A:608:THR:C	1:A:610:PRO:CD	2.50	0.71
18:R:151:LEU:HD12	18:R:163:LEU:CG	2.20	0.71
18:R:195:PRO:CB	18:R:199:LYS:HB2	2.14	0.71
1:A:926:ASN:HA	1:A:931:ARG:HG3	1.73	0.70
17:Q:187:ILE:CD1	18:R:210:PHE:O	2.29	0.70
18:R:193:ASN:ND2	18:R:197:LYS:O	2.22	0.70
20:T:8:ASP:OD2	20:T:10:THR:OG1	2.08	0.70
14:N:32:ASP:HB3	14:N:34:VAL:HG23	1.73	0.70
14:N:317:GLU:HG3	16:P:235:ARG:HG2	1.71	0.70
1:A:18:ILE:HB	1:A:1460:LEU:HD21	1.70	0.70
5:E:25:GLY:O	5:E:65:ASN:CA	2.34	0.70
8:H:65:TYR:CZ	8:H:70:LEU:HD13	2.25	0.70
2:B:721:ARG:HG3	2:B:939:HIS:O	1.91	0.70
2:B:812:ARG:HD3	2:B:814:TYR:OH	1.92	0.70
3:C:24:GLU:HG2	3:C:228:ARG:HG3	1.73	0.70
1:A:505:LEU:O	2:B:1106:ARG:NH2	2.24	0.70
1:A:298:ALA:O	17:Q:60:ARG:NE	2.24	0.70
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.21	0.70
1:A:932:ARG:HB3	1:A:940:LYS:CB	2.22	0.70
11:K:111:ASP:O	11:K:113:GLN:N	2.19	0.70
1:A:609:HIS:N	1:A:610:PRO:HD3	2.07	0.70
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.73	0.70
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.24	0.69
18:R:195:PRO:HG2	18:R:199:LYS:C	2.12	0.69
19:S:115:LYS:HB2	19:S:143:TRP:HB3	1.73	0.69
1:A:926:ASN:CB	1:A:931:ARG:HG3	2.22	0.69
3:C:56:SER:HG	3:C:158:GLU:H	1.37	0.69
17:Q:184:ILE:HG12	18:R:211:SER:HB2	1.74	0.69
18:R:201:LEU:HB3	18:R:203:PHE:HE1	1.57	0.69
2:B:274:ARG:NH1	2:B:281:ASP:OD1	2.25	0.69
9:I:84:HIS:H	9:I:84:HIS:CD2	2.10	0.69
1:A:1162:GLU:HG2	1:A:1306:LYS:HB2	1.74	0.69
1:A:1309:MET:HB2	21:U:252:LYS:HE2	1.74	0.69
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLY:O	1:A:521:VAL:HG23	1.93	0.69
13:M:238:LYS:HD2	13:M:299:LEU:HA	1.74	0.69
16:P:267:PRO:HB2	16:P:337:LYS:HD2	1.73	0.69
1:A:1162:GLU:HG2	1:A:1306:LYS:CB	2.23	0.69
3:C:272:LEU:HD21	11:K:84:GLN:HG2	1.74	0.69
1:A:608:THR:OG1	1:A:610:PRO:HG2	1.92	0.68
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.76	0.68
1:A:932:ARG:HG3	1:A:943:LEU:HG	1.74	0.68
13:M:34:CYS:HB3	13:M:39:LEU:HB3	1.73	0.68
1:A:1319:LYS:HE2	1:A:1333:GLU:OE2	1.93	0.68
1:A:60:PRO:HD2	1:A:62:GLN:HG2	1.75	0.68
16:P:206:GLU:OE2	16:P:206:GLU:HA	1.91	0.68
18:R:202:PHE:O	18:R:203:PHE:CD1	2.47	0.68
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.25	0.68
1:A:729:PRO:HG2	21:U:250:MET:HB2	1.76	0.68
2:B:1062:ARG:HH21	2:B:1065:GLY:H	1.41	0.68
18:R:127:ASN:HD21	18:R:140:LYS:HD3	1.57	0.68
1:A:1306:LYS:O	1:A:1308:TYR:N	2.27	0.68
17:Q:113:ARG:NH2	18:R:218:LYS:CG	2.57	0.68
20:T:177:ARG:N	20:T:178:ALA:O	2.27	0.68
13:M:10:LEU:HD13	13:M:10:LEU:N	2.04	0.67
17:Q:68:GLY:O	18:R:226:ASP:CG	2.31	0.67
18:R:205:ASP:O	18:R:206:LYS:CD	2.42	0.67
1:A:1052:ARG:NH1	1:A:1056:GLU:OE1	2.28	0.67
1:A:1162:GLU:CB	1:A:1306:LYS:CB	2.62	0.67
12:L:35:ARG:HH12	12:L:42:ARG:HH21	1.39	0.67
16:P:206:GLU:C	16:P:208:ARG:H	1.98	0.67
2:B:198:GLU:OE1	2:B:388:TYR:OH	2.07	0.67
1:A:199:TYR:CE2	13:M:93:PHE:HZ	2.13	0.67
13:M:34:CYS:CB	13:M:39:LEU:HB3	2.23	0.67
17:Q:184:ILE:HG12	18:R:211:SER:CB	2.25	0.67
13:M:89:GLY:O	13:M:90:ALA:HB2	1.93	0.67
17:Q:109:HIS:CE1	18:R:233:ILE:HG21	2.30	0.67
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.60	0.67
1:A:1154:ALA:HB1	1:A:1310:HIS:HE1	1.59	0.67
1:A:926:ASN:CA	1:A:931:ARG:HG3	2.25	0.67
2:B:57:ARG:NH1	2:B:537:GLN:OE1	2.27	0.67
1:A:67:ARG:NH2	13:M:45:VAL:O	2.28	0.67
1:A:1022:ILE:HG23	1:A:1023:VAL:HG23	1.77	0.66
9:I:84:HIS:CG	9:I:85:PRO:CD	2.65	0.66
11:K:82:SER:OG	11:K:84:GLN:OE1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:226:GLU:HA	21:U:226:GLU:OE2	1.93	0.66
1:A:931:ARG:O	1:A:933:THR:N	2.28	0.66
1:A:1162:GLU:CG	1:A:1306:LYS:CB	2.74	0.66
16:P:297:LYS:O	16:P:299:ARG:N	2.26	0.66
1:A:156:GLY:HA2	1:A:181:HIS:CG	2.29	0.66
1:A:181:HIS:H	1:A:181:HIS:CD2	2.13	0.66
21:U:284:PRO:O	21:U:286:THR:N	2.28	0.66
3:C:148:ILE:HG13	10:J:5:VAL:HG22	1.77	0.66
5:E:29:THR:HB	5:E:32:GLU:HG3	1.77	0.66
18:R:195:PRO:HG3	18:R:199:LYS:HB3	1.72	0.66
1:A:1471:PHE:CE1	6:F:64:ARG:HD3	2.30	0.66
3:C:134:ASN:N	3:C:136:ASP:OD1	2.28	0.66
20:T:139:VAL:CG1	20:T:142:SER:HB2	2.26	0.66
1:A:487:SER:HB2	1:A:673:GLN:HE22	1.59	0.66
1:A:912:SER:H	1:A:1327:GLU:HB3	1.61	0.66
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.25	0.66
22:X:14:DA:H2"	22:X:15:DA:C8	2.30	0.66
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.12	0.66
3:C:56:SER:OG	3:C:158:GLU:N	2.21	0.66
4:D:26:PHE:HZ	7:G:42:TYR:HA	1.60	0.66
17:Q:141:ALA:HB1	17:Q:152:PHE:HE2	1.60	0.66
9:I:65:LEU:O	9:I:122:ARG:NH2	2.29	0.66
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.13	0.66
18:R:195:PRO:CD	18:R:199:LYS:HB2	2.25	0.66
1:A:202:TRP:H	1:A:212:LYS:HA	1.60	0.66
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.96	0.66
12:L:35:ARG:HH12	12:L:42:ARG:HE	1.44	0.65
1:A:541:THR:O	1:A:545:VAL:HG23	1.96	0.65
1:A:1177:TYR:OH	9:I:28:GLU:OE2	2.14	0.65
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.78	0.65
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.77	0.65
1:A:157:GLY:N	1:A:181:HIS:CE1	2.65	0.65
1:A:274:ASP:O	1:A:277:THR:N	2.29	0.65
8:H:17:PRO:O	8:H:19:GLY:N	2.28	0.65
17:Q:105:TYR:CE1	18:R:234:GLU:OE1	2.40	0.65
17:Q:23:ARG:HH21	18:R:206:LYS:CB	2.10	0.65
18:R:195:PRO:O	18:R:196:ASP:HB3	1.95	0.65
1:A:79:THR:CG2	13:M:43:ASP:CG	2.65	0.65
2:B:685:LYS:HD2	2:B:691:SER:HA	1.76	0.65
12:L:35:ARG:NH1	12:L:42:ARG:HE	1.94	0.65
21:U:255:GLY:O	21:U:256:THR:OG1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ARG:HB3	1:A:940:LYS:HB2	1.79	0.65
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.89	0.65
1:A:42:LYS:HE3	1:A:56:GLY:HA3	1.79	0.65
1:A:640:LEU:HD23	1:A:645:LEU:HD11	1.79	0.65
1:A:367:ILE:HG13	1:A:496:PHE:HD1	1.62	0.64
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.78	0.64
6:F:48:ASN:ND2	6:F:51:ARG:O	2.26	0.64
1:A:190:ARG:NH2	22:X:58:DT:OP2	2.29	0.64
1:A:358:ARG:HH21	2:B:1076:GLU:HA	1.62	0.64
2:B:333:GLU:OE1	19:S:53:ASN:ND2	2.27	0.64
2:B:881:GLU:C	2:B:883:THR:H	2.00	0.64
18:R:202:PHE:C	18:R:203:PHE:CD1	2.70	0.64
1:A:549:THR:O	1:A:589:LYS:NZ	2.27	0.64
1:A:608:THR:HB	1:A:610:PRO:CD	2.27	0.64
1:A:1162:GLU:HA	1:A:1305:SER:O	1.97	0.64
7:G:78:ARG:NH1	7:G:79:PRO:O	2.31	0.64
17:Q:180:PHE:CZ	18:R:212:VAL:C	2.71	0.64
18:R:222:SER:C	18:R:224:THR:H	1.99	0.64
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.79	0.64
20:T:20:LEU:HD23	20:T:113:ARG:HG2	1.79	0.64
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.63	0.64
13:M:90:ALA:HB2	13:M:100:LYS:HE3	1.80	0.64
1:A:1116:ASN:OD1	1:A:1136:THR:HB	1.97	0.64
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.79	0.64
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.33	0.64
2:B:823:PHE:HA	13:M:140:ASN:HD21	1.63	0.64
2:B:906:GLN:HG2	12:L:45:TYR:OH	1.98	0.64
1:A:673:GLN:O	1:A:677:ASN:HB2	1.98	0.64
3:C:157:GLN:OE1	10:J:65:LEU:HD22	1.98	0.64
17:Q:25:PHE:O	18:R:219:LEU:HD21	1.98	0.64
1:A:285:LYS:HE3	13:M:80:LEU:HD23	1.80	0.63
9:I:63:ASP:OD1	9:I:66:THR:OG1	2.16	0.63
15:O:75:VAL:HG22	15:O:94:LYS:HG2	1.81	0.63
2:B:52:GLN:N	20:T:141:LEU:HD12	2.14	0.63
2:B:247:ALA:O	19:S:169:LYS:NZ	2.25	0.63
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.32	0.63
2:B:1062:ARG:HH12	2:B:1075:MET:H	1.45	0.63
18:R:195:PRO:HB2	18:R:199:LYS:HB3	1.77	0.63
1:A:1319:LYS:HB3	1:A:1331:LEU:HB3	1.81	0.63
2:B:761:THR:H	2:B:764:MET:CE	2.11	0.63
8:H:85:ALA:HB1	8:H:88:PHE:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:O	1:A:135:GLY:N	2.31	0.63
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.87	0.63
18:R:181:ALA:HA	18:R:184:ALA:HB3	1.80	0.63
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.32	0.63
2:B:76:GLY:O	2:B:78:VAL:HG22	1.98	0.63
2:B:588:ARG:NH1	2:B:669:GLU:OE2	2.31	0.63
2:B:747:LEU:HD11	2:B:810:PHE:CZ	2.34	0.63
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.64	0.63
2:B:998:ASP:OD1	2:B:999:ALA:N	2.32	0.63
1:A:1246:ILE:HD11	1:A:1258:ARG:HD2	1.81	0.62
13:M:86:LYS:NZ	22:X:40:DT:C4	2.66	0.62
1:A:924:TYR:O	1:A:926:ASN:ND2	2.32	0.62
1:A:1158:LEU:HD13	1:A:1336:LEU:HD22	1.81	0.62
17:Q:60:ARG:O	17:Q:64:ASN:ND2	2.28	0.62
1:A:157:GLY:H	1:A:181:HIS:CE1	2.16	0.62
3:C:157:GLN:CD	10:J:65:LEU:HD22	2.19	0.62
8:H:108:ALA:O	8:H:110:THR:N	2.32	0.62
1:A:95:PHE:N	1:A:311:GLN:OE1	2.31	0.62
1:A:201:GLU:HG3	1:A:212:LYS:HB3	1.81	0.62
1:A:1312:PRO:HB3	1:A:1334:TRP:HZ3	1.65	0.62
1:A:1316:ASN:ND2	1:A:1318:LYS:HE3	2.14	0.62
5:E:65:ASN:CG	5:E:66:ASP:H	2.00	0.62
1:A:51:ARG:H	1:A:52:PRO:HD2	1.65	0.62
2:B:898:THR:O	2:B:900:GLU:HG3	2.00	0.62
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.80	0.62
17:Q:109:HIS:HE1	18:R:233:ILE:HG21	1.63	0.62
17:Q:113:ARG:CZ	18:R:218:LYS:HG3	2.29	0.62
18:R:205:ASP:O	18:R:206:LYS:HB2	1.98	0.62
2:B:1144:THR:O	2:B:1146:ILE:N	2.33	0.62
10:J:64:PRO:C	10:J:66:GLU:H	2.02	0.62
20:T:141:LEU:O	20:T:142:SER:HB3	1.99	0.62
1:A:455:ILE:HD13	1:A:520:MET:HE3	1.81	0.62
20:T:139:VAL:HG12	20:T:142:SER:CB	2.25	0.62
1:A:157:GLY:CA	1:A:181:HIS:NE2	2.62	0.61
1:A:786:ALA:O	1:A:826:SER:HB3	2.00	0.61
2:B:749:HIS:CD2	2:B:810:PHE:CD1	2.88	0.61
18:R:151:LEU:HD11	18:R:163:LEU:HD13	1.82	0.61
1:A:263:ALA:HB1	1:A:272:ASN:HB3	1.82	0.61
1:A:1162:GLU:HA	1:A:1306:LYS:HA	1.82	0.61
1:A:1163:HIS:N	1:A:1306:LYS:N	2.37	0.61
8:H:137:VAL:HG22	8:H:138:ASP:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:881:GLU:C	2:B:883:THR:N	2.51	0.61
1:A:344:LYS:HA	1:A:1435:THR:HG21	1.82	0.61
1:A:379:GLY:HA2	1:A:475:ARG:O	2.01	0.61
16:P:153:THR:N	16:P:326:GLU:OE2	2.34	0.61
2:B:529:MET:SD	2:B:623:ARG:HB2	2.41	0.61
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.00	0.61
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.81	0.61
17:Q:105:TYR:HE1	18:R:234:GLU:CD	1.78	0.61
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.33	0.61
7:G:52:ASP:H	7:G:72:TYR:HA	1.64	0.61
9:I:105:GLU:O	9:I:106:ASP:CB	2.49	0.61
1:A:883:ILE:HG13	1:A:885:GLN:HG3	1.83	0.61
1:A:1307:VAL:O	1:A:1308:TYR:C	2.40	0.61
5:E:46:ASP:C	5:E:48:PRO:HD3	2.20	0.61
1:A:1309:MET:CB	21:U:252:LYS:HE2	2.31	0.60
2:B:880:LEU:O	2:B:881:GLU:CB	2.24	0.60
13:M:178:LYS:HZ2	20:T:156:VAL:HG11	1.65	0.60
22:X:49:DT:H3'	22:X:50:DT:H5''	1.83	0.60
3:C:157:GLN:CD	10:J:65:LEU:HB3	2.22	0.60
17:Q:70:LYS:O	17:Q:102:VAL:HG11	2.01	0.60
2:B:676:ALA:HB2	2:B:693:TYR:CD1	2.36	0.60
9:I:105:GLU:O	9:I:106:ASP:HB3	2.02	0.60
1:A:199:TYR:CZ	13:M:93:PHE:HZ	2.19	0.60
1:A:608:THR:CA	1:A:610:PRO:HD2	2.30	0.60
8:H:66:GLU:HA	8:H:66:GLU:OE2	2.00	0.60
13:M:50:SER:O	13:M:53:ARG:HB2	2.01	0.60
13:M:90:ALA:HB2	13:M:100:LYS:CE	2.31	0.60
13:M:91:ALA:O	13:M:93:PHE:N	2.34	0.60
18:R:195:PRO:CG	18:R:199:LYS:C	2.69	0.60
1:A:685:HIS:HB3	2:B:784:SER:OG	2.01	0.60
2:B:380:ARG:NE	2:B:609:GLU:OE2	2.34	0.60
1:A:623:PRO:C	1:A:625:ASP:H	2.05	0.60
2:B:841:ARG:NH2	2:B:893:SER:O	2.35	0.60
16:P:297:LYS:CB	16:P:298:PRO:HD3	2.15	0.60
18:R:205:ASP:O	18:R:206:LYS:CB	2.48	0.60
22:X:32:DT:H4'	22:X:33:DT:H5'	1.82	0.60
17:Q:112:ARG:HD3	18:R:237:LEU:CD1	2.22	0.60
18:R:118:TRP:NE1	18:R:122:GLU:OE1	2.34	0.60
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.84	0.60
2:B:898:THR:O	2:B:900:GLU:N	2.35	0.60
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:25:PHE:CD1	18:R:210:PHE:CZ	2.90	0.60
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.83	0.60
2:B:52:GLN:CA	20:T:141:LEU:HD13	2.28	0.60
2:B:819:SER:HB3	2:B:821:LYS:HG3	1.84	0.60
2:B:823:PHE:HA	13:M:140:ASN:ND2	2.16	0.60
6:F:88:ASP:OD2	6:F:91:LEU:N	2.35	0.60
1:A:540:ASP:CB	2:B:790:GLN:HE21	2.15	0.59
1:A:1116:ASN:O	1:A:1117:VAL:CB	2.49	0.59
5:E:41:LYS:HG3	5:E:46:ASP:CG	2.23	0.59
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.84	0.59
9:I:65:LEU:HD22	9:I:122:ARG:HG2	1.82	0.59
12:L:26:ASN:O	12:L:27:GLU:HB3	2.02	0.59
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.84	0.59
17:Q:52:LEU:HB3	17:Q:54:PHE:CD2	2.33	0.59
1:A:386:ALA:O	1:A:449:HIS:ND1	2.35	0.59
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.66	0.59
13:M:218:PHE:HD1	13:M:277:ILE:HG22	1.67	0.59
1:A:354:LEU:O	1:A:357:LYS:HE2	2.02	0.59
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.84	0.59
18:R:204:ASN:CG	18:R:205:ASP:H	2.06	0.59
1:A:621:ILE:O	1:A:621:ILE:HG22	2.02	0.59
1:A:1102:MET:HG2	21:U:277:GLN:HB2	1.85	0.59
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.85	0.59
7:G:110:ARG:NH2	7:G:118:GLU:OE2	2.36	0.59
9:I:80:ARG:HD3	9:I:95:VAL:HG12	1.83	0.59
1:A:180:GLY:C	1:A:182:GLY:H	2.04	0.59
1:A:271:ARG:O	1:A:272:ASN:CB	2.48	0.59
2:B:160:TYR:OH	20:T:141:LEU:HD13	2.02	0.59
2:B:249:LYS:O	2:B:250:SER:HB2	2.02	0.59
2:B:489:ILE:HG21	2:B:522:LEU:HD13	1.83	0.59
5:E:52:ARG:HG3	5:E:54:ARG:HG3	1.85	0.59
14:N:318:ASP:OD1	16:P:239:ARG:NH2	2.36	0.59
17:Q:98:THR:HG22	17:Q:100:VAL:H	1.67	0.59
1:A:932:ARG:HG3	1:A:940:LYS:HA	1.84	0.59
1:A:998:PRO:HA	1:A:1059:ARG:HG2	1.85	0.59
17:Q:180:PHE:CE1	18:R:213:ASP:CA	2.75	0.59
1:A:26:LEU:HD23	2:B:1168:ALA:HB2	1.84	0.59
1:A:575:PRO:HG2	1:A:594:LEU:HD11	1.83	0.59
5:E:133:GLN:N	5:E:133:GLN:OE1	2.36	0.59
9:I:61:GLU:C	9:I:63:ASP:N	2.52	0.59
18:R:214:GLU:OE1	18:R:217:GLN:NE2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ILE:HG13	1:A:866:LYS:N	2.17	0.59
2:B:42:GLN:HG2	2:B:43:GLN:N	2.15	0.59
8:H:146:LYS:O	8:H:148:LEU:N	2.29	0.59
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.36	0.59
17:Q:112:ARG:NE	18:R:237:LEU:HD12	2.13	0.59
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.04	0.58
2:B:690:CYS:SG	2:B:691:SER:N	2.76	0.58
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.84	0.58
19:S:115:LYS:NZ	19:S:117:GLY:O	2.28	0.58
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.86	0.58
2:B:790:GLN:HA	2:B:968:ASN:HD22	1.67	0.58
3:C:60:HIS:NE2	3:C:63:PHE:HB2	2.18	0.58
1:A:601:ASN:HD21	1:A:632:ASN:H	1.52	0.58
1:A:832:THR:N	1:A:835:GLU:OE1	2.25	0.58
3:C:6:GLN:CG	11:K:100:LEU:HD23	2.29	0.58
16:P:171:THR:HG22	16:P:220:VAL:HG13	1.85	0.58
17:Q:24:GLY:HA2	18:R:209:GLN:HG2	1.84	0.58
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.84	0.58
2:B:857:GLY:HA2	2:B:903:ILE:HD11	1.86	0.58
13:M:10:LEU:N	13:M:10:LEU:HD22	2.19	0.58
1:A:624:GLY:O	1:A:626:THR:N	2.35	0.58
2:B:438:ARG:NE	2:B:442:ASP:OD2	2.31	0.58
11:K:39:ASP:OD1	11:K:39:ASP:N	2.37	0.58
18:R:212:VAL:O	18:R:213:ASP:CG	2.41	0.58
2:B:290:TYR:CE2	2:B:562:ALA:HA	2.39	0.58
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.37	0.58
3:C:85:SER:HB2	3:C:166:LYS:HE3	1.86	0.58
11:K:63:VAL:HB	11:K:71:ILE:HG22	1.86	0.58
21:U:224:THR:O	21:U:226:GLU:N	2.36	0.58
1:A:121:SER:HA	1:A:126:ILE:HG21	1.86	0.58
2:B:1062:ARG:NH1	2:B:1074:PRO:HB3	2.19	0.58
8:H:65:TYR:CE2	8:H:70:LEU:HD13	2.39	0.58
1:A:264:VAL:O	1:A:266:MET:N	2.36	0.57
1:A:271:ARG:O	1:A:272:ASN:HB2	2.04	0.57
1:A:641:CYS:SG	1:A:643:LYS:N	2.77	0.57
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.04	0.57
16:P:205:ARG:O	16:P:206:GLU:C	2.42	0.57
1:A:1127:LEU:HD21	1:A:1381:GLU:HB3	1.84	0.57
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.39	0.57
17:Q:25:PHE:CD1	18:R:210:PHE:HZ	2.23	0.57
1:A:1303:GLN:O	1:A:1304:ILE:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.86	0.57
2:B:921:ILE:HG13	2:B:921:ILE:O	2.03	0.57
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.38	0.57
1:A:200:ALA:O	1:A:213:LYS:HA	2.03	0.57
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.85	0.57
1:A:1112:VAL:O	21:U:252:LYS:CB	2.49	0.57
1:A:926:ASN:HB3	1:A:931:ARG:CB	2.34	0.57
1:A:927:GLU:O	1:A:929:ALA:N	2.37	0.57
2:B:230:ARG:HD2	2:B:405:ARG:HH12	1.69	0.57
9:I:104:ALA:O	9:I:106:ASP:N	2.37	0.57
13:M:89:GLY:O	13:M:90:ALA:HB3	2.01	0.57
13:M:178:LYS:HB3	20:T:154:LYS:CD	2.35	0.57
18:R:154:LEU:CD2	18:R:163:LEU:HD23	2.23	0.57
1:A:305:GLU:OE1	13:M:102:GLN:NE2	2.38	0.57
2:B:798:ARG:HD3	2:B:950:ARG:HG2	1.86	0.57
5:E:15:LYS:NZ	5:E:33:LEU:O	2.31	0.57
12:L:35:ARG:HH12	12:L:42:ARG:NH2	2.02	0.57
20:T:58:LEU:HD23	20:T:63:ALA:HB2	1.87	0.57
9:I:104:ALA:C	9:I:106:ASP:H	2.08	0.57
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.38	0.57
1:A:47:THR:HG23	1:A:53:LYS:HG2	1.86	0.56
1:A:606:HIS:CG	1:A:607:SER:N	2.72	0.56
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.02	0.56
2:B:812:ARG:HH22	23:Y:52:DT:P	2.26	0.56
23:Y:39:DG:H2'	23:Y:40:DT:C6	2.40	0.56
2:B:52:GLN:N	20:T:141:LEU:CD1	2.67	0.56
13:M:179:GLU:HG3	20:T:154:LYS:HE2	1.87	0.56
18:R:142:LYS:HD3	18:R:145:VAL:HG23	1.87	0.56
