



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 5IYD / pdb_00005iyd
EMDB ID : EMD-8138
Title : Human core-PIC in the initial transcribing state (no IIS)
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

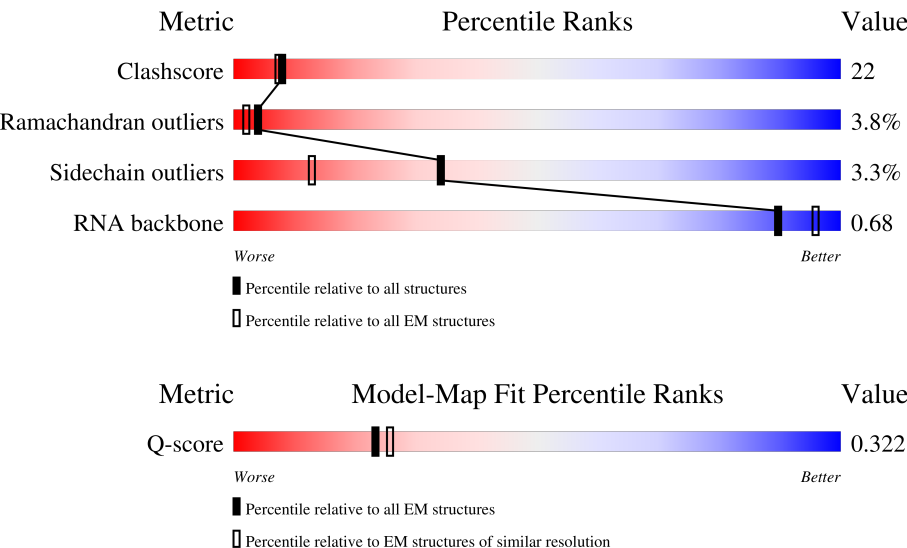
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	1970	47% 23% 26%
2	B	1174	57% 36% 5%
3	C	275	64% 32%

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	X	80	
22	Y	80	
23	Z	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	ZN	B	1201	-	-	X	-
25	ZN	I	202	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 46709 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 DNA chain called SCP-X.

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

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

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

- Molecule 23 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	6	Total	C	N	O	P	0	0
			125	57	23	40	5		

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

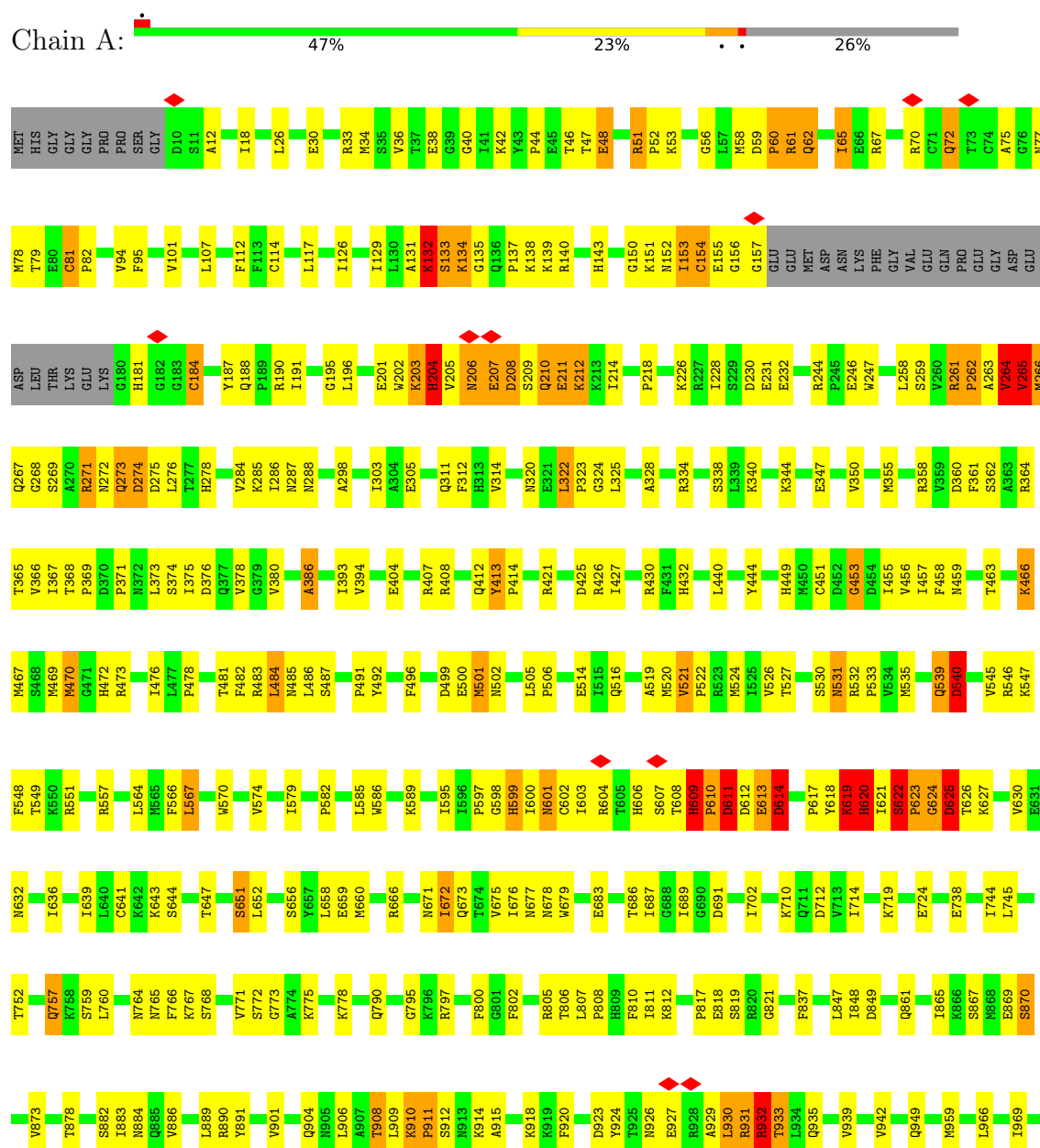
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	3	Total	Zn	0
			3	3	
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	

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



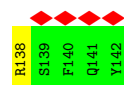
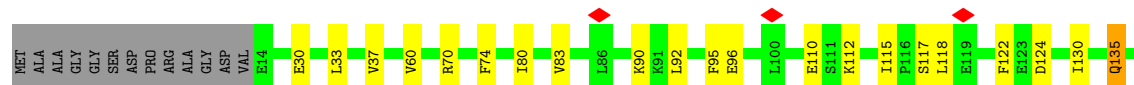
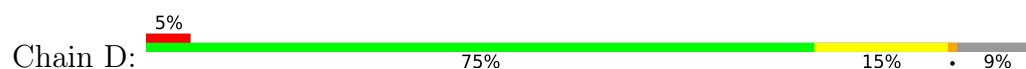


Frequency	Percentage
Daily	57%
Weekly	36%
Monthly	5%

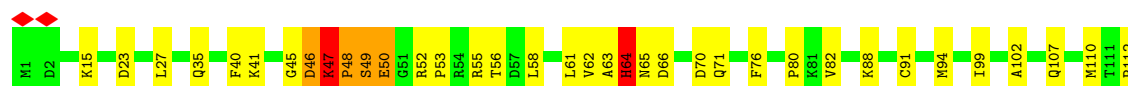
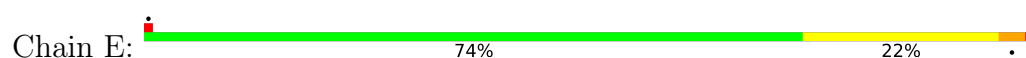




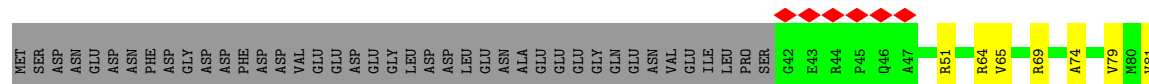
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



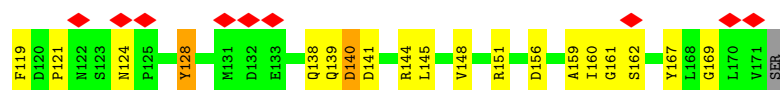
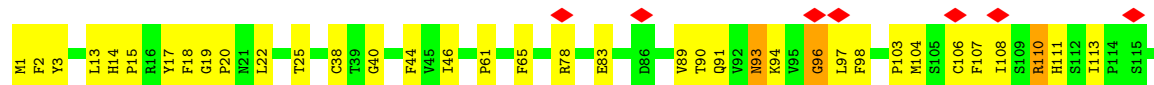
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



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

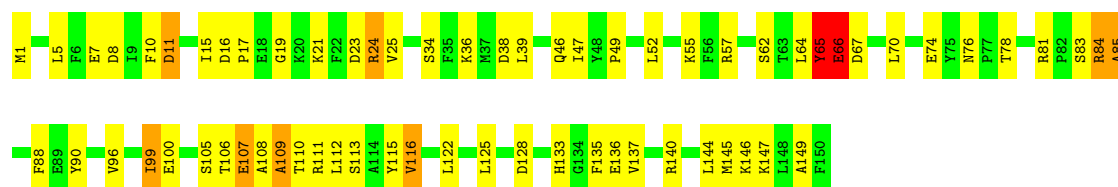


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



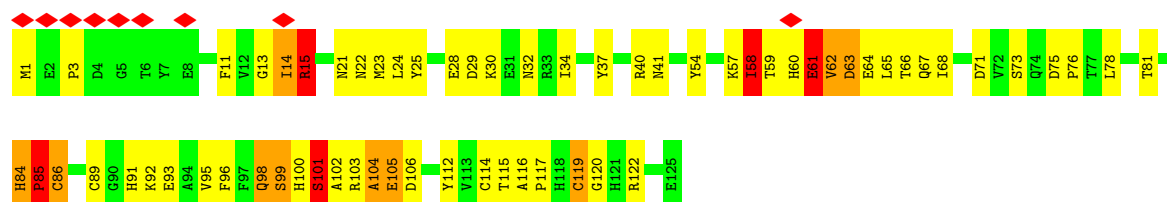
- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

Chain H:  56% 37% 5% .



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

Chain I:  7% 49% 39% 8% .



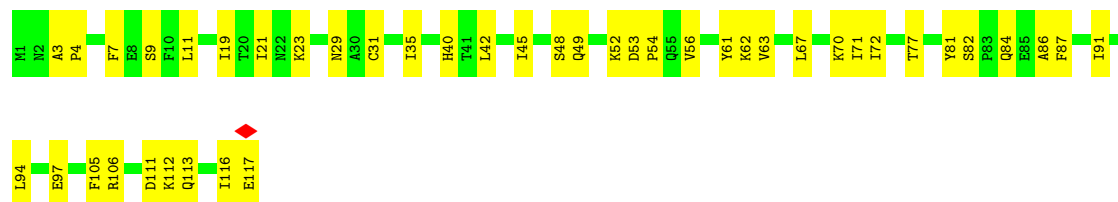
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10

Chain J:  57% 33% 9% .

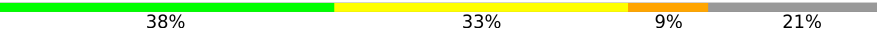


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  63% 37% .



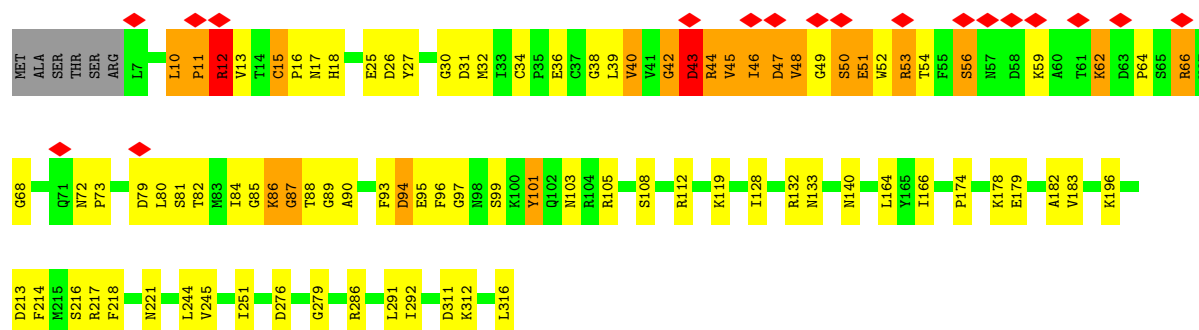
- Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L:  38% 33% 9% 21%

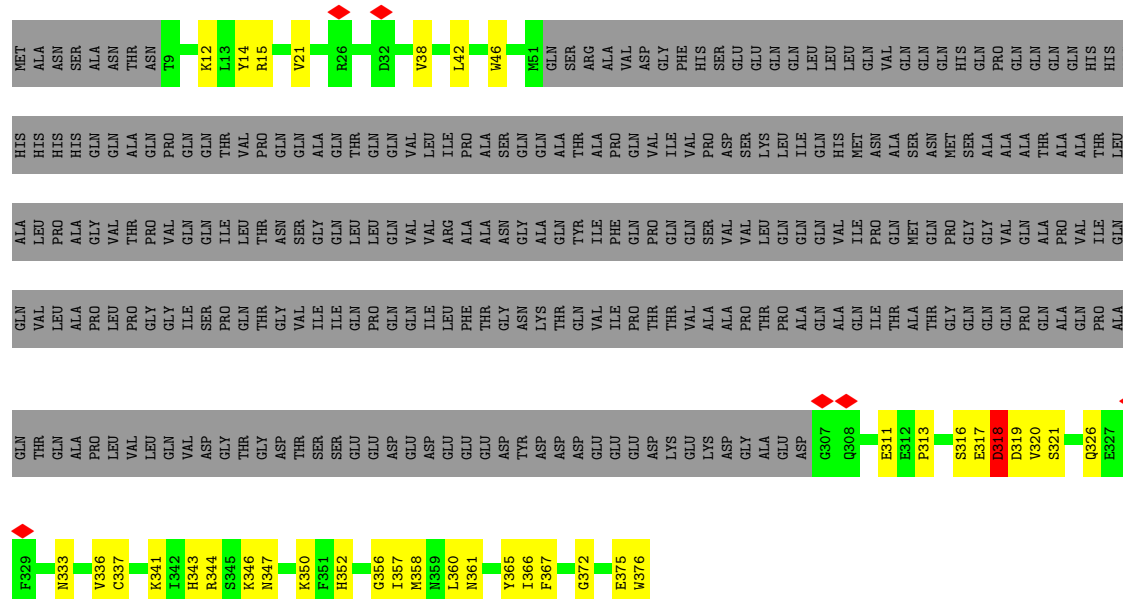


- Molecule 13: Transcription initiation factor IIB

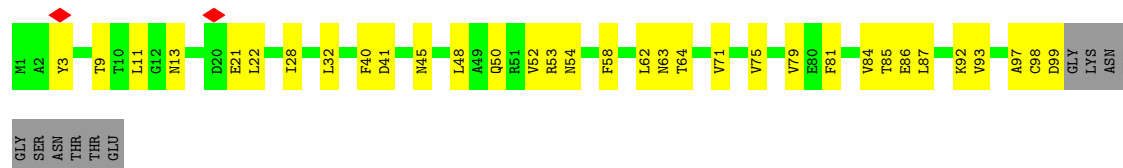
Chain M:  6% 69% 22% 6% ..



• Molecule 14: Transcription initiation factor IIA subunit 1



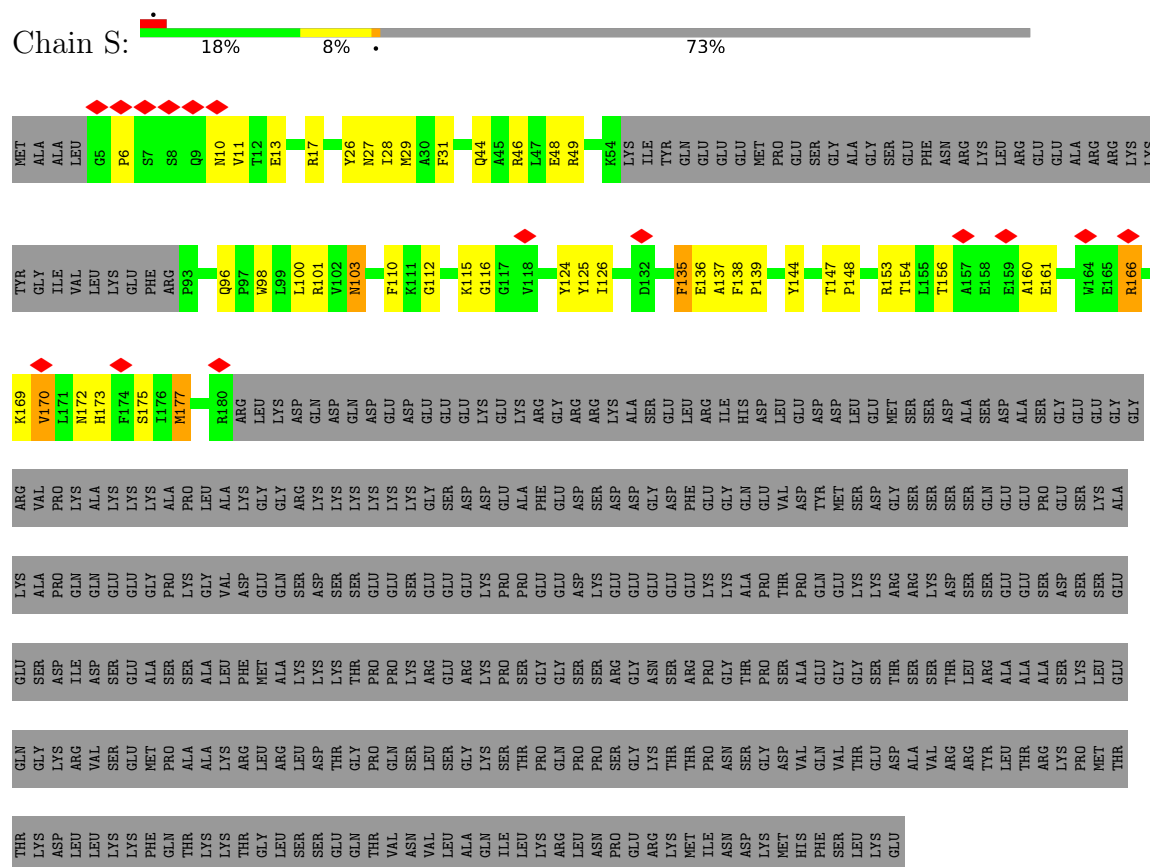
• Molecule 15: Transcription initiation factor IIA subunit 2



ASP
ILE
THR
SER
SER
LYS

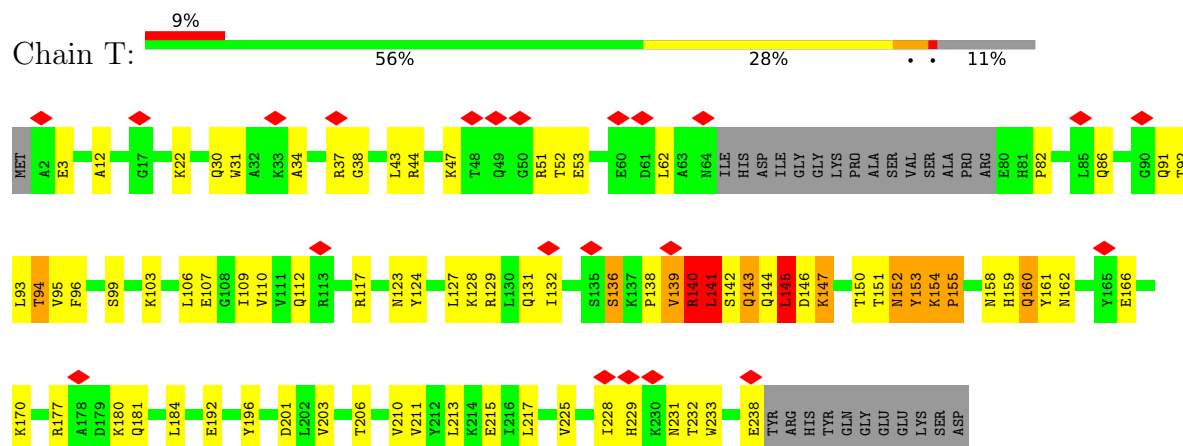
• Molecule 19: General transcription factor IIF subunit 1

Chain S:



• Molecule 20: General transcription factor IIF subunit 2

Chain T:



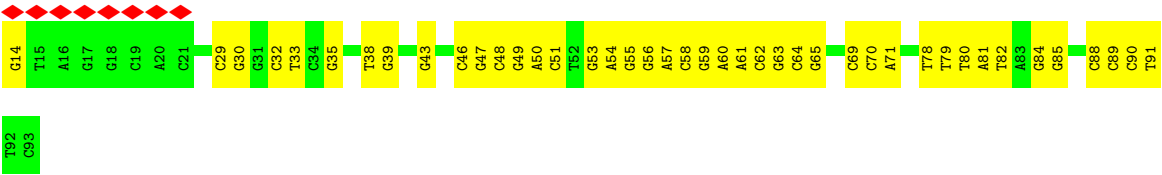
• Molecule 21: SCP-X

Chain X:

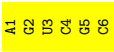
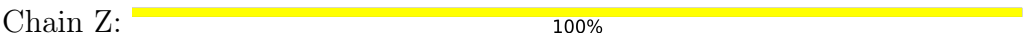




• Molecule 22: SCP-Y



• Molecule 23: RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99929	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	0.149	Depositor
Minimum map value	-0.087	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	4/11727 (0.0%)	1.22	102/15833 (0.6%)
2	B	0.85	1/9503 (0.0%)	1.24	60/12831 (0.5%)
3	C	0.74	0/2259	1.23	15/3073 (0.5%)
4	D	0.34	0/1077	0.91	2/1446 (0.1%)
5	E	0.55	0/1753	1.11	6/2368 (0.3%)
6	F	0.58	0/700	1.04	2/946 (0.2%)
7	G	0.41	0/1382	0.99	9/1874 (0.5%)
8	H	0.53	0/1227	1.03	3/1654 (0.2%)
9	I	0.45	0/1038	1.19	8/1407 (0.6%)
10	J	0.77	0/542	1.26	5/730 (0.7%)
11	K	0.66	0/956	1.08	6/1294 (0.5%)
12	L	0.63	0/394	0.99	2/524 (0.4%)
13	M	0.55	0/2429	1.17	21/3281 (0.6%)
14	N	0.31	0/945	0.90	1/1274 (0.1%)
15	O	0.33	0/816	0.84	0/1105
16	P	0.41	0/1489	1.04	6/2005 (0.3%)
17	Q	0.39	0/1507	1.03	7/2023 (0.3%)
18	R	0.74	2/1380 (0.1%)	1.45	22/1854 (1.2%)
19	S	0.34	0/1167	0.85	3/1576 (0.2%)
20	T	0.36	0/1817	0.97	5/2445 (0.2%)
21	X	0.29	0/1843	0.53	0/2847
22	Y	0.26	0/1817	0.46	0/2800
23	Z	0.20	0/139	0.32	0/215
All	All	0.64	7/47907 (0.0%)	1.11	285/65405 (0.4%)