21:U:243:GLU:CD	21:U:246:ARG:HH12	2.08	0.56
1:A:537:ILE:HG13	1:A:672:ILE:HD13	1.86	0.56
1:A:789:GLY:HA2	1:A:822:PHE:CE1	2.40	0.56
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.86	0.56
2:B:223:SER:OG	2:B:232:THR:O	2.23	0.56
17:Q:105:TYR:CD1	18:R:234:GLU:HB2	2.40	0.56
22:X:53:DA:H2'	22:X:54:DA:C8	2.40	0.56
1:A:1117:VAL:O	1:A:1117:VAL:HG12	2.04	0.56
1:A:1128:ILE:HG23	1:A:1414:ILE:HD11	1.87	0.56
2:B:1040:GLN:H	2:B:1040:GLN:CD	2.08	0.56
5:E:46:ASP:C	5:E:48:PRO:CD	2.73	0.56
13:M:60:ALA:HB1	23:Y:54:DA:H2	1.70	0.56
18:R:204:ASN:CG	18:R:205:ASP:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:O	1:A:209:SER:N	2.39	0.56
1:A:926:ASN:HB3	1:A:931:ARG:CG	2.36	0.56
2:B:1069:ILE:HD11	13:M:45:VAL:HG22	1.87	0.56
11:K:16:GLU:OE1	11:K:36:ASN:ND2	2.39	0.56
14:N:319:ASP:C	14:N:321:SER:H	2.08	0.56
1:A:608:THR:CB	1:A:610:PRO:CD	2.82	0.56
22:X:47:DT:H3'	22:X:48:DT:H5''	1.88	0.56
1:A:205:VAL:O	1:A:206:ASN:HB2	2.06	0.56
17:Q:113:ARG:CZ	18:R:218:LYS:CG	2.84	0.56
18:R:204:ASN:ND2	18:R:205:ASP:H	2.03	0.56
13:M:183:VAL:HG12	20:T:152:ASN:HD21	1.71	0.56
1:A:157:GLY:C	1:A:181:HIS:NE2	2.59	0.56
2:B:499:ARG:NH2	2:B:522:LEU:HD11	2.20	0.56
2:B:1094:GLN:NE2	2:B:1102:PHE:HD2	2.04	0.56
5:E:94:MET:HB2	5:E:99:ILE:HD11	1.88	0.56
16:P:167:ASN:ND2	23:Y:79:DT:O2	2.34	0.56
1:A:623:PRO:O	1:A:625:ASP:N	2.39	0.55
2:B:255:ARG:NE	2:B:307:GLU:OE2	2.38	0.55
2:B:1076:GLU:HB2	13:M:54:THR:OG1	2.06	0.55
3:C:154:ARG:HB3	10:J:65:LEU:HD21	1.88	0.55
2:B:513:GLU:CD	2:B:707:CYS:HB2	2.26	0.55
3:C:134:ASN:H	3:C:136:ASP:CG	2.10	0.55
1:A:1143:LEU:HD11	1:A:1336:LEU:HG	1.88	0.55
2:B:873:LEU:CB	2:B:874:PRO:CD	2.85	0.55
8:H:64:LEU:H	8:H:70:LEU:HD21	1.71	0.55
8:H:106:THR:O	8:H:108:ALA:N	2.37	0.55
9:I:41:ASN:HA	19:S:177:MET:HE1	1.87	0.55
12:L:35:ARG:NH1	12:L:42:ARG:HH21	2.04	0.55
16:P:239:ARG:NH1	16:P:242:GLN:OE1	2.40	0.55
20:T:82:PRO:HG2	20:T:117:ARG:HB2	1.89	0.55
1:A:293:ASN:OD1	1:A:298:ALA:HA	2.06	0.55
1:A:522:PRO:HB3	1:A:666:ARG:CG	2.36	0.55
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.89	0.55
1:A:625:ASP:O	1:A:638:GLY:HA2	2.06	0.55
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.67	0.55
1:A:622:SER:C	1:A:624:GLY:N	2.56	0.55
1:A:930:LEU:O	1:A:931:ARG:C	2.44	0.55
1:A:1223:ASP:OD1	1:A:1224:ARG:NH1	2.39	0.55
19:S:46:ARG:NH2	20:T:2:ALA:O	2.39	0.55
1:A:522:PRO:HB3	1:A:666:ARG:HG3	1.89	0.55
13:M:34:CYS:CB	13:M:39:LEU:CB	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.36	0.55
1:A:1306:LYS:C	1:A:1308:TYR:N	2.57	0.55
4:D:90:LYS:HE3	4:D:130:ILE:HD11	1.88	0.55
19:S:46:ARG:HB2	19:S:101:ARG:HB2	1.89	0.55
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.46	0.55
1:A:116:LYS:HE2	1:A:181:HIS:CB	2.36	0.55
1:A:1109:TYR:HE2	1:A:1113:SER:H	1.55	0.55
13:M:179:GLU:N	20:T:154:LYS:HE3	2.22	0.55
16:P:256:GLN:O	16:P:316:LYS:NZ	2.32	0.55
20:T:140:ARG:O	20:T:141:LEU:CB	2.55	0.55
1:A:415:GLY:C	1:A:449:HIS:HD2	2.11	0.54
1:A:181:HIS:CD2	1:A:181:HIS:N	2.74	0.54
2:B:248:LYS:HA	19:S:169:LYS:HG2	1.89	0.54
13:M:90:ALA:CB	13:M:100:LYS:HE3	2.37	0.54
16:P:298:PRO:O	16:P:299:ARG:C	2.43	0.54
1:A:61:ARG:HB3	1:A:72:GLN:HE21	1.72	0.54
1:A:469:MET:HE3	2:B:1094:GLN:HG2	1.89	0.54
1:A:1222:THR:HB	21:U:241:THR:HG21	1.88	0.54
19:S:31:PHE:HB2	20:T:92:THR:HB	1.89	0.54
19:S:172:ASN:OD1	19:S:173:HIS:N	2.37	0.54
2:B:360:LYS:HG3	2:B:553:LEU:HD23	1.88	0.54
5:E:67:ASP:O	5:E:69:THR:N	2.41	0.54
13:M:52:TRP:CD1	13:M:52:TRP:O	2.60	0.54
16:P:294:ARG:NH1	22:X:14:DA:OP1	2.28	0.54
1:A:459:ASN:O	1:A:501:MET:HE2	2.07	0.54
1:A:1281:ASP:O	1:A:1285:LEU:N	2.35	0.54
2:B:232:THR:OG1	2:B:233:SER:N	2.38	0.54
6:F:102:ILE:HG22	6:F:104:ILE:HG12	1.89	0.54
20:T:139:VAL:CG1	20:T:142:SER:OG	2.55	0.54
1:A:936:GLU:HA	1:A:1002:SER:HB2	1.89	0.54
1:A:1113:SER:HB3	1:A:1309:MET:HE3	1.90	0.54
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.72	0.54
17:Q:153:ARG:HH11	17:Q:158:HIS:HB3	1.71	0.54
2:B:992:ASN:ND2	2:B:1018:TYR:CD2	2.74	0.54
2:B:1078:ARG:NH1	23:Y:50:DA:O3'	2.41	0.54
1:A:926:ASN:HB3	1:A:931:ARG:HG3	1.89	0.54
1:A:261:ARG:C	1:A:263:ALA:H	2.11	0.54
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.43	0.54
1:A:894:ASP:OD1	1:A:895:GLY:N	2.41	0.54
19:S:51:LEU:HD21	19:S:54:LYS:HD3	1.90	0.54
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:SER:C	1:A:624:GLY:H	2.01	0.54
3:C:30:VAL:HG22	11:K:45:ILE:HD11	1.90	0.54
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.43	0.54
13:M:193:ARG:NH1	23:Y:75:DC:OP1	2.41	0.54
1:A:522:PRO:HA	1:A:666:ARG:NE	2.09	0.53
2:B:529:MET:HG2	2:B:530:ALA:N	2.22	0.53
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.90	0.53
2:B:73:HIS:C	2:B:75:SER:N	2.61	0.53
2:B:109:MET:HG3	2:B:174:LEU:HD11	1.89	0.53
2:B:529:MET:HG3	2:B:624:PRO:HD2	1.90	0.53
5:E:6:GLU:OE2	5:E:9:ARG:NH1	2.39	0.53
9:I:103:ARG:O	9:I:105:GLU:HG2	2.09	0.53
3:C:47:ILE:H	3:C:47:ILE:HD12	1.73	0.53
3:C:154:ARG:HB3	10:J:65:LEU:CD2	2.38	0.53
12:L:35:ARG:HH12	12:L:42:ARG:NE	2.07	0.53
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.90	0.53
18:R:151:LEU:HB2	18:R:163:LEU:HD21	1.90	0.53
1:A:484:LEU:HD12	1:A:484:LEU:O	2.08	0.53
5:E:14:ARG:O	5:E:17:ILE:HG13	2.09	0.53
14:N:314:LEU:HD21	16:P:250:PHE:HB2	1.90	0.53
14:N:332:GLU:HB2	15:O:92:LYS:O	2.09	0.53
18:R:162:GLY:O	18:R:163:LEU:CB	2.56	0.53
1:A:269:SER:O	1:A:270:ALA:CB	2.55	0.53
3:C:70:LEU:HD23	10:J:5:VAL:O	2.07	0.53
3:C:82:LEU:HD23	3:C:167:LYS:HB2	1.90	0.53
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.42	0.53
6:F:56:TYR:CE1	6:F:124:ILE:HB	2.43	0.53
13:M:13:VAL:HG12	13:M:20:ASP:HB3	1.90	0.53
18:R:195:PRO:HB2	18:R:199:LYS:CG	2.38	0.53
1:A:299:ALA:HA	17:Q:60:ARG:NH2	2.23	0.53
1:A:1304:ILE:HG22	1:A:1340:GLY:HA3	1.91	0.53
3:C:147:ASP:O	10:J:16:ASN:HB3	2.08	0.53
1:A:270:ALA:O	1:A:272:ASN:N	2.42	0.53
2:B:386:ASP:OD2	2:B:502:HIS:HB2	2.09	0.53
1:A:297:GLY:HA3	17:Q:57:LYS:HB3	1.90	0.53
2:B:675:LEU:HD11	2:B:697:GLU:OE2	2.09	0.53
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.91	0.53
21:U:248:HIS:O	21:U:252:LYS:NZ	2.37	0.53
1:A:263:ALA:O	1:A:264:VAL:CG2	2.57	0.52
1:A:542:LEU:HD21	1:A:642:LYS:HB2	1.91	0.52
2:B:733:MET:HE1	2:B:1054:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.92	0.52
1:A:521:VAL:HB	1:A:522:PRO:HD3	1.90	0.52
18:R:80:LYS:HD3	20:T:188:PHE:HE2	1.74	0.52
20:T:12:ALA:HB2	20:T:106:LEU:HD13	1.90	0.52
1:A:1316:ASN:ND2	1:A:1318:LYS:CE	2.72	0.52
2:B:1163:MET:HA	2:B:1168:ALA:H	1.73	0.52
6:F:79:VAL:HG12	6:F:81:VAL:H	1.74	0.52
13:M:25:GLU:OE1	13:M:44:ARG:NH2	2.36	0.52
17:Q:25:PHE:HA	18:R:219:LEU:HD13	1.90	0.52
17:Q:180:PHE:CZ	18:R:213:ASP:N	2.76	0.52
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.43	0.52
20:T:208:GLN:HE21	20:T:213:LEU:HB2	1.74	0.52
21:U:279:ARG:NH1	21:U:280:SER:O	2.43	0.52
1:A:389:THR:HG21	1:A:417:LYS:HD2	1.90	0.52
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.91	0.52
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.77	0.52
18:R:151:LEU:HD12	18:R:163:LEU:HD21	1.89	0.52
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.24	0.52
6:F:73:ILE:HD11	6:F:96:GLU:OE2	2.08	0.52
17:Q:25:PHE:HD1	18:R:210:PHE:CZ	2.27	0.52
1:A:116:LYS:HE2	1:A:181:HIS:HB2	1.92	0.52
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.91	0.52
1:A:729:PRO:CG	21:U:250:MET:HB2	2.38	0.52
6:F:69:ARG:HG3	6:F:102:ILE:HD12	1.91	0.52
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.52
9:I:61:GLU:C	9:I:63:ASP:H	2.13	0.52
10:J:52:HIS:HE1	10:J:54:ASP:HA	1.75	0.52
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.92	0.52
2:B:483:ARG:NH1	2:B:527:ALA:O	2.43	0.52
2:B:906:GLN:HB3	12:L:45:TYR:HE1	1.75	0.52
2:B:976:MET:O	2:B:978:ILE:N	2.41	0.52
17:Q:75:ARG:HH21	17:Q:95:ASN:HD22	1.57	0.52
20:T:177:ARG:N	20:T:178:ALA:HB3	2.24	0.52
22:X:44:DT:H3'	22:X:45:DT:H5''	1.91	0.52
1:A:358:ARG:NH2	2:B:1076:GLU:HA	2.25	0.52
6:F:88:ASP:CG	6:F:91:LEU:H	2.12	0.52
17:Q:23:ARG:CZ	18:R:207:SER:O	2.48	0.52
1:A:263:ALA:O	1:A:264:VAL:HG22	2.10	0.52
1:A:467:MET:SD	1:A:524:MET:HB3	2.49	0.52
3:C:60:HIS:CD2	3:C:63:PHE:HB2	2.45	0.52
17:Q:105:TYR:HD1	18:R:234:GLU:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:45:DT:H5"	23:Y:46:DC:H5"	1.92	0.52
13:M:245:VAL:HG12	13:M:291:LEU:HD23	1.92	0.52
1:A:608:THR:HB	1:A:610:PRO:HD2	1.92	0.51
2:B:931:ILE:HD11	2:B:947:ILE:HA	1.92	0.51
9:I:119:CYS:HB3	9:I:121:HIS:HB2	1.90	0.51
13:M:178:LYS:HB3	20:T:154:LYS:CE	2.40	0.51
20:T:191:PHE:HZ	20:T:237:PRO:HG3	1.74	0.51
2:B:62:ALA:N	2:B:63:PRO:HD3	2.25	0.51
2:B:552:ASN:OD1	2:B:553:LEU:N	2.43	0.51
17:Q:44:LYS:HG3	17:Q:47:ASP:H	1.76	0.51
1:A:790:GLN:NE2	1:A:797:ARG:HG2	2.25	0.51
1:A:1316:ASN:CG	1:A:1318:LYS:HE2	2.31	0.51
2:B:490:GLY:O	2:B:491:ARG:CG	2.59	0.51
3:C:157:GLN:CG	10:J:65:LEU:CB	2.85	0.51
5:E:172:ARG:HD3	5:E:210:GLN:HG2	1.92	0.51
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.93	0.51
18:R:212:VAL:O	18:R:213:ASP:OD1	2.28	0.51
1:A:255:VAL:HG13	1:A:280:LEU:HD21	1.91	0.51
1:A:972:THR:HA	1:A:1320:ILE:HG21	1.91	0.51
2:B:50:PHE:O	2:B:54:SER:HB2	2.11	0.51
2:B:363:TYR:CD2	2:B:553:LEU:HD21	2.45	0.51
3:C:267:ILE:HG13	3:C:272:LEU:HB3	1.92	0.51
17:Q:109:HIS:CE1	18:R:233:ILE:CG2	2.93	0.51
1:A:1158:LEU:HD11	1:A:1308:TYR:HD2	1.76	0.51
9:I:61:GLU:O	9:I:63:ASP:HB2	2.10	0.51
17:Q:25:PHE:CD2	18:R:219:LEU:CD1	2.94	0.51
21:U:227:GLU:O	21:U:228:MET:HE3	2.04	0.51
1:A:334:ARG:NH2	13:M:66:ARG:O	2.44	0.51
2:B:749:HIS:CD2	2:B:810:PHE:HD1	2.27	0.51
5:E:52:ARG:NH2	5:E:54:ARG:HD3	2.26	0.51
5:E:149:VAL:HG23	5:E:192:LYS:HB3	1.92	0.51
13:M:94:ASP:O	13:M:97:GLY:N	2.42	0.51
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.93	0.51
2:B:309:PHE:CZ	9:I:40:ARG:HB2	2.46	0.51
9:I:65:LEU:CA	9:I:122:ARG:HE	2.24	0.51
14:N:366:ILE:O	15:O:54:ASN:ND2	2.44	0.51
1:A:362:SER:OG	2:B:1084:LEU:HB2	2.11	0.51
1:A:859:TYR:OH	1:A:863:ARG:NH2	2.41	0.51
1:A:1162:GLU:HB3	1:A:1306:LYS:CA	2.40	0.51
5:E:63:ALA:O	5:E:64:HIS:CG	2.64	0.51
8:H:95:LYS:HB2	8:H:139:SER:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:ARG:O	9:I:105:GLU:N	2.44	0.51
10:J:66:GLU:HG3	12:L:23:HIS:CG	2.46	0.51
17:Q:180:PHE:HE1	18:R:212:VAL:C	2.12	0.51
22:X:42:DT:H2''	22:X:43:DT:H5''	1.92	0.51
1:A:604:ARG:HG3	1:A:606:HIS:HE1	1.76	0.51
13:M:178:LYS:HG2	20:T:156:VAL:HG12	1.91	0.51
17:Q:141:ALA:HB1	17:Q:152:PHE:CE2	2.44	0.51
1:A:261:ARG:HD2	1:A:277:THR:OG1	2.11	0.51
1:A:678:ASN:O	1:A:681:LEU:HB3	2.10	0.51
2:B:914:GLU:OE1	2:B:914:GLU:N	2.40	0.51
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.46	0.51
12:L:26:ASN:HD21	12:L:28:ILE:HD12	1.76	0.51
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.91	0.51
1:A:11:SER:O	2:B:1135:TYR:OH	2.27	0.50
2:B:553:LEU:HB2	2:B:573:TRP:HZ3	1.75	0.50
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.26	0.50
3:C:49:TRP:CZ3	12:L:54:VAL:HG21	2.46	0.50
9:I:61:GLU:O	9:I:62:VAL:C	2.46	0.50
15:O:64:THR:HG22	15:O:75:VAL:HB	1.92	0.50
19:S:26:TYR:CD1	20:T:97:THR:HG22	2.46	0.50
22:X:52:DG:H2''	22:X:53:DA:O4'	2.11	0.50
1:A:201:GLU:CG	1:A:212:LYS:HB3	2.40	0.50
2:B:499:ARG:CZ	2:B:522:LEU:HD11	2.41	0.50
2:B:1040:GLN:CD	2:B:1040:GLN:N	2.63	0.50
17:Q:17:LEU:HD21	17:Q:191:LEU:HB3	1.93	0.50
2:B:716:HIS:CE1	2:B:1007:ASN:HD21	2.29	0.50
2:B:867:ILE:O	2:B:893:SER:HB2	2.11	0.50
2:B:1060:HIS:HB2	2:B:1078:ARG:HE	1.75	0.50
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.92	0.50
1:A:604:ARG:HG3	1:A:606:HIS:CE1	2.45	0.50
2:B:1072:ARG:HG3	2:B:1072:ARG:O	2.10	0.50
2:B:240:LEU:O	2:B:253:GLY:HA2	2.11	0.50
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.50
2:B:891:ASP:OD1	2:B:892:CYS:N	2.44	0.50
7:G:158:PHE:N	7:G:158:PHE:CD1	2.80	0.50
21:U:286:THR:HG21	21:U:299:LYS:HD2	1.93	0.50
2:B:72:GLN:HB3	2:B:76:GLY:HA3	1.92	0.50
2:B:1101:GLN:HE22	6:F:64:ARG:HG2	1.76	0.50
22:X:19:DG:N2	23:Y:76:DC:O2	2.44	0.50
1:A:366:VAL:O	1:A:481:THR:HB	2.12	0.50
2:B:483:ARG:HG3	2:B:526:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:855:ALA:HB2	12:L:46:LYS:HE2	1.93	0.50
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.93	0.50
17:Q:25:PHE:O	18:R:219:LEU:CD2	2.59	0.50
1:A:1407:CYS:SG	1:A:1408:ARG:N	2.84	0.50
2:B:957:THR:O	2:B:960:GLY:N	2.36	0.50
2:B:1132:THR:HG23	2:B:1133:HIS:ND1	2.27	0.50
3:C:49:TRP:O	3:C:163:ALA:HA	2.12	0.50
8:H:108:ALA:O	8:H:109:ALA:C	2.47	0.50
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	2.11	0.50
20:T:166:GLU:HA	20:T:169:LYS:HE3	1.92	0.50
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.12	0.50
1:A:673:GLN:O	1:A:677:ASN:CB	2.60	0.50
1:A:1276:VAL:HG12	1:A:1279:MET:HB2	1.93	0.50
2:B:326:ALA:HB2	2:B:338:TYR:HE2	1.76	0.50
17:Q:188:TYR:HD1	17:Q:191:LEU:HD22	1.77	0.50
18:R:227:SER:O	18:R:228:MET:O	2.30	0.50
2:B:489:ILE:HG13	2:B:490:GLY:H	1.77	0.49
19:S:26:TYR:HD1	20:T:97:THR:HG22	1.76	0.49
22:X:13:DT:H2''	22:X:14:DA:H8	1.77	0.49
22:X:45:DT:H4'	22:X:45:DT:OP1	2.12	0.49
23:Y:62:DC:H1'	23:Y:63:DG:H4'	1.93	0.49
1:A:930:LEU:C	1:A:931:ARG:O	2.49	0.49
1:A:1158:LEU:HD11	1:A:1308:TYR:CD2	2.47	0.49
1:A:1471:PHE:HE1	6:F:64:ARG:HD3	1.77	0.49
8:H:74:GLU:C	8:H:76:ASN:N	2.57	0.49
13:M:7:LEU:HG	13:M:10:LEU:HD11	1.94	0.49
17:Q:164:ASP:O	17:Q:166:SER:N	2.45	0.49
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.46	0.49
1:A:621:ILE:C	1:A:623:PRO:N	2.62	0.49
1:A:893:GLU:HG2	5:E:203:TYR:CD1	2.46	0.49
1:A:375:ILE:HG21	1:A:666:ARG:NH1	2.26	0.49
2:B:626:LEU:HG	2:B:698:ILE:HG22	1.95	0.49
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.93	0.49
12:L:19:CYS:HB3	12:L:22:CYS:SG	2.53	0.49
13:M:276:ASP:HA	20:T:153:TYR:CE1	2.47	0.49
17:Q:95:ASN:OD1	17:Q:96:TYR:N	2.45	0.49
18:R:80:LYS:HB2	20:T:188:PHE:CE2	2.47	0.49
19:S:15:VAL:HA	20:T:42:LYS:HG2	1.93	0.49
1:A:133:SER:HG	1:A:136:GLN:CB	2.13	0.49
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.23	0.49
2:B:935:PHE:CE1	2:B:1050:ARG:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:HIS:CE1	2:B:1078:ARG:HG3	2.47	0.49
3:C:116:THR:HB	3:C:146:ASP:HB2	1.93	0.49
12:L:56:ASP:OD1	12:L:56:ASP:N	2.46	0.49
20:T:140:ARG:O	20:T:141:LEU:HB2	2.13	0.49
20:T:175:ARG:HE	22:X:21:DG:P	2.36	0.49
1:A:1306:LYS:O	1:A:1307:VAL:C	2.49	0.49
13:M:178:LYS:HB3	20:T:154:LYS:HE3	1.93	0.49
2:B:555:GLU:OE1	19:S:124:TYR:OH	2.18	0.49
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.94	0.49
5:E:48:PRO:O	5:E:52:ARG:NH1	2.45	0.49
9:I:57:LYS:O	9:I:58:ILE:HG12	2.13	0.49
2:B:1092:ASP:HA	2:B:1095:ILE:HD12	1.94	0.49
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.94	0.49
17:Q:23:ARG:HD3	18:R:207:SER:O	2.12	0.49
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.43	0.49
1:A:522:PRO:CA	1:A:666:ARG:HE	2.10	0.49
1:A:1167:ARG:HA	1:A:1293:LEU:HD22	1.93	0.49
2:B:177:CYS:HB3	2:B:180:ASP:HB2	1.95	0.49
2:B:324:ARG:NH1	19:S:162:GLU:OE2	2.46	0.49
14:N:323:GLU:HG2	14:N:325:GLY:HA3	1.94	0.49
20:T:177:ARG:H	20:T:178:ALA:HB3	1.76	0.49
1:A:53:LYS:HE3	1:A:59:ASP:HB3	1.95	0.49
1:A:560:VAL:HG21	1:A:586:TRP:CE3	2.48	0.49
2:B:677:MET:HG3	2:B:678:THR:HG23	1.95	0.49
2:B:871:VAL:HG13	2:B:890:ARG:HB2	1.95	0.49
17:Q:112:ARG:CG	18:R:237:LEU:HD11	2.37	0.49
1:A:932:ARG:HE	1:A:943:LEU:HD22	1.78	0.48
3:C:169:PHE:HE1	3:C:171:LYS:HB3	1.78	0.48
3:C:169:PHE:CE1	3:C:171:LYS:HB3	2.47	0.48
7:G:1:MET:N	7:G:78:ARG:O	2.45	0.48
8:H:85:ALA:HB1	8:H:88:PHE:CD2	2.47	0.48
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.95	0.48
19:S:124:TYR:HB3	20:T:20:LEU:HD11	1.95	0.48
2:B:418:TYR:CD1	2:B:434:ALA:HB2	2.48	0.48
3:C:75:SER:HB3	3:C:79:VAL:HB	1.95	0.48
22:X:29:DC:H2''	22:X:30:DG:H5'	1.94	0.48
1:A:1065:PHE:CE2	1:A:1069:LEU:HD11	2.49	0.48
2:B:598:VAL:C	2:B:600:GLU:H	2.16	0.48
3:C:7:PRO:O	3:C:8:THR:OG1	2.29	0.48
13:M:300:PHE:HD2	13:M:306:PHE:HE1	1.62	0.48
17:Q:188:TYR:CE1	18:R:210:PHE:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:139:VAL:HG13	20:T:142:SER:OG	2.12	0.48
1:A:1162:GLU:CG	1:A:1306:LYS:HB2	2.38	0.48
2:B:422:PHE:HD1	2:B:428:ASP:H	1.62	0.48
2:B:810:PHE:CD2	2:B:927:ARG:NH2	2.81	0.48
2:B:1101:GLN:NE2	6:F:64:ARG:CG	2.77	0.48
17:Q:184:ILE:HD11	18:R:213:ASP:OD2	2.14	0.48
22:X:46:DT:H2'	22:X:47:DT:C5	2.48	0.48
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.77	0.48
2:B:798:ARG:O	2:B:801:VAL:HG22	2.14	0.48
2:B:852:GLY:O	2:B:868:GLY:N	2.30	0.48
10:J:6:ARG:HA	10:J:13:ILE:HA	1.96	0.48