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	3
2	B	0	1
8	H	0	1
9	I	0	1
16	P	0	1
17	Q	0	1
18	R	0	4
20	T	0	1
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	939	HIS	CA-C	-6.64	1.44	1.53
1	A	1291	ASN	CA-CB	6.44	1.63	1.53
1	A	484	LEU	CA-C	-5.71	1.45	1.52
1	A	1290	SER	C-O	5.67	1.30	1.24
1	A	806	THR	CA-CB	-5.57	1.44	1.53
18	R	205	ASP	N-CA	5.49	1.51	1.46
18	R	206	LYS	CA-C	5.06	1.59	1.52

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	GLN	C-N-CD	-17.90	51.61	125.00
9	I	104	ALA	N-CA-C	-17.08	92.38	112.87
3	C	137	ASN	N-CA-C	-16.86	89.41	110.65
13	M	94	ASP	N-CA-C	-15.26	90.44	114.09
9	I	84	HIS	C-N-CD	-14.61	65.08	125.00
1	A	413	TYR	CA-C-N	-13.87	106.68	120.83
1	A	413	TYR	C-N-CA	-13.87	106.68	120.83
18	R	194	ARG	C-N-CD	-12.75	72.73	125.00
16	P	206	GLU	C-N-CD	-12.65	73.12	125.00
1	A	1306	LYS	N-CA-C	-11.44	98.08	112.72
18	R	205	ASP	N-CA-C	11.16	125.16	109.31
13	M	11	PRO	N-CA-C	-11.11	97.48	112.48
1	A	622	SER	N-CA-C	-10.75	86.06	109.81
5	E	47	LYS	C-N-CD	-10.49	82.01	125.00
1	A	1307	VAL	N-CA-C	9.62	129.36	109.34
18	R	224	THR	N-CA-C	9.19	130.38	110.80
2	B	132	VAL	N-CA-C	9.00	115.84	106.21
2	B	492	ASP	N-CA-C	8.89	124.28	111.56
1	A	203	LYS	N-CA-C	8.88	123.57	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ASP	N-CA-C	8.84	129.62	110.80
1	A	211	GLU	N-CA-C	-8.77	100.90	111.69
1	A	1314	THR	N-CA-C	-8.75	103.19	114.04
8	H	85	ALA	N-CA-C	-8.63	96.67	109.62
1	A	601	ASN	N-CA-C	8.48	122.47	107.80
13	M	43	ASP	N-CA-C	-8.31	93.09	110.80
2	B	1008	VAL	N-CA-C	8.19	118.23	110.53
1	A	672	ILE	N-CA-C	7.95	118.73	110.62
8	H	84	ARG	N-CA-C	7.92	121.71	110.23
2	B	62	ALA	CA-C-N	-7.89	112.25	120.38
2	B	62	ALA	C-N-CA	-7.89	112.25	120.38
1	A	150	GLY	N-CA-C	7.86	123.91	113.37
1	A	744	ILE	N-CA-C	7.86	117.96	110.42
3	C	6	GLN	N-CA-C	7.84	127.14	109.81
7	G	46	ILE	N-CA-C	7.84	117.90	110.53
16	P	162	VAL	CA-C-N	7.81	127.87	119.90
16	P	162	VAL	C-N-CA	7.81	127.87	119.90
13	M	51	GLU	N-CA-C	7.79	119.77	111.28
9	I	84	HIS	CA-C-N	7.78	129.57	119.84
9	I	84	HIS	C-N-CA	7.78	129.57	119.84
9	I	84	HIS	N-CA-C	7.76	126.96	109.81
1	A	1385	VAL	N-CA-C	7.73	118.50	110.62
1	A	476	ILE	N-CA-C	7.72	118.95	109.30
1	A	1483	GLY	N-CA-C	7.71	122.64	112.77
2	B	883	THR	CA-C-N	-7.66	106.91	121.54
2	B	883	THR	C-N-CA	-7.66	106.91	121.54
1	A	932	ARG	CA-C-N	-7.51	106.94	121.58
1	A	932	ARG	C-N-CA	-7.51	106.94	121.58
1	A	620	HIS	N-CA-C	7.49	126.74	110.80
2	B	882	SER	N-CA-C	-7.49	101.17	111.28
17	Q	100	VAL	N-CA-C	7.43	124.80	109.34
2	B	223	SER	N-CA-C	7.37	120.31	110.88
2	B	294	ASP	CA-C-N	7.24	127.24	119.28
2	B	294	ASP	C-N-CA	7.24	127.24	119.28
13	M	93	PHE	N-CA-C	7.19	120.66	110.23
2	B	46	SER	N-CA-C	7.13	119.05	111.28
3	C	42	VAL	CA-C-N	-7.12	113.33	120.31
3	C	42	VAL	C-N-CA	-7.12	113.33	120.31
13	M	50	SER	CA-C-N	7.05	129.73	120.28
13	M	50	SER	C-N-CA	7.05	129.73	120.28
13	M	62	LYS	N-CA-C	-6.89	105.42	114.31
8	H	66	GLU	N-CA-C	6.81	125.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ASN	CA-C-N	-6.80	108.54	121.54
1	A	206	ASN	C-N-CA	-6.80	108.54	121.54
2	B	802	ASP	N-CA-C	6.80	118.35	111.07
1	A	548	PHE	N-CA-C	6.79	118.77	111.36
13	M	251	ILE	N-CA-C	6.70	116.85	110.42
1	A	1199	MET	CA-C-N	6.70	128.21	119.84
1	A	1199	MET	C-N-CA	6.70	128.21	119.84
1	A	1405	MET	N-CA-C	6.68	119.57	111.82
12	L	19	CYS	N-CA-C	6.67	118.46	110.19
17	Q	99	LEU	N-CA-C	-6.62	105.12	113.72
1	A	133	SER	N-CA-C	6.61	124.87	110.80
17	Q	172	ASP	N-CA-C	6.61	124.87	110.80
10	J	50	LEU	N-CA-C	6.57	118.44	111.28
1	A	1470	CYS	N-CA-C	6.47	121.03	113.20
1	A	1454	VAL	N-CA-C	6.46	116.60	110.53
1	A	807	LEU	CA-C-N	-6.46	113.16	119.87
1	A	807	LEU	C-N-CA	-6.46	113.16	119.87
1	A	527	THR	CA-C-N	6.45	127.00	120.04
1	A	527	THR	C-N-CA	6.45	127.00	120.04
1	A	501	MET	CA-CB-CG	6.45	126.99	114.10
1	A	539	GLN	CA-C-N	6.42	128.88	120.28
1	A	539	GLN	C-N-CA	6.42	128.88	120.28
17	Q	66	LEU	N-CA-C	6.42	118.27	111.28
9	I	98	GLN	N-CA-C	6.41	119.16	108.96
2	B	58	ILE	N-CA-C	6.41	116.57	110.42
2	B	962	THR	CA-C-N	6.41	126.36	119.76
2	B	962	THR	C-N-CA	6.41	126.36	119.76
13	M	12	ARG	CA-C-N	-6.37	114.62	123.10
13	M	12	ARG	C-N-CA	-6.37	114.62	123.10
18	R	206	LYS	N-CA-C	6.37	124.36	110.80
2	B	711	ILE	CA-C-N	6.36	126.86	119.99
2	B	711	ILE	C-N-CA	6.36	126.86	119.99
7	G	110	ARG	N-CA-C	6.36	119.89	111.75
11	K	9	SER	N-CA-C	6.35	120.12	112.38
10	J	65	LEU	N-CA-C	-6.33	105.31	113.16
3	C	221	ASP	CA-C-N	6.25	125.88	119.56
3	C	221	ASP	C-N-CA	6.25	125.88	119.56
1	A	886	VAL	CB-CA-C	-6.25	103.77	111.08
2	B	421	LYS	N-CA-C	6.22	118.06	111.28
2	B	844	ILE	N-CA-C	6.21	117.36	107.98
11	K	62	LYS	CA-C-N	-6.21	118.38	122.60
11	K	62	LYS	C-N-CA	-6.21	118.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	115	ILE	CA-C-N	6.21	126.67	119.47
4	D	115	ILE	C-N-CA	6.21	126.67	119.47
1	A	456	VAL	CA-C-N	-6.18	115.14	122.93
1	A	456	VAL	C-N-CA	-6.18	115.14	122.93
1	A	1190	GLN	N-CA-C	6.17	118.01	111.28
7	G	107	PHE	N-CA-C	6.17	119.01	109.07
3	C	92	GLU	CB-CA-C	-6.17	109.45	116.54
18	R	225	VAL	N-CA-C	6.16	122.15	109.34
1	A	672	ILE	CB-CA-C	-6.09	103.92	112.14
2	B	919	CYS	N-CA-C	6.06	119.36	109.24
1	A	496	PHE	N-CA-C	-6.05	104.07	112.30
2	B	164	ASN	N-CA-C	6.03	119.73	112.38
2	B	922	ARG	N-CA-C	6.02	119.05	109.24
3	C	225	LYS	CA-C-N	-6.00	113.35	120.13
3	C	225	LYS	C-N-CA	-6.00	113.35	120.13
13	M	81	SER	N-CA-C	6.00	116.16	108.24
1	A	759	SER	N-CA-C	5.99	119.85	112.54
19	S	147	THR	CA-C-N	5.99	125.95	119.78
19	S	147	THR	C-N-CA	5.99	125.95	119.78
1	A	622	SER	C-N-CD	-5.98	100.49	125.00
18	R	224	THR	CA-C-N	5.96	132.69	121.97
18	R	224	THR	C-N-CA	5.96	132.69	121.97
1	A	322	LEU	CA-C-N	5.95	125.89	119.76
1	A	322	LEU	C-N-CA	5.95	125.89	119.76
1	A	910	LYS	CA-C-N	5.95	127.27	119.84
1	A	910	LYS	C-N-CA	5.95	127.27	119.84
18	R	163	LEU	CA-C-N	-5.95	109.76	121.41
18	R	163	LEU	C-N-CA	-5.95	109.76	121.41
3	C	66	HIS	N-CA-C	5.93	117.42	111.07
2	B	79	GLU	CA-C-N	-5.93	107.33	121.80
2	B	79	GLU	C-N-CA	-5.93	107.33	121.80
16	P	158	SER	N-CA-C	-5.93	105.04	112.93
2	B	435	ILE	N-CA-C	5.92	116.06	108.12
10	J	45	CYS	N-CA-C	-5.92	104.95	111.82
2	B	497	LYS	CA-C-N	-5.91	110.71	120.88
2	B	497	LYS	C-N-CA	-5.91	110.71	120.88
1	A	986	MET	N-CA-C	5.91	117.39	111.07
1	A	539	GLN	N-CA-C	5.90	116.73	108.00
1	A	1160	ARG	N-CA-C	5.90	117.71	111.28
17	Q	174	ARG	N-CA-C	5.88	117.69	111.28
1	A	920	PHE	N-CA-C	5.85	120.59	112.45
1	A	678	ASN	N-CA-C	5.85	117.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	19	GLY	CA-C-N	5.83	125.21	118.85
7	G	19	GLY	C-N-CA	5.83	125.21	118.85
1	A	848	ILE	N-CA-C	5.82	116.60	110.72
13	M	42	GLY	N-CA-C	5.82	126.97	113.18
2	B	1162	LEU	N-CA-C	5.80	117.60	111.28
1	A	72	GLN	CB-CA-C	-5.79	109.35	117.23
1	A	521	VAL	N-CA-C	5.76	121.33	108.88
5	E	102	ALA	N-CA-C	5.76	117.81	108.41
18	R	127	ASN	OD1-CG-ND2	-5.76	116.84	122.60
18	R	163	LEU	N-CA-C	5.75	123.06	110.80
1	A	677	ASN	N-CA-C	5.75	117.55	111.28
2	B	785	TYR	CA-C-N	-5.75	113.52	122.37
2	B	785	TYR	C-N-CA	-5.75	113.52	122.37
13	M	34	CYS	CA-C-N	5.74	127.02	119.84
13	M	34	CYS	C-N-CA	5.74	127.02	119.84
20	T	136	SER	N-CA-C	5.74	117.88	110.65
2	B	1082	GLY	N-CA-C	5.73	122.07	112.85
1	A	273	GLN	N-CA-C	-5.71	101.05	109.62
3	C	123	ASN	N-CA-C	-5.70	105.14	111.36
1	A	151	LYS	N-CA-C	5.67	119.90	112.92
13	M	44	ARG	N-CA-C	5.66	118.53	110.10
1	A	847	LEU	N-CA-C	5.65	117.44	111.28
18	R	139	PHE	CA-C-N	5.64	131.86	121.70
18	R	139	PHE	C-N-CA	5.64	131.86	121.70
5	E	145	VAL	N-CA-C	5.64	113.45	107.76
18	R	115	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	432	HIS	CA-C-N	5.62	125.73	119.32
1	A	432	HIS	C-N-CA	5.62	125.73	119.32
2	B	163	LEU	N-CA-C	5.60	119.21	112.38
2	B	77	GLU	N-CA-C	5.59	122.72	110.80
10	J	43	TYR	N-CA-C	5.59	119.36	112.54
7	G	124	ASN	CA-C-N	-5.59	114.62	120.38
7	G	124	ASN	C-N-CA	-5.59	114.62	120.38
18	R	223	VAL	N-CA-C	-5.59	104.49	110.36
16	P	325	PHE	N-CA-C	5.56	117.42	111.36
18	R	207	SER	N-CA-C	5.55	117.12	109.29
1	A	101	VAL	N-CA-C	5.52	115.72	110.42
5	E	126	ILE	N-CA-C	5.50	115.87	108.17
1	A	886	VAL	N-CA-C	5.48	116.65	108.54
1	A	75	ALA	CB-CA-C	-5.47	110.25	116.54
7	G	96	GLY	N-CA-C	5.47	117.56	110.45
10	J	7	CYS	N-CA-C	5.46	118.39	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	90	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	394	VAL	N-CA-C	5.46	116.09	108.89
1	A	675	VAL	CB-CA-C	-5.46	104.99	111.97
2	B	192	LYS	N-CA-C	-5.43	99.58	108.76
18	R	207	SER	CA-C-N	-5.43	113.28	122.67
18	R	207	SER	C-N-CA	-5.43	113.28	122.67
2	B	95	LYS	CA-C-N	5.42	126.61	119.84
2	B	95	LYS	C-N-CA	5.42	126.61	119.84
1	A	609	HIS	C-N-CD	-5.42	102.80	125.00
1	A	660	MET	N-CA-C	5.41	119.87	113.16
2	B	407	MET	N-CA-C	5.41	117.26	111.36
2	B	161	CYS	N-CA-C	-5.40	103.56	110.53
1	A	267	GLN	CB-CA-C	-5.40	110.37	116.63
9	I	15	ARG	N-CA-C	-5.40	99.30	110.80
1	A	566	PHE	N-CA-C	5.40	119.49	113.01
2	B	1087	GLY	N-CA-C	5.39	119.48	112.25
1	A	380	VAL	CA-C-N	5.39	125.39	119.89
1	A	380	VAL	C-N-CA	5.39	125.39	119.89
1	A	1306	LYS	CA-C-N	5.39	131.67	121.97
1	A	1306	LYS	C-N-CA	5.39	131.67	121.97
1	A	867	SER	N-CA-C	5.39	117.01	111.03
1	A	540	ASP	CB-CA-C	5.39	119.73	110.79
1	A	614	ASP	CA-C-N	-5.38	112.18	121.66
1	A	614	ASP	C-N-CA	-5.38	112.18	121.66
1	A	470	MET	N-CA-C	5.38	117.37	109.24
6	F	88	ASP	CA-C-N	5.38	125.03	119.05
6	F	88	ASP	C-N-CA	5.38	125.03	119.05
14	N	346	LYS	CB-CA-C	-5.37	109.93	117.23
2	B	39	LEU	N-CA-C	5.36	118.92	112.38
2	B	963	PRO	CA-C-O	-5.36	115.23	121.34
1	A	386	ALA	N-CA-C	5.36	118.03	111.82
1	A	288	ASN	N-CA-C	-5.35	105.53	111.36
1	A	539	GLN	CB-CA-C	-5.34	108.86	116.34
13	M	25	GLU	N-CA-C	5.34	117.33	108.20
1	A	1121	VAL	N-CA-C	5.32	120.38	108.88
1	A	1482	TYR	CA-C-N	5.32	125.85	120.00
1	A	1482	TYR	C-N-CA	5.32	125.85	120.00
1	A	636	ILE	N-CA-C	5.31	115.97	110.82
7	G	93	ASN	N-CA-C	5.31	117.25	109.24
2	B	1006	VAL	CA-C-N	5.30	131.67	121.54
2	B	1006	VAL	C-N-CA	5.30	131.67	121.54
1	A	1093	GLN	N-CA-C	5.30	117.97	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	CYS	CA-C-N	5.28	125.36	119.87
1	A	81	CYS	C-N-CA	5.28	125.36	119.87
9	I	85	PRO	N-CA-C	5.27	123.32	112.47
1	A	1369	LEU	N-CA-C	5.27	119.70	113.28
1	A	60	PRO	N-CA-C	-5.25	107.29	113.86
2	B	757	PRO	CA-C-O	-5.25	115.43	121.36
1	A	1076	PHE	N-CA-C	5.24	117.00	111.28
2	B	1054	MET	N-CA-C	5.24	117.94	109.40
1	A	206	ASN	N-CA-C	5.23	121.94	110.80
3	C	71	ILE	CA-C-N	5.23	124.99	119.76
3	C	71	ILE	C-N-CA	5.23	124.99	119.76
11	K	82	SER	CA-C-N	5.23	124.73	119.19
11	K	82	SER	C-N-CA	5.23	124.73	119.19
1	A	651	SER	N-CA-C	5.23	117.27	110.53
2	B	667	THR	N-CA-C	5.22	117.71	111.71
13	M	216	SER	N-CA-C	5.22	116.66	110.97
2	B	788	TYR	CA-C-N	-5.21	114.34	122.73
2	B	788	TYR	C-N-CA	-5.21	114.34	122.73
2	B	997	GLY	N-CA-C	5.21	120.85	111.62
2	B	388	TYR	CA-CB-CG	-5.20	104.55	113.90
18	R	139	PHE	O-C-N	-5.19	116.56	122.89
1	A	933	THR	N-CA-C	-5.18	106.91	113.18
20	T	94	THR	CA-C-N	-5.18	115.92	123.06
20	T	94	THR	C-N-CA	-5.18	115.92	123.06
20	T	136	SER	CA-C-N	-5.17	115.90	122.98
20	T	136	SER	C-N-CA	-5.17	115.90	122.98
1	A	287	ASN	N-CA-C	5.17	116.91	111.28
2	B	169	ARG	N-CA-C	5.15	116.98	111.36
2	B	79	GLU	N-CA-C	5.15	121.78	114.16
2	B	866	ILE	N-CA-C	5.15	116.61	111.00
18	R	218	LYS	CA-C-N	5.13	127.11	120.44
18	R	218	LYS	C-N-CA	5.13	127.11	120.44
5	E	64	HIS	N-CA-C	5.12	120.93	113.40
1	A	1128	ILE	N-CA-C	5.12	115.34	110.42
2	B	780	VAL	N-CA-C	5.11	115.84	108.48
17	Q	184	ILE	N-CA-C	5.11	115.83	110.62
13	M	166	ILE	CB-CA-C	-5.10	105.44	111.97
17	Q	103	VAL	N-CA-C	5.09	116.55	111.00
2	B	942	LYS	N-CA-C	-5.09	102.22	110.32
3	C	83	GLN	N-CA-C	5.09	117.37	110.35
19	S	103	ASN	CB-CA-C	-5.08	110.32	117.23
12	L	29	LYS	N-CA-C	-5.08	107.59	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	15	CYS	CA-C-N	5.07	124.67	119.05
13	M	15	CYS	C-N-CA	5.07	124.67	119.05
1	A	204	HIS	N-CA-C	5.06	121.58	110.80
1	A	1141	VAL	N-CA-C	5.06	115.37	107.99
1	A	639	ILE	N-CA-C	5.05	116.09	109.58
2	B	364	PHE	N-CA-C	5.04	116.78	111.28
2	B	531	TYR	CA-C-N	-5.03	115.45	122.75
2	B	531	TYR	C-N-CA	-5.03	115.45	122.75
11	K	21	ILE	N-CA-C	5.03	115.09	107.75
16	P	160	GLY	N-CA-C	-5.02	106.56	112.64
1	A	848	ILE	CB-CA-C	-5.02	105.29	112.22
1	A	1372	GLU	N-CA-C	5.01	116.83	111.36
2	B	205	VAL	N-CA-C	5.01	115.50	108.89
5	E	50	GLU	N-CA-C	5.01	121.46	110.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1291	ASN	Sidechain
1	A	1308	TYR	Peptide
1	A	210	GLN	Mainchain
2	B	873	LEU	Mainchain
8	H	99	ILE	Peptide
9	I	101	SER	Mainchain
16	P	242	GLN	Sidechain
17	Q	125	ALA	Peptide
18	R	109	LEU	Mainchain
18	R	139	PHE	Peptide,Mainchain
18	R	215	GLU	Mainchain
20	T	123	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11615	559	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9317	0	9312	482	0
3	C	2213	0	2157	104	0
4	D	1062	0	1042	14	0
5	E	1723	0	1745	52	0
6	F	689	0	715	11	0
7	G	1351	0	1358	43	0
8	H	1205	0	1168	67	0
9	I	1013	0	939	84	0
10	J	533	0	557	44	0
11	K	937	0	959	27	0
12	L	388	0	397	31	0
13	M	2391	0	2413	164	0
14	N	930	0	888	32	0
15	O	806	0	818	27	0
16	P	1462	0	1548	51	0
17	Q	1484	0	1501	230	0
18	R	1357	0	1381	231	0
19	S	1138	0	1103	43	0
20	T	1788	0	1817	154	0
21	X	1645	0	908	53	0
22	Y	1624	0	899	47	0
23	Z	125	0	67	10	0
24	A	2	0	0	0	0
25	A	3	0	0	0	0
25	B	1	0	0	2	0
25	C	1	0	0	0	0
25	I	2	0	0	2	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
All	All	46709	0	45307	2013	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 22.