2:B:250:SER:O	2:B:251:ALA:C	2.52	0.48
2:B:464:ALA:HB1	13:M:62:LYS:NZ	2.28	0.48
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.95	0.48
5:E:13:ILE:HG22	5:E:136:LEU:HA	1.94	0.48
5:E:64:HIS:HE1	5:E:68:PRO:CB	2.21	0.48
8:H:93:TYR:HE1	8:H:140:ARG:HA	1.79	0.48
1:A:455:ILE:HD13	1:A:520:MET:CE	2.43	0.48
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.96	0.48
5:E:71:GLN:HE21	5:E:99:ILE:HG22	1.79	0.48
1:A:30:GLU:CD	1:A:33:ARG:HH21	2.16	0.48
1:A:265:VAL:HG23	1:A:266:MET:H	1.79	0.48
1:A:1162:GLU:CB	1:A:1306:LYS:CA	2.91	0.48
2:B:474:THR:HG23	2:B:732:ALA:O	2.13	0.48
2:B:881:GLU:OE1	2:B:883:THR:OG1	2.23	0.48
3:C:148:ILE:HG12	3:C:149:LEU:N	2.28	0.48
11:K:47:LYS:HD2	11:K:61:TYR:HD1	1.78	0.48
17:Q:113:ARG:NH2	18:R:218:LYS:HG3	2.29	0.48
22:X:50:DT:H4'	22:X:50:DT:OP1	2.13	0.48
1:A:686:THR:OG1	1:A:687:ILE:N	2.46	0.48
1:A:868:MET:HE1	1:A:1400:LEU:HG	1.96	0.48
2:B:356:PHE:O	19:S:116:GLY:HA2	2.13	0.48
2:B:726:SER:O	2:B:730:LYS:HE2	2.14	0.48
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.78	0.48
2:B:964:ASP:OD1	2:B:964:ASP:N	2.47	0.48
17:Q:69:ASP:HA	18:R:226:ASP:CG	2.34	0.48
1:A:117:LEU:HB2	1:A:232:GLU:HG2	1.96	0.48
1:A:621:ILE:O	1:A:623:PRO:CD	2.61	0.48
16:P:156:SER:O	16:P:158:SER:N	2.47	0.48
18:R:195:PRO:HB2	18:R:199:LYS:HG3	1.95	0.48
18:R:222:SER:C	18:R:224:THR:N	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLY:C	1:A:182:GLY:N	2.67	0.47
1:A:807:LEU:HB3	1:A:809:HIS:HD2	1.78	0.47
2:B:964:ASP:O	2:B:965:ILE:HG13	2.14	0.47
3:C:157:GLN:HG3	10:J:65:LEU:CB	2.44	0.47
13:M:86:LYS:NZ	22:X:40:DT:N3	2.61	0.47
16:P:293:TYR:HD2	16:P:302:LEU:HD13	1.78	0.47
17:Q:68:GLY:C	18:R:226:ASP:CG	2.73	0.47
17:Q:105:TYR:CD1	18:R:234:GLU:CB	2.97	0.47
18:R:167:LEU:HD22	18:R:200:ILE:HB	1.96	0.47
20:T:81:HIS:HB3	20:T:116:CYS:SG	2.54	0.47
23:Y:52:DT:H2''	23:Y:53:DG:O4'	2.13	0.47
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.96	0.47
2:B:812:ARG:NH2	23:Y:52:DT:OP1	2.38	0.47
2:B:1000:THR:HG23	2:B:1001:PRO:HD2	1.96	0.47
5:E:129:GLN:OE1	5:E:130:PHE:N	2.47	0.47
13:M:45:VAL:C	13:M:47:ASP:H	2.15	0.47
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.49	0.47
2:B:94:SER:OG	2:B:95:LYS:N	2.47	0.47
2:B:455:ASP:O	2:B:457:LYS:N	2.40	0.47
4:D:30:GLU:O	7:G:3:TYR:HA	2.13	0.47
18:R:119:LEU:HA	18:R:123:ALA:HB3	1.95	0.47
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.95	0.47
1:A:1138:SER:OG	1:A:1139:LEU:N	2.46	0.47
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.79	0.47
2:B:628:VAL:HG21	2:B:682:LEU:HD11	1.97	0.47
3:C:184:PHE:HD1	3:C:231:TYR:CE1	2.33	0.47
13:M:75:LEU:HD22	13:M:139:ASN:OD1	2.14	0.47
17:Q:153:ARG:HD3	17:Q:158:HIS:HB3	1.94	0.47
1:A:275:ASP:OD1	1:A:276:LEU:N	2.47	0.47
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	2.33	0.47
2:B:676:ALA:HB2	2:B:693:TYR:CG	2.50	0.47
5:E:26:TYR:HA	5:E:64:HIS:C	2.14	0.47
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.97	0.47
13:M:9:ALA:CA	13:M:10:LEU:HD13	2.37	0.47
13:M:32:MET:O	13:M:40:VAL:HA	2.15	0.47
1:A:889:LEU:HD21	5:E:206:TYR:HE1	1.80	0.47
2:B:124:LEU:HD23	2:B:149:ILE:HD11	1.95	0.47
2:B:947:ILE:HG12	2:B:948:GLN:N	2.29	0.47
2:B:1124:ILE:HG22	2:B:1126:ALA:H	1.78	0.47
3:C:86:ARG:HH22	11:K:10:PHE:HE1	1.62	0.47
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:GLN:O	9:I:100:HIS:N	2.48	0.47
17:Q:173:ALA:O	17:Q:177:LEU:HD23	2.15	0.47
18:R:195:PRO:O	18:R:196:ASP:CB	2.59	0.47
1:A:557:ARG:HB3	1:A:557:ARG:HH11	1.79	0.47
1:A:616:GLY:O	1:A:619:LYS:HB2	2.15	0.47
1:A:790:GLN:CD	1:A:797:ARG:HG2	2.34	0.47
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.97	0.47
1:A:1263:ASN:HB2	1:A:1268:LYS:HD2	1.96	0.47
1:A:1320:ILE:HD12	1:A:1329:LYS:O	2.14	0.47
2:B:960:GLY:O	2:B:962:THR:N	2.48	0.47
20:T:141:LEU:HB3	20:T:142:SER:H	1.50	0.47
1:A:119:VAL:HG21	1:A:147:LEU:HD21	1.97	0.47
1:A:1319:LYS:HA	1:A:1319:LYS:HD3	1.69	0.47
2:B:1091:ARG:O	2:B:1095:ILE:HG13	2.14	0.47
13:M:30:GLY:HA2	13:M:44:ARG:HG2	1.96	0.47
1:A:1171:ALA:O	9:I:59:THR:HG23	2.15	0.47
2:B:796:MET:O	2:B:948:GLN:HA	2.14	0.47
2:B:1066:PRO:HB2	2:B:1075:MET:HG3	1.97	0.47
9:I:73:SER:HA	9:I:95:VAL:HG21	1.97	0.47
17:Q:101:ASN:ND2	17:Q:202:GLU:OE2	2.40	0.47
20:T:80:GLU:O	20:T:119:ALA:HB2	2.14	0.47
1:A:264:VAL:CG2	1:A:272:ASN:OD1	2.44	0.47
1:A:1189:ASP:O	1:A:1192:TRP:N	2.48	0.47
10:J:40:LEU:HD11	10:J:49:LEU:HD13	1.97	0.47
18:R:164:GLY:CA	18:R:203:PHE:HZ	1.88	0.47
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.97	0.47
1:A:365:THR:HG22	2:B:1059:ILE:HG22	1.98	0.46
1:A:576:GLN:HG3	1:A:577:PRO:HD2	1.97	0.46
3:C:35:ARG:HG2	3:C:36:ARG:N	2.30	0.46
3:C:76:ASP:OD1	3:C:243:THR:HG21	2.15	0.46
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.28	0.46
10:J:63:ALA:N	10:J:64:PRO:CD	2.77	0.46
15:O:77:ASN:OD1	15:O:78:ASP:N	2.48	0.46
20:T:198:ASN:OD1	20:T:199:LEU:N	2.49	0.46
1:A:578:ALA:HB3	1:A:587:THR:HG23	1.96	0.46
1:A:1116:ASN:O	1:A:1117:VAL:HB	2.14	0.46
2:B:213:SER:HA	2:B:242:ARG:HD2	1.96	0.46
2:B:282:ARG:HD2	9:I:21:ASN:HD21	1.81	0.46
13:M:196:LYS:NZ	22:X:13:DT:OP1	2.41	0.46
18:R:224:THR:OG1	18:R:225:VAL:N	2.48	0.46
1:A:367:ILE:HA	1:A:482:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:HIS:NE2	9:I:100:HIS:HA	2.31	0.46
1:A:966:LEU:HD13	1:A:1043:ILE:HD11	1.96	0.46
2:B:348:LEU:HD13	2:B:364:PHE:HD2	1.79	0.46
8:H:65:TYR:CE2	8:H:70:LEU:HD22	2.50	0.46
8:H:65:TYR:CG	8:H:70:LEU:HD22	2.50	0.46
19:S:122:THR:HA	20:T:24:PRO:HA	1.97	0.46
1:A:511:THR:HG21	2:B:1105:GLU:OE2	2.16	0.46
1:A:525:ILE:HG12	1:A:666:ARG:NH2	2.30	0.46
1:A:623:PRO:C	1:A:625:ASP:N	2.68	0.46
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.79	0.46
1:A:1224:ARG:HH22	1:A:1306:LYS:HD3	1.72	0.46
1:A:1319:LYS:O	1:A:1321:ILE:HG23	2.15	0.46
1:A:1472:ASP:HB2	6:F:107:ARG:HB3	1.97	0.46
2:B:224:CYS:O	2:B:225:LEU:C	2.54	0.46
2:B:950:ARG:HB2	2:B:952:GLU:OE1	2.15	0.46
2:B:1101:GLN:HE22	6:F:64:ARG:CG	2.29	0.46
3:C:6:GLN:O	11:K:104:ARG:NH1	2.49	0.46
3:C:157:GLN:NE2	10:J:65:LEU:HB3	2.31	0.46
17:Q:180:PHE:CE1	18:R:213:ASP:N	2.84	0.46
18:R:163:LEU:HD12	18:R:163:LEU:O	2.15	0.46
2:B:526:LEU:HD12	2:B:526:LEU:HA	1.48	0.46
1:A:42:LYS:NZ	1:A:43:TYR:O	2.49	0.46
1:A:1158:LEU:O	1:A:1162:GLU:HG3	2.15	0.46
1:A:1162:GLU:CB	1:A:1306:LYS:HA	2.45	0.46
1:A:1185:VAL:HG21	9:I:51:SER:OG	2.16	0.46
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	2.36	0.46
5:E:65:ASN:OD1	5:E:67:ASP:N	2.42	0.46
16:P:206:GLU:C	16:P:208:ARG:N	2.67	0.46
1:A:196:LEU:HG	1:A:325:LEU:HD21	1.98	0.46
1:A:1128:ILE:HD12	1:A:1414:ILE:HD11	1.98	0.46
1:A:1162:GLU:CA	1:A:1306:LYS:HA	2.46	0.46
1:A:1318:LYS:HE2	1:A:1318:LYS:HB2	1.70	0.46
1:A:1408:ARG:O	1:A:1410:HIS:N	2.48	0.46
9:I:58:ILE:C	9:I:60:HIS:H	2.18	0.46
11:K:111:ASP:C	11:K:113:GLN:H	2.15	0.46
17:Q:188:TYR:CE1	18:R:210:PHE:CG	3.04	0.46
19:S:128:THR:HG22	19:S:136:GLU:HB3	1.98	0.46
23:Y:54:DA:H3'	23:Y:55:DG:H5''	1.97	0.46
1:A:116:LYS:HE2	1:A:181:HIS:HB3	1.98	0.46
1:A:608:THR:CB	1:A:610:PRO:HG2	2.45	0.46
13:M:183:VAL:HG12	20:T:152:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:104:LYS:HE3	17:Q:105:TYR:CZ	2.50	0.46
18:R:80:LYS:HG2	18:R:108:HIS:HE1	1.81	0.46
18:R:151:LEU:HB3	18:R:154:LEU:HB3	1.97	0.46
2:B:248:LYS:O	2:B:249:LYS:HB2	2.16	0.46
2:B:422:PHE:CD1	2:B:427:LYS:HA	2.50	0.46
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.94	0.46
10:J:3:ILE:HD13	10:J:18:TRP:CD2	2.50	0.46
10:J:64:PRO:C	10:J:66:GLU:N	2.56	0.46
10:J:66:GLU:HG3	12:L:23:HIS:CE1	2.49	0.46
14:N:313:PRO:HD2	16:P:250:PHE:HB3	1.98	0.46
17:Q:185:GLU:HB3	17:Q:186:PRO:HD3	1.97	0.46
20:T:229:HIS:CD2	22:X:28:DG:H21	2.33	0.46
22:X:59:DC:H2''	22:X:60:DG:O5'	2.16	0.46
1:A:818:GLU:H	1:A:818:GLU:CD	2.19	0.46
12:L:16:ILE:HG21	12:L:47:LYS:HD2	1.98	0.46
18:R:116:LYS:HA	18:R:119:LEU:HD12	1.98	0.46
19:S:18:VAL:HG22	19:S:137:ALA:HB3	1.98	0.46
21:U:243:GLU:O	21:U:247:GLU:N	2.46	0.46
23:Y:58:DC:H1'	23:Y:59:DG:C4	2.51	0.46
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.45
2:B:972:ILE:O	2:B:976:MET:N	2.48	0.45
2:B:1062:ARG:HH12	2:B:1075:MET:N	2.11	0.45
5:E:41:LYS:HG3	5:E:46:ASP:HB2	1.97	0.45
5:E:91:CYS:HA	5:E:94:MET:HG2	1.98	0.45
8:H:74:GLU:C	8:H:76:ASN:H	2.13	0.45
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.81	0.45
14:N:333:ASN:HB3	14:N:359:ASN:O	2.16	0.45
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.56	0.45
17:Q:128:LYS:HG3	17:Q:129:CYS:N	2.31	0.45
19:S:166:ARG:HH11	19:S:166:ARG:CG	2.28	0.45
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.99	0.45
2:B:934:LYS:HE2	2:B:942:LYS:HD2	1.99	0.45
3:C:31:ALA:HB1	3:C:184:PHE:HE1	1.80	0.45
3:C:68:LEU:HA	3:C:68:LEU:HD12	1.66	0.45
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.34	0.45
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.51	0.45
10:J:3:ILE:HG13	10:J:52:HIS:CD2	2.51	0.45
17:Q:112:ARG:NH2	18:R:237:LEU:O	2.50	0.45
1:A:26:LEU:O	1:A:26:LEU:HD12	2.17	0.45
1:A:375:ILE:HA	1:A:375:ILE:HD13	1.69	0.45
1:A:672:ILE:HD13	1:A:672:ILE:HG21	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:THR:HG1	1:A:880:ARG:HE	1.64	0.45
1:A:963:ARG:O	1:A:967:ARG:HG3	2.16	0.45
1:A:1128:ILE:HD13	1:A:1128:ILE:HA	1.80	0.45
1:A:1158:LEU:HD21	1:A:1308:TYR:CD2	2.51	0.45
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.97	0.45
2:B:226:GLU:OE2	2:B:617:ASP:CB	2.57	0.45
2:B:1001:PRO:HB2	2:B:1002:PHE:CE1	2.51	0.45
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.52	0.45
16:P:263:ASP:OD1	16:P:264:VAL:N	2.49	0.45
1:A:43:TYR:O	1:A:45:GLU:N	2.49	0.45
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.90	0.45
1:A:931:ARG:C	1:A:933:THR:H	2.20	0.45
4:D:140:PHE:CZ	4:D:142:TYR:HB3	2.52	0.45
5:E:116:GLN:O	5:E:119:VAL:HB	2.16	0.45
9:I:41:ASN:HB2	19:S:153:ARG:HD2	1.99	0.45
13:M:157:ASP:OD2	13:M:185:ARG:NH2	2.49	0.45
16:P:298:PRO:O	16:P:300:ILE:N	2.49	0.45
17:Q:184:ILE:HD11	18:R:218:LYS:NZ	2.19	0.45
19:S:127:PHE:HB2	20:T:19:TRP:HB2	1.98	0.45
1:A:208:ASP:OD1	1:A:209:SER:N	2.38	0.45
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.45	0.45
1:A:618:TYR:C	1:A:620:HIS:H	2.20	0.45
2:B:333:GLU:CD	19:S:53:ASN:HD21	2.17	0.45
3:C:212:ASP:O	3:C:213:GLU:C	2.53	0.45
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.97	0.45
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.82	0.45
13:M:130:LEU:HA	13:M:131:PRO:HD3	1.82	0.45
14:N:312:GLU:C	14:N:314:LEU:H	2.20	0.45
18:R:171:ILE:HG12	18:R:177:ASN:H	1.81	0.45
18:R:205:ASP:O	18:R:206:LYS:HE3	2.16	0.45
1:A:263:ALA:C	1:A:264:VAL:HG22	2.37	0.45
1:A:516:GLN:HA	1:A:520:MET:CE	2.46	0.45
1:A:516:GLN:HA	1:A:520:MET:HE2	1.97	0.45
1:A:873:VAL:HG22	1:A:1083:PRO:HA	1.99	0.45
18:R:123:ALA:O	18:R:127:ASN:HB2	2.16	0.45
1:A:197:GLU:CD	13:M:93:PHE:CE2	2.89	0.45
1:A:267:GLN:O	1:A:268:GLY:C	2.55	0.45
1:A:375:ILE:HD12	1:A:375:ILE:HG23	1.54	0.45
1:A:451:CYS:SG	1:A:452:ASP:N	2.88	0.45
1:A:524:MET:N	1:A:524:MET:SD	2.82	0.45
1:A:865:ILE:HD12	2:B:1092:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ASP:O	1:A:1031:ARG:NH2	2.49	0.45
1:A:1119:LEU:HD13	1:A:1388:PHE:CG	2.52	0.45
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	1.98	0.45
1:A:1162:GLU:HG2	1:A:1306:LYS:CA	2.47	0.45
1:A:1408:ARG:HH22	1:A:1421:ARG:HB2	1.81	0.45
1:A:1451:MET:CE	1:A:1456:GLU:HB3	2.47	0.45
3:C:85:SER:CB	3:C:166:LYS:HE3	2.47	0.45
3:C:149:LEU:HD21	3:C:152:LYS:HG3	1.98	0.45
13:M:178:LYS:NZ	20:T:156:VAL:HG11	2.31	0.45
17:Q:36:ILE:HG23	17:Q:39:ARG:NH2	2.32	0.45
1:A:529:GLN:HG3	1:A:1094:SER:HB3	1.98	0.45
1:A:610:PRO:HB3	1:A:626:THR:CG2	2.47	0.45
2:B:79:GLU:O	2:B:80:GLU:HG2	2.17	0.45
2:B:180:ASP:OD1	2:B:181:PRO:HD2	2.16	0.45
2:B:531:TYR:CD2	2:B:532:ILE:N	2.85	0.45
7:G:116:GLU:O	7:G:130:THR:HA	2.16	0.45
9:I:92:LYS:HG3	9:I:93:GLU:HG2	1.99	0.45
17:Q:25:PHE:CE1	18:R:210:PHE:CZ	3.05	0.45
17:Q:187:ILE:HG21	18:R:210:PHE:O	2.16	0.45
21:U:255:GLY:C	21:U:256:THR:HG23	2.37	0.45
1:A:599:HIS:O	1:A:992:LYS:NZ	2.50	0.45
1:A:1103:THR:HG23	1:A:1106:THR:OG1	2.17	0.45
2:B:91:ILE:HD11	2:B:124:LEU:HD11	1.98	0.45
2:B:109:MET:O	2:B:112:GLU:N	2.50	0.45
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.99	0.45
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.49	0.45
5:E:47:LYS:HA	5:E:47:LYS:HD3	1.63	0.45
11:K:5:PRO:HB2	11:K:7:PHE:CE2	2.52	0.45
1:A:205:VAL:O	1:A:206:ASN:CB	2.66	0.44
1:A:1429:LYS:HB2	1:A:1438:VAL:HG21	2.00	0.44
2:B:936:ALA:O	2:B:1049:GLN:N	2.42	0.44
2:B:1028:LEU:C	2:B:1029:TYR:HD1	2.21	0.44
2:B:1062:ARG:HH21	2:B:1065:GLY:N	2.10	0.44
5:E:11:TRP:CE3	5:E:37:LEU:HD13	2.51	0.44
10:J:3:ILE:HG22	10:J:15:GLY:HA2	1.99	0.44
17:Q:188:TYR:CE2	18:R:211:SER:HB3	2.52	0.44
22:X:48:DT:OP1	22:X:48:DT:H4'	2.16	0.44
1:A:932:ARG:NE	1:A:943:LEU:HD22	2.30	0.44
1:A:1468:THR:HA	6:F:60:TYR:HB3	1.98	0.44
2:B:573:TRP:O	2:B:573:TRP:HE3	2.00	0.44
3:C:275:ASN:ND2	11:K:23:LYS:HA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:ARG:NH2	5:E:54:ARG:HH11	2.15	0.44
14:N:25:VAL:HG11	15:O:36:VAL:HG13	1.97	0.44
16:P:297:LYS:C	16:P:299:ARG:N	2.71	0.44
1:A:186:ARG:HH11	1:A:208:ASP:HB2	1.82	0.44
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.52	0.44
2:B:322:GLY:O	2:B:326:ALA:N	2.34	0.44
14:N:376:TRP:HD1	15:O:62:LEU:O	2.01	0.44
20:T:194:HIS:N	20:T:197:TYR:OH	2.50	0.44
21:U:134:PRO:HG2	21:U:174:GLU:HG2	1.99	0.44
2:B:747:LEU:HD11	2:B:810:PHE:HZ	1.79	0.44
2:B:899:SER:O	2:B:901:THR:N	2.51	0.44
7:G:18:PHE:HA	7:G:22:LEU:HD13	2.00	0.44
8:H:71:ASP:OD1	8:H:71:ASP:N	2.48	0.44
1:A:729:PRO:O	21:U:252:LYS:O	2.36	0.44
1:A:893:GLU:O	5:E:200:ALA:HB2	2.17	0.44
1:A:1103:THR:HG21	1:A:1119:LEU:HG	1.99	0.44
1:A:1112:VAL:HG12	21:U:254:GLY:HA2	2.00	0.44
2:B:41:ARG:HD2	2:B:41:ARG:HA	1.36	0.44
2:B:271:ILE:HD12	2:B:311:ILE:HD11	2.00	0.44
6:F:105:ILE:HG22	6:F:119:GLY:HA2	2.00	0.44
13:M:34:CYS:HB2	13:M:39:LEU:HB3	1.99	0.44
15:O:7:ARG:HB3	15:O:16:GLN:NE2	2.32	0.44
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.99	0.44
2:B:809:VAL:HG23	2:B:924:ARG:HG3	1.99	0.44
2:B:1055:VAL:HG13	2:B:1056:ASP:N	2.33	0.44
2:B:1162:LEU:O	2:B:1167:ILE:HB	2.18	0.44
3:C:134:ASN:C	3:C:136:ASP:OD1	2.56	0.44
13:M:52:TRP:O	13:M:54:THR:N	2.45	0.44
17:Q:126:SER:O	17:Q:164:ASP:HB2	2.18	0.44
18:R:88:ARG:NH1	18:R:97:LEU:HD11	2.33	0.44
1:A:263:ALA:CB	1:A:272:ASN:HB3	2.46	0.44
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.17	0.44
1:A:1407:CYS:SG	1:A:1408:ARG:HG2	2.58	0.44
2:B:289:ILE:HG12	2:B:291:ASP:H	1.82	0.44
4:D:70:ARG:NE	7:G:142:GLU:OE2	2.42	0.44
9:I:84:HIS:CD2	9:I:84:HIS:N	2.81	0.44
15:O:80:GLU:HG3	15:O:89:LYS:HG2	1.98	0.44
1:A:614:ASP:OD2	21:U:267:LYS:HG3	2.17	0.44
1:A:1306:LYS:C	1:A:1308:TYR:H	2.20	0.44
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.00	0.44
2:B:783:ALA:HB2	2:B:1041:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLU:HG2	3:C:228:ARG:CG	2.46	0.44
4:D:26:PHE:CE2	7:G:78:ARG:HG2	2.53	0.44
18:R:157:GLN:HG3	18:R:159:ASP:H	1.82	0.44
1:A:932:ARG:HB3	1:A:940:LYS:HA	2.00	0.44
1:A:987:ILE:HD13	1:A:1058:PHE:CD2	2.53	0.44
2:B:758:LEU:HD23	2:B:758:LEU:HA	1.68	0.44
3:C:45:ILE:HD11	3:C:82:LEU:HD22	2.00	0.44
10:J:4:PRO:O	10:J:14:VAL:HG12	2.18	0.44
13:M:60:ALA:HB1	23:Y:54:DA:C2	2.51	0.44
16:P:317:VAL:HG12	16:P:319:ALA:H	1.83	0.44
1:A:231:GLU:OE1	1:A:231:GLU:N	2.41	0.43
1:A:415:GLY:O	1:A:449:HIS:HD2	2.00	0.43
1:A:514:GLU:OE1	2:B:1099:ALA:HB1	2.18	0.43
2:B:1068:GLN:HB3	13:M:51:GLU:HB3	1.99	0.43
9:I:65:LEU:HA	9:I:122:ARG:HE	1.83	0.43
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.83	0.43
16:P:204:ILE:HD12	16:P:206:GLU:HB2	1.98	0.43
17:Q:100:VAL:O	17:Q:103:VAL:HG23	2.18	0.43
2:B:294:ASP:HA	2:B:295:PRO:HD2	1.79	0.43
2:B:529:MET:HE2	2:B:624:PRO:O	2.19	0.43
5:E:3:ASP:O	5:E:6:GLU:HB2	2.18	0.43
10:J:46:ARG:HH11	10:J:46:ARG:HD3	1.59	0.43
13:M:57:ASN:HA	23:Y:51:DC:N4	2.33	0.43
13:M:179:GLU:HA	20:T:154:LYS:HZ1	1.82	0.43
1:A:376:ASP:HB3	1:A:521:VAL:HB	2.00	0.43
1:A:522:PRO:HG3	1:A:666:ARG:HG3	1.99	0.43
1:A:1371:ILE:HD13	1:A:1409:GLY:O	2.17	0.43
2:B:759:VAL:CG1	2:B:999:ALA:HB2	2.48	0.43
2:B:926:VAL:HG23	2:B:926:VAL:O	2.17	0.43
3:C:71:ILE:CG2	3:C:148:ILE:HG21	2.48	0.43
4:D:48:ASN:ND2	4:D:57:LEU:HG	2.24	0.43
7:G:44:PHE:HE2	7:G:104:MET:HB2	1.83	0.43
8:H:96:VAL:HG22	8:H:116:VAL:HG13	2.00	0.43
16:P:178:LEU:HB3	16:P:183:ILE:HD11	2.00	0.43
21:U:256:THR:O	21:U:257:GLN:CB	2.59	0.43
1:A:133:SER:O	1:A:136:GLN:N	2.37	0.43
2:B:52:GLN:HB2	2:B:160:TYR:OH	2.19	0.43
2:B:967:ILE:HD12	2:B:968:ASN:H	1.83	0.43
16:P:329:TYR:N	16:P:330:PRO:HD2	2.33	0.43
21:U:251:ALA:O	21:U:252:LYS:CB	2.36	0.43
1:A:264:VAL:HG22	1:A:272:ASN:CG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD23	1:A:507:GLN:HE22	1.84	0.43
2:B:290:TYR:HE2	2:B:562:ALA:HA	1.83	0.43
5:E:41:LYS:HG3	5:E:46:ASP:CB	2.48	0.43
5:E:45:GLY:C	5:E:46:ASP:O	2.54	0.43
7:G:63:ARG:C	7:G:65:PHE:H	2.21	0.43
9:I:50:ASN:OD1	9:I:51:SER:N	2.51	0.43
11:K:53:ASP:OD1	11:K:54:PRO:HD2	2.18	0.43
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.99	0.43
18:R:148:LYS:HD3	18:R:174:ALA:HB2	2.00	0.43
1:A:156:GLY:CA	1:A:181:HIS:CE1	3.02	0.43
1:A:264:VAL:HB	13:M:52:TRP:CE3	2.53	0.43
1:A:866:LYS:HG2	1:A:1432:PHE:CD1	2.54	0.43
1:A:1307:VAL:CG1	1:A:1339:ASP:H	2.32	0.43
2:B:76:GLY:O	2:B:78:VAL:CG2	2.66	0.43
10:J:66:GLU:HG3	12:L:23:HIS:ND1	2.34	0.43
13:M:178:LYS:HG2	20:T:156:VAL:CG1	2.48	0.43
13:M:184:SER:OG	13:M:185:ARG:N	2.52	0.43
17:Q:137:THR:OG1	17:Q:139:LEU:HG	2.18	0.43
1:A:612:ASP:O	1:A:613:GLU:C	2.57	0.43
2:B:422:PHE:CD1	2:B:422:PHE:C	2.91	0.43
2:B:1072:ARG:HD3	2:B:1153:TYR:CD2	2.53	0.43
3:C:74:ILE:O	3:C:128:ILE:HG13	2.19	0.43
5:E:121:MET:HG2	5:E:127:LEU:HD13	2.00	0.43
12:L:26:ASN:O	12:L:27:GLU:CB	2.62	0.43
2:B:1124:ILE:HD11	2:B:1170:ARG:HD3	2.00	0.43
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.54	0.43
13:M:91:ALA:O	13:M:92:SER:C	2.55	0.43
1:A:477:LEU:HD23	1:A:477:LEU:HA	1.82	0.43
1:A:505:LEU:HA	1:A:506:PRO:HD2	1.93	0.43
1:A:540:ASP:CB	2:B:790:GLN:NE2	2.79	0.43
1:A:779:ILE:O	1:A:783:GLN:HG3	2.19	0.43
1:A:922:PHE:HA	1:A:1052:ARG:HD3	2.01	0.43
1:A:924:TYR:CE2	1:A:949:GLN:HG2	2.54	0.43
1:A:932:ARG:O	1:A:940:LYS:HB3	2.18	0.43
2:B:598:VAL:O	2:B:600:GLU:N	2.49	0.43
8:H:11:ASP:HB2	8:H:55:LYS:HG2	2.00	0.43
20:T:82:PRO:HD2	20:T:117:ARG:O	2.19	0.43
20:T:124:TYR:O	20:T:127:LEU:HB3	2.19	0.43
20:T:168:LYS:C	20:T:170:LYS:H	2.22	0.43
21:U:133:ALA:HA	21:U:134:PRO:HD3	1.89	0.43
21:U:139:SER:O	21:U:143:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:GLU:HG2	1:A:1306:LYS:HA	2.01	0.43
1:A:1218:ARG:HG2	21:U:237:ARG:NH2	2.34	0.43
2:B:285:LEU:HD22	9:I:16:PHE:HZ	1.84	0.43
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.54	0.43
8:H:34:SER:O	8:H:36:LYS:HG3	2.19	0.43
13:M:178:LYS:HD3	20:T:154:LYS:HD3	2.01	0.43
17:Q:170:LYS:O	17:Q:174:ARG:N	2.47	0.43
20:T:59:ASN:OD1	20:T:60:GLU:N	2.52	0.43
1:A:326:PRO:HD3	13:M:92:SER:OG	2.18	0.42
1:A:370:ASP:HA	1:A:371:PRO:HD2	1.91	0.42
1:A:609:HIS:O	1:A:610:PRO:O	2.36	0.42
1:A:766:PHE:CD1	1:A:781:ILE:HD11	2.54	0.42
1:A:1301:ILE:HG13	1:A:1302:GLU:HG2	2.01	0.42
2:B:510:CYS:SG	2:B:511:PRO:HD2	2.60	0.42
2:B:613:ARG:HD3	2:B:615:TYR:OH	2.19	0.42
2:B:978:ILE:HD12	2:B:978:ILE:HG23	1.83	0.42
2:B:1071:ASN:O	2:B:1072:ARG:HG2	2.19	0.42
3:C:71:ILE:HG22	3:C:148:ILE:HG21	2.00	0.42
16:P:288:PHE:CD1	16:P:289:PRO:HD2	2.53	0.42
20:T:229:HIS:HD2	22:X:28:DG:H21	1.65	0.42
22:X:33:DT:H2''	22:X:34:DT:C5	2.54	0.42
1:A:617:PRO:O	1:A:621:ILE:HG12	2.18	0.42
1:A:937:ASP:O	1:A:940:LYS:HD2	2.19	0.42
3:C:225:LYS:O	3:C:227:GLU:HG2	2.19	0.42
5:E:56:THR:N	5:E:78:GLU:OE2	2.52	0.42
20:T:93:LEU:HD11	20:T:113:ARG:HD2	2.01	0.42
22:X:51:DC:H2'	22:X:52:DG:C4	2.53	0.42
1:A:15:LEU:HD12	2:B:1148:LEU:O	2.19	0.42
1:A:156:GLY:O	1:A:180:GLY:HA2	2.19	0.42
1:A:206:ASN:C	1:A:208:ASP:H	2.23	0.42
1:A:478:PRO:O	1:A:479:TRP:HB2	2.19	0.42
1:A:483:ARG:HH12	2:B:788:TYR:HE2	1.68	0.42
1:A:799:PRO:O	1:A:806:THR:HG22	2.19	0.42
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.54	0.42
19:S:177:MET:HE3	19:S:177:MET:HB3	1.88	0.42
1:A:924:TYR:OH	1:A:952:LEU:HD12	2.19	0.42
1:A:1156:ASP:OD1	1:A:1225:LYS:NZ	2.40	0.42
2:B:79:GLU:C	2:B:80:GLU:HG2	2.39	0.42
2:B:566:LYS:HD3	2:B:573:TRP:NE1	2.23	0.42
3:C:67:ARG:NH1	3:C:150:ILE:HA	2.35	0.42
7:G:117:MET:HG2	7:G:128:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:ASP:OD2	9:I:32:ASN:ND2	2.37	0.42
1:A:22:GLN:OE1	1:A:1448:SER:OG	2.32	0.42
1:A:197:GLU:CD	13:M:93:PHE:CD2	2.92	0.42
2:B:79:GLU:O	2:B:80:GLU:CG	2.67	0.42
2:B:106:SER:HB2	2:B:107:PRO:HD2	2.00	0.42
7:G:21:ASN:O	7:G:25:THR:OG1	2.31	0.42
14:N:319:ASP:C	14:N:321:SER:N	2.72	0.42
17:Q:163:GLU:HB3	17:Q:164:ASP:H	1.62	0.42
1:A:954:ARG:HD3	1:A:954:ARG:HA	1.84	0.42
1:A:1251:ASN:HB3	21:U:234:LYS:HE2	2.01	0.42
1:A:1307:VAL:C	1:A:1308:TYR:O	2.50	0.42
2:B:187:ILE:HG22	2:B:188:ASN:OD1	2.20	0.42
2:B:202:THR:OG1	2:B:226:GLU:OE1	2.38	0.42
2:B:235:ILE:CD1	2:B:261:PRO:HD3	2.50	0.42
9:I:66:THR:O	9:I:68:ILE:HG22	2.20	0.42
9:I:103:ARG:C	9:I:105:GLU:N	2.72	0.42
13:M:263:GLN:HA	13:M:268:LYS:HG2	2.01	0.42
18:R:77:VAL:HG21	18:R:111:ILE:HD11	2.01	0.42
18:R:113:LEU:HA	18:R:116:LYS:HE3	2.01	0.42
21:U:194:ARG:HD3	21:U:194:ARG:HA	1.61	0.42
21:U:200:ASP:OD2	21:U:203:ASN:N	2.52	0.42
22:X:45:DT:H6	22:X:45:DT:H2'	1.73	0.42
23:Y:70:DC:H2''	23:Y:71:DA:C8	2.54	0.42
1:A:611:ASP:HB3	1:A:612:ASP:H	1.31	0.42
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.20	0.42
2:B:629:GLU:O	2:B:631:GLN:N	2.53	0.42
2:B:800:ALA:O	2:B:805:PHE:HB2	2.20	0.42
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	2.00	0.42
3:C:6:GLN:HG2	3:C:6:GLN:O	2.17	0.42
3:C:73:LEU:O	3:C:238:SER:HB3	2.20	0.42
9:I:58:ILE:O	9:I:59:THR:OG1	2.36	0.42
9:I:60:HIS:C	9:I:62:VAL:N	2.71	0.42
10:J:35:LEU:HD13	10:J:46:ARG:HG2	2.00	0.42
12:L:17:TYR:HE1	12:L:46:LYS:HG3	1.84	0.42
13:M:218:PHE:CD1	13:M:277:ILE:HG22	2.51	0.42
13:M:245:VAL:HB	13:M:248:ARG:HB2	2.01	0.42
19:S:51:LEU:HG	19:S:54:LYS:HB2	2.00	0.42
22:X:70:DG:H2''	22:X:71:DA:C8	2.54	0.42
1:A:36:VAL:HG11	1:A:72:GLN:HE22	1.85	0.42
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.54	0.42
2:B:793:SER:CA	2:B:944:THR:O	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:THR:HG22	8:H:140:ARG:NH1	2.35	0.42
9:I:81:THR:HG22	9:I:94:ALA:O	2.19	0.42
13:M:15:CYS:HA	13:M:16:PRO:HD3	1.75	0.42
13:M:45:VAL:HG12	13:M:47:ASP:H	1.84	0.42
17:Q:184:ILE:HG12	18:R:211:SER:HB3	2.02	0.42
20:T:128:LYS:O	20:T:132:ILE:N	2.44	0.42
1:A:932:ARG:CG	1:A:940:LYS:HA	2.49	0.42
1:A:1376:LYS:HA	1:A:1376:LYS:HD2	1.80	0.42
2:B:343:LEU:O	2:B:347:MET:HB3	2.20	0.42
3:C:19:VAL:HB	3:C:241:PRO:HB2	2.02	0.42
3:C:47:ILE:HD12	3:C:47:ILE:N	2.34	0.42
8:H:65:TYR:CD1	8:H:65:TYR:N	2.88	0.42
20:T:26:TYR:CE2	20:T:127:LEU:HD21	2.54	0.42
21:U:226:GLU:HB3	21:U:227:GLU:H	1.56	0.42
23:Y:70:DC:H2''	23:Y:71:DA:H8	1.85	0.42
23:Y:79:DT:H6	23:Y:79:DT:H2'	1.69	0.42
1:A:244:ARG:HA	1:A:245:PRO:HD3	1.87	0.42
1:A:460:ARG:NH2	1:A:499:ASP:HB3	2.35	0.42
1:A:779:ILE:O	1:A:782:SER:HB2	2.20	0.42
2:B:146:LYS:HB2	2:B:146:LYS:HE2	1.83	0.42
2:B:198:GLU:HA	2:B:393:LEU:HD23	2.02	0.42
2:B:203:ASN:O	2:B:571:GLY:HA3	2.20	0.42
2:B:838:GLN:OE1	2:B:886:ARG:NH1	2.53	0.42
2:B:1027:VAL:HG12	2:B:1029:TYR:HE1	1.84	0.42
8:H:81:ARG:HA	8:H:82:PRO:HD3	1.83	0.42
9:I:75:ASP:HA	9:I:76:PRO:HD3	1.87	0.42
17:Q:25:PHE:HA	18:R:219:LEU:CD1	2.50	0.42
17:Q:28:ILE:HA	17:Q:31:ALA:HB3	2.02	0.42
20:T:3:GLU:H	20:T:3:GLU:CD	2.24	0.42
22:X:61:DA:H2''	22:X:62:DG:C8	2.54	0.42
1:A:482:PHE:HE2	1:A:501:MET:O	2.03	0.41
1:A:641:CYS:SG	1:A:642:LYS:N	2.93	0.41
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	0.41
1:A:1389:ASP:O	21:U:297:ARG:NH2	2.53	0.41
2:B:198:GLU:OE2	2:B:391:LYS:HD3	2.20	0.41
2:B:1008:VAL:HG13	2:B:1009:GLN:N	2.35	0.41
6:F:102:ILE:CG2	6:F:104:ILE:HG12	2.49	0.41
10:J:6:ARG:HG2	10:J:13:ILE:HG22	2.02	0.41
13:M:65:SER:O	13:M:67:VAL:N	2.53	0.41
1:A:124:PRO:HA	1:A:127:LYS:HE3	2.02	0.41
1:A:455:ILE:HG12	1:A:473:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ASN:OD1	1:A:792:ASN:N	2.53	0.41
2:B:623:ARG:NH2	2:B:675:LEU:HD21	2.35	0.41
2:B:721:ARG:HA	2:B:721:ARG:NE	2.34	0.41
3:C:6:GLN:HG3	11:K:104:ARG:CZ	2.50	0.41
3:C:157:GLN:HG2	10:J:65:LEU:HB3	1.95	0.41
8:H:108:ALA:C	8:H:110:THR:N	2.72	0.41
13:M:10:LEU:H	13:M:11:PRO:HD3	1.60	0.41
18:R:166:ILE:HG22	18:R:168:LEU:H	1.84	0.41
1:A:79:THR:HG23	13:M:43:ASP:CG	2.40	0.41
1:A:261:ARG:HB2	1:A:274:ASP:CB	2.50	0.41
1:A:597:PRO:HB2	1:A:660:MET:HG3	2.01	0.41
1:A:666:ARG:HD3	1:A:666:ARG:HA	1.79	0.41
1:A:999:ARG:CZ	8:H:99:ILE:HG21	2.49	0.41
1:A:1117:VAL:O	1:A:1118:THR:C	2.57	0.41
1:A:1191:GLU:HA	1:A:1194:ASN:ND2	2.35	0.41
2:B:193:VAL:HG21	2:B:482:LEU:HD23	2.03	0.41
2:B:278:PHE:HZ	2:B:359:THR:HG22	1.86	0.41
2:B:588:ARG:NH2	2:B:663:GLU:OE1	2.51	0.41
2:B:1001:PRO:HB2	2:B:1002:PHE:CD1	2.56	0.41
16:P:206:GLU:O	16:P:208:ARG:N	2.53	0.41
20:T:155:PRO:C	20:T:157:ALA:N	2.73	0.41
20:T:229:HIS:CD2	23:Y:67:DC:HI'	2.55	0.41
1:A:199:TYR:CE2	13:M:93:PHE:CZ	3.02	0.41
1:A:570:TRP:CZ3	1:A:572:GLY:HA2	2.56	0.41
1:A:890:ARG:HD3	1:A:890:ARG:HA	1.87	0.41
1:A:932:ARG:HD3	1:A:932:ARG:HA	1.38	0.41
1:A:1113:SER:HB3	1:A:1114:ALA:H	1.69	0.41
2:B:33:TYR:CE1	2:B:37:LYS:HG3	2.55	0.41
2:B:1029:TYR:CD1	2:B:1029:TYR:N	2.85	0.41
2:B:1142:ASN:ND2	2:B:1145:GLN:HG2	2.36	0.41
20:T:143:GLN:OE1	20:T:143:GLN:N	2.53	0.41
21:U:260:LEU:HB3	21:U:261:PHE:H	1.61	0.41
1:A:209:SER:O	1:A:210:GLN:HG2	2.21	0.41
1:A:612:ASP:O	1:A:613:GLU:O	2.38	0.41
2:B:802:ASP:C	2:B:804:GLY:H	2.24	0.41
2:B:1060:HIS:CD2	2:B:1078:ARG:HD2	2.56	0.41
7:G:108:ILE:HG21	7:G:163:LEU:HG	2.02	0.41
8:H:92:MET:CE	8:H:143:LEU:HD23	2.51	0.41
14:N:347:ASN:HB3	16:P:208:ARG:HH11	1.84	0.41
20:T:140:ARG:HH11	20:T:140:ARG:CG	2.32	0.41
22:X:43:DT:H2'	22:X:44:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:GLU:HG2	1:A:819:SER:N	2.36	0.41
1:A:1175:ILE:HG23	1:A:1285:LEU:HD23	2.01	0.41
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.50	0.41
2:B:192:LYS:HE2	2:B:449:ALA:O	2.20	0.41
2:B:230:ARG:HB2	2:B:405:ARG:CZ	2.50	0.41
2:B:520:VAL:HG13	2:B:520:VAL:O	2.20	0.41
9:I:65:LEU:HD22	9:I:122:ARG:O	2.21	0.41
9:I:65:LEU:CB	9:I:122:ARG:HE	2.33	0.41
15:O:66:ARG:N	15:O:73:THR:O	2.54	0.41
18:R:88:ARG:HH21	18:R:95:HIS:HB3	1.85	0.41
19:S:111:LYS:O	19:S:146:PHE:HA	2.20	0.41
22:X:11:DT:H6	22:X:11:DT:H2'	1.71	0.41
1:A:630:VAL:HG12	1:A:635:LEU:CD1	2.51	0.41
1:A:926:ASN:HA	1:A:931:ARG:CG	2.48	0.41
1:A:1411:LEU:HD23	1:A:1411:LEU:HA	1.92	0.41
2:B:78:VAL:HB	2:B:79:GLU:H	1.62	0.41
3:C:242:GLU:OE1	3:C:242:GLU:N	2.54	0.41
5:E:45:GLY:O	5:E:48:PRO:HD3	2.21	0.41
14:N:360:LEU:HD21	15:O:81:PHE:HE2	1.84	0.41
20:T:166:GLU:HA	20:T:169:LYS:CE	2.50	0.41
22:X:20:DG:N2	23:Y:75:DC:O2	2.54	0.41
1:A:133:SER:C	1:A:135:GLY:N	2.74	0.41
1:A:413:TYR:OH	1:A:451:CYS:HA	2.21	0.41
1:A:522:PRO:O	1:A:525:ILE:HG13	2.21	0.41
2:B:25:ALA:HA	2:B:28:ILE:HD12	2.01	0.41
2:B:51:ILE:HB	2:B:160:TYR:CE2	2.56	0.41
2:B:470:LEU:HD23	2:B:472:ARG:HH11	1.85	0.41
2:B:759:VAL:HG13	2:B:999:ALA:HB2	2.03	0.41
2:B:783:ALA:HB2	2:B:1041:ILE:HG21	2.01	0.41
2:B:928:ILE:HG21	2:B:928:ILE:HD13	1.83	0.41
7:G:14:HIS:HA	7:G:15:PRO:HD3	1.93	0.41
17:Q:30:HIS:O	17:Q:34:LEU:HB2	2.20	0.41
18:R:181:ALA:O	18:R:185:LEU:N	2.52	0.41
1:A:530:SER:O	1:A:532:ARG:N	2.54	0.41
1:A:626:THR:OG1	1:A:627:LYS:N	2.54	0.41
1:A:880:ARG:HH11	1:A:880:ARG:HD3	1.76	0.41
1:A:1029:LEU:H	5:E:162:ARG:HH12	1.66	0.41
2:B:115:LEU:HA	2:B:115:LEU:HD23	1.93	0.41
2:B:175:ASN:HD21	10:J:64:PRO:HG2	1.86	0.41
2:B:197:GLN:NE2	2:B:466:VAL:HG22	2.36	0.41
2:B:778:SER:O	2:B:1045:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1022:LEU:HD11	2:B:1023:ARG:CZ	2.51	0.41
3:C:59:LEU:HA	3:C:59:LEU:HD12	1.73	0.41
8:H:34:SER:HB3	8:H:36:LYS:NZ	2.36	0.41
8:H:84:ARG:HB3	8:H:86:ASP:HB2	2.03	0.41
12:L:35:ARG:HH12	12:L:42:ARG:CZ	2.34	0.41
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.56	0.41
19:S:15:VAL:HG22	20:T:42:LYS:HE2	2.03	0.41
20:T:175:ARG:HB3	20:T:208:GLN:HA	2.02	0.41
23:Y:50:DA:H2''	23:Y:51:DC:O5'	2.20	0.41
1:A:408:ARG:HG2	1:A:412:GLN:OE1	2.22	0.41
1:A:522:PRO:CG	1:A:666:ARG:HG3	2.50	0.41
1:A:728:THR:HG23	1:A:736:THR:HG23	2.02	0.41
1:A:790:GLN:HA	1:A:822:PHE:HA	2.03	0.41
1:A:893:GLU:HG2	5:E:203:TYR:CE1	2.56	0.41
1:A:1194:ASN:O	1:A:1197:TYR:HD2	2.04	0.41
2:B:254:GLN:HG3	2:B:303:PRO:CG	2.50	0.41
2:B:363:TYR:CG	2:B:553:LEU:HD21	2.56	0.41
2:B:699:HIS:CE1	2:B:701:SER:OG	2.74	0.41
2:B:749:HIS:HD2	2:B:810:PHE:HD1	1.66	0.41
2:B:906:GLN:HB3	12:L:45:TYR:CE1	2.54	0.41
4:D:75:LYS:HE2	4:D:141:GLN:HB3	2.03	0.41
5:E:160:LEU:HD11	5:E:167:GLU:HG2	2.03	0.41
8:H:13:LYS:HE2	8:H:31:GLU:HB2	2.02	0.41
8:H:139:SER:HB3	8:H:140:ARG:H	1.60	0.41
15:O:80:GLU:OE2	15:O:82:ARG:NE	2.44	0.41
16:P:246:PHE:HA	16:P:247:PRO:HD3	1.95	0.41
17:Q:28:ILE:HD12	18:R:192:VAL:HG12	2.03	0.41
17:Q:45:GLU:OE2	17:Q:56:ARG:NH1	2.52	0.41
17:Q:138:ASP:OD1	17:Q:138:ASP:N	2.54	0.41
18:R:129:LYS:HE2	18:R:140:LYS:O	2.21	0.41
23:Y:57:DA:H5''	23:Y:58:DC:H2'	2.02	0.41
1:A:117:LEU:H	1:A:232:GLU:CD	2.24	0.40
1:A:286:ILE:HG13	1:A:287:ASN:N	2.36	0.40
1:A:464:LEU:HA	1:A:464:LEU:HD23	1.87	0.40
1:A:787:VAL:HG23	1:A:824:GLU:C	2.42	0.40
1:A:931:ARG:HD3	1:A:931:ARG:HA	1.43	0.40
2:B:121:SER:HB2	2:B:152:ILE:O	2.21	0.40
2:B:544:PHE:HD1	2:B:544:PHE:HA	1.78	0.40
2:B:602:SER:OG	2:B:620:ARG:NH1	2.54	0.40
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.50	0.40
7:G:99:THR:HG21	7:G:143:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:ASN:OD1	13:M:57:ASN:N	2.54	0.40
13:M:92:SER:O	13:M:93:PHE:C	2.59	0.40
13:M:107:MET:HG3	13:M:108:SER:H	1.87	0.40
13:M:178:LYS:O	20:T:154:LYS:HE3	2.21	0.40
14:N:337:CYS:HB2	14:N:355:ASP:O	2.22	0.40
16:P:283:TYR:CZ	16:P:285:PRO:HB3	2.56	0.40
1:A:375:ILE:HG13	1:A:666:ARG:NH1	2.36	0.40
1:A:607:SER:HB2	1:A:643:LYS:CD	2.52	0.40
2:B:51:ILE:HA	2:B:51:ILE:HD13	1.75	0.40
2:B:347:MET:CE	2:B:365:LEU:HD13	2.51	0.40
2:B:966:ILE:HG21	2:B:966:ILE:HD13	1.83	0.40
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.40
3:C:133:ARG:HA	3:C:136:ASP:CG	2.23	0.40
16:P:199:ALA:HB2	16:P:214:PHE:CE1	2.56	0.40
22:X:24:DG:H2'	22:X:25:DG:C8	2.56	0.40
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.33	0.40
1:A:689:ILE:HD11	2:B:982:ILE:HD13	2.03	0.40
1:A:1350:LYS:HE2	5:E:8:TYR:CG	2.57	0.40
13:M:12:ARG:O	13:M:12:ARG:CG	2.69	0.40
16:P:162:VAL:HA	16:P:163:PRO:HD2	1.79	0.40
18:R:205:ASP:O	18:R:206:LYS:CE	2.69	0.40
1:A:642:LYS:O	1:A:646:GLY:N	2.49	0.40
1:A:728:THR:H	1:A:728:THR:HG1	1.66	0.40
1:A:837:PHE:HB2	2:B:506:TRP:CZ3	2.56	0.40
1:A:1320:ILE:HD11	1:A:1328:PHE:HB3	2.03	0.40
3:C:189:ASP:N	3:C:189:ASP:OD1	2.53	0.40
3:C:267:ILE:HG13	3:C:272:LEU:CB	2.51	0.40
7:G:144:ARG:HE	7:G:171:VAL:HG11	1.86	0.40
10:J:5:VAL:O	10:J:6:ARG:HB2	2.22	0.40
13:M:17:ASN:CG	13:M:18:HIS:HD1	2.23	0.40
13:M:70:SER:C	13:M:72:ASN:H	2.25	0.40
16:P:203:ARG:NH2	23:Y:79:DT:OP1	2.45	0.40
1:A:780:ASN:ND2	2:B:976:MET:SD	2.94	0.40
1:A:1295:ASP:O	1:A:1297:THR:HG23	2.21	0.40
2:B:269:ILE:HD13	2:B:269:ILE:HA	1.82	0.40
2:B:552:ASN:O	2:B:555:GLU:HG2	2.20	0.40
2:B:1043:ILE:HD13	2:B:1043:ILE:HG21	1.86	0.40
3:C:25:ASN:HA	3:C:227:GLU:OE1	2.21	0.40
9:I:12:VAL:HG11	9:I:15:ARG:HH21	1.85	0.40
9:I:99:SER:OG	9:I:100:HIS:N	2.52	0.40
17:Q:128:LYS:HE3	17:Q:133:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:112:GLY:HA2	19:S:145:ASN:O	2.21	0.40
22:X:24:DG:H2''	22:X:25:DG:H5'	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1450/1970 (74%)	1270 (88%)	118 (8%)	62 (4%)	2	26
2	B	1163/1174 (99%)	1001 (86%)	110 (10%)	52 (4%)	2	25
3	C	273/275 (99%)	242 (89%)	24 (9%)	7 (3%)	5	35
4	D	127/142 (89%)	120 (94%)	7 (6%)	0	100	100
5	E	208/210 (99%)	191 (92%)	8 (4%)	9 (4%)	2	26
6	F	84/127 (66%)	80 (95%)	4 (5%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	148/150 (99%)	117 (79%)	14 (10%)	17 (12%)	0	7
9	I	123/125 (98%)	90 (73%)	22 (18%)	11 (9%)	1	13
10	J	65/67 (97%)	56 (86%)	5 (8%)	4 (6%)	1	20
11	K	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17	54
12	L	44/58 (76%)	32 (73%)	9 (20%)	3 (7%)	1	18
13	M	308/316 (98%)	262 (85%)	28 (9%)	18 (6%)	1	21
14	N	109/376 (29%)	95 (87%)	11 (10%)	3 (3%)	5	34
15	O	97/109 (89%)	96 (99%)	1 (1%)	0	100	100
16	P	183/339 (54%)	170 (93%)	7 (4%)	6 (3%)	4	31
17	Q	176/439 (40%)	160 (91%)	8 (4%)	8 (4%)	2	25
18	R	163/291 (56%)	142 (87%)	15 (9%)	6 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	134/517 (26%)	119 (89%)	11 (8%)	4 (3%)	4	33
20	T	218/249 (88%)	190 (87%)	16 (7%)	12 (6%)	2	22
21	U	168/301 (56%)	142 (84%)	18 (11%)	8 (5%)	2	24
All	All	5525/7524 (73%)	4842 (88%)	452 (8%)	231 (4%)	5	26