All (2013) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:224:THR:CG2	18:R:225:VAL:HG23	1.23	1.56
1:A:1290:SER:CB	2:B:250:SER:CB	1.84	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:SER:CB	2:B:250:SER:HB3	1.12	1.54
1:A:1307:VAL:HG21	1:A:1339:ASP:CB	1.35	1.50
2:B:92:TYR:CD1	20:T:141:LEU:HD11	1.45	1.48
2:B:56:GLN:HG2	20:T:140:ARG:CD	1.45	1.44
3:C:157:GLN:NE2	10:J:65:LEU:HB3	1.20	1.44
17:Q:113:ARG:NE	18:R:222:SER:HB3	1.24	1.44
5:E:47:LYS:HB3	5:E:48:PRO:CD	1.39	1.43
1:A:608:THR:C	1:A:610:PRO:HD2	1.41	1.42
8:H:65:TYR:CE2	8:H:70:LEU:HB3	1.51	1.42
17:Q:184:ILE:HD11	18:R:213:ASP:CG	1.42	1.42
1:A:458:PHE:HE1	1:A:501:MET:SD	1.40	1.41
17:Q:109:HIS:CE1	18:R:225:VAL:HG21	1.58	1.39
17:Q:113:ARG:HE	18:R:222:SER:CB	1.33	1.38
13:M:44:ARG:NH1	13:M:46:ILE:HG22	1.37	1.37
17:Q:23:ARG:HH12	18:R:206:LYS:CG	1.35	1.37
17:Q:113:ARG:HD3	18:R:221:ARG:C	1.50	1.36
3:C:5:ASN:O	3:C:7:PRO:HD3	1.20	1.36
1:A:1290:SER:OG	2:B:250:SER:HB3	1.18	1.35
17:Q:188:TYR:CE2	18:R:210:PHE:CD1	2.15	1.35
1:A:427:ILE:HG12	13:M:38:GLY:O	1.25	1.34
3:C:157:GLN:CD	10:J:65:LEU:HB3	1.52	1.34
13:M:27:TYR:CE2	13:M:46:ILE:HD13	1.64	1.33
17:Q:109:HIS:ND1	18:R:225:VAL:HG21	1.43	1.32
1:A:1307:VAL:CG2	1:A:1339:ASP:HB3	1.59	1.30
16:P:159:SER:HB2	16:P:329:TYR:CD2	1.66	1.30
1:A:264:VAL:C	1:A:272:ASN:HD22	1.40	1.29
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.12	1.28
1:A:152:ASN:O	1:A:153:ILE:HG12	1.32	1.28
13:M:178:LYS:O	20:T:154:LYS:HB2	1.18	1.27
17:Q:21:VAL:O	18:R:210:PHE:CE2	1.87	1.27
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.62	1.27
1:A:156:GLY:HA2	1:A:181:HIS:ND1	1.47	1.27
17:Q:184:ILE:CD1	18:R:213:ASP:OD2	1.80	1.27
13:M:178:LYS:O	20:T:154:LYS:CB	1.83	1.27
1:A:202:TRP:HE3	1:A:212:LYS:O	1.11	1.26
18:R:224:THR:CG2	18:R:225:VAL:H	1.40	1.26
5:E:47:LYS:CB	5:E:48:PRO:HD2	1.63	1.26
17:Q:113:ARG:CD	18:R:221:ARG:C	2.06	1.26
13:M:182:ALA:HB2	20:T:154:LYS:CB	1.64	1.25
2:B:92:TYR:CB	20:T:145:LEU:HD12	1.66	1.25
9:I:62:VAL:O	9:I:64:GLU:N	1.71	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:113:ARG:HD3	18:R:221:ARG:O	1.36	1.23
1:A:425:ASP:OD2	13:M:39:LEU:CD1	1.85	1.23
18:R:224:THR:CG2	18:R:225:VAL:CG2	2.16	1.22
17:Q:188:TYR:CE2	18:R:210:PHE:HD1	1.51	1.21
9:I:57:LYS:O	9:I:58:ILE:HG12	1.40	1.21
17:Q:188:TYR:CZ	18:R:210:PHE:CD1	2.29	1.21
17:Q:113:ARG:HD2	18:R:221:ARG:CB	1.70	1.20
16:P:159:SER:HB2	16:P:329:TYR:CE2	1.75	1.20
17:Q:23:ARG:NH1	18:R:206:LYS:CG	2.03	1.19
16:P:159:SER:CB	16:P:329:TYR:CD2	2.23	1.19
17:Q:23:ARG:HH12	18:R:206:LYS:CB	1.55	1.19
2:B:883:THR:O	2:B:885:ARG:N	1.74	1.19
1:A:265:VAL:N	1:A:272:ASN:HB2	1.58	1.18
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.41	1.18
17:Q:113:ARG:NE	18:R:222:SER:CB	1.97	1.18
2:B:882:SER:HB3	2:B:887:TYR:CE1	1.79	1.17
1:A:458:PHE:CE1	1:A:501:MET:SD	2.32	1.17
17:Q:184:ILE:CG1	18:R:213:ASP:OD1	1.93	1.17
17:Q:188:TYR:CZ	18:R:210:PHE:HD1	1.61	1.17
1:A:622:SER:O	1:A:624:GLY:N	1.77	1.16
1:A:1290:SER:HB3	2:B:250:SER:OG	1.46	1.16
3:C:157:GLN:NE2	10:J:65:LEU:CB	2.08	1.16
2:B:882:SER:HB3	2:B:887:TYR:CZ	1.80	1.15
2:B:132:VAL:CG2	2:B:141:GLN:HG3	1.75	1.15
17:Q:113:ARG:CZ	18:R:222:SER:HB3	1.76	1.15
9:I:85:PRO:O	9:I:86:CYS:O	1.62	1.14
1:A:609:HIS:N	1:A:610:PRO:CD	2.09	1.14
1:A:202:TRP:HB2	1:A:212:LYS:HB3	1.27	1.14
2:B:92:TYR:CD1	20:T:141:LEU:CD1	2.30	1.14
1:A:1307:VAL:CG2	1:A:1339:ASP:CB	2.21	1.13
2:B:56:GLN:HG2	20:T:140:ARG:HD3	1.23	1.13
9:I:85:PRO:O	9:I:86:CYS:C	1.89	1.13
1:A:608:THR:C	1:A:610:PRO:CD	2.22	1.13
17:Q:188:TYR:OH	18:R:210:PHE:CE1	2.02	1.13
1:A:262:PRO:HG3	2:B:1070:LEU:HG	1.14	1.13
1:A:425:ASP:OD2	13:M:39:LEU:HD11	0.96	1.12
1:A:608:THR:OG1	1:A:610:PRO:CG	1.97	1.12
2:B:883:THR:O	2:B:884:ASN:C	1.83	1.13
16:P:159:SER:CB	16:P:329:TYR:CE2	2.32	1.12
3:C:157:GLN:CG	10:J:65:LEU:CB	2.28	1.12
13:M:182:ALA:HB2	20:T:154:LYS:HB3	1.24	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:GLY:O	1:A:625:ASP:HB2	1.46	1.11
2:B:132:VAL:HG23	2:B:141:GLN:HG3	1.20	1.11
17:Q:187:ILE:HG21	18:R:211:SER:HA	1.20	1.11
1:A:264:VAL:C	1:A:272:ASN:ND2	2.08	1.11
1:A:264:VAL:HB	1:A:272:ASN:CG	1.75	1.10
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.32	1.10
1:A:1290:SER:HB3	2:B:250:SER:CB	1.64	1.10
17:Q:184:ILE:HD11	18:R:213:ASP:OD2	0.94	1.10
18:R:224:THR:HG23	18:R:225:VAL:HG23	1.32	1.10
13:M:11:PRO:HD2	13:M:13:VAL:HG22	1.11	1.10
18:R:224:THR:HG22	18:R:225:VAL:HG23	1.27	1.10
2:B:298:MET:SD	9:I:13:GLY:O	2.10	1.10
2:B:882:SER:O	2:B:887:TYR:CD2	2.02	1.10
1:A:202:TRP:CE3	1:A:212:LYS:O	2.03	1.09
1:A:1290:SER:HB2	2:B:250:SER:HB3	1.22	1.09
2:B:92:TYR:HB2	20:T:145:LEU:HD12	1.33	1.09
17:Q:187:ILE:HG22	18:R:210:PHE:O	1.49	1.09
1:A:265:VAL:N	1:A:272:ASN:CB	2.15	1.08
8:H:66:GLU:HG3	8:H:67:ASP:N	1.60	1.08
17:Q:110:MET:HG2	18:R:222:SER:HB2	1.08	1.08
13:M:44:ARG:HH11	13:M:46:ILE:CG2	1.67	1.08
18:R:224:THR:HG21	18:R:225:VAL:HG23	1.27	1.08
17:Q:113:ARG:NH1	18:R:218:LYS:O	1.86	1.07
2:B:56:GLN:CG	20:T:140:ARG:CD	2.32	1.07
20:T:139:VAL:O	20:T:141:LEU:N	1.86	1.07
5:E:47:LYS:CB	5:E:48:PRO:CD	2.13	1.07
18:R:224:THR:HG22	18:R:225:VAL:N	1.50	1.07
13:M:11:PRO:HD2	13:M:13:VAL:CG2	1.85	1.07
1:A:262:PRO:CG	2:B:1070:LEU:HG	1.85	1.06
1:A:131:ALA:O	1:A:133:SER:N	1.86	1.06
2:B:74:ALA:O	2:B:75:SER:OG	1.72	1.06
2:B:92:TYR:HD1	20:T:141:LEU:CD1	1.66	1.06
1:A:425:ASP:CG	13:M:39:LEU:HD11	1.79	1.05
3:C:157:GLN:CG	10:J:65:LEU:HB3	1.83	1.05
17:Q:184:ILE:HG12	18:R:213:ASP:OD1	1.56	1.05
1:A:610:PRO:O	1:A:611:ASP:HB2	1.55	1.05
13:M:94:ASP:OD2	13:M:97:GLY:O	1.75	1.04
16:P:297:LYS:CB	16:P:298:PRO:CD	2.34	1.04
17:Q:184:ILE:HD13	18:R:211:SER:HB2	1.36	1.04
17:Q:187:ILE:HG21	18:R:211:SER:CA	1.88	1.04
17:Q:113:ARG:HD2	18:R:221:ARG:HB2	1.32	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:23:ARG:NH1	18:R:206:LYS:HG2	1.70	1.03
3:C:5:ASN:C	3:C:7:PRO:HD3	1.73	1.02
17:Q:188:TYR:CE1	18:R:211:SER:HB3	1.93	1.02
2:B:56:GLN:CD	20:T:140:ARG:NH1	2.17	1.02
2:B:292:PHE:CD2	9:I:14:ILE:HD13	1.94	1.01
1:A:273:GLN:O	1:A:274:ASP:O	1.77	1.01
17:Q:188:TYR:OH	18:R:210:PHE:CD1	2.07	1.01
2:B:882:SER:CB	2:B:887:TYR:CZ	2.44	1.00
18:R:225:VAL:O	18:R:230:GLU:OE1	1.78	1.00
2:B:92:TYR:CE1	20:T:141:LEU:HD11	1.96	1.00
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.03	1.00
1:A:265:VAL:CA	1:A:272:ASN:HB2	1.91	1.00
3:C:210:GLU:O	3:C:213:GLU:HG3	1.60	1.00
1:A:609:HIS:N	1:A:610:PRO:HD3	1.77	1.00
1:A:67:ARG:NH2	13:M:45:VAL:O	1.94	1.00
18:R:224:THR:CG2	18:R:225:VAL:N	2.08	1.00
17:Q:184:ILE:CD1	18:R:213:ASP:CG	2.27	0.99
1:A:1290:SER:OG	2:B:250:SER:O	1.79	0.99
3:C:157:GLN:CD	10:J:65:LEU:CB	2.32	0.99
13:M:94:ASP:CB	13:M:99:SER:H	1.76	0.99
17:Q:20:TYR:O	18:R:210:PHE:CD2	2.14	0.99
17:Q:105:TYR:OH	18:R:234:GLU:OE1	1.80	0.99
17:Q:113:ARG:CD	18:R:222:SER:N	2.25	0.99
13:M:27:TYR:HE2	13:M:46:ILE:HD13	0.95	0.98
13:M:94:ASP:HB2	13:M:99:SER:H	1.26	0.98
1:A:1117:VAL:O	1:A:1118:THR:C	2.06	0.98
2:B:56:GLN:HG2	20:T:140:ARG:HD2	1.45	0.98
17:Q:109:HIS:ND1	18:R:225:VAL:CG2	2.25	0.98
1:A:133:SER:O	1:A:135:GLY:N	1.96	0.98
16:P:298:PRO:O	16:P:300:ILE:HG12	1.63	0.98
1:A:610:PRO:O	1:A:626:THR:HG21	1.62	0.98
17:Q:112:ARG:NH2	18:R:237:LEU:HB2	1.78	0.98
3:C:5:ASN:O	3:C:7:PRO:CD	2.12	0.97
5:E:48:PRO:O	5:E:50:GLU:CG	2.12	0.97
17:Q:113:ARG:CZ	18:R:218:LYS:O	2.12	0.97
17:Q:188:TYR:HE2	18:R:210:PHE:CD1	1.76	0.97
3:C:157:GLN:CG	10:J:65:LEU:HB2	1.94	0.97
13:M:44:ARG:HH11	13:M:46:ILE:HG22	0.82	0.97
3:C:157:GLN:HG2	10:J:65:LEU:CB	1.95	0.96
13:M:182:ALA:CB	20:T:154:LYS:HB3	1.95	0.96
17:Q:109:HIS:HB3	18:R:224:THR:HG21	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:CA	1:A:181:HIS:ND1	2.28	0.96
1:A:79:THR:HG21	13:M:43:ASP:HB2	1.45	0.95
18:R:224:THR:HG23	18:R:225:VAL:H	1.30	0.95
8:H:65:TYR:CE2	8:H:70:LEU:HB2	2.00	0.95
17:Q:21:VAL:O	18:R:210:PHE:HE2	1.36	0.95
17:Q:184:ILE:HD12	18:R:218:LYS:NZ	1.81	0.95
2:B:1137:CYS:HG	25:B:1201:ZN:ZN	0.68	0.95
1:A:79:THR:CG2	13:M:43:ASP:HB2	1.96	0.95
17:Q:24:GLY:N	18:R:210:PHE:CD2	2.35	0.95
17:Q:187:ILE:CG2	18:R:210:PHE:O	2.15	0.94
1:A:152:ASN:O	1:A:153:ILE:CG1	2.16	0.94
9:I:15:ARG:O	9:I:24:LEU:HD12	1.67	0.94
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.51	0.94
1:A:266:MET:HG2	1:A:272:ASN:ND2	1.82	0.94
13:M:11:PRO:CD	13:M:13:VAL:HG22	1.97	0.94
2:B:225:LEU:HB2	2:B:228:SER:HB3	1.48	0.93
1:A:1290:SER:OG	2:B:250:SER:CB	1.97	0.93
17:Q:109:HIS:CE1	18:R:225:VAL:CG2	2.50	0.93
2:B:92:TYR:HB3	20:T:145:LEU:HD12	1.49	0.93
17:Q:113:ARG:NE	18:R:222:SER:CA	2.31	0.93
17:Q:113:ARG:HE	18:R:222:SER:CA	1.82	0.93
1:A:156:GLY:HA2	1:A:181:HIS:CG	2.02	0.93
1:A:1171:ALA:HB1	9:I:59:THR:CG2	1.98	0.93
5:E:47:LYS:HE2	5:E:47:LYS:HA	1.47	0.93
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.04	0.93
5:E:46:ASP:O	5:E:47:LYS:HB2	1.65	0.93
9:I:57:LYS:C	9:I:58:ILE:HG12	1.92	0.93
9:I:116:ALA:CB	25:I:202:ZN:ZN	1.46	0.92
17:Q:113:ARG:HD2	18:R:221:ARG:C	1.90	0.92
17:Q:23:ARG:HH12	18:R:206:LYS:HB3	1.34	0.92
17:Q:24:GLY:N	18:R:210:PHE:CE2	2.38	0.92
17:Q:110:MET:HG2	18:R:222:SER:CB	1.98	0.92
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.50	0.91
17:Q:23:ARG:HH12	18:R:206:LYS:HG2	1.28	0.91
17:Q:113:ARG:HH22	18:R:218:LYS:HG2	1.35	0.91
1:A:926:ASN:OD1	1:A:931:ARG:HG2	1.71	0.91
13:M:44:ARG:NH1	13:M:46:ILE:CG2	2.29	0.91
2:B:549:SER:HG	2:B:577:HIS:HE2	1.17	0.91
5:E:47:LYS:CB	5:E:48:PRO:HD3	2.00	0.91
13:M:27:TYR:HE2	13:M:46:ILE:CD1	1.82	0.91
17:Q:188:TYR:CE2	18:R:210:PHE:CE1	2.58	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:O	1:A:272:ASN:ND2	2.03	0.91
2:B:878:ASP:O	2:B:879:GLU:O	1.89	0.90
8:H:65:TYR:HE2	8:H:70:LEU:CB	1.69	0.90
5:E:48:PRO:O	5:E:50:GLU:HG3	1.71	0.89
1:A:262:PRO:HG3	2:B:1070:LEU:CG	2.03	0.89
1:A:1115:LYS:O	1:A:1116:ASN:O	1.89	0.89
2:B:90:GLN:HG2	20:T:141:LEU:HD12	1.53	0.89
2:B:56:GLN:CG	20:T:140:ARG:HD3	2.01	0.89
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.54	0.89
17:Q:188:TYR:CE1	18:R:211:SER:CB	2.55	0.89
13:M:182:ALA:CB	20:T:154:LYS:CB	2.52	0.88
2:B:882:SER:O	2:B:887:TYR:CG	2.27	0.88
1:A:608:THR:OG1	1:A:610:PRO:HG3	1.72	0.88
1:A:929:ALA:O	1:A:931:ARG:N	2.06	0.88
16:P:159:SER:HB3	16:P:329:TYR:CD2	2.08	0.88
3:C:56:SER:O	10:J:65:LEU:O	1.90	0.87
17:Q:21:VAL:C	18:R:210:PHE:CE2	2.52	0.87
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.09	0.87
1:A:203:LYS:O	1:A:204:HIS:HB2	1.74	0.87
1:A:211:GLU:O	1:A:212:LYS:HB2	1.71	0.87
17:Q:187:ILE:HD13	18:R:211:SER:HA	1.57	0.87
1:A:133:SER:C	1:A:135:GLY:H	1.80	0.87
5:E:48:PRO:O	5:E:50:GLU:N	2.06	0.87
13:M:178:LYS:C	20:T:154:LYS:HB2	1.99	0.87
17:Q:110:MET:CG	18:R:222:SER:HB2	1.99	0.87
2:B:716:HIS:HD2	2:B:982:ILE:HG13	1.38	0.86
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.57	0.86
1:A:1116:ASN:HD21	1:A:1138:SER:HB3	1.39	0.86
5:E:15:LYS:NZ	5:E:35:GLN:O	2.07	0.86
20:T:140:ARG:HA	20:T:140:ARG:NE	1.90	0.86
2:B:225:LEU:O	2:B:227:ASN:N	2.08	0.86
20:T:139:VAL:C	20:T:141:LEU:H	1.83	0.86
2:B:56:GLN:CG	20:T:140:ARG:HD2	2.01	0.86
13:M:94:ASP:HB2	13:M:97:GLY:O	1.74	0.86
17:Q:24:GLY:HA2	18:R:209:GLN:CG	2.05	0.86
1:A:1307:VAL:HG21	1:A:1339:ASP:HB2	1.54	0.86
1:A:1116:ASN:HD21	1:A:1138:SER:CB	1.88	0.86
1:A:1171:ALA:HB1	9:I:59:THR:HG22	1.57	0.86
13:M:179:GLU:HA	20:T:154:LYS:CG	2.05	0.85
16:P:159:SER:HB3	16:P:329:TYR:CG	2.10	0.85
14:N:313:PRO:HG2	16:P:235:ARG:HH22	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:GLN:HG2	20:T:140:ARG:NE	1.91	0.85
1:A:79:THR:HG21	13:M:43:ASP:CB	2.06	0.85
17:Q:35:ASP:OD2	18:R:161:ARG:NH2	2.10	0.85
1:A:266:MET:HG2	1:A:272:ASN:HD21	1.35	0.85
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.00	0.85
2:B:803:ARG:NH2	3:C:177:ASN:OD1	2.10	0.85
5:E:47:LYS:HA	5:E:47:LYS:CE	2.07	0.85
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.59	0.84
17:Q:101:ASN:C	17:Q:103:VAL:H	1.80	0.84
17:Q:188:TYR:HE1	18:R:211:SER:CB	1.89	0.84
20:T:154:LYS:HE3	20:T:154:LYS:H	1.42	0.84
20:T:140:ARG:HA	20:T:140:ARG:CZ	2.05	0.84
1:A:1290:SER:HB2	2:B:250:SER:CB	1.83	0.84
1:A:156:GLY:HA2	1:A:181:HIS:HD1	1.43	0.84
3:C:157:GLN:HG2	10:J:65:LEU:HB2	1.57	0.84
17:Q:112:ARG:HH21	18:R:237:LEU:HD22	1.41	0.84
17:Q:109:HIS:CB	18:R:224:THR:HG21	2.07	0.84
17:Q:113:ARG:NH2	18:R:222:SER:HB3	1.92	0.84
5:E:126:ILE:HD13	5:E:186:LYS:HE3	1.60	0.83
16:P:159:SER:HB3	16:P:329:TYR:CD1	2.12	0.83
17:Q:112:ARG:HH22	18:R:237:LEU:HB2	1.39	0.83
2:B:225:LEU:HB3	2:B:228:SER:HB2	1.60	0.83
13:M:182:ALA:HB2	20:T:154:LYS:CG	2.07	0.83
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.42	0.83
17:Q:21:VAL:O	18:R:210:PHE:CZ	2.32	0.83
1:A:427:ILE:CG1	13:M:38:GLY:O	2.20	0.83
2:B:289:ILE:HG12	2:B:297:MET:HG2	1.60	0.83
17:Q:20:TYR:O	18:R:210:PHE:HD2	1.57	0.83
13:M:39:LEU:O	13:M:40:VAL:HG22	1.78	0.83
3:C:157:GLN:HE21	10:J:65:LEU:HB3	1.03	0.83
1:A:623:PRO:O	1:A:625:ASP:N	2.12	0.82
17:Q:184:ILE:CD1	18:R:213:ASP:OD1	2.25	0.82
20:T:141:LEU:O	20:T:143:GLN:N	2.12	0.82
1:A:426:ARG:O	13:M:39:LEU:HA	1.79	0.82
2:B:56:GLN:CD	20:T:140:ARG:HH11	1.85	0.82
8:H:65:TYR:CZ	8:H:70:LEU:HB2	2.13	0.82
18:R:224:THR:HG22	18:R:225:VAL:CG2	1.95	0.82
18:R:213:ASP:C	18:R:215:GLU:H	1.82	0.82
1:A:1246:ILE:HD11	1:A:1258:ARG:HD2	1.60	0.81
8:H:66:GLU:CG	8:H:67:ASP:N	2.42	0.81
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:58:GLN:OE1	18:R:194:ARG:HD2	1.80	0.81
2:B:61:ASP:HB3	2:B:63:PRO:HD3	1.61	0.81
17:Q:24:GLY:HA2	18:R:209:GLN:HG2	1.61	0.81
19:S:31:PHE:HB2	20:T:92:THR:HB	1.60	0.81
20:T:141:LEU:C	20:T:143:GLN:OE1	2.23	0.81
1:A:1307:VAL:HG21	1:A:1339:ASP:CA	2.10	0.81
1:A:1304:ILE:O	1:A:1307:VAL:HG12	1.80	0.81
13:M:182:ALA:CB	20:T:154:LYS:CG	2.59	0.81
1:A:608:THR:CA	1:A:610:PRO:HD2	2.10	0.81
1:A:1307:VAL:HG21	1:A:1339:ASP:HB3	0.83	0.81
5:E:48:PRO:O	5:E:50:GLU:HG2	1.78	0.81
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.13	0.80
2:B:225:LEU:O	2:B:226:GLU:C	2.22	0.80
16:P:159:SER:CB	16:P:329:TYR:CG	2.64	0.80
18:R:194:ARG:C	18:R:196:ASP:H	1.88	0.80
16:P:159:SER:HB3	16:P:329:TYR:CE2	2.15	0.80
17:Q:113:ARG:NH2	18:R:222:SER:CB	2.45	0.80
17:Q:105:TYR:CZ	18:R:234:GLU:OE1	2.33	0.80
17:Q:113:ARG:HD2	18:R:221:ARG:CA	2.10	0.80
1:A:926:ASN:HD22	1:A:932:ARG:HG3	1.47	0.80
2:B:957:THR:O	2:B:960:GLY:N	2.10	0.80
5:E:64:HIS:C	5:E:66:ASP:H	1.89	0.80
1:A:153:ILE:O	1:A:154:CYS:O	2.00	0.80
1:A:609:HIS:ND1	1:A:609:HIS:O	2.14	0.80
17:Q:23:ARG:NH1	18:R:206:LYS:HG3	1.95	0.80
1:A:926:ASN:OD1	1:A:931:ARG:CG	2.30	0.80
17:Q:184:ILE:CD1	18:R:218:LYS:NZ	2.45	0.80
1:A:263:ALA:O	1:A:265:VAL:N	2.15	0.79
8:H:65:TYR:CZ	8:H:70:LEU:CB	2.64	0.79
17:Q:23:ARG:HH22	18:R:206:LYS:HB3	1.47	0.79
17:Q:113:ARG:HD3	18:R:222:SER:N	1.90	0.79
17:Q:113:ARG:HE	18:R:222:SER:HB3	0.69	0.79
2:B:225:LEU:HB2	2:B:228:SER:CB	2.12	0.79
13:M:178:LYS:O	20:T:154:LYS:HB3	1.80	0.79
17:Q:113:ARG:HH21	18:R:222:SER:CB	1.96	0.79
2:B:958:CYS:SG	2:B:959:GLU:N	2.56	0.79
17:Q:113:ARG:CD	18:R:221:ARG:O	2.22	0.79
2:B:496:ALA:HB1	2:B:498:PRO:HD2	1.65	0.79
17:Q:24:GLY:H	18:R:210:PHE:HD2	1.28	0.79
14:N:317:GLU:O	14:N:318:ASP:O	2.01	0.78
20:T:141:LEU:O	20:T:143:GLN:OE1	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PRO:O	1:A:483:ARG:NH2	2.16	0.78
16:P:159:SER:HB3	16:P:329:TYR:CE1	2.18	0.78
16:P:208:ARG:HH21	16:P:208:ARG:HG3	1.47	0.78
17:Q:23:ARG:NH1	18:R:206:LYS:HB3	1.96	0.78
1:A:926:ASN:ND2	1:A:932:ARG:CG	2.47	0.78
13:M:94:ASP:CB	13:M:97:GLY:O	2.32	0.78
1:A:608:THR:OG1	1:A:610:PRO:HG2	1.84	0.78
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.65	0.78
18:R:195:PRO:O	18:R:196:ASP:CB	2.31	0.78
5:E:40:PHE:CE2	5:E:46:ASP:OD2	2.37	0.78
2:B:225:LEU:O	2:B:228:SER:N	2.17	0.78
1:A:926:ASN:HD21	1:A:932:ARG:HG2	1.48	0.78
2:B:490:GLY:O	2:B:491:ARG:HB2	1.84	0.78
16:P:159:SER:HB3	16:P:329:TYR:CZ	2.19	0.77
2:B:92:TYR:CE1	20:T:141:LEU:CD1	2.63	0.77
2:B:1137:CYS:SG	25:B:1201:ZN:ZN	1.72	0.77
18:R:195:PRO:O	18:R:196:ASP:HB2	1.81	0.77
1:A:360:ASP:OD1	1:A:361:PHE:N	2.17	0.77
2:B:874:PRO:O	2:B:875:GLU:HB2	1.82	0.77
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.13	0.77
17:Q:184:ILE:HD11	18:R:213:ASP:OD1	1.83	0.77
2:B:222:ARG:HB3	2:B:222:ARG:HH11	1.49	0.77
17:Q:113:ARG:CZ	18:R:222:SER:CB	2.51	0.77
9:I:103:ARG:C	9:I:105:GLU:H	1.92	0.77
1:A:129:ILE:O	1:A:132:LYS:HB2	1.84	0.77
1:A:612:ASP:C	1:A:614:ASP:H	1.91	0.77
17:Q:23:ARG:NH1	18:R:206:LYS:CB	2.38	0.77
17:Q:188:TYR:HE2	18:R:210:PHE:CE1	2.00	0.77
5:E:45:GLY:O	5:E:46:ASP:O	2.02	0.77
9:I:103:ARG:C	9:I:105:GLU:N	2.34	0.77
21:X:41:DT:H3'	21:X:42:DT:H4'	1.67	0.76
13:M:182:ALA:HB2	20:T:154:LYS:CA	2.15	0.76
1:A:622:SER:C	1:A:624:GLY:H	1.93	0.76
1:A:1307:VAL:CG2	1:A:1339:ASP:HB2	2.10	0.76
2:B:428:ASP:OD1	20:T:158:ASN:ND2	2.18	0.76
17:Q:113:ARG:NE	18:R:222:SER:N	2.33	0.76
17:Q:184:ILE:HD13	18:R:211:SER:CB	2.15	0.76
2:B:1080:ARG:HH21	13:M:50:SER:HB3	1.49	0.76
17:Q:109:HIS:CG	18:R:224:THR:HG21	2.20	0.76
17:Q:113:ARG:CD	18:R:221:ARG:CB	2.60	0.76
13:M:44:ARG:HE	13:M:46:ILE:HG23	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:343:HIS:NE2	21:X:9:DC:OP1	2.19	0.76
17:Q:24:GLY:HA2	18:R:209:GLN:CD	2.11	0.76
1:A:153:ILE:O	1:A:154:CYS:C	2.28	0.75
3:C:157:GLN:HE21	10:J:65:LEU:CB	1.80	0.75
8:H:65:TYR:CD2	8:H:70:LEU:HB3	2.20	0.75
2:B:225:LEU:CB	2:B:228:SER:CB	2.64	0.75
13:M:44:ARG:CZ	13:M:46:ILE:HG22	2.14	0.75
17:Q:187:ILE:CD1	18:R:212:VAL:H	1.99	0.75
18:R:194:ARG:O	18:R:196:ASP:N	2.19	0.75
1:A:18:ILE:HD12	2:B:1171:MET:HB2	1.69	0.75
1:A:265:VAL:HA	1:A:272:ASN:HB2	1.67	0.75
1:A:679:TRP:CH2	1:A:683:GLU:HG3	2.22	0.75
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.69	0.75
13:M:94:ASP:CG	13:M:97:GLY:O	2.30	0.75
17:Q:101:ASN:C	17:Q:103:VAL:N	2.43	0.75
2:B:1040:GLN:OE1	2:B:1040:GLN:N	2.20	0.75
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.52	0.74
13:M:39:LEU:O	13:M:40:VAL:CG2	2.35	0.74
1:A:1192:TRP:HE1	1:A:1249:ASP:H	1.35	0.74
7:G:151:ARG:HG3	17:Q:139:LEU:HD22	1.67	0.74
1:A:61:ARG:HB3	1:A:72:GLN:HG2	1.69	0.74
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.31	0.74
1:A:157:GLY:H	1:A:181:HIS:CE1	2.05	0.74
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.21	0.74
17:Q:113:ARG:NH2	18:R:222:SER:OG	2.21	0.74
17:Q:184:ILE:HD12	18:R:218:LYS:HZ3	1.52	0.74
2:B:91:ILE:O	20:T:141:LEU:HD12	1.87	0.74
1:A:157:GLY:N	1:A:181:HIS:CE1	2.56	0.74
19:S:49:ARG:NH1	19:S:96:GLN:O	2.21	0.74
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.62	0.73
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.69	0.73
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.69	0.73
17:Q:122:THR:HA	17:Q:169:PRO:HD2	1.70	0.73
1:A:608:THR:OG1	1:A:610:PRO:CD	2.35	0.73
2:B:310:VAL:HG13	19:S:161:GLU:HB3	1.69	0.73
10:J:3:ILE:H	10:J:3:ILE:HD12	1.54	0.73
1:A:1116:ASN:C	1:A:1118:THR:H	1.97	0.73
7:G:97:LEU:HB2	7:G:108:ILE:HB	1.71	0.73
8:H:1:MET:HE1	8:H:85:ALA:HB2	1.71	0.73
1:A:926:ASN:ND2	1:A:932:ARG:HG3	2.03	0.73
14:N:333:ASN:HB3	14:N:360:LEU:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLU:HB3	2:B:127:ASP:HB3	1.70	0.73
9:I:92:LYS:NZ	9:I:93:GLU:OE2	2.20	0.72
13:M:279:GLY:HA2	20:T:153:TYR:CE2	2.24	0.72
13:M:53:ARG:HH22	22:Y:54:DA:H61	1.34	0.72
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.22	0.72
8:H:99:ILE:HG22	8:H:136:GLU:HG3	1.70	0.72
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.71	0.72
2:B:356:PHE:HB3	19:S:116:GLY:HA2	1.71	0.72
1:A:608:THR:CB	1:A:610:PRO:CD	2.67	0.72
3:C:193:ARG:HH12	3:C:218:ALA:HB1	1.54	0.72
8:H:65:TYR:OH	8:H:70:LEU:HB2	1.89	0.72
13:M:279:GLY:HA2	20:T:153:TYR:HE2	1.55	0.72
18:R:224:THR:HG23	18:R:225:VAL:CG2	2.00	0.72
14:N:311:GLU:HG2	16:P:251:LEU:HD21	1.72	0.72
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.70	0.72
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.70	0.72
1:A:1171:ALA:CB	9:I:59:THR:HG22	2.18	0.72
2:B:487:SER:OG	2:B:524:LYS:NZ	2.22	0.72
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.72
14:N:316:SER:OG	16:P:235:ARG:NH1	2.23	0.72
2:B:514:THR:HG22	2:B:524:LYS:HA	1.72	0.72
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.72	0.72
18:R:224:THR:HG22	18:R:225:VAL:CB	2.19	0.72
16:P:160:GLY:O	16:P:162:VAL:HG13	1.90	0.71
2:B:225:LEU:CB	2:B:228:SER:HB2	2.19	0.71
22:Y:49:DG:H2'	22:Y:50:DA:H8	1.56	0.71
9:I:85:PRO:C	9:I:86:CYS:O	2.31	0.71
17:Q:187:ILE:CG2	18:R:210:PHE:C	2.62	0.71
13:M:179:GLU:HA	20:T:154:LYS:CD	2.20	0.71
1:A:491:PRO:HG3	1:A:535:MET:HE2	1.73	0.71
2:B:873:LEU:H	2:B:874:PRO:HD2	1.54	0.71
13:M:10:LEU:N	13:M:10:LEU:HD22	2.05	0.71
18:R:224:THR:HG22	18:R:225:VAL:CA	2.20	0.71
1:A:264:VAL:C	1:A:272:ASN:CB	2.64	0.71
1:A:926:ASN:ND2	1:A:932:ARG:HG2	2.06	0.71
21:X:47:DT:H3'	21:X:48:DT:H5''	1.71	0.71
1:A:47:THR:HG23	1:A:53:LYS:HA	1.72	0.71
2:B:854:ILE:HD11	2:B:921:ILE:HD12	1.73	0.70
17:Q:23:ARG:NH2	18:R:206:LYS:HB3	2.05	0.70
1:A:929:ALA:C	1:A:931:ARG:H	2.00	0.70
2:B:56:GLN:CG	20:T:140:ARG:NH1	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASP:OD1	2:B:103:GLY:N	2.24	0.70
5:E:41:LYS:NZ	5:E:47:LYS:HE3	2.06	0.70
17:Q:188:TYR:CE1	18:R:211:SER:OG	2.42	0.70
1:A:358:ARG:NH2	2:B:1076:GLU:OE1	2.23	0.70
2:B:132:VAL:HG23	2:B:141:GLN:CG	2.12	0.70
1:A:1307:VAL:HG11	1:A:1340:GLY:H	1.57	0.70
2:B:56:GLN:HG2	20:T:140:ARG:NH1	2.07	0.70
9:I:15:ARG:HD3	9:I:37:TYR:CD2	2.27	0.70
21:X:42:DT:H3'	21:X:43:DT:H5''	1.72	0.70
2:B:92:TYR:HD1	20:T:141:LEU:HD11	0.83	0.70
3:C:212:ASP:O	3:C:214:ASP:N	2.24	0.70
17:Q:187:ILE:HD13	18:R:212:VAL:H	1.56	0.70
2:B:132:VAL:HG21	2:B:141:GLN:HG3	1.69	0.70
17:Q:114:ILE:HD11	18:R:218:LYS:HE3	1.74	0.70
20:T:154:LYS:HE3	20:T:154:LYS:N	2.07	0.70
1:A:79:THR:HG21	13:M:43:ASP:CA	2.22	0.70
2:B:56:GLN:HG2	20:T:140:ARG:CZ	2.20	0.70
17:Q:184:ILE:HG13	18:R:213:ASP:OD1	1.91	0.70
2:B:1066:PRO:HB3	13:M:46:ILE:HG12	1.74	0.70
9:I:84:HIS:HB3	9:I:92:LYS:CB	2.22	0.70
13:M:94:ASP:HB3	13:M:99:SER:H	1.57	0.70
1:A:622:SER:C	1:A:624:GLY:N	2.50	0.69
2:B:851:ASP:HB2	12:L:14:PRO:HG3	1.72	0.69
8:H:147:LYS:HE2	8:H:149:ALA:HA	1.73	0.69
1:A:155:GLU:C	1:A:181:HIS:HD1	2.01	0.69
8:H:66:GLU:HG3	8:H:67:ASP:H	1.52	0.69
1:A:211:GLU:O	1:A:212:LYS:CB	2.41	0.69
9:I:119:CYS:SG	9:I:120:GLY:N	2.64	0.69
1:A:1116:ASN:ND2	1:A:1138:SER:CB	2.54	0.69
2:B:1076:GLU:HG3	13:M:54:THR:OG1	1.92	0.69
9:I:15:ARG:O	9:I:24:LEU:CD1	2.39	0.69
9:I:84:HIS:CB	9:I:92:LYS:HB3	2.23	0.69
1:A:131:ALA:C	1:A:133:SER:H	1.99	0.69
1:A:190:ARG:NH2	21:X:58:DT:OP2	2.24	0.69
1:A:202:TRP:HB2	1:A:212:LYS:CB	2.16	0.69
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.58	0.69
18:R:213:ASP:C	18:R:215:GLU:N	2.46	0.69
20:T:228:ILE:HG22	21:X:29:DC:H1'	1.75	0.69
22:Y:53:DG:H2''	22:Y:55:DG:H5'	1.73	0.69
17:Q:184:ILE:CD1	18:R:211:SER:HB2	2.20	0.68
1:A:228:ILE:O	1:A:244:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:MET:O	1:A:1088:GLY:N	2.27	0.68
17:Q:188:TYR:CZ	18:R:210:PHE:CE1	2.65	0.68
2:B:73:HIS:C	2:B:75:SER:H	2.01	0.68
3:C:157:GLN:HG3	10:J:65:LEU:HB2	1.73	0.68
14:N:319:ASP:C	14:N:321:SER:H	2.01	0.68
1:A:618:TYR:C	1:A:620:HIS:H	2.01	0.68
2:B:92:TYR:CB	20:T:145:LEU:CD1	2.59	0.68
2:B:298:MET:SD	9:I:13:GLY:C	2.77	0.68
2:B:329:GLY:H	2:B:335:ARG:HH21	1.39	0.68
7:G:93:ASN:ND2	17:Q:151:THR:HA	2.08	0.68
13:M:62:LYS:HB2	23:Z:1:A:H5''	1.76	0.68
16:P:159:SER:CB	16:P:329:TYR:CZ	2.75	0.68
1:A:264:VAL:HB	1:A:272:ASN:ND2	2.08	0.68
13:M:44:ARG:NE	13:M:46:ILE:HG23	2.09	0.68
2:B:1029:TYR:HE1	2:B:1036:LYS:HE2	1.59	0.67
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.75	0.67
2:B:56:GLN:CG	20:T:140:ARG:HH11	2.07	0.67
1:A:152:ASN:C	1:A:153:ILE:HG12	2.16	0.67
2:B:73:HIS:O	2:B:75:SER:N	2.27	0.67
2:B:801:VAL:HA	2:B:805:PHE:HB3	1.77	0.67
3:C:267:ILE:HG21	11:K:84:GLN:HE22	1.60	0.67
17:Q:184:ILE:CD1	18:R:218:LYS:HZ2	2.05	0.67
12:L:28:ILE:HG23	12:L:32:ASP:OD1	1.94	0.67
1:A:112:PHE:H	1:A:188:GLN:HE22	1.42	0.67
3:C:212:ASP:C	3:C:214:ASP:N	2.50	0.67
1:A:207:GLU:O	1:A:209:SER:N	2.27	0.67
1:A:265:VAL:C	1:A:272:ASN:ND2	2.52	0.67
2:B:490:GLY:O	2:B:491:ARG:CB	2.43	0.67
1:A:265:VAL:N	1:A:272:ASN:HB3	2.08	0.67
2:B:91:ILE:O	20:T:141:LEU:CD1	2.42	0.67
2:B:895:PHE:O	2:B:897:ARG:NE	2.25	0.67
2:B:292:PHE:CD2	9:I:14:ILE:CD1	2.75	0.66
1:A:923:ASP:O	1:A:932:ARG:NH1	2.28	0.66
2:B:775:GLY:N	2:B:1047:TYR:OH	2.28	0.66
1:A:1117:VAL:O	1:A:1118:THR:O	2.12	0.66
1:A:1481:LYS:HA	1:A:1484:MET:HE2	1.78	0.66
2:B:225:LEU:C	2:B:227:ASN:N	2.52	0.66
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.59	0.66
18:R:194:ARG:C	18:R:196:ASP:N	2.54	0.66
1:A:775:LYS:HB3	2:B:974:SER:OG	1.96	0.66
11:K:111:ASP:O	11:K:113:GLN:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:112:ARG:NH2	18:R:237:LEU:CB	2.58	0.66
20:T:141:LEU:C	20:T:141:LEU:HD22	2.18	0.66
1:A:610:PRO:C	1:A:626:THR:HG21	2.20	0.66
17:Q:42:CYS:C	17:Q:95:ASN:HD21	2.04	0.66
1:A:611:ASP:OD1	1:A:626:THR:HG23	1.96	0.66
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.31	0.66
3:C:3:TYR:O	11:K:52:LYS:HE3	1.96	0.66
17:Q:113:ARG:NH2	18:R:218:LYS:HG2	2.10	0.66
1:A:486:LEU:HD22	2:B:790:GLN:CD	2.22	0.65
5:E:47:LYS:HB3	5:E:48:PRO:HD2	0.67	0.65
16:P:239:ARG:NH1	16:P:242:GLN:OE1	2.29	0.65
1:A:355:MET:HE1	1:A:1431:SER:HB2	1.78	0.65
2:B:834:ARG:O	2:B:885:ARG:NH1	2.24	0.65
2:B:1005:ALA:C	2:B:1007:ASN:H	2.04	0.65
1:A:265:VAL:H	1:A:272:ASN:HB2	1.57	0.65
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.61	0.65
1:A:421:ARG:NH2	1:A:425:ASP:OD2	2.29	0.65
1:A:608:THR:CB	1:A:610:PRO:HD2	2.26	0.65
1:A:686:THR:OG1	1:A:687:ILE:N	2.26	0.65
2:B:241:ALA:HA	2:B:253:GLY:HA2	1.78	0.65
2:B:489:ILE:HG21	2:B:522:LEU:HD13	1.79	0.65
3:C:212:ASP:C	3:C:214:ASP:H	2.03	0.65
13:M:86:LYS:HA	13:M:86:LYS:NZ	2.12	0.65
17:Q:68:GLY:O	18:R:226:ASP:OD2	2.14	0.65
2:B:908:MET:HE3	2:B:920:LYS:HB2	1.77	0.65
13:M:27:TYR:HD2	13:M:46:ILE:HB	1.61	0.65
2:B:250:SER:O	2:B:251:ALA:HB2	1.96	0.65
3:C:67:ARG:NH2	10:J:3:ILE:O	2.28	0.65
13:M:179:GLU:HA	20:T:154:LYS:HD3	1.78	0.65
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.12	0.65
8:H:64:LEU:C	8:H:66:GLU:H	2.05	0.65
18:R:227:SER:O	18:R:228:MET:O	2.14	0.65
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.79	0.65
17:Q:113:ARG:HD2	18:R:221:ARG:HB3	1.75	0.65
1:A:738:GLU:OE2	1:A:797:ARG:HD3	1.97	0.65
2:B:225:LEU:CB	2:B:228:SER:HB3	2.24	0.65
17:Q:113:ARG:HH12	18:R:218:LYS:CG	2.09	0.65
1:A:258:LEU:HA	1:A:261:ARG:HG3	1.79	0.64
1:A:467:MET:SD	1:A:524:MET:HB3	2.38	0.64
13:M:179:GLU:HG2	20:T:154:LYS:HD3	1.79	0.64
2:B:312:GLN:HB3	19:S:153:ARG:HH22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:HB2	13:M:39:LEU:HG	1.79	0.64
2:B:934:LYS:NZ	23:Z:6:C:OP1	2.31	0.64
2:B:1124:ILE:HG22	2:B:1126:ALA:H	1.63	0.64
1:A:1116:ASN:O	1:A:1118:THR:N	2.31	0.64
14:N:358:MET:HB2	14:N:365:TYR:HB2	1.78	0.64