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	70	ARG
1	A	133	SER
1	A	205	VAL
1	A	208	ASP
1	A	264	VAL
1	A	265	VAL
1	A	272	ASN
1	A	531	ASN
1	A	607	SER
1	A	610	PRO
1	A	622	SER
1	A	623	PRO
1	A	931	ARG
1	A	932	ARG
1	A	1087	VAL
1	A	1117	VAL
1	A	1200	PRO
1	A	1304	ILE
1	A	1308	TYR
2	B	74	ALA
2	B	78	VAL
2	B	225	LEU
2	B	226	GLU
2	B	231	PRO
2	B	249	LYS
2	B	251	ALA
2	B	452	ASN
2	B	460	HIS
2	B	491	ARG
2	B	513	GLU
2	B	526	LEU
2	B	879	GLU

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Mol	Chain	Res	Type
2	B	898	THR
2	B	1108	PHE
3	C	6	GLN
3	C	7	PRO
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	64	HIS
5	E	65	ASN
5	E	68	PRO
8	H	18	GLU
8	H	67	ASP
8	H	75	TYR
9	I	85	PRO
9	I	99	SER
9	I	103	ARG
10	J	2	ILE
11	K	112	LYS
12	L	17	TYR
13	M	11	PRO
13	M	90	ALA
13	M	92	SER
13	M	93	PHE
13	M	94	ASP
13	M	95	GLU
14	N	355	ASP
16	P	206	GLU
16	P	297	LYS
16	P	299	ARG
17	Q	126	SER
18	R	163	LEU
18	R	195	PRO
18	R	206	LYS
18	R	223	VAL
18	R	226	ASP
18	R	228	MET
19	S	160	ALA
20	T	124	TYR
20	T	151	THR
20	T	153	TYR
20	T	156	VAL
20	T	180	LYS

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Mol	Chain	Res	Type
21	U	228	MET
21	U	285	MET
21	U	300	PHE
1	A	48	GLU
1	A	66	GLU
1	A	204	HIS
1	A	263	ALA
1	A	613	GLU
1	A	624	GLY
1	A	625	ASP
1	A	912	SER
1	A	926	ASN
1	A	928	ARG
1	A	935	GLN
1	A	1307	VAL
1	A	1409	GLY
2	B	76	GLY
2	B	456	GLN
2	B	599	SER
2	B	705	GLY
2	B	873	LEU
2	B	881	GLU
2	B	899	SER
2	B	1145	GLN
3	C	143	VAL
3	C	211	LEU
3	C	272	LEU
5	E	124	LYS
8	H	35	PHE
8	H	73	GLY
8	H	109	ALA
8	H	111	ARG
8	H	139	SER
9	I	62	VAL
9	I	105	GLU
10	J	41	LYS
12	L	16	ILE
13	M	10	LEU
13	M	47	ASP
13	M	48	VAL
13	M	53	ARG
13	M	66	ARG

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Mol	Chain	Res	Type
13	M	91	ALA
13	M	110	SER
14	N	320	VAL
16	P	157	GLU
16	P	208	ARG
17	Q	125	ALA
17	Q	158	HIS
20	T	169	LYS
20	T	178	ALA
21	U	225	ALA
21	U	252	LYS
21	U	256	THR
1	A	49	GLY
1	A	54	LEU
1	A	134	LYS
1	A	156	GLY
1	A	195	GLY
1	A	614	ASP
1	A	724	GLU
1	A	1085	GLU
1	A	1265	ASP
1	A	1274	GLU
1	A	1299	GLN
1	A	1316	ASN
2	B	63	PRO
2	B	242	ARG
2	B	250	SER
2	B	548	TRP
2	B	630	LYS
2	B	691	SER
2	B	839	GLY
2	B	892	CYS
2	B	1136	GLU
8	H	21	LYS
8	H	66	GLU
8	H	70	LEU
8	H	138	ASP
8	H	140	ARG
8	H	148	LEU
9	I	106	ASP
9	I	118	HIS
13	M	12	ARG