1:A:79:THR:HG21	13:M:43:ASP:HA	1.78	0.64
1:A:691:ASP:OD2	1:A:765:ASN:HB2	1.98	0.64
2:B:602:SER:OG	2:B:620:ARG:NH1	2.31	0.64
2:B:882:SER:CB	2:B:887:TYR:CE2	2.80	0.64
13:M:39:LEU:O	13:M:40:VAL:O	2.15	0.64
2:B:326:ALA:HB2	2:B:338:TYR:HE2	1.61	0.64
13:M:17:ASN:OD1	13:M:18:HIS:N	2.30	0.64
20:T:153:TYR:HA	20:T:154:LYS:HE3	1.78	0.64
1:A:265:VAL:H	1:A:272:ASN:CB	2.07	0.64
1:A:610:PRO:O	1:A:611:ASP:CB	2.40	0.64
1:A:1290:SER:HG	2:B:250:SER:HB3	1.43	0.64
2:B:92:TYR:CG	20:T:145:LEU:HD12	2.32	0.64
7:G:94:LYS:NZ	17:Q:162:GLU:OE2	2.30	0.63
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.31	0.63
2:B:74:ALA:C	2:B:75:SER:OG	2.40	0.63
2:B:95:LYS:HD3	2:B:162:LEU:HD21	1.81	0.63
17:Q:113:ARG:HH22	18:R:218:LYS:CG	2.11	0.63
2:B:132:VAL:HG21	2:B:141:GLN:OE1	1.98	0.63
8:H:57:ARG:HD3	8:H:146:LYS:HD3	1.78	0.63
1:A:367:ILE:HG21	1:A:501:MET:CG	2.28	0.63
2:B:453:TRP:CE3	2:B:466:VAL:HG21	2.33	0.63
13:M:10:LEU:HD22	13:M:10:LEU:H	1.62	0.63
17:Q:114:ILE:CD1	18:R:218:LYS:HE3	2.29	0.63
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.61	0.63
12:L:28:ILE:HD12	12:L:34:ILE:HA	1.80	0.63
18:R:127:ASN:ND2	20:T:238:GLU:OE1	2.31	0.63
1:A:47:THR:O	1:A:48:GLU:HB2	1.97	0.63
2:B:956:PHE:HB3	2:B:962:THR:HG22	1.81	0.63
21:X:32:DT:H4'	21:X:33:DT:H5'	1.78	0.63
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.81	0.63
2:B:90:GLN:HG2	20:T:141:LEU:CD1	2.24	0.63
2:B:882:SER:HB2	2:B:887:TYR:CZ	2.33	0.63
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.32	0.63
1:A:619:LYS:C	1:A:620:HIS:CG	2.76	0.62
8:H:64:LEU:HB3	8:H:84:ARG:CD	2.27	0.62
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:23:ASP:O	8:H:25:VAL:N	2.31	0.62
2:B:899:SER:O	2:B:901:THR:N	2.33	0.62
5:E:46:ASP:O	5:E:47:LYS:CB	2.40	0.62
13:M:39:LEU:C	13:M:40:VAL:HG22	2.24	0.62
1:A:375:ILE:HB	1:A:666:ARG:HD2	1.80	0.62
2:B:422:PHE:CD1	2:B:422:PHE:C	2.77	0.62
6:F:125:ILE:HG22	6:F:127:ASP:H	1.63	0.62
13:M:94:ASP:CB	13:M:99:SER:N	2.58	0.62
1:A:264:VAL:CA	1:A:272:ASN:HB3	2.30	0.62
5:E:166:ARG:HB2	5:E:169:GLN:HG3	1.80	0.62
17:Q:180:PHE:CD2	18:R:213:ASP:OD1	2.33	0.62
19:S:28:ILE:HD13	20:T:95:VAL:HG22	1.82	0.62
1:A:1192:TRP:CD1	1:A:1248:ASN:HA	2.34	0.62
8:H:65:TYR:HE2	8:H:70:LEU:CA	2.12	0.62
1:A:202:TRP:CB	1:A:212:LYS:HB3	2.16	0.62
1:A:531:ASN:HD22	1:A:901:VAL:HG23	1.65	0.62
1:A:935:GLN:HG2	1:A:1059:ARG:HH12	1.65	0.62
1:A:264:VAL:HB	1:A:272:ASN:CB	2.30	0.62
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.82	0.62
2:B:489:ILE:HG13	2:B:490:GLY:H	1.65	0.62
5:E:41:LYS:HE3	5:E:47:LYS:CE	2.30	0.62
12:L:35:ARG:NH1	12:L:42:ARG:HH21	1.98	0.62
17:Q:165:GLU:HB3	17:Q:170:LYS:HE2	1.82	0.62
10:J:67:LYS:NZ	12:L:20:GLY:O	2.32	0.62
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	1.82	0.61
9:I:15:ARG:O	9:I:15:ARG:HG3	2.00	0.61
13:M:86:LYS:HA	13:M:86:LYS:CE	2.29	0.61
17:Q:188:TYR:HE1	18:R:211:SER:OG	1.80	0.61
16:P:208:ARG:HG3	16:P:208:ARG:NH2	2.15	0.61
2:B:461:GLN:NE2	21:X:43:DT:O2	2.34	0.61
2:B:529:MET:HE2	2:B:623:ARG:HB2	1.82	0.61
9:I:116:ALA:HB2	25:I:202:ZN:ZN	1.26	0.61
21:X:42:DT:H2'	21:X:43:DT:H71	1.81	0.61
1:A:1480:CYS:O	1:A:1484:MET:HG3	1.99	0.61
2:B:1115:GLN:HB2	2:B:1148:LEU:HD21	1.82	0.61
9:I:15:ARG:HD3	9:I:37:TYR:CE2	2.35	0.61
15:O:41:ASP:OD1	15:O:45:ASN:ND2	2.33	0.61
17:Q:108:ASP:OD2	18:R:237:LEU:HD22	2.01	0.61
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.81	0.61
1:A:608:THR:O	1:A:610:PRO:HD2	1.94	0.61
1:A:1290:SER:HB2	2:B:250:SER:HB2	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ILE:HG13	10:J:52:HIS:CE1	2.36	0.61
17:Q:23:ARG:CZ	18:R:206:LYS:HB3	2.30	0.61
2:B:329:GLY:O	2:B:335:ARG:NE	2.34	0.61
2:B:810:PHE:N	2:B:925:SER:O	2.29	0.61
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.32	0.61
4:D:70:ARG:NH2	7:G:140:ASP:O	2.33	0.61
9:I:14:ILE:HG23	9:I:14:ILE:O	1.99	0.61
1:A:265:VAL:N	1:A:272:ASN:HD22	1.95	0.61
13:M:59:LYS:HB2	23:Z:1:A:H5'	1.83	0.61
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.65	0.61
1:A:153:ILE:O	1:A:153:ILE:HG22	2.01	0.61
1:A:263:ALA:C	1:A:265:VAL:H	2.09	0.61
1:A:865:ILE:O	1:A:869:GLU:HB3	2.01	0.61
2:B:861:SER:N	2:B:864:ASP:OD2	2.34	0.61
6:F:65:VAL:HG22	6:F:104:ILE:HD11	1.81	0.61
12:L:28:ILE:O	12:L:28:ILE:HG22	2.01	0.61
17:Q:23:ARG:NH2	18:R:207:SER:O	2.33	0.61
2:B:56:GLN:HG2	20:T:140:ARG:HH11	1.64	0.60
9:I:99:SER:OG	9:I:100:HIS:N	2.32	0.60
22:Y:49:DG:N2	23:Z:4:C:O2	2.34	0.60
2:B:959:GLU:OE2	2:B:961:ILE:HB	2.01	0.60
13:M:44:ARG:HE	13:M:46:ILE:CG2	2.14	0.60
20:T:94:THR:HG23	20:T:109:ILE:HG22	1.83	0.60
3:C:42:VAL:HB	3:C:178:PRO:HG2	1.81	0.60
3:C:157:GLN:HG2	10:J:65:LEU:HB3	1.62	0.60
13:M:36:GLU:N	13:M:36:GLU:OE1	2.34	0.60
20:T:82:PRO:HG2	20:T:117:ARG:HB2	1.83	0.60
2:B:712:PRO:O	2:B:939:HIS:HE1	1.84	0.60
3:C:4:ALA:HA	11:K:52:LYS:HZ1	1.66	0.60
13:M:46:ILE:HD12	13:M:46:ILE:O	2.00	0.60
17:Q:171:LYS:O	17:Q:173:ALA:N	2.35	0.60
1:A:208:ASP:OD1	1:A:209:SER:N	2.32	0.60
1:A:156:GLY:CA	1:A:181:HIS:CE1	2.84	0.60
1:A:264:VAL:C	1:A:272:ASN:CG	2.70	0.60
1:A:930:LEU:O	1:A:931:ARG:O	2.20	0.60
18:R:206:LYS:HA	18:R:206:LYS:NZ	2.16	0.60
2:B:40:VAL:O	2:B:44:LEU:HD13	2.01	0.60
9:I:29:ASP:OD2	9:I:32:ASN:ND2	2.28	0.60
13:M:27:TYR:CE2	13:M:46:ILE:CD1	2.60	0.60
17:Q:187:ILE:HG21	18:R:210:PHE:C	2.27	0.60
18:R:166:ILE:HG22	18:R:168:LEU:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:LEU:HD13	2:B:573:TRP:CZ3	2.36	0.60
8:H:85:ALA:CB	8:H:144:LEU:CD2	2.80	0.60
12:L:26:ASN:HB2	12:L:44:MET:CE	2.31	0.60
1:A:114:CYS:HB2	1:A:184:CYS:SG	2.42	0.60
2:B:866:ILE:HD12	2:B:921:ILE:HD11	1.82	0.60
2:B:882:SER:HB3	2:B:887:TYR:CD1	2.33	0.60
8:H:85:ALA:HB1	8:H:144:LEU:HD22	1.81	0.60
2:B:52:GLN:OE1	2:B:160:TYR:OH	2.15	0.60
1:A:1022:ILE:HG23	1:A:1023:VAL:HG23	1.84	0.59
12:L:15:MET:HB3	12:L:29:LYS:HB3	1.83	0.59
22:Y:48:DC:H2'	22:Y:49:DG:C8	2.37	0.59
2:B:1079:SER:O	2:B:1080:ARG:HD2	2.02	0.59
3:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.67	0.59
9:I:61:GLU:C	9:I:63:ASP:H	2.08	0.59
17:Q:113:ARG:CD	18:R:222:SER:CA	2.77	0.59
18:R:163:LEU:O	18:R:164:GLY:C	2.42	0.59
1:A:268:GLY:HA3	1:A:271:ARG:HB2	1.84	0.59
2:B:1130:THR:HB	2:B:1133:HIS:HB2	1.83	0.59
3:C:56:SER:OG	3:C:158:GLU:N	2.28	0.59
3:C:147:ASP:O	10:J:16:ASN:HB3	2.03	0.59
9:I:101:SER:O	9:I:104:ALA:HB2	2.02	0.59
17:Q:109:HIS:CG	18:R:225:VAL:CG2	2.85	0.59
19:S:10:ASN:OD1	19:S:11:VAL:N	2.36	0.59
19:S:44:GLN:HB2	19:S:103:ASN:HA	1.84	0.59
1:A:1036:ASN:ND2	5:E:202:ARG:O	2.29	0.59
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.31	0.59
2:B:552:ASN:OD1	2:B:553:LEU:N	2.35	0.59
20:T:154:LYS:H	20:T:154:LYS:CE	2.13	0.59
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.36	0.59
1:A:1188:GLU:HG3	9:I:1:MET:HG2	1.83	0.59
2:B:470:LEU:HD21	2:B:478:THR:HG23	1.83	0.59
13:M:94:ASP:O	13:M:96:PHE:N	2.35	0.59
1:A:931:ARG:O	1:A:933:THR:N	2.35	0.59
1:A:935:GLN:HA	1:A:1059:ARG:HH22	1.67	0.59
2:B:631:GLN:HB3	2:B:685:LYS:NZ	2.18	0.59
8:H:96:VAL:HG22	8:H:116:VAL:HG13	1.84	0.59
13:M:196:LYS:NZ	21:X:13:DT:OP1	2.32	0.59
17:Q:109:HIS:CG	18:R:225:VAL:HG21	2.33	0.59
1:A:51:ARG:H	1:A:52:PRO:HD2	1.66	0.59
1:A:60:PRO:HD2	1:A:62:GLN:HG2	1.83	0.59
1:A:486:LEU:HD22	2:B:790:GLN:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:VAL:HG22	1:A:676:ILE:HG13	1.84	0.59
2:B:419:ALA:O	2:B:423:ILE:HG12	2.03	0.59
13:M:59:LYS:HG3	13:M:64:PRO:HG2	1.84	0.59
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.85	0.58
2:B:290:TYR:OH	2:B:566:LYS:NZ	2.36	0.58
2:B:357:CYS:HB2	2:B:360:LYS:HD2	1.86	0.58
13:M:311:ASP:OD2	13:M:312:LYS:NZ	2.36	0.58
1:A:621:ILE:HG22	1:A:621:ILE:O	2.01	0.58
2:B:1117:HIS:HB2	2:B:1127:ILE:HG12	1.84	0.58
14:N:347:ASN:ND2	14:N:375:GLU:OE2	2.35	0.58
17:Q:113:ARG:NH1	18:R:218:LYS:C	2.59	0.58
22:Y:49:DG:H2'	22:Y:50:DA:C8	2.37	0.58
1:A:1464:ALA:O	1:A:1469:GLY:HA3	2.03	0.58
1:A:320:ASN:HB2	1:A:338:SER:OG	2.03	0.58
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.67	0.58
1:A:926:ASN:OD1	1:A:931:ARG:CB	2.51	0.58
2:B:510:CYS:HB2	2:B:705:GLY:HA3	1.84	0.58
12:L:26:ASN:HB2	12:L:44:MET:HE2	1.86	0.58
17:Q:106:LYS:NZ	18:R:223:VAL:O	2.33	0.58
20:T:147:LYS:HG2	20:T:147:LYS:O	2.04	0.58
20:T:158:ASN:HB3	20:T:161:TYR:HB2	1.84	0.58
17:Q:46:GLU:OE2	17:Q:56:ARG:NH1	2.34	0.58
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.85	0.58
1:A:1211:LEU:HD11	1:A:1258:ARG:HG3	1.86	0.58
5:E:64:HIS:O	5:E:66:ASP:N	2.37	0.58
7:G:144:ARG:N	7:G:169:GLY:O	2.34	0.58
8:H:106:THR:O	8:H:107:GLU:HB2	2.03	0.58
12:L:17:TYR:HB3	12:L:44:MET:HE3	1.86	0.58
13:M:44:ARG:CZ	13:M:46:ILE:CG2	2.80	0.58
1:A:67:ARG:H	1:A:78:MET:HE1	1.67	0.58
1:A:612:ASP:C	1:A:614:ASP:N	2.62	0.58
1:A:1307:VAL:HG21	1:A:1339:ASP:N	2.18	0.58
9:I:62:VAL:O	9:I:63:ASP:C	2.45	0.58
17:Q:77:ARG:HB2	17:Q:93:PHE:HB3	1.86	0.58
2:B:90:GLN:CG	20:T:141:LEU:HD12	2.31	0.58
3:C:4:ALA:HA	11:K:52:LYS:NZ	2.18	0.58
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.39	0.58
17:Q:23:ARG:HH11	18:R:206:LYS:HG2	1.66	0.58
1:A:386:ALA:HA	1:A:449:HIS:CD2	2.38	0.58
2:B:798:ARG:O	2:B:801:VAL:HG22	2.03	0.58
5:E:62:VAL:O	5:E:63:ALA:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.69	0.58
1:A:620:HIS:O	1:A:621:ILE:HB	2.05	0.57
3:C:274:ILE:HD11	11:K:31:CYS:SG	2.43	0.57
1:A:567:LEU:HG	1:A:671:ASN:OD1	2.04	0.57
3:C:90:CYS:SG	3:C:94:CYS:HB3	2.43	0.57
17:Q:58:GLN:NE2	18:R:194:ARG:NH1	2.52	0.57
1:A:805:ARG:NH2	2:B:671:GLU:O	2.37	0.57
2:B:446:TYR:HB2	22:Y:59:DG:OP1	2.05	0.57
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.39	0.57
22:Y:48:DC:O2	23:Z:5:G:N2	2.26	0.57
1:A:79:THR:HG23	13:M:43:ASP:HB2	1.81	0.57
1:A:1123:ARG:NH2	1:A:1360:ASN:HB2	2.19	0.57
1:A:1372:GLU:OE2	5:E:207:ARG:NH1	2.36	0.57
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.86	0.57
2:B:1162:LEU:HD23	2:B:1165:MET:HE3	1.86	0.57
1:A:1290:SER:OG	2:B:250:SER:C	2.48	0.57
2:B:132:VAL:HG21	2:B:141:GLN:CD	2.29	0.57
2:B:882:SER:HB2	2:B:887:TYR:CE2	2.38	0.57
20:T:138:PRO:O	20:T:140:ARG:N	2.37	0.57
2:B:232:THR:HG23	2:B:233:SER:H	1.69	0.57
2:B:761:THR:OG1	2:B:764:MET:HG3	2.05	0.57
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.86	0.57
13:M:182:ALA:CB	20:T:154:LYS:HG3	2.33	0.57
2:B:1029:TYR:CE1	2:B:1036:LYS:HE2	2.38	0.57
1:A:298:ALA:H	17:Q:60:ARG:HE	1.53	0.57
2:B:474:THR:HG23	2:B:732:ALA:O	2.05	0.57
21:X:49:DT:H2'	21:X:50:DT:H4'	1.85	0.57
1:A:264:VAL:N	1:A:272:ASN:HB3	2.20	0.57
5:E:41:LYS:CE	5:E:47:LYS:HE3	2.35	0.57
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.86	0.57
17:Q:113:ARG:HH21	18:R:222:SER:HB3	1.62	0.57
1:A:334:ARG:NH2	13:M:66:ARG:O	2.37	0.57
1:A:375:ILE:HB	1:A:666:ARG:CD	2.35	0.57
1:A:1098:PRO:O	1:A:1101:GLN:CD	2.48	0.57
2:B:1075:MET:HE1	13:M:51:GLU:HG2	1.87	0.57
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.87	0.56
1:A:264:VAL:CB	1:A:272:ASN:ND2	2.67	0.56
1:A:355:MET:CE	1:A:1431:SER:HB2	2.35	0.56
1:A:1289:GLU:HG2	1:A:1292:MET:HE2	1.87	0.56
2:B:94:SER:O	2:B:122:ALA:HB1	2.05	0.56
1:A:133:SER:C	1:A:135:GLY:N	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG21	13:M:48:VAL:HB	1.88	0.56
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.20	0.56
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.87	0.56
2:B:895:PHE:O	2:B:897:ARG:HG3	2.05	0.56
3:C:157:GLN:HG3	10:J:65:LEU:CB	2.30	0.56
17:Q:21:VAL:HA	18:R:210:PHE:CE2	2.39	0.56
1:A:264:VAL:CB	1:A:272:ASN:CG	2.65	0.56
1:A:425:ASP:HB2	13:M:39:LEU:CG	2.35	0.56
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	0.56
8:H:17:PRO:C	8:H:19:GLY:H	2.13	0.56
17:Q:113:ARG:HD3	18:R:222:SER:CA	2.34	0.56
18:R:155:LEU:HD13	18:R:204:ASN:HD22	1.70	0.56
1:A:455:ILE:HG12	1:A:473:ARG:HG2	1.87	0.56
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.87	0.56
1:A:30:GLU:OE1	1:A:33:ARG:NH2	2.24	0.56
2:B:56:GLN:CB	20:T:140:ARG:CD	2.83	0.56
2:B:166:LEU:HB3	2:B:170:ASP:HB2	1.87	0.56
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.87	0.56
1:A:266:MET:HG2	1:A:272:ASN:CG	2.29	0.56
1:A:546:ARG:NH1	1:A:768:SER:OG	2.39	0.56
2:B:132:VAL:HG21	2:B:141:GLN:CG	2.31	0.56
3:C:157:GLN:CD	10:J:65:LEU:CG	2.79	0.56
13:M:44:ARG:NE	13:M:46:ILE:CG2	2.68	0.56
18:R:184:ALA:HA	18:R:187:ASP:HB3	1.87	0.56
1:A:1154:ALA:HB1	1:A:1310:HIS:CE1	2.41	0.56
5:E:91:CYS:HA	5:E:94:MET:HE3	1.87	0.56
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.88	0.56
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.88	0.56
2:B:906:GLN:CG	12:L:45:TYR:HE1	2.17	0.56
2:B:1053:HIS:CE1	2:B:1058:LYS:HG3	2.40	0.56
10:J:65:LEU:H	10:J:65:LEU:HD22	1.70	0.56
17:Q:108:ASP:O	17:Q:111:ARG:HG2	2.06	0.56
1:A:138:LYS:N	1:A:1445:HIS:HE1	2.03	0.56
1:A:139:LYS:HE2	1:A:143:HIS:NE2	2.20	0.56
1:A:619:LYS:O	1:A:620:HIS:CG	2.59	0.56
2:B:270:ILE:HG21	2:B:308:ALA:HB2	1.87	0.56
2:B:852:GLY:O	2:B:868:GLY:N	2.31	0.56
17:Q:58:GLN:HE22	18:R:194:ARG:HH11	1.54	0.56
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.87	0.55
10:J:7:CYS:SG	10:J:48:MET:HE3	2.45	0.55
13:M:72:ASN:HB2	22:Y:58:DC:H42	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD12	1:A:323:PRO:HD2	1.87	0.55
2:B:92:TYR:HE2	2:B:146:LYS:HE2	1.69	0.55
3:C:154:ARG:NH2	10:J:61:ASN:OD1	2.35	0.55
3:C:154:ARG:NH1	10:J:61:ASN:HA	2.21	0.55
13:M:10:LEU:HD23	13:M:10:LEU:O	2.06	0.55
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.39	0.55