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Mol	Chain	Res	Type
13	M	14	THR
13	M	101	TYR
14	N	325	GLY
17	Q	40	ASN
17	Q	164	ASP
17	Q	165	GLU
19	S	156	THR
20	T	141	LEU
21	U	251	ALA
1	A	44	PRO
1	A	62	GLN
1	A	75	ALA
1	A	132	LYS
1	A	184	CYS
1	A	726	GLU
1	A	894	ASP
1	A	1103	THR
2	B	427	LYS
2	B	527	ALA
2	B	823	PHE
3	C	217	GLN
5	E	27	LEU
8	H	22	PHE
8	H	149	ALA
9	I	104	ALA
12	L	45	TYR
13	M	56	SER
13	M	71	GLN
17	Q	25	PHE
17	Q	100	VAL
19	S	154	THR
20	T	154	LYS
1	A	56	GLY
1	A	210	GLN
1	A	1271	GLU
2	B	232	THR
2	B	511	PRO
2	B	631	GLN
2	B	803	ARG
2	B	875	GLU
2	B	876	ASN
2	B	886	ARG

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Mol	Chain	Res	Type
2	B	900	GLU
9	I	67	GLN
10	J	5	VAL
16	P	162	VAL
20	T	148	VAL
21	U	257	GLN
1	A	299	ALA
1	A	1414	ILE
2	B	61	ASP
2	B	685	LYS
2	B	884	ASN
2	B	1069	ILE
9	I	58	ILE
10	J	6	ARG
19	S	121	ASN
20	T	171	GLU
1	A	1275	VAL
9	I	117	PRO
2	B	136	GLY
2	B	330	VAL
2	B	561	ILE
1	A	1312	PRO
2	B	253	GLY
5	E	48	PRO
8	H	82	PRO
2	B	931	ILE
3	C	151	VAL
20	T	38	GLY
1	A	55	GLY
1	A	371	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	1279/1748 (73%)	1224 (96%)	55 (4%)	29 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1020/1028 (99%)	982 (96%)	38 (4%)	34	60
3	C	252/252 (100%)	243 (96%)	9 (4%)	35	61
4	D	119/126 (94%)	119 (100%)	0	100	100
5	E	192/192 (100%)	187 (97%)	5 (3%)	46	68
6	F	74/111 (67%)	72 (97%)	2 (3%)	44	67
7	G	152/153 (99%)	151 (99%)	1 (1%)	84	90
8	H	131/131 (100%)	127 (97%)	4 (3%)	40	64
9	I	112/112 (100%)	109 (97%)	3 (3%)	44	67
10	J	56/56 (100%)	49 (88%)	7 (12%)	4	23
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	66
12	L	43/55 (78%)	41 (95%)	2 (5%)	26	55
13	M	263/268 (98%)	253 (96%)	10 (4%)	33	59
14	N	105/324 (32%)	101 (96%)	4 (4%)	33	59
15	O	90/98 (92%)	88 (98%)	2 (2%)	52	71
16	P	159/293 (54%)	157 (99%)	2 (1%)	69	82
17	Q	164/373 (44%)	158 (96%)	6 (4%)	34	60
18	R	150/261 (58%)	143 (95%)	7 (5%)	26	55
19	S	121/448 (27%)	117 (97%)	4 (3%)	38	63
20	T	196/218 (90%)	193 (98%)	3 (2%)	65	80
21	U	148/266 (56%)	140 (95%)	8 (5%)	22	52
All	All	4932/6619 (74%)	4757 (96%)	175 (4%)	39	62

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	74	CYS
1	A	117	LEU
1	A	146	ASP
1	A	181	HIS
1	A	204	HIS
1	A	205	VAL
1	A	212	LYS
1	A	227	ARG
1	A	272	ASN

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Mol	Chain	Res	Type
1	A	436	SER
1	A	463	THR
1	A	484	LEU
1	A	488	VAL
1	A	524	MET
1	A	534	VAL
1	A	538	VAL
1	A	545	VAL
1	A	607	SER
1	A	613	GLU
1	A	619	LYS
1	A	621	ILE
1	A	625	ASP
1	A	644	SER
1	A	687	ILE
1	A	691	ASP
1	A	766	PHE
1	A	792	ASN
1	A	818	GLU
1	A	849	ASP
1	A	853	LYS
1	A	864	LEU
1	A	873	VAL
1	A	908	THR
1	A	930	LEU
1	A	931	ARG
1	A	932	ARG
1	A	940	LYS
1	A	1036	ASN
1	A	1077	ASN
1	A	1128	ILE
1	A	1160	ARG
1	A	1165	THR
1	A	1168	LYS
1	A	1203	ASP
1	A	1281	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1304	ILE
1	A	1306	LYS
1	A	1308	TYR
1	A	1309	MET

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	1318	LYS
1	A	1341	VAL
1	A	1485	GLU
2	B	41	ARG
2	B	57	ARG
2	B	61	ASP
2	B	67	LEU
2	B	78	VAL
2	B	79	GLU
2	B	132	VAL
2	B	225	LEU
2	B	250	SER
2	B	269	ILE
2	B	282	ARG
2	B	330	VAL
2	B	371	ARG
2	B	388	TYR
2	B	416	ARG
2	B	422	PHE
2	B	448	LEU
2	B	485	LEU
2	B	621	ILE
2	B	655	ASP
2	B	667	THR
2	B	711	ILE
2	B	733	MET
2	B	735	VAL
2	B	737	ILE
2	B	747	LEU
2	B	784	SER
2	B	785	TYR
2	B	853	LEU
2	B	880	LEU
2	B	921	ILE
2	B	958	CYS
2	B	1018	TYR
2	B	1035	ARG
2	B	1071	ASN
2	B	1091	ARG
2	B	1092	ASP
2	B	1156	LYS
3	C	6	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
3	C	35	ARG
3	C	58	VAL
3	C	63	PHE
3	C	70	LEU
3	C	135	ARG
3	C	136	ASP
3	C	148	ILE
3	C	242	GLU
5	E	38	GLU
5	E	47	LYS
5	E	64	HIS
5	E	113	SER
5	E	205	THR
6	F	54	THR
6	F	64	ARG
7	G	158	PHE
8	H	65	TYR
8	H	66	GLU
8	H	107	GLU
8	H	144	LEU
9	I	60	HIS
9	I	61	GLU
9	I	111	TYR
10	J	7	CYS
10	J	14	VAL
10	J	46	ARG
10	J	47	ARG
10	J	54	ASP
10	J	59	LEU
10	J	65	LEU
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
12	L	16	ILE
12	L	27	GLU
13	M	10	LEU
13	M	12	ARG
13	M	39	LEU
13	M	43	ASP
13	M	47	ASP
13	M	48	VAL
13	M	111	ASP

*Continued on next page...*

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Mol	Chain	Res	Type
13	M	132	ARG
13	M	133	ASN
13	M	282	ASP
14	N	20	ASP
14	N	318	ASP
14	N	351	PHE
14	N	360	LEU
15	O	63	ASN
15	O	88	ILE
16	P	180	LEU
16	P	297	LYS
17	Q	17	LEU
17	Q	76	MET
17	Q	138	ASP
17	Q	171	LYS
17	Q	177	LEU
17	Q	191	LEU
18	R	163	LEU
18	R	169	GLU
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
18	R	223	VAL
18	R	235	GLU
19	S	135	PHE
19	S	163	GLU
19	S	166	ARG
19	S	177	MET
20	T	140	ARG
20	T	148	VAL
20	T	154	LYS
21	U	194	ARG
21	U	226	GLU
21	U	232	GLU
21	U	248	HIS
21	U	252	LYS
21	U	253	THR
21	U	257	GLN
21	U	276	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	122	ASN
1	A	222	HIS
1	A	273	GLN
1	A	507	GLN
1	A	529	GLN
1	A	673	GLN
1	A	757	GLN
1	A	989	ASN
1	A	1194	ASN
1	A	1445	HIS
2	B	175	ASN
2	B	319	ASN
2	B	452	ASN
2	B	790	GLN
2	B	941	GLN
2	B	1101	GLN
3	C	6	GLN
3	C	25	ASN
3	C	275	ASN
4	D	48	ASN
5	E	64	HIS
9	I	21	ASN
9	I	22	ASN
9	I	41	ASN
9	I	84	HIS
10	J	52	HIS
11	K	89	ASN
12	L	26	ASN
13	M	71	GLN
13	M	102	GLN
17	Q	109	HIS
18	R	204	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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](#)

There are no chain breaks in this entry.

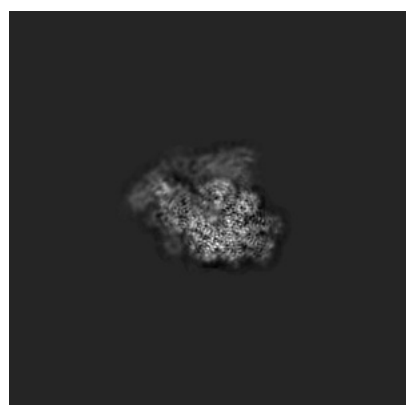
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8137. These allow visual inspection of the internal detail of the map and identification of artifacts.

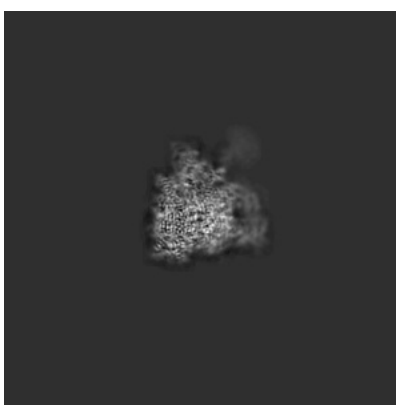
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

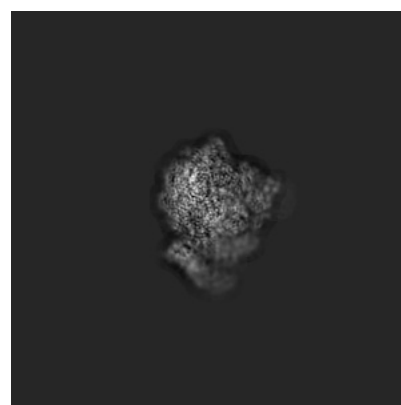
#### 6.1.1 Primary map



X



Y

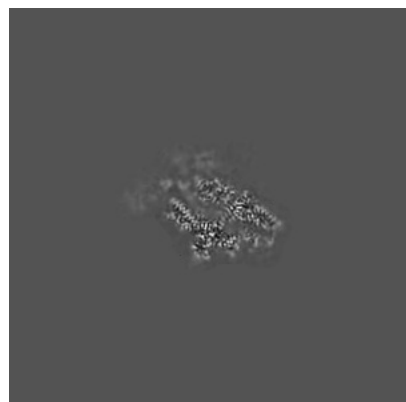


Z

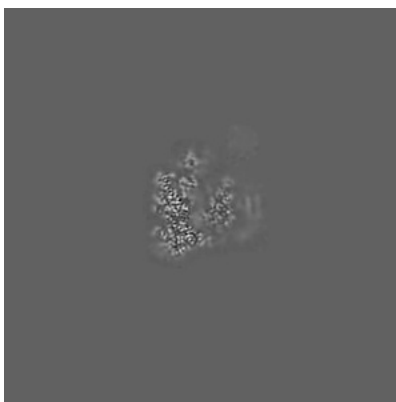
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

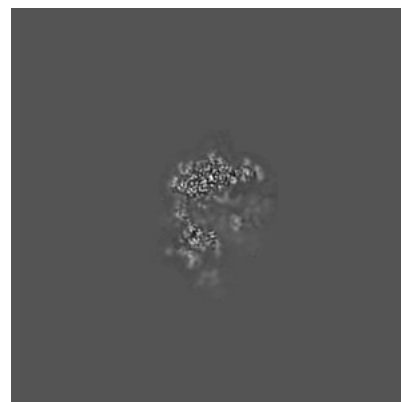
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

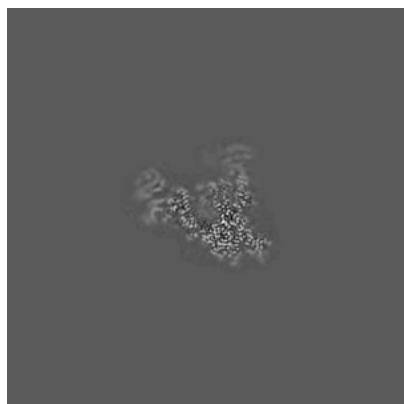


Z Index: 192

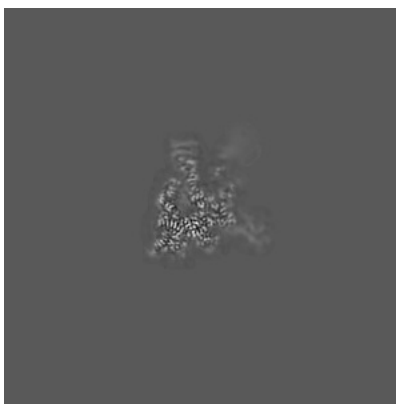
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

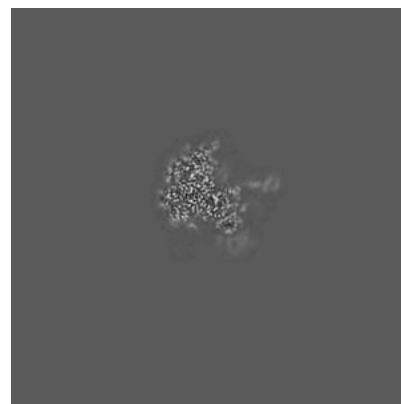
### 6.3.1 Primary map



X Index: 175



Y Index: 210

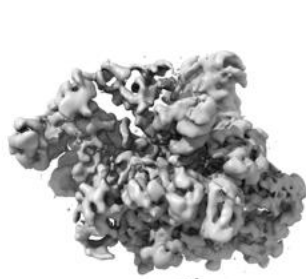


Z Index: 163

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

## 6.4 Orthogonal surface views [i](#)

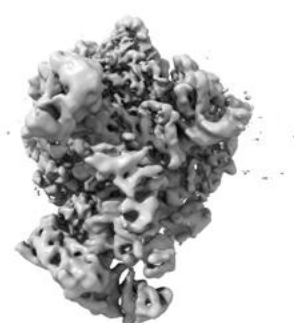
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

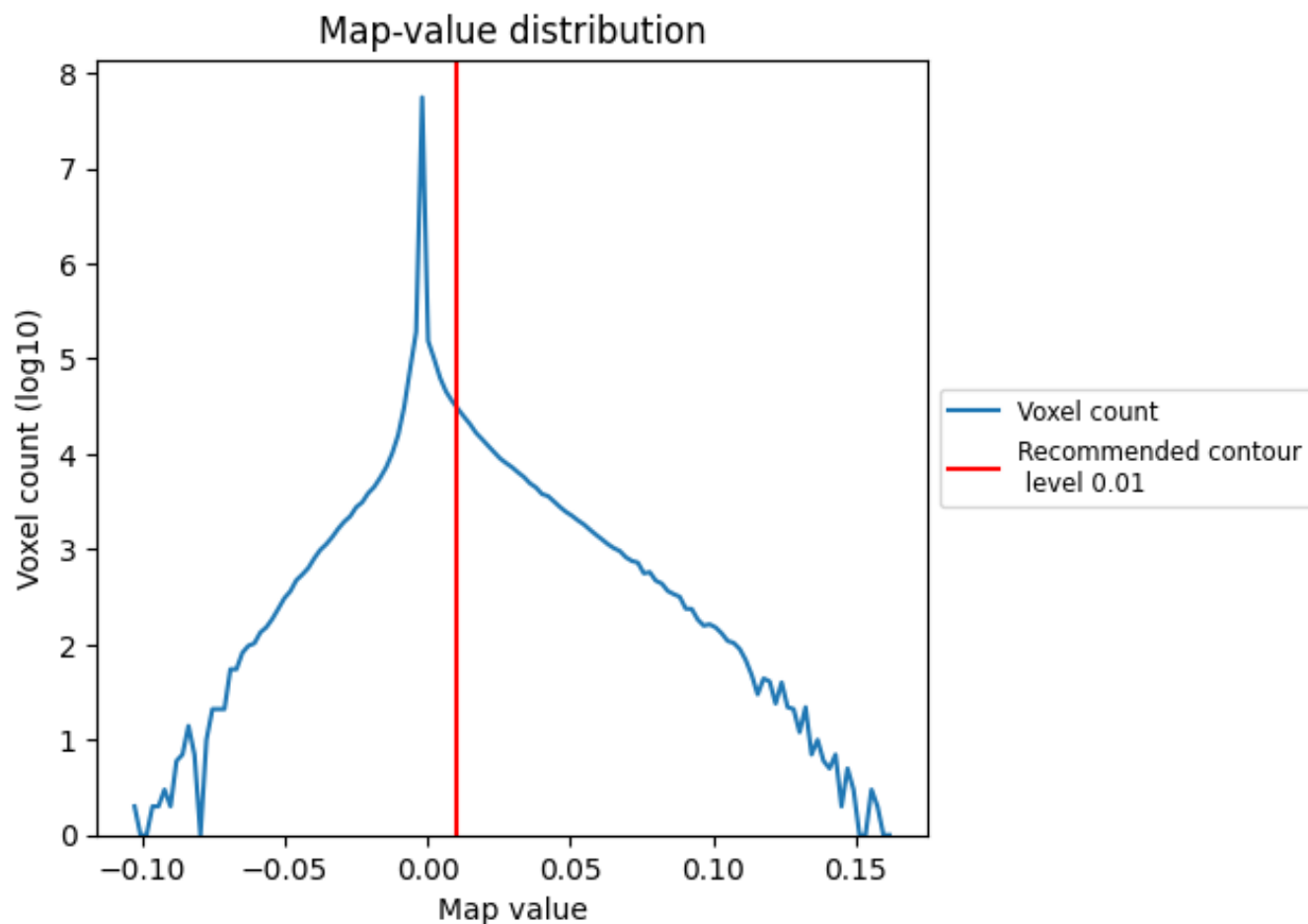
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

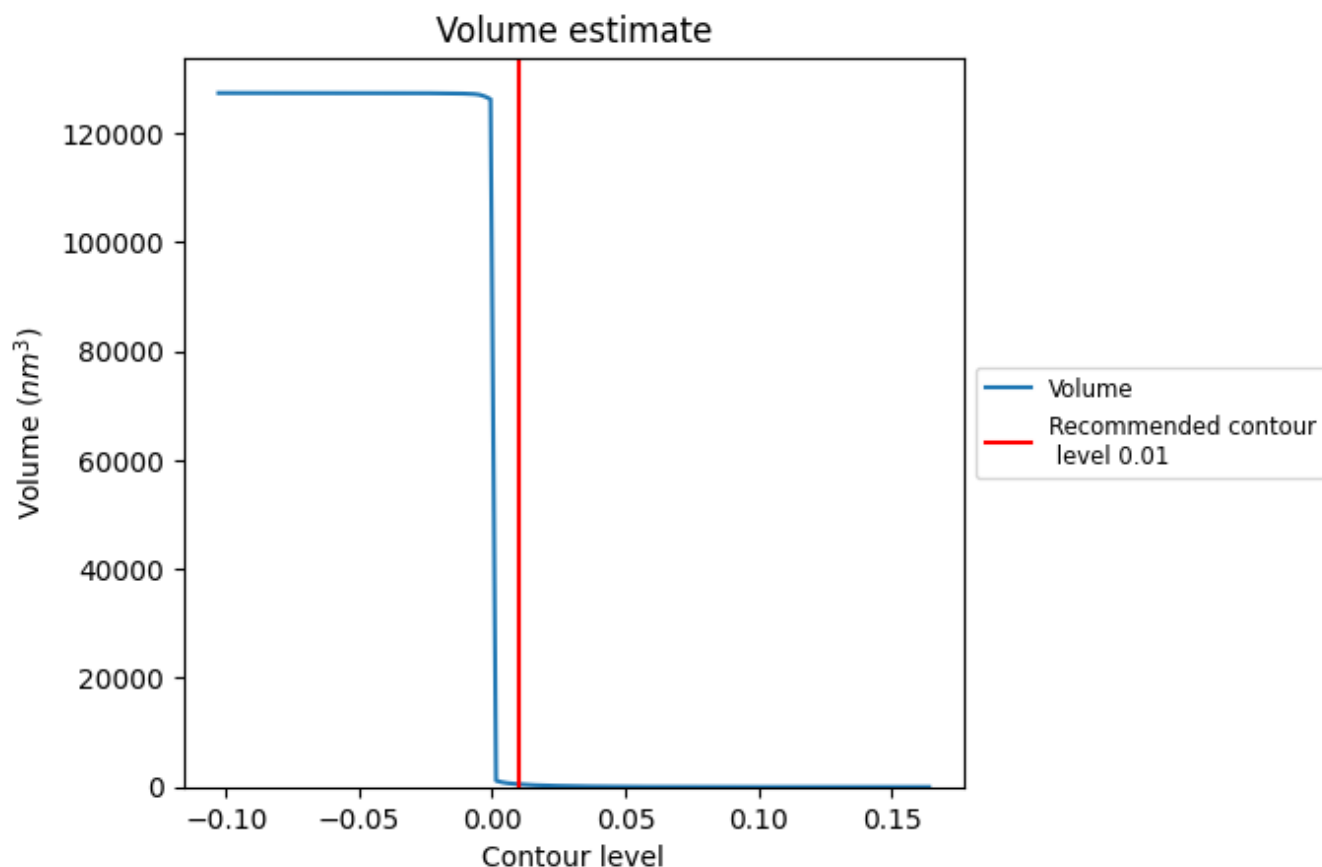
This section contains the results of statistical analysis of the map.