13:M:94:ASP:HB3	13:M:99:SER:N	2.21	0.55
13:M:182:ALA:HB3	20:T:154:LYS:CG	2.34	0.55
17:Q:105:TYR:OH	18:R:234:GLU:CD	2.50	0.55
17:Q:187:ILE:HG21	18:R:211:SER:N	2.21	0.55
19:S:6:PRO:HG3	19:S:10:ASN:HD22	1.71	0.55
1:A:1253:GLU:HG2	9:I:3:PRO:HB2	1.89	0.55
2:B:758:LEU:HD13	2:B:991:ALA:HB2	1.88	0.55
2:B:894:THR:HG23	2:B:897:ARG:NH1	2.22	0.55
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.87	0.55
19:S:27:ASN:O	20:T:95:VAL:HG13	2.06	0.55
2:B:855:ALA:O	2:B:858:VAL:HG12	2.07	0.55
8:H:85:ALA:HB3	8:H:144:LEU:CD2	2.36	0.55
9:I:96:PHE:HB3	9:I:112:TYR:HD1	1.72	0.55
17:Q:115:GLU:HA	17:Q:118:GLU:HB3	1.87	0.55
17:Q:170:LYS:HG2	17:Q:171:LYS:H	1.72	0.55
1:A:425:ASP:CB	13:M:39:LEU:HD11	2.35	0.55
16:P:257:ASN:ND2	21:X:14:DA:N3	2.54	0.55
1:A:930:LEU:O	1:A:931:ARG:C	2.49	0.55
1:A:1373:ALA:HB2	5:E:145:VAL:HG22	1.88	0.55
2:B:90:GLN:CG	20:T:141:LEU:CD1	2.83	0.55
3:C:157:GLN:HE21	10:J:65:LEU:CA	2.20	0.55
21:X:24:DG:H2''	21:X:25:DG:H5'	1.89	0.55
13:M:174:PRO:HD2	13:M:213:ASP:HB3	1.89	0.55
2:B:605:ARG:NH2	9:I:71:ASP:OD2	2.39	0.55
2:B:1087:GLY:HA3	22:Y:48:DC:OP1	2.07	0.55
6:F:88:ASP:OD1	6:F:91:LEU:N	2.33	0.55
13:M:94:ASP:HB2	13:M:99:SER:N	2.09	0.55
19:S:172:ASN:HD21	19:S:175:SER:HB2	1.72	0.55
16:P:163:PRO:HA	16:P:262:CYS:HB3	1.88	0.55
2:B:625:LEU:HD13	2:B:675:LEU:HD11	1.88	0.55
18:R:181:ALA:HA	18:R:184:ALA:HB3	1.88	0.55
1:A:269:SER:H	1:A:271:ARG:HD3	1.73	0.54
1:A:328:ALA:HA	13:M:84:ILE:HG22	1.89	0.54
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.47	0.54
13:M:45:VAL:CG1	13:M:48:VAL:HG13	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:188:TYR:OH	18:R:210:PHE:HE1	1.79	0.54
20:T:203:VAL:HG11	20:T:210:VAL:HG22	1.88	0.54
1:A:65:ILE:HA	1:A:78:MET:HE2	1.89	0.54
1:A:522:PRO:HB3	1:A:666:ARG:HB2	1.89	0.54
1:A:1158:LEU:HD11	1:A:1308:TYR:CG	2.41	0.54
2:B:92:TYR:CD2	20:T:145:LEU:HD11	2.42	0.54
2:B:225:LEU:O	2:B:227:ASN:C	2.51	0.54
3:C:212:ASP:O	3:C:213:GLU:C	2.50	0.54
8:H:106:THR:O	8:H:108:ALA:N	2.37	0.54
9:I:62:VAL:C	9:I:64:GLU:H	2.10	0.54
17:Q:25:PHE:N	18:R:210:PHE:CE2	2.74	0.54
1:A:152:ASN:OD1	1:A:188:GLN:HB2	2.06	0.54
1:A:196:LEU:HB2	1:A:325:LEU:HD21	1.90	0.54
2:B:549:SER:OG	2:B:577:HIS:NE2	2.25	0.54
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.72	0.54
17:Q:149:THR:HG23	17:Q:151:THR:H	1.72	0.54
1:A:273:GLN:O	1:A:274:ASP:C	2.49	0.54
1:A:285:LYS:HD2	13:M:80:LEU:HD23	1.89	0.54
1:A:1264:SER:OG	1:A:1267:ASN:ND2	2.38	0.54
2:B:708:ALA:O	2:B:711:ILE:HG23	2.08	0.54
13:M:119:LYS:HD3	22:Y:60:DA:H62	1.72	0.54
20:T:177:ARG:HH22	21:X:19:DG:P	2.31	0.54
21:X:42:DT:H3'	21:X:43:DT:C5'	2.37	0.54
1:A:47:THR:OG1	1:A:53:LYS:HG2	2.07	0.54
1:A:129:ILE:HG22	1:A:140:ARG:HG3	1.90	0.54
1:A:644:SER:O	1:A:651:SER:HB3	2.06	0.54
1:A:760:LEU:HD13	1:A:767:LYS:HB2	1.89	0.54
2:B:252:ILE:O	2:B:254:GLN:N	2.35	0.54
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.89	0.54
2:B:473:LEU:HD21	2:B:1052:LYS:HB2	1.90	0.54
2:B:883:THR:O	2:B:885:ARG:CA	2.55	0.54
21:X:45:DT:O2	21:X:46:DT:N3	2.41	0.54
2:B:206:TYR:HD1	2:B:208:PHE:HE1	1.54	0.54
2:B:649:ASN:OD1	2:B:650:ASN:N	2.40	0.54
13:M:52:TRP:C	13:M:54:THR:H	2.16	0.54
22:Y:64:DC:H2''	22:Y:65:DG:H5'	1.89	0.54
1:A:131:ALA:C	1:A:133:SER:N	2.56	0.54
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.89	0.54
3:C:209:SER:O	3:C:212:ASP:OD1	2.25	0.54
7:G:106:CYS:HA	7:G:159:ALA:O	2.08	0.54
7:G:108:ILE:HG23	7:G:162:SER:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:21:VAL:CA	18:R:210:PHE:CE2	2.91	0.54
1:A:266:MET:HE2	13:M:52:TRP:CE2	2.43	0.54
20:T:177:ARG:NH2	21:X:19:DG:OP1	2.39	0.54
1:A:264:VAL:HG21	13:M:68:GLY:HA3	1.88	0.53
1:A:358:ARG:HE	2:B:1076:GLU:CD	2.16	0.53
1:A:790:GLN:HE22	1:A:821:GLY:HA3	1.71	0.53
1:A:1204:VAL:HA	1:A:1207:ILE:HG12	1.89	0.53
2:B:92:TYR:CE2	2:B:146:LYS:HE2	2.42	0.53
5:E:64:HIS:C	5:E:66:ASP:N	2.56	0.53
17:Q:112:ARG:NH2	18:R:237:LEU:HD22	2.17	0.53
1:A:1188:GLU:HA	9:I:1:MET:HE2	1.91	0.53
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.90	0.53
2:B:292:PHE:HD2	9:I:14:ILE:HD13	1.68	0.53
2:B:1053:HIS:HE1	2:B:1058:LYS:HG3	1.73	0.53
7:G:94:LYS:O	7:G:110:ARG:NH1	2.34	0.53
1:A:455:ILE:HG21	1:A:520:MET:HE1	1.91	0.53
2:B:914:GLU:HG3	13:M:132:ARG:HB3	1.91	0.53
8:H:66:GLU:CG	8:H:67:ASP:H	2.16	0.53
17:Q:144:LEU:HD22	17:Q:154:CYS:HA	1.91	0.53
1:A:95:PHE:CE1	1:A:218:PRO:HG3	2.44	0.53
1:A:152:ASN:O	1:A:153:ILE:CB	2.56	0.53
1:A:1477:ALA:HB2	7:G:22:LEU:HD23	1.90	0.53
2:B:352:GLY:HA3	2:B:357:CYS:SG	2.48	0.53
17:Q:25:PHE:HZ	18:R:223:VAL:HG22	1.72	0.53
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.41	0.53
1:A:601:ASN:HD21	1:A:632:ASN:H	1.55	0.53
2:B:489:ILE:HA	21:X:47:DT:O2	2.09	0.53
2:B:716:HIS:CD2	2:B:982:ILE:HG13	2.30	0.53
2:B:752:TYR:CG	3:C:63:PHE:HE1	2.26	0.53
17:Q:113:ARG:HD3	18:R:222:SER:HA	1.91	0.53
23:Z:1:A:H2'	23:Z:2:G:O4'	2.09	0.53
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.91	0.53
22:Y:53:DG:H4'	22:Y:54:DA:OP1	2.09	0.53
1:A:373:LEU:O	1:A:485:ASN:ND2	2.41	0.53
1:A:469:MET:HE3	2:B:1094:GLN:OE1	2.09	0.53
1:A:930:LEU:C	1:A:931:ARG:O	2.50	0.53
1:A:1116:ASN:C	1:A:1118:THR:N	2.57	0.53
1:A:1466:ALA:O	1:A:1469:GLY:N	2.39	0.53
2:B:309:PHE:HE2	9:I:40:ARG:HD2	1.72	0.53
2:B:824:ASP:OD2	2:B:875:GLU:HG3	2.09	0.53
12:L:35:ARG:HH11	12:L:42:ARG:HH21	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:GLY:O	1:A:625:ASP:CB	2.33	0.53
2:B:356:PHE:HB3	19:S:116:GLY:CA	2.39	0.53
7:G:138:GLN:HG2	7:G:139:GLN:HG2	1.89	0.53
16:P:309:LYS:HD3	22:Y:82:DT:H5"	1.91	0.53
19:S:13:GLU:OE1	20:T:44:ARG:NH1	2.41	0.53
1:A:611:ASP:O	1:A:612:ASP:HB2	2.09	0.53
1:A:623:PRO:C	1:A:625:ASP:N	2.67	0.53
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.39	0.53
2:B:712:PRO:HD2	2:B:939:HIS:CE1	2.44	0.53
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.89	0.53
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.39	0.53
8:H:16:ASP:HB3	8:H:19:GLY:HA2	1.89	0.53
21:X:26:DG:N2	22:Y:69:DC:N3	2.57	0.53
1:A:426:ARG:HD2	13:M:40:VAL:HG11	1.91	0.52
1:A:557:ARG:HA	1:A:586:TRP:CZ3	2.44	0.52
1:A:679:TRP:CZ3	1:A:683:GLU:HG3	2.44	0.52
1:A:870:SER:HB2	1:A:882:SER:HB3	1.90	0.52
2:B:800:ALA:O	2:B:805:PHE:HB2	2.09	0.52
3:C:56:SER:HG	3:C:158:GLU:H	1.55	0.52
2:B:1073:GLN:NE2	2:B:1154:ALA:HB2	2.25	0.52
3:C:157:GLN:NE2	10:J:65:LEU:CG	2.70	0.52
12:L:13:GLN:C	12:L:15:MET:H	2.17	0.52
1:A:203:LYS:O	1:A:204:HIS:CB	2.53	0.52
2:B:344:GLN:O	2:B:361:LYS:NZ	2.38	0.52
2:B:844:ILE:HG22	2:B:846:ASP:H	1.74	0.52
4:D:33:LEU:HD12	4:D:80:ILE:HG23	1.91	0.52
14:N:317:GLU:C	14:N:318:ASP:O	2.52	0.52
17:Q:25:PHE:HA	18:R:219:LEU:HD13	1.91	0.52
1:A:44:PRO:HG3	1:A:284:VAL:HG13	1.91	0.52
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.74	0.52
4:D:135:GLN:HA	4:D:138:ARG:HG2	1.91	0.52
17:Q:203:ILE:HG23	17:Q:204:LEU:HG	1.91	0.52
1:A:40:GLY:O	1:A:42:LYS:HG2	2.10	0.52
2:B:822:GLY:HA3	2:B:825:GLN:HG2	1.92	0.52
6:F:64:ARG:HH12	7:G:61:PRO:HB3	1.75	0.52
17:Q:70:LYS:HZ2	18:R:226:ASP:HA	1.75	0.52
1:A:440:LEU:HB2	1:A:444:TYR:HD2	1.73	0.52
1:A:530:SER:O	1:A:532:ARG:N	2.43	0.52
1:A:1305:SER:OG	1:A:1307:VAL:HB	2.10	0.52
1:A:1313:GLN:OE1	1:A:1316:ASN:ND2	2.43	0.52
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:GLN:CB	20:T:140:ARG:HD2	2.38	0.52
2:B:1016:SER:HB3	2:B:1022:LEU:CB	2.40	0.52
7:G:111:HIS:CE1	17:Q:125:ALA:H	2.28	0.52
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.23	0.52
1:A:367:ILE:HG21	1:A:501:MET:HG2	1.91	0.52
1:A:367:ILE:HG12	1:A:499:ASP:O	2.10	0.52
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.45	0.52
1:A:1128:ILE:HG23	1:A:1414:ILE:HG13	1.92	0.52
2:B:92:TYR:CD2	20:T:145:LEU:CD1	2.92	0.52
2:B:312:GLN:HB3	19:S:153:ARG:NH2	2.24	0.52
9:I:62:VAL:O	9:I:64:GLU:HG2	2.10	0.52
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.52
1:A:26:LEU:HB2	2:B:1168:ALA:HB2	1.92	0.52
1:A:485:ASN:C	1:A:485:ASN:OD1	2.52	0.52
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.74	0.52
2:B:553:LEU:O	2:B:556:ILE:HG12	2.10	0.52
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.75	0.52
2:B:882:SER:HB3	2:B:887:TYR:CE2	2.35	0.52
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.44	0.52
2:B:331:THR:O	2:B:333:GLU:N	2.42	0.52
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.90	0.52
2:B:1075:MET:CE	13:M:51:GLU:HG2	2.40	0.52
5:E:53:PRO:HB2	5:E:56:THR:HB	1.92	0.52
13:M:27:TYR:CD2	13:M:46:ILE:HB	2.44	0.52
17:Q:28:ILE:HD12	18:R:190:LEU:HD21	1.92	0.52
17:Q:172:ASP:HA	17:Q:175:THR:HB	1.91	0.52
1:A:1207:ILE:HG22	1:A:1262:MET:HG3	1.92	0.52
1:A:1290:SER:CB	2:B:250:SER:HB2	2.21	0.52
2:B:1053:HIS:ND1	2:B:1058:LYS:HE3	2.25	0.52
6:F:51:ARG:HA	6:F:116:GLU:OE1	2.10	0.52
13:M:179:GLU:CG	20:T:154:LYS:HD3	2.39	0.52
21:X:24:DG:H2'	21:X:25:DG:C8	2.45	0.52
1:A:360:ASP:CG	2:B:1064:ARG:H	2.17	0.51
1:A:926:ASN:OD1	1:A:931:ARG:HB3	2.10	0.51
2:B:56:GLN:CB	20:T:140:ARG:HD3	2.39	0.51
2:B:203:ASN:O	2:B:204:THR:OG1	2.27	0.51
2:B:896:LEU:C	2:B:897:ARG:HG3	2.34	0.51
2:B:1053:HIS:CE1	2:B:1058:LYS:HE3	2.45	0.51
14:N:313:PRO:HG2	16:P:235:ARG:NH2	2.17	0.51
16:P:193:ASN:HD21	16:P:196:ARG:HD3	1.74	0.51
1:A:924:TYR:CZ	1:A:949:GLN:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:LYS:O	2:B:240:LEU:HD12	2.11	0.51
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.25	0.51
9:I:91:HIS:ND1	9:I:92:LYS:O	2.43	0.51
14:N:333:ASN:CG	14:N:361:ASN:H	2.19	0.51
20:T:132:ILE:O	20:T:136:SER:OG	2.26	0.51
1:A:201:GLU:OE2	1:A:203:LYS:NZ	2.43	0.51
1:A:1323:THR:HG23	1:A:1325:ASP:H	1.75	0.51
16:P:203:ARG:NH2	16:P:210:THR:OG1	2.43	0.51
16:P:206:GLU:OE1	16:P:207:PRO:HD3	2.10	0.51
1:A:926:ASN:CG	1:A:931:ARG:HB3	2.35	0.51
3:C:5:ASN:N	11:K:97:GLU:OE2	2.43	0.51
3:C:99:VAL:HG13	3:C:124:SER:OG	2.10	0.51
20:T:181:GLN:HA	20:T:184:LEU:HD12	1.93	0.51
1:A:112:PHE:H	1:A:188:GLN:NE2	2.09	0.51
1:A:710:LYS:O	1:A:714:ILE:HG12	2.11	0.51
2:B:295:PRO:HB3	9:I:11:PHE:HD2	1.75	0.51
11:K:116:ILE:HG13	11:K:117:GLU:HG3	1.90	0.51
13:M:45:VAL:HG11	13:M:48:VAL:HG13	1.92	0.51
21:X:23:DT:H2''	21:X:24:DG:H8	1.75	0.51
22:Y:80:DT:H2''	22:Y:81:DA:C8	2.45	0.51
1:A:613:GLU:O	1:A:614:ASP:HB3	2.10	0.51
2:B:56:GLN:NE2	2:B:60:GLU:OE2	2.44	0.51
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.44	0.51
10:J:54:ASP:OD2	10:J:57:GLU:HG2	2.11	0.51
2:B:838:GLN:O	2:B:891:ASP:N	2.43	0.51
9:I:61:GLU:C	9:I:63:ASP:N	2.69	0.51
17:Q:23:ARG:NH2	18:R:207:SER:N	2.58	0.51
17:Q:101:ASN:O	17:Q:103:VAL:N	2.43	0.51
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.46	0.51
1:A:264:VAL:CG1	13:M:52:TRP:CD1	2.94	0.51
2:B:234:THR:O	2:B:236:TRP:HD1	1.93	0.51
22:Y:48:DC:H2'	22:Y:49:DG:H8	1.76	0.51
1:A:927:GLU:HB3	1:A:931:ARG:HD3	1.93	0.51
2:B:988:LYS:O	2:B:992:ASN:HB2	2.11	0.51
14:N:347:ASN:O	14:N:375:GLU:HA	2.11	0.51
16:P:298:PRO:O	16:P:299:ARG:C	2.53	0.51
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.41	0.51
1:A:265:VAL:C	1:A:272:ASN:HD22	2.19	0.51
1:A:298:ALA:N	17:Q:60:ARG:HE	2.09	0.51
1:A:1020:LEU:HD13	1:A:1041:PHE:HE2	1.76	0.51
1:A:1115:LYS:C	1:A:1116:ASN:O	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ALA:HB2	20:T:201:ASP:CG	2.35	0.51
3:C:157:GLN:CD	10:J:65:LEU:HG	2.36	0.51
8:H:65:TYR:N	8:H:65:TYR:CD1	2.77	0.51
1:A:1319:LYS:HB2	1:A:1333:GLU:OE2	2.11	0.50
2:B:854:ILE:HG13	2:B:866:ILE:O	2.10	0.50
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.46	0.50
9:I:93:GLU:O	9:I:115:THR:HG22	2.11	0.50
17:Q:36:ILE:HG21	17:Q:48:MET:HG2	1.92	0.50
20:T:229:HIS:NE2	21:X:28:DG:H1'	2.25	0.50
1:A:1022:ILE:HD13	1:A:1080:ILE:HD12	1.92	0.50
7:G:93:ASN:HD22	17:Q:151:THR:HA	1.73	0.50
8:H:85:ALA:HB1	8:H:144:LEU:CD2	2.41	0.50
8:H:85:ALA:HB3	8:H:144:LEU:HD21	1.93	0.50
13:M:94:ASP:HB3	13:M:99:SER:C	2.36	0.50
2:B:1029:TYR:CE1	2:B:1036:LYS:HG3	2.46	0.50
9:I:81:THR:HB	9:I:96:PHE:CE2	2.46	0.50
17:Q:44:LYS:HG3	17:Q:46:GLU:H	1.76	0.50
17:Q:109:HIS:HB3	18:R:224:THR:CG2	2.33	0.50
19:S:26:TYR:HB2	19:S:139:PRO:O	2.12	0.50
21:X:50:DT:H3'	21:X:51:DC:H5''	1.92	0.50
1:A:710:LYS:HE3	1:A:818:GLU:OE2	2.11	0.50
3:C:137:ASN:ND2	3:C:137:ASN:H	2.09	0.50
5:E:41:LYS:HE3	5:E:47:LYS:HE3	1.91	0.50
7:G:13:LEU:HD21	7:G:22:LEU:HD11	1.93	0.50
8:H:108:ALA:O	8:H:109:ALA:C	2.55	0.50
13:M:276:ASP:O	20:T:153:TYR:HB2	2.11	0.50
17:Q:24:GLY:CA	18:R:209:GLN:HG2	2.38	0.50
17:Q:188:TYR:OH	18:R:211:SER:OG	2.19	0.50
21:X:3:DA:H1'	21:X:4:DG:H5'	1.94	0.50
21:X:36:DT:H71	21:X:37:DT:H3	1.77	0.50
1:A:138:LYS:H	1:A:1445:HIS:HE1	1.60	0.50
2:B:92:TYR:HE1	20:T:141:LEU:HG	1.77	0.50
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.35	0.50
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.92	0.50
1:A:36:VAL:HG11	1:A:72:GLN:NE2	2.27	0.50
1:A:366:VAL:O	1:A:481:THR:HB	2.12	0.50
1:A:603:ILE:HG12	1:A:604:ARG:H	1.76	0.50
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.45	0.50
3:C:259:LEU:HD22	11:K:42:LEU:HD21	1.94	0.50
13:M:10:LEU:C	13:M:12:ARG:N	2.69	0.50
19:S:172:ASN:OD1	19:S:173:HIS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:13:DT:H3	22:Y:81:DA:H61	1.60	0.50
1:A:137:PRO:HB2	1:A:1445:HIS:CE1	2.46	0.50
1:A:451:CYS:O	1:A:453:GLY:N	2.38	0.50
1:A:516:GLN:HA	1:A:520:MET:HE2	1.94	0.50
8:H:64:LEU:C	8:H:66:GLU:N	2.69	0.50
13:M:182:ALA:HB2	20:T:154:LYS:HA	1.92	0.50
18:R:82:VAL:HG22	18:R:140:LYS:HE2	1.94	0.50
3:C:142:TYR:O	3:C:144:GLU:N	2.45	0.50