### 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.

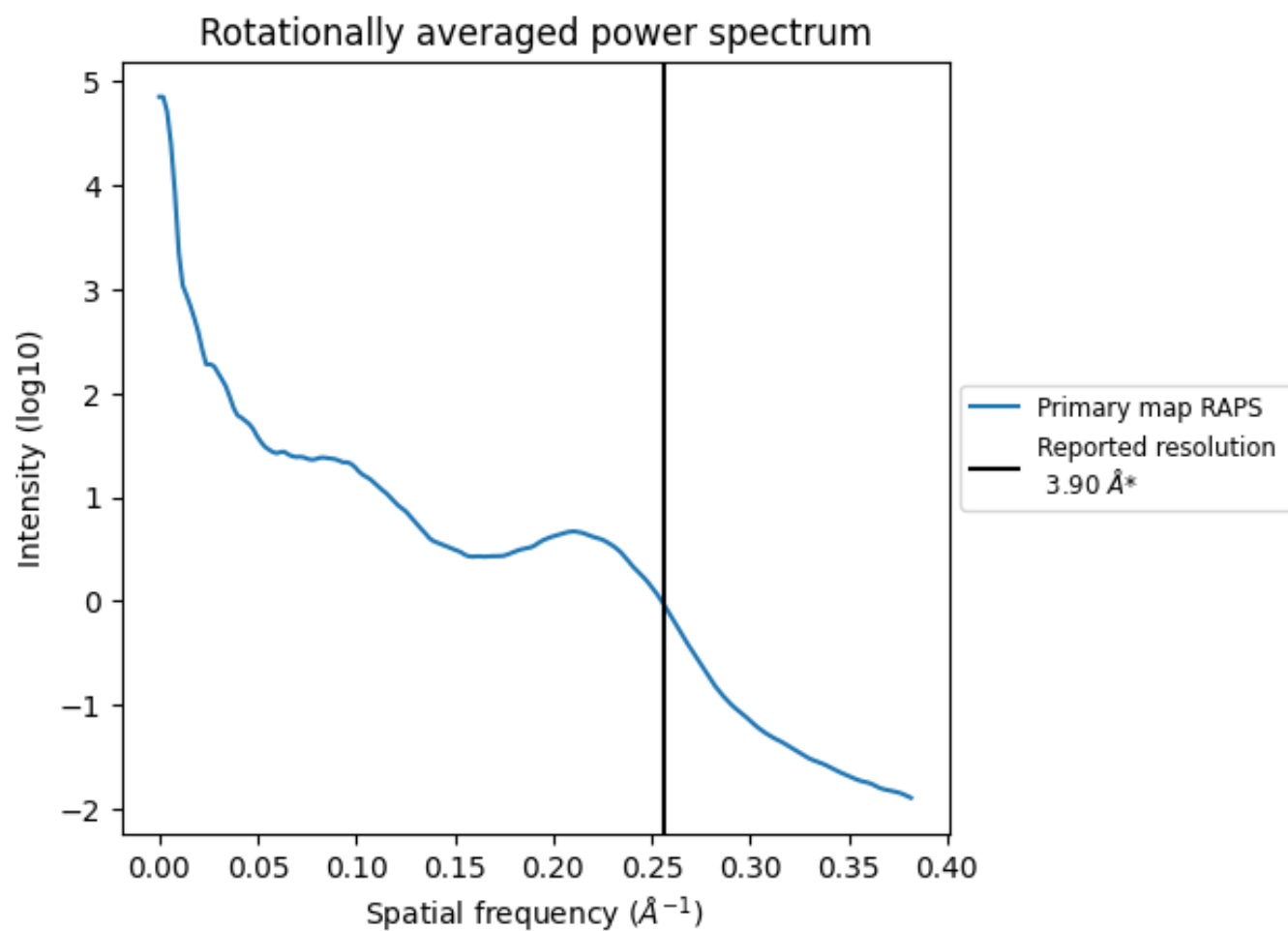
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm<sup>3</sup>; this corresponds to an approximate mass of 451 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 ⓘ

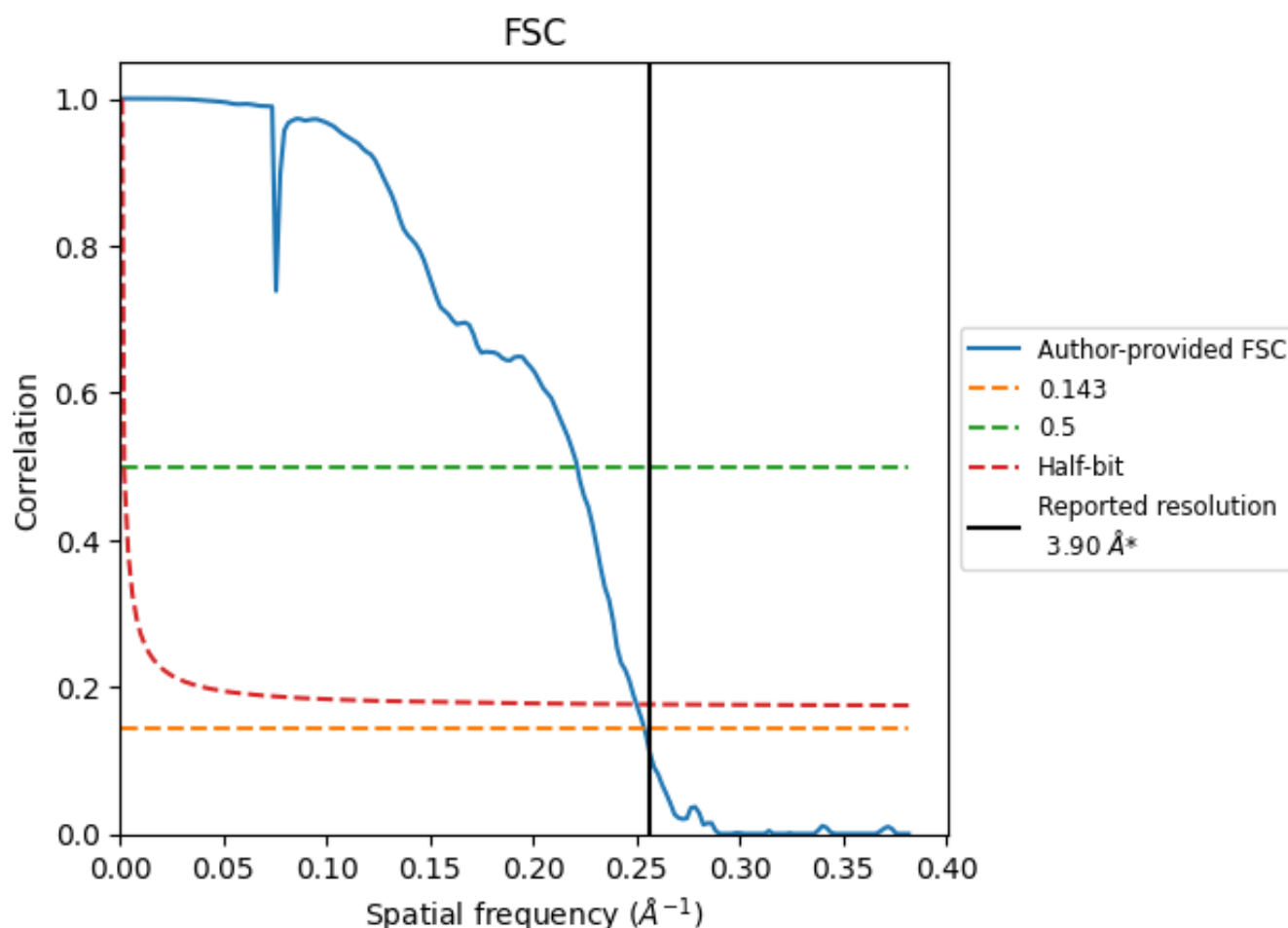


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

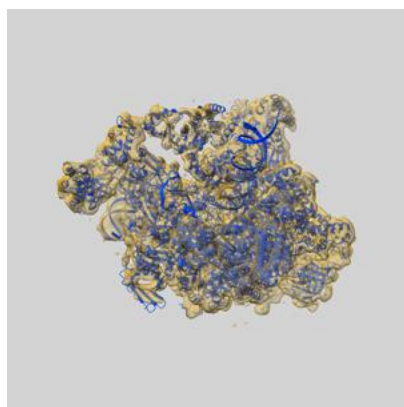
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.52	4.00
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

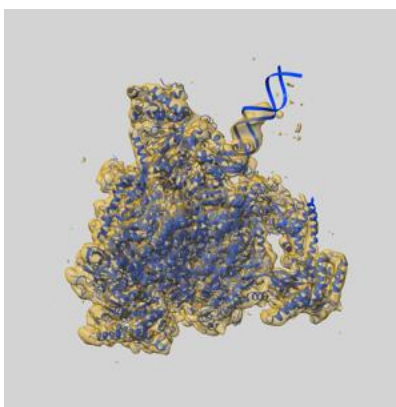
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8137 and PDB model 5IYC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

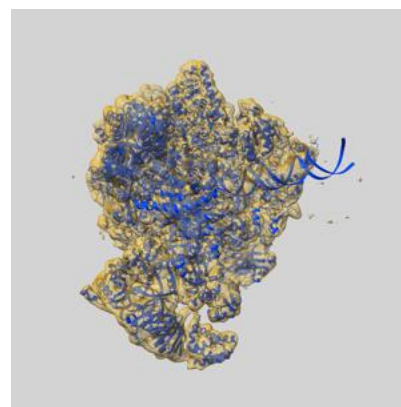
### 9.1 Map-model overlay [i](#)



X



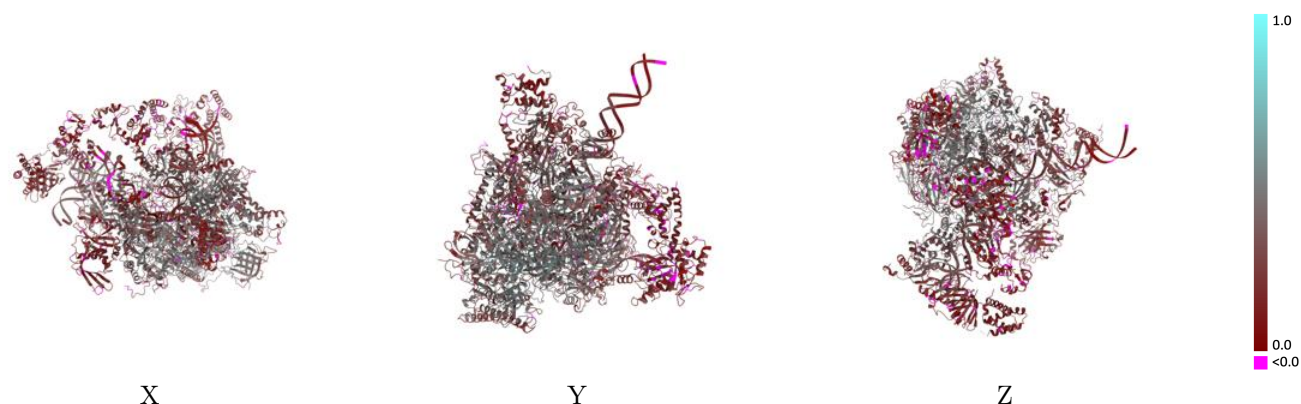
Y



Z

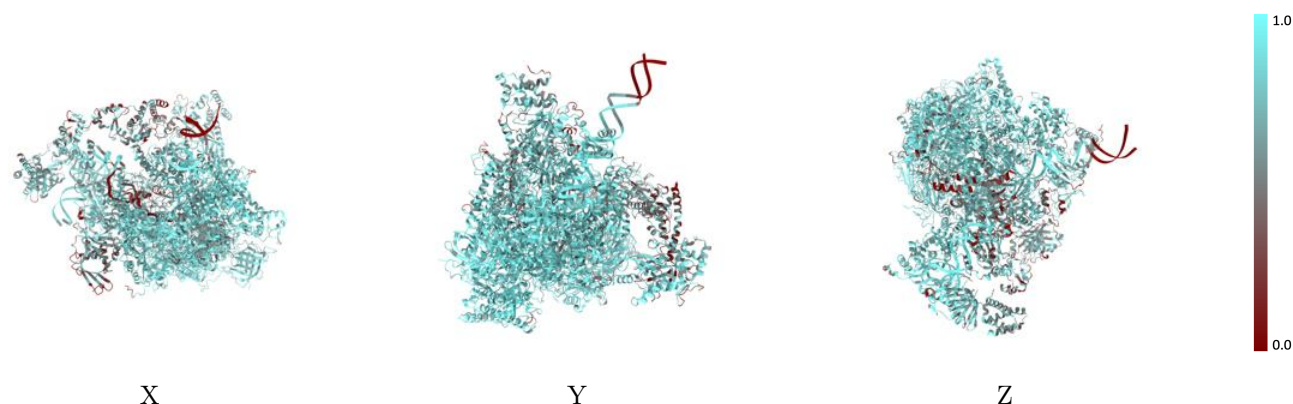
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



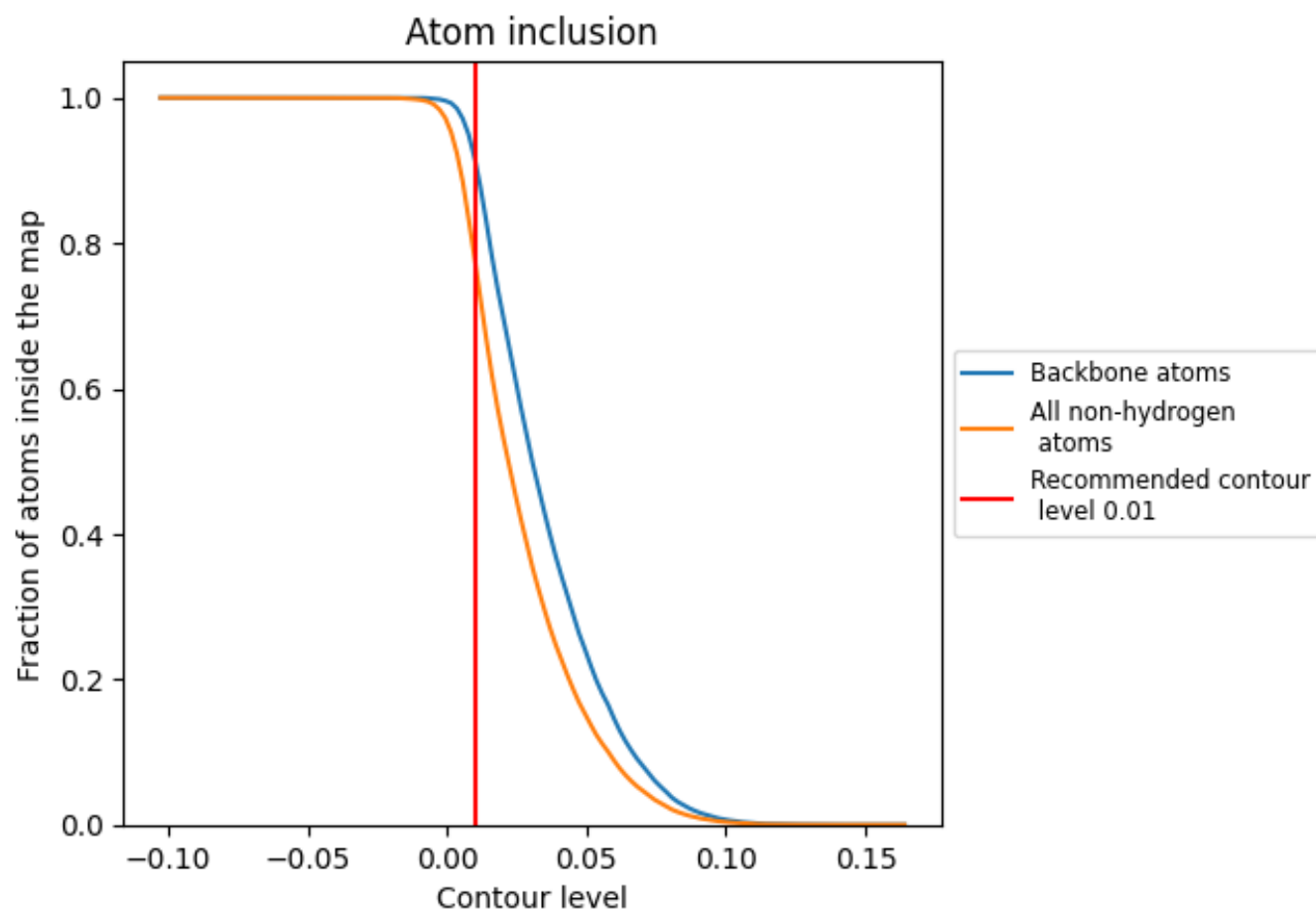
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7756	 0.3060
A	 0.8488	 0.3730
B	 0.8491	 0.3980
C	 0.8745	 0.3840
D	 0.7113	 0.1630
E	 0.8389	 0.3450
F	 0.8308	 0.3900
G	 0.7447	 0.2050
H	 0.8438	 0.3320
I	 0.7835	 0.2840
J	 0.8772	 0.3930
K	 0.8751	 0.3840
L	 0.8817	 0.3710
M	 0.7866	 0.3020
N	 0.6692	 0.1670
O	 0.6878	 0.1690
P	 0.8193	 0.2500
Q	 0.4571	 0.1260
R	 0.4906	 0.1260
S	 0.4995	 0.1530
T	 0.5522	 0.1590
U	 0.5858	 0.1460
X	 0.6790	 0.2090
Y	 0.7802	 0.2350