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.77	0.50
17:Q:113:ARG:HH12	18:R:218:LYS:CA	2.25	0.50
17:Q:180:PHE:CE1	18:R:212:VAL:O	2.65	0.50
1:A:1076:PHE:CE2	1:A:1080:ILE:HD11	2.47	0.49
1:A:1304:ILE:HA	1:A:1340:GLY:HA3	1.93	0.49
1:A:1361:ASP:OD2	1:A:1364:GLU:HB2	2.12	0.49
2:B:98:HIS:HB2	2:B:108:MET:HE3	1.93	0.49
2:B:285:LEU:HD21	2:B:298:MET:HE2	1.94	0.49
13:M:85:GLY:O	13:M:86:LYS:HB2	2.11	0.49
1:A:196:LEU:HD22	1:A:325:LEU:HD21	1.94	0.49
1:A:262:PRO:CB	2:B:1070:LEU:HG	2.38	0.49
1:A:606:HIS:HB3	1:A:627:LYS:HA	1.94	0.49
1:A:802:PHE:CE2	1:A:808:PRO:HD3	2.47	0.49
1:A:1305:SER:OG	1:A:1306:LYS:N	2.46	0.49
2:B:92:TYR:HB3	20:T:145:LEU:CD1	2.30	0.49
2:B:838:GLN:HG3	2:B:886:ARG:NH2	2.27	0.49
9:I:86:CYS:HB2	9:I:114:CYS:SG	2.51	0.49
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.47	0.49
18:R:213:ASP:O	18:R:215:GLU:N	2.44	0.49
20:T:34:ALA:O	20:T:37:ARG:HG3	2.12	0.49
20:T:144:GLN:O	20:T:145:LEU:HB2	2.13	0.49
22:Y:46:DC:H2'	22:Y:47:DG:C8	2.48	0.49
22:Y:46:DC:H2'	22:Y:47:DG:H8	1.77	0.49
1:A:1290:SER:CB	2:B:250:SER:OG	2.24	0.49
2:B:628:VAL:HG12	2:B:633:LEU:HA	1.95	0.49
8:H:65:TYR:HE1	8:H:84:ARG:HH21	1.60	0.49
1:A:371:PRO:HD2	2:B:788:TYR:CE1	2.48	0.49
1:A:622:SER:O	1:A:623:PRO:C	2.48	0.49
2:B:899:SER:C	2:B:901:THR:H	2.21	0.49
17:Q:70:LYS:NZ	18:R:230:GLU:OE2	2.46	0.49
1:A:1473:LEU:HD13	6:F:104:ILE:HD12	1.94	0.49
14:N:317:GLU:O	14:N:318:ASP:C	2.56	0.49
15:O:48:LEU:HD23	15:O:52:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:57:DA:H5''	22:Y:58:DC:H2'	1.95	0.49
1:A:60:PRO:O	1:A:61:ARG:HG3	2.12	0.49
1:A:374:SER:C	1:A:485:ASN:HD22	2.20	0.49
1:A:883:ILE:HG21	1:A:1424:THR:HA	1.93	0.49
2:B:302:LYS:HG3	9:I:23:MET:HE1	1.93	0.49
2:B:878:ASP:C	2:B:879:GLU:O	2.55	0.49
13:M:56:SER:O	22:Y:51:DC:N4	2.45	0.49
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.95	0.49
1:A:133:SER:O	1:A:134:LYS:HB2	2.12	0.49
3:C:146:ASP:O	3:C:148:ILE:N	2.45	0.49
17:Q:25:PHE:H	18:R:210:PHE:HE2	1.61	0.49
17:Q:75:ARG:HB3	17:Q:95:ASN:HB3	1.95	0.49
17:Q:187:ILE:HD13	18:R:212:VAL:N	2.25	0.49
20:T:95:VAL:O	20:T:107:GLU:N	2.45	0.49
20:T:166:GLU:O	20:T:170:LYS:HG3	2.13	0.49
1:A:263:ALA:O	1:A:265:VAL:HG22	2.12	0.49
2:B:89:GLU:HG3	2:B:90:GLN:H	1.78	0.49
12:L:25:GLU:OE1	12:L:25:GLU:N	2.36	0.49
19:S:126:ILE:O	19:S:137:ALA:HA	2.13	0.49
20:T:141:LEU:C	20:T:141:LEU:CD2	2.86	0.49
2:B:1162:LEU:HD23	2:B:1165:MET:CE	2.43	0.49
3:C:36:ARG:NH2	11:K:40:HIS:HB2	2.28	0.49
9:I:66:THR:O	9:I:68:ILE:N	2.44	0.49
15:O:86:GLU:HG3	15:O:87:LEU:N	2.28	0.49
2:B:62:ALA:N	2:B:63:PRO:HD3	2.28	0.49
2:B:323:SER:HB3	2:B:335:ARG:NH1	2.27	0.49
20:T:139:VAL:C	20:T:141:LEU:N	2.50	0.49
20:T:180:LYS:HE3	20:T:184:LEU:HD11	1.95	0.49
1:A:1158:LEU:HD11	1:A:1308:TYR:CD1	2.47	0.48
2:B:422:PHE:CE2	2:B:429:PHE:HB2	2.48	0.48
2:B:631:GLN:HB3	2:B:685:LYS:HZ3	1.77	0.48
3:C:154:ARG:HG2	3:C:155:LYS:H	1.77	0.48
2:B:1079:SER:C	2:B:1080:ARG:HD2	2.38	0.48
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.95	0.48
8:H:10:PHE:CE2	8:H:39:LEU:HD22	2.47	0.48
21:X:33:DT:H2''	21:X:34:DT:C5	2.47	0.48
1:A:266:MET:HB3	13:M:52:TRP:CE3	2.49	0.48
1:A:458:PHE:HE2	1:A:482:PHE:CD2	2.31	0.48
1:A:1298:LEU:C	1:A:1300:GLY:H	2.21	0.48
1:A:1319:LYS:HD3	1:A:1333:GLU:OE1	2.13	0.48
2:B:497:LYS:O	2:B:500:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:ARG:NH1	13:M:53:ARG:HD2	2.28	0.48
9:I:28:GLU:HG2	9:I:30:LYS:HG3	1.94	0.48
17:Q:191:LEU:HD21	18:R:210:PHE:HB2	1.95	0.48
18:R:75:PHE:HD2	20:T:192:GLU:OE2	1.96	0.48
1:A:347:GLU:OE1	1:A:347:GLU:N	2.42	0.48
2:B:58:ILE:O	2:B:61:ASP:HB2	2.13	0.48
2:B:422:PHE:O	2:B:425:ARG:N	2.46	0.48
6:F:79:VAL:HG12	6:F:81:VAL:H	1.78	0.48
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.94	0.48
8:H:65:TYR:HE2	8:H:70:LEU:HA	1.76	0.48
22:Y:29:DC:H2"	22:Y:30:DG:C8	2.48	0.48
1:A:264:VAL:C	1:A:272:ASN:HB3	2.37	0.48
1:A:312:PHE:HB2	13:M:101:TYR:OH	2.14	0.48
1:A:492:TYR:CD2	1:A:501:MET:HE1	2.49	0.48
1:A:609:HIS:H	1:A:610:PRO:HD3	1.73	0.48
2:B:248:LYS:HG2	19:S:170:VAL:HG23	1.96	0.48
2:B:378:GLY:O	9:I:102:ALA:HB3	2.14	0.48
2:B:728:MET:HA	2:B:731:GLN:HB2	1.95	0.48
2:B:881:GLU:HB3	2:B:883:THR:HG23	1.94	0.48
2:B:1029:TYR:HE1	2:B:1036:LYS:CE	2.25	0.48
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.14	0.48
5:E:49:SER:O	5:E:52:ARG:NH1	2.36	0.48
17:Q:127:PHE:HA	17:Q:163:GLU:C	2.39	0.48
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.48	0.48
1:A:266:MET:HE2	13:M:52:TRP:CZ2	2.48	0.48
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.48
1:A:745:LEU:HD21	1:A:817:PRO:HB3	1.95	0.48
2:B:225:LEU:HB3	2:B:228:SER:CB	2.31	0.48
2:B:819:SER:HB3	2:B:821:LYS:HB2	1.94	0.48
7:G:97:LEU:HG	7:G:113:ILE:HD11	1.95	0.48
8:H:99:ILE:HD11	8:H:112:LEU:HD21	1.94	0.48
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.29	0.48
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.49	0.48
1:A:1020:LEU:HD22	1:A:1076:PHE:CD2	2.48	0.48
1:A:1463:LEU:HA	2:B:1104:ARG:HD3	1.96	0.48
2:B:274:ARG:NH2	2:B:279:VAL:O	2.47	0.48
2:B:363:TYR:CD2	2:B:553:LEU:HD11	2.48	0.48
3:C:100:GLU:HG3	3:C:164:TYR:CE1	2.48	0.48
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.96	0.48
1:A:231:GLU:H	1:A:231:GLU:CD	2.19	0.48
1:A:540:ASP:HB3	2:B:790:GLN:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:SER:OG	1:A:773:GLY:N	2.45	0.48
2:B:23:GLN:OE1	2:B:23:GLN:N	2.40	0.48
2:B:73:HIS:C	2:B:75:SER:N	2.66	0.48
2:B:752:TYR:O	10:J:1:MET:HG3	2.13	0.48
2:B:799:SER:HB2	2:B:951:GLN:HB2	1.95	0.48
2:B:952:GLU:OE2	3:C:40:ALA:HB2	2.13	0.48
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.95	0.48
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.48	0.48
20:T:138:PRO:HB2	20:T:140:ARG:HH21	1.79	0.48
1:A:459:ASN:C	1:A:459:ASN:OD1	2.56	0.48
1:A:522:PRO:HG3	1:A:666:ARG:HG2	1.95	0.48
1:A:719:LYS:HG2	1:A:724:GLU:OE1	2.13	0.48
1:A:882:SER:C	1:A:884:ASN:H	2.22	0.48
1:A:1147:SER:HB3	1:A:1157:ILE:HD11	1.95	0.48
2:B:573:TRP:O	2:B:573:TRP:HE3	1.97	0.48
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.96	0.48
20:T:150:THR:C	20:T:152:ASN:H	2.22	0.48
1:A:567:LEU:HD11	1:A:595:ILE:HG12	1.96	0.48
1:A:891:TYR:CE1	1:A:1087:VAL:HG13	2.49	0.48
2:B:1163:MET:HA	2:B:1167:ILE:O	2.14	0.48
17:Q:21:VAL:HA	18:R:210:PHE:CD2	2.49	0.48
17:Q:184:ILE:CD1	18:R:211:SER:CB	2.86	0.48
19:S:110:PHE:CD1	19:S:148:PRO:HA	2.48	0.48
1:A:1130:ILE:HD13	1:A:1411:LEU:HB3	1.95	0.47
2:B:312:GLN:O	19:S:153:ARG:NH2	2.47	0.47
2:B:950:ARG:HH12	3:C:171:LYS:HG3	1.79	0.47
2:B:1060:HIS:CE1	2:B:1078:ARG:HG2	2.48	0.47
4:D:60:VAL:HG13	7:G:103:PRO:HG3	1.95	0.47
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.78	0.47
20:T:47:LYS:HG2	20:T:52:THR:HG23	1.95	0.47
1:A:77:ASN:OD1	1:A:77:ASN:N	2.47	0.47
1:A:613:GLU:O	1:A:614:ASP:CB	2.62	0.47
2:B:733:MET:HG2	2:B:1050:ARG:O	2.14	0.47
5:E:48:PRO:C	5:E:50:GLU:N	2.72	0.47
5:E:173:ILE:CG2	5:E:209:VAL:HG22	2.44	0.47
20:T:141:LEU:C	20:T:143:GLN:N	2.72	0.47
1:A:344:LYS:NZ	22:Y:43:DG:H5"	2.28	0.47
1:A:702:ILE:HG12	1:A:752:THR:HG23	1.94	0.47
1:A:1067:TRP:CZ2	1:A:1071:GLU:HG3	2.50	0.47
2:B:861:SER:O	2:B:896:LEU:HD23	2.15	0.47
3:C:100:GLU:HG3	3:C:164:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:LYS:HD2	4:D:124:ASP:OD1	2.14	0.47
5:E:27:LEU:HB2	5:E:64:HIS:HB3	1.96	0.47
7:G:40:GLY:O	7:G:78:ARG:NH1	2.48	0.47
11:K:87:PHE:CE1	11:K:91:ILE:HD11	2.49	0.47
13:M:245:VAL:HG12	13:M:291:LEU:HD23	1.95	0.47
14:N:344:ARG:HH21	22:Y:78:DT:H3'	1.77	0.47
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.96	0.47
17:Q:169:PRO:HA	17:Q:174:ARG:HG2	1.96	0.47
18:R:161:ARG:HG3	18:R:161:ARG:O	2.13	0.47
1:A:156:GLY:CA	1:A:181:HIS:HD1	2.08	0.47
2:B:52:GLN:O	20:T:140:ARG:HG3	2.14	0.47
2:B:531:TYR:HE2	2:B:599:SER:HB3	1.79	0.47
2:B:878:ASP:O	2:B:879:GLU:C	2.56	0.47
9:I:21:ASN:O	9:I:22:ASN:ND2	2.47	0.47
13:M:182:ALA:HB3	20:T:154:LYS:HG2	1.96	0.47
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.79	0.47
17:Q:24:GLY:HA2	18:R:209:GLN:OE1	2.13	0.47
1:A:1304:ILE:HB	1:A:1307:VAL:CG1	2.44	0.47
20:T:143:GLN:O	20:T:144:GLN:C	2.58	0.47
1:A:810:PHE:CZ	1:A:819:SER:HA	2.50	0.47
1:A:1290:SER:OG	2:B:250:SER:CA	2.61	0.47
2:B:494:LYS:HG3	21:X:49:DT:C2	2.50	0.47
2:B:804:GLY:HA2	2:B:807:ARG:HE	1.79	0.47
3:C:117:SER:OG	3:C:147:ASP:HB3	2.15	0.47
17:Q:58:GLN:HE22	18:R:194:ARG:NH1	2.10	0.47
17:Q:113:ARG:HH11	18:R:221:ARG:HB2	1.79	0.47
18:R:194:ARG:HD3	18:R:194:ARG:HA	1.39	0.47
18:R:204:ASN:OD1	18:R:205:ASP:N	2.48	0.47
20:T:141:LEU:CA	20:T:143:GLN:OE1	2.63	0.47
1:A:362:SER:OG	2:B:1084:LEU:HD13	2.15	0.47
1:A:597:PRO:O	1:A:599:HIS:N	2.48	0.47
2:B:348:LEU:N	2:B:349:PRO:HD3	2.30	0.47
2:B:886:ARG:NH2	13:M:12:ARG:HH22	2.13	0.47
10:J:65:LEU:HD22	10:J:65:LEU:N	2.29	0.47
13:M:217:ARG:O	13:M:221:ASN:ND2	2.46	0.47
17:Q:188:TYR:CD2	17:Q:191:LEU:HD22	2.50	0.47
8:H:24:ARG:NH1	8:H:46:GLN:OE1	2.48	0.47
9:I:61:GLU:HG3	9:I:103:ARG:NH2	2.30	0.47
12:L:26:ASN:ND2	12:L:44:MET:HE2	2.30	0.47
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.40	0.47
17:Q:108:ASP:CG	18:R:237:LEU:HD22	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:140:LYS:H	18:R:141:PRO:HD2	1.79	0.47
18:R:157:GLN:O	18:R:161:ARG:N	2.46	0.47
19:S:136:GLU:HG2	19:S:138:PHE:CE1	2.49	0.47
22:Y:63:DG:H5'	22:Y:65:DG:OP1	2.15	0.47
1:A:519:ALA:HA	1:A:524:MET:HE3	1.97	0.47
3:C:1:MET:O	3:C:3:TYR:N	2.37	0.47
3:C:14:LEU:HD13	3:C:19:VAL:HG23	1.95	0.47
4:D:95:PHE:HZ	7:G:83:GLU:HG3	1.80	0.47
7:G:139:GLN:O	7:G:141:ASP:N	2.47	0.47
8:H:81:ARG:C	8:H:83:SER:H	2.23	0.47
9:I:57:LYS:C	9:I:58:ILE:CG1	2.75	0.47
19:S:135:PHE:HE2	20:T:43:LEU:HD23	1.79	0.47
21:X:48:DT:OP1	21:X:48:DT:H4'	2.15	0.47
1:A:156:GLY:N	1:A:181:HIS:ND1	2.63	0.47
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.96	0.47
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.50	0.47
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.97	0.47
3:C:175:LYS:NZ	12:L:57:ALA:HB3	2.30	0.47
18:R:209:GLN:NE2	18:R:215:GLU:OE1	2.48	0.47
1:A:322:LEU:HD23	1:A:325:LEU:HD22	1.97	0.46
1:A:334:ARG:HE	13:M:66:ARG:HD3	1.79	0.46
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.55	0.46
1:A:606:HIS:O	1:A:608:THR:N	2.44	0.46
2:B:295:PRO:HB3	9:I:11:PHE:CD2	2.49	0.46
2:B:561:ILE:HD11	2:B:576:ILE:HG21	1.97	0.46
2:B:588:ARG:HH11	2:B:588:ARG:HB2	1.79	0.46
2:B:924:ARG:O	2:B:924:ARG:HG3	2.15	0.46
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.96	0.46
2:B:1080:ARG:NH2	13:M:50:SER:HB3	2.26	0.46
9:I:98:GLN:O	9:I:100:HIS:N	2.47	0.46
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.30	0.46
17:Q:105:TYR:CE1	18:R:234:GLU:CD	2.93	0.46
17:Q:118:GLU:HB2	17:Q:181:ASN:ND2	2.29	0.46
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.47	0.46
2:B:206:TYR:HD1	2:B:208:PHE:CE1	2.32	0.46
2:B:584:MET:HG3	2:B:605:ARG:HD2	1.97	0.46
2:B:756:LYS:HG2	10:J:51:ALA:O	2.16	0.46
7:G:94:LYS:HA	7:G:119:PHE:CD2	2.49	0.46
12:L:35:ARG:NH1	12:L:42:ARG:NH2	2.62	0.46
16:P:183:ILE:HG12	16:P:244:LEU:HD13	1.96	0.46
16:P:297:LYS:HB2	16:P:298:PRO:HD2	1.91	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:HG22	2:B:1059:ILE:HG22	1.97	0.46
1:A:426:ARG:O	13:M:39:LEU:CA	2.59	0.46
1:A:472:HIS:NE2	1:A:521:VAL:HG21	2.31	0.46
1:A:601:ASN:ND2	1:A:992:LYS:HD2	2.30	0.46
1:A:1252:ALA:HB1	9:I:3:PRO:HB3	1.96	0.46
2:B:92:TYR:CG	20:T:145:LEU:CD1	2.97	0.46
2:B:874:PRO:HG2	2:B:875:GLU:H	1.81	0.46
3:C:169:PHE:CE1	3:C:171:LYS:HB3	2.51	0.46
5:E:146:PRO:O	5:E:148:HIS:ND1	2.48	0.46
5:E:173:ILE:HG23	5:E:209:VAL:HG22	1.97	0.46
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.98	0.46
14:N:333:ASN:O	15:O:93:VAL:HG23	2.14	0.46
14:N:337:CYS:O	15:O:97:ALA:HA	2.14	0.46
16:P:249:LYS:HB3	16:P:251:LEU:HG	1.97	0.46
17:Q:24:GLY:CA	18:R:209:GLN:OE1	2.63	0.46
20:T:127:LEU:O	20:T:131:GLN:N	2.44	0.46
20:T:153:TYR:CD1	20:T:153:TYR:C	2.93	0.46
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.54	0.46
1:A:156:GLY:N	1:A:181:HIS:HD1	2.12	0.46
1:A:687:ILE:HG13	1:A:691:ASP:OD2	2.16	0.46
1:A:1192:TRP:NE1	1:A:1249:ASP:H	2.10	0.46
3:C:100:GLU:CG	3:C:164:TYR:HE1	2.28	0.46
11:K:61:TYR:HA	11:K:72:ILE:O	2.15	0.46
17:Q:113:ARG:CD	18:R:221:ARG:HB3	2.40	0.46
21:X:60:DG:N3	22:Y:35:DG:N2	2.64	0.46
2:B:127:ASP:HA	2:B:145:GLN:O	2.16	0.46
3:C:274:ILE:O	11:K:23:LYS:NZ	2.33	0.46
9:I:41:ASN:CG	19:S:153:ARG:HD2	2.40	0.46
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.15	0.46
20:T:211:VAL:O	20:T:215:GLU:HG2	2.15	0.46
9:I:84:HIS:ND1	9:I:85:PRO:CD	2.77	0.46
20:T:128:LYS:HA	20:T:131:GLN:HB3	1.97	0.46
1:A:46:THR:HG23	1:A:58:MET:HG2	1.98	0.46
1:A:608:THR:OG1	1:A:610:PRO:HD2	2.13	0.46
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.81	0.46
1:A:939:VAL:O	1:A:942:VAL:HG22	2.16	0.46
2:B:250:SER:O	2:B:251:ALA:CB	2.61	0.46
2:B:972:ILE:HG12	2:B:981:LEU:HD21	1.97	0.46
3:C:136:ASP:OD1	3:C:136:ASP:N	2.49	0.46
9:I:62:VAL:C	9:I:64:GLU:N	2.57	0.46
11:K:49:GLN:HG3	11:K:94:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:HG2	18:R:201:LEU:HD21	1.98	0.46
18:R:198:LYS:HE3	18:R:199:LYS:HE3	1.98	0.46
19:S:98:TRP:HB2	19:S:112:GLY:HA3	1.98	0.46
1:A:618:TYR:C	1:A:620:HIS:N	2.71	0.46
1:A:795:GLY:HA3	1:A:1107:PHE:HD2	1.80	0.46
1:A:800:PHE:HD1	1:A:805:ARG:C	2.23	0.46
1:A:908:THR:C	1:A:910:LYS:H	2.24	0.46
1:A:1128:ILE:HG23	1:A:1414:ILE:CG1	2.46	0.46
2:B:1135:TYR:O	2:B:1136:GLU:HG2	2.16	0.46
3:C:68:LEU:HD12	3:C:71:ILE:HD12	1.97	0.46
8:H:23:ASP:OD1	8:H:23:ASP:N	2.37	0.46
14:N:46:TRP:CZ2	15:O:11:LEU:HD11	2.51	0.46
15:O:84:VAL:HG13	15:O:85:THR:HG23	1.97	0.46
16:P:165:LEU:HD21	16:P:258:MET:HE2	1.98	0.46
21:X:24:DG:H4'	21:X:25:DG:OP1	2.16	0.46
21:X:30:DG:N2	22:Y:64:DC:O2	2.49	0.46
21:X:31:DT:H2'	21:X:32:DT:C2	2.50	0.46
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.70	0.46
1:A:455:ILE:CG2	1:A:520:MET:HE1	2.46	0.46
1:A:574:VAL:O	8:H:74:GLU:HA	2.16	0.46
1:A:601:ASN:ND2	1:A:988:TRP:HZ3	2.14	0.46
1:A:1176:TYR:HB2	1:A:1211:LEU:HD23	1.98	0.46
2:B:234:THR:O	2:B:236:TRP:CD1	2.69	0.46
2:B:257:VAL:HA	2:B:268:PRO:HA	1.97	0.46
2:B:853:LEU:HD13	2:B:907:VAL:HG11	1.97	0.46
2:B:959:GLU:OE2	10:J:42:ARG:HB3	2.15	0.46
3:C:246:LEU:HD11	11:K:106:ARG:NH2	2.31	0.46
16:P:297:LYS:HA	16:P:297:LYS:HD3	1.30	0.46
2:B:952:GLU:OE1	2:B:952:GLU:N	2.46	0.46
2:B:1108:PHE:CD2	2:B:1109:GLU:HG3	2.51	0.46
13:M:53:ARG:NH1	22:Y:55:DG:O6	2.49	0.46
14:N:376:TRP:HD1	15:O:62:LEU:O	1.98	0.46
17:Q:202:GLU:C	17:Q:204:LEU:H	2.23	0.46
18:R:119:LEU:HA	18:R:123:ALA:HB3	1.97	0.46
1:A:196:LEU:HD21	1:A:311:GLN:HG3	1.99	0.45
1:A:687:ILE:HA	1:A:691:ASP:OD2	2.15	0.45
1:A:1210:TRP:CD1	1:A:1281:ASP:HB3	2.52	0.45
2:B:594:MET:O	20:T:129:ARG:NH1	2.49	0.45
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.48	0.45
2:B:1151:MET:HE1	2:B:1171:MET:SD	2.56	0.45
3:C:131:THR:HB	3:C:147:ASP:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:177:ARG:NH1	21:X:19:DG:H3'	2.31	0.45
1:A:324:GLY:HA2	13:M:90:ALA:HB3	1.99	0.45
1:A:455:ILE:HD13	1:A:520:MET:CE	2.46	0.45
2:B:489:ILE:HD12	21:X:47:DT:O2	2.17	0.45
2:B:551:GLU:HB2	2:B:576:ILE:HD11	1.97	0.45
2:B:1123:GLY:HA3	2:B:1170:ARG:HB3	1.97	0.45
3:C:72:PRO:HG3	10:J:13:ILE:HD13	1.97	0.45
12:L:19:CYS:HB3	12:L:23:HIS:H	1.81	0.45
17:Q:114:ILE:CG1	18:R:218:LYS:HE3	2.47	0.45
20:T:30:GLN:NE2	20:T:62:LEU:O	2.48	0.45
21:X:37:DT:H1'	21:X:38:DT:O5'	2.16	0.45
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.47	0.45
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.98	0.45
2:B:258:ALA:N	2:B:267:VAL:O	2.42	0.45
8:H:96:VAL:HG13	8:H:115:TYR:O	2.16	0.45
17:Q:99:LEU:O	17:Q:101:ASN:N	2.42	0.45
17:Q:112:ARG:O	17:Q:115:GLU:HB2	2.16	0.45
1:A:187:TYR:HD2	1:A:202:TRP:CD1	2.35	0.45
1:A:350:VAL:HG21	1:A:1435:THR:HG23	1.98	0.45
1:A:539:GLN:HB3	1:A:540:ASP:H	1.44	0.45
2:B:65:ILE:HD11	2:B:86:LEU:HD12	1.99	0.45
2:B:92:TYR:HB2	20:T:145:LEU:CD1	2.24	0.45
2:B:489:ILE:HG13	2:B:490:GLY:N	2.29	0.45
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.51	0.45
8:H:85:ALA:CB	8:H:144:LEU:HD22	2.46	0.45
9:I:32:ASN:HB2	9:I:34:ILE:HG12	1.98	0.45
9:I:61:GLU:H	9:I:61:GLU:HG2	1.45	0.45
16:P:160:GLY:O	16:P:162:VAL:CG1	2.57	0.45
20:T:31:TRP:HD1	20:T:62:LEU:HD21	1.82	0.45
1:A:485:ASN:O	1:A:487:SER:N	2.49	0.45
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.31	0.45
2:B:497:LYS:HE2	2:B:497:LYS:HB3	1.77	0.45
2:B:561:ILE:HD11	2:B:576:ILE:HG12	1.97	0.45
2:B:957:THR:HG23	2:B:961:ILE:HG23	1.98	0.45
3:C:10:ARG:HH21	3:C:24:GLU:CD	2.23	0.45
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.97	0.45
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.51	0.45
17:Q:144:LEU:O	17:Q:153:ARG:N	2.44	0.45
18:R:198:LYS:HG3	18:R:199:LYS:HG3	1.98	0.45
22:Y:61:DA:H3'	22:Y:62:DC:H5''	1.98	0.45
1:A:275:ASP:OD1	1:A:276:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1484:MET:SD	7:G:20:PRO:HA	2.57	0.45
2:B:309:PHE:HA	2:B:312:GLN:NE2	2.31	0.45
10:J:35:LEU:HD13	10:J:46:ARG:HG2	1.99	0.45
13:M:86:LYS:N	13:M:86:LYS:HD2	2.31	0.45
13:M:244:LEU:HD21	13:M:292:ILE:HA	1.98	0.45
17:Q:92:TYR:CE2	17:Q:94:ILE:HB	2.52	0.45
1:A:393:ILE:CG2	6:F:74:ALA:HB1	2.47	0.45
1:A:408:ARG:HD3	1:A:412:GLN:OE1	2.17	0.45
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.52	0.45
1:A:470:MET:HG2	1:A:524:MET:HG3	1.98	0.45
1:A:1102:MET:HE2	1:A:1102:MET:HB2	1.78	0.45
2:B:56:GLN:HB3	20:T:140:ARG:HD2	1.98	0.45
2:B:102:ASP:OD1	2:B:104:ALA:N	2.38	0.45
2:B:402:PHE:C	2:B:402:PHE:CD1	2.95	0.45
2:B:882:SER:CB	2:B:887:TYR:CE1	2.72	0.45
2:B:968:ASN:OD1	2:B:970:HIS:N	2.34	0.45
5:E:55:ARG:NE	5:E:107:GLN:OE1	2.46	0.45
11:K:67:LEU:HA	11:K:67:LEU:HD23	1.63	0.45
15:O:50:GLN:O	15:O:53:ARG:NH1	2.49	0.45
17:Q:69:ASP:HB3	17:Q:71:PHE:CD2	2.52	0.45
18:R:225:VAL:HG12	18:R:230:GLU:OE1	2.17	0.45
1:A:285:LYS:HE3	1:A:285:LYS:HB3	1.83	0.45
1:A:1057:GLU:O	1:A:1059:ARG:HG3	2.17	0.45
2:B:420:GLN:HA	2:B:423:ILE:HG12	1.99	0.45
5:E:88:LYS:O	5:E:91:CYS:HB2	2.17	0.45
20:T:51:ARG:NE	20:T:53:GLU:OE2	2.39	0.45
20:T:196:TYR:HB2	20:T:232:THR:HB	1.98	0.45
21:X:37:DT:H4'	21:X:38:DT:OP1	2.15	0.45
1:A:206:ASN:HB3	1:A:208:ASP:OD2	2.17	0.45
1:A:810:PHE:CE2	1:A:819:SER:HA	2.52	0.45
2:B:556:ILE:O	20:T:91:GLN:NE2	2.49	0.45
2:B:588:ARG:NH1	2:B:603:MET:HE2	2.32	0.45
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.98	0.45
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.94	0.45
13:M:73:PRO:HB3	13:M:79:ASP:OD1	2.17	0.45
2:B:931:ILE:HD11	2:B:947:ILE:HA	1.99	0.45
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.51	0.45
4:D:74:PHE:CZ	4:D:83:VAL:HG21	2.51	0.45
13:M:87:GLY:O	13:M:88:THR:CB	2.64	0.45
16:P:295:MET:HG2	16:P:297:LYS:H	1.81	0.45
1:A:202:TRP:HZ3	1:A:214:ILE:HG12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:ARG:NH1	1:A:1349:GLU:OE2	2.50	0.44
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.82	0.44
13:M:286:ARG:HG3	13:M:316:LEU:HD23	1.98	0.44
17:Q:17:LEU:HD11	17:Q:191:LEU:HB3	1.99	0.44
17:Q:114:ILE:HD11	18:R:218:LYS:CE	2.43	0.44
1:A:404:GLU:CD	1:A:407:ARG:HH12	2.22	0.44
1:A:601:ASN:ND2	1:A:632:ASN:H	2.15	0.44
2:B:1021:HIS:HB2	3:C:203:TRP:CZ3	2.53	0.44
8:H:15:ILE:HD11	8:H:52:LEU:N	2.32	0.44
8:H:108:ALA:O	8:H:110:THR:N	2.49	0.44
18:R:222:SER:O	18:R:223:VAL:C	2.61	0.44
20:T:146:ASP:HB3	20:T:147:LYS:H	1.64	0.44
21:X:53:DA:C6	21:X:54:DA:C6	3.05	0.44
1:A:611:ASP:CG	1:A:626:THR:HG23	2.42	0.44
2:B:32:SER:OG	2:B:643:LEU:HD22	2.17	0.44
2:B:203:ASN:O	2:B:571:GLY:HA3	2.18	0.44
2:B:1005:ALA:C	2:B:1007:ASN:N	2.73	0.44
7:G:96:GLY:O	7:G:128:TYR:HE2	2.00	0.44
18:R:139:PHE:HA	18:R:140:LYS:HB2	1.98	0.44
19:S:17:ARG:HG2	20:T:38:GLY:O	2.17	0.44
1:A:526:VAL:HA	1:A:533:PRO:HA	2.00	0.44
1:A:567:LEU:HD22	1:A:570:TRP:HB2	2.00	0.44
1:A:1298:LEU:O	1:A:1300:GLY:N	2.50	0.44
1:A:1477:ALA:O	1:A:1480:CYS:HB2	2.18	0.44
2:B:854:ILE:HD13	2:B:904:VAL:HG21	1.99	0.44
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.48	0.44
3:C:6:GLN:O	3:C:7:PRO:CB	2.62	0.44
12:L:16:ILE:HG21	12:L:47:LYS:CD	2.48	0.44
13:M:59:LYS:HA	23:Z:1:A:N7	2.32	0.44
13:M:86:LYS:HB3	13:M:87:GLY:H	1.66	0.44
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.82	0.44
20:T:99:SER:HB2	20:T:103:LYS:H	1.81	0.44
21:X:29:DC:H2''	21:X:30:DG:H5'	1.99	0.44
2:B:119:THR:HG23	2:B:187:ILE:HD13	1.99	0.44
2:B:536:SER:HB2	2:B:600:GLU:CD	2.43	0.44
2:B:838:GLN:HG3	2:B:886:ARG:HH22	1.82	0.44
2:B:1080:ARG:HH21	13:M:50:SER:CB	2.27	0.44
7:G:1:MET:HB3	7:G:3:TYR:CZ	2.53	0.44
13:M:10:LEU:N	13:M:10:LEU:CD2	2.76	0.44
14:N:372:GLY:HA3	15:O:58:PHE:CZ	2.53	0.44
15:O:64:THR:HA	16:P:189:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:171:THR:HG21	21:X:16:DA:H4'	1.99	0.44
22:Y:70:DC:H2''	22:Y:71:DA:H8	1.82	0.44
1:A:278:HIS:HB3	13:M:82:THR:HG23	2.00	0.44
2:B:74:ALA:HB2	20:T:201:ASP:CB	2.47	0.44
2:B:244:GLY:O	2:B:246:GLY:N	2.50	0.44
2:B:281:ASP:H	9:I:22:ASN:HD22	1.66	0.44
2:B:818:GLU:OE2	2:B:828:VAL:HA	2.17	0.44
2:B:867:ILE:O	2:B:893:SER:HB2	2.17	0.44
2:B:903:ILE:O	2:B:923:VAL:HG13	2.18	0.44
9:I:65:LEU:HD23	9:I:122:ARG:NH2	2.32	0.44
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.53	0.44
16:P:304:ILE:HD12	16:P:304:ILE:N	2.33	0.44
19:S:124:TYR:HE1	20:T:22:LYS:HG3	1.83	0.44
20:T:159:HIS:CG	20:T:160:GLN:N	2.85	0.44
2:B:99:TRP:NE1	2:B:105:PRO:HB3	2.31	0.44
2:B:1029:TYR:HD1	2:B:1036:LYS:HA	1.82	0.44
8:H:64:LEU:HB3	8:H:84:ARG:NE	2.32	0.44
12:L:26:ASN:CB	12:L:44:MET:HE2	2.46	0.44
17:Q:69:ASP:HB3	17:Q:71:PHE:HD2	1.83	0.44
17:Q:114:ILE:HG12	18:R:218:LYS:HE3	2.00	0.44
17:Q:187:ILE:CD1	18:R:211:SER:HA	2.36	0.44
20:T:94:THR:HA	20:T:109:ILE:HA	1.99	0.44
20:T:225:VAL:HA	20:T:231:ASN:HA	1.99	0.44
22:Y:56:DG:N2	22:Y:58:DC:OP1	2.51	0.44
1:A:264:VAL:CB	1:A:272:ASN:HB3	2.47	0.44
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.44
1:A:1254:LYS:HE3	9:I:3:PRO:HA	2.00	0.44
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.00	0.44
2:B:226:GLU:OE1	2:B:226:GLU:N	2.51	0.44
11:K:35:ILE:HB	11:K:71:ILE:HG12	1.98	0.44
22:Y:60:DA:H2''	22:Y:61:DA:C8	2.53	0.44
22:Y:88:DC:H2''	22:Y:89:DC:O4'	2.18	0.44
1:A:600:ILE:HD12	1:A:656:SER:HA	1.99	0.44
1:A:800:PHE:HA	1:A:805:ARG:O	2.18	0.44
1:A:1127:LEU:HD11	1:A:1381:GLU:HB3	2.00	0.44
2:B:56:GLN:NE2	20:T:140:ARG:NH1	2.65	0.44
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.47	0.44
2:B:1030:ASN:N	2:B:1035:ARG:O	2.42	0.44
7:G:89:VAL:HA	7:G:98:PHE:O	2.17	0.44
11:K:63:VAL:HG13	11:K:70:LYS:O	2.18	0.44
12:L:19:CYS:HB3	12:L:23:HIS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:79:DT:H6	22:Y:79:DT:H2'	1.62	0.44
1:A:564:LEU:HA	1:A:564:LEU:HD23	1.76	0.43
3:C:45:ILE:HG22	3:C:73:LEU:HD12	2.00	0.43
3:C:161:LEU:C	3:C:161:LEU:HD12	2.42	0.43
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.43
7:G:14:HIS:CD2	7:G:65:PHE:HE1	2.35	0.43
8:H:11:ASP:OD2	8:H:55:LYS:HG2	2.17	0.43
14:N:326:GLN:OE1	15:O:92:LYS:NZ	2.30	0.43
15:O:71:VAL:HG22	15:O:98:CYS:HB3	1.99	0.43
17:Q:113:ARG:HH12	18:R:218:LYS:HA	1.83	0.43
22:Y:58:DC:H2'	22:Y:58:DC:H6	1.65	0.43
1:A:246:GLU:HG3	1:A:247:TRP:CD1	2.53	0.43
1:A:263:ALA:C	1:A:265:VAL:N	2.70	0.43
2:B:271:ILE:HG12	2:B:311:ILE:HD11	2.00	0.43
2:B:725:GLN:HG2	2:B:938:ARG:O	2.18	0.43
2:B:894:THR:HG23	2:B:897:ARG:HH11	1.83	0.43
8:H:17:PRO:C	8:H:19:GLY:N	2.76	0.43
12:L:26:ASN:CG	12:L:44:MET:HE2	2.43	0.43
15:O:64:THR:HG22	15:O:75:VAL:HB	2.00	0.43
16:P:267:PRO:HG2	16:P:337:LYS:HB2	2.00	0.43
1:A:134:LYS:HA	1:A:140:ARG:NH2	2.33	0.43
1:A:861:GLN:HE22	1:A:1093:GLN:HA	1.83	0.43
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.47	0.43
2:B:329:GLY:C	2:B:331:THR:H	2.26	0.43
2:B:403:LEU:HD21	2:B:447:SER:HB2	2.00	0.43
2:B:625:LEU:CD1	2:B:675:LEU:HD11	2.49	0.43
4:D:118:LEU:HB2	4:D:122:PHE:CD2	2.52	0.43
8:H:5:LEU:HD11	8:H:62:SER:HB3	2.00	0.43
8:H:135:PHE:O	8:H:137:VAL:HG22	2.19	0.43
1:A:81:CYS:HA	1:A:82:PRO:HD2	1.87	0.43
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.34	0.43
1:A:931:ARG:C	1:A:933:THR:N	2.75	0.43
1:A:1451:MET:HE2	1:A:1451:MET:HB3	1.56	0.43
2:B:558:PRO:C	2:B:560:ALA:H	2.26	0.43
2:B:632:LYS:HA	2:B:682:LEU:HD21	1.99	0.43
2:B:875:GLU:O	2:B:876:ASN:HB2	2.18	0.43
8:H:34:SER:O	8:H:36:LYS:HG2	2.18	0.43
16:P:305:PHE:CZ	22:Y:82:DT:H1'	2.54	0.43
1:A:1307:VAL:CG2	1:A:1339:ASP:N	2.81	0.43
2:B:874:PRO:CG	2:B:875:GLU:H	2.30	0.43
8:H:38:ASP:OD1	8:H:39:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.48	0.43
20:T:86:GLN:O	20:T:112:GLN:NE2	2.52	0.43
2:B:754:PRO:HB2	2:B:773:PRO:HB2	1.99	0.43
2:B:797:ASN:HB2	2:B:964:ASP:HA	2.00	0.43
2:B:906:GLN:NE2	12:L:45:TYR:CE1	2.84	0.43
3:C:18:ASN:HB2	3:C:234:GLU:HG2	1.99	0.43
3:C:44:ILE:O	3:C:167:LYS:HA	2.18	0.43
3:C:45:ILE:O	3:C:73:LEU:HB2	2.18	0.43
1:A:924:TYR:CE1	1:A:949:GLN:HG3	2.53	0.43
1:A:1301:ILE:O	1:A:1345:ARG:HD3	2.19	0.43
2:B:25:ALA:HA	2:B:28:ILE:HD12	2.00	0.43
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.49	0.43
2:B:573:TRP:CZ3	2:B:575:GLY:HA2	2.54	0.43
3:C:9:VAL:HG21	11:K:105:PHE:HA	2.00	0.43
13:M:48:VAL:HA	13:M:51:GLU:CD	2.43	0.43
14:N:38:VAL:HG13	15:O:22:LEU:HD22	1.99	0.43
16:P:207:PRO:O	16:P:209:THR:HG23	2.18	0.43
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.51	0.43
1:A:1103:THR:HG21	1:A:1106:THR:OG1	2.18	0.43
2:B:41:ARG:HD2	2:B:41:ARG:HA	1.75	0.43
2:B:931:ILE:CD1	2:B:947:ILE:HA	2.48	0.43
5:E:41:LYS:HZ1	5:E:47:LYS:HE3	1.78	0.43
12:L:26:ASN:CG	12:L:28:ILE:HG13	2.43	0.43
17:Q:108:ASP:CG	18:R:237:LEU:CD2	2.92	0.43
17:Q:113:ARG:NH1	18:R:218:LYS:HA	2.33	0.43
21:X:2:DA:N6	22:Y:91:DT:O4	2.52	0.43
1:A:367:ILE:HG21	1:A:501:MET:HG3	1.99	0.43
1:A:805:ARG:HG2	1:A:812:LYS:HA	2.01	0.43
2:B:74:ALA:CB	20:T:201:ASP:HB3	2.49	0.43
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.19	0.43
17:Q:105:TYR:CZ	18:R:234:GLU:CD	2.96	0.43
21:X:30:DG:H5''	21:X:31:DT:O4'	2.18	0.43
1:A:62:GLN:NE2	1:A:261:ARG:HH21	2.17	0.43
1:A:94:VAL:HG21	1:A:314:VAL:HG21	2.01	0.43
1:A:273:GLN:C	1:A:274:ASP:O	2.56	0.43
1:A:375:ILE:HG13	1:A:666:ARG:NH1	2.34	0.43
1:A:546:ARG:O	1:A:546:ARG:HG2	2.18	0.43
1:A:603:ILE:HG12	1:A:604:ARG:N	2.34	0.43
1:A:1132:LYS:HE3	21:X:53:DA:H5'	2.01	0.43
4:D:90:LYS:HE3	4:D:130:ILE:HD11	2.01	0.43
8:H:108:ALA:C	8:H:110:THR:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:75:ASP:OD2	9:I:78:LEU:HG	2.18	0.43
17:Q:15:LYS:HE3	17:Q:38:ILE:HG23	2.01	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.19	0.43
1:A:931:ARG:C	1:A:933:THR:H	2.26	0.42
1:A:1192:TRP:O	1:A:1195:VAL:HB	2.19	0.42
2:B:40:VAL:HG21	2:B:181:PRO:HB2	2.00	0.42
2:B:993:LYS:HA	2:B:1018:TYR:OH	2.19	0.42
7:G:104:MET:HE2	7:G:159:ALA:HB2	2.00	0.42
20:T:154:LYS:H	20:T:154:LYS:CD	2.31	0.42
1:A:117:LEU:HB2	1:A:232:GLU:CD	2.44	0.42
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.18	0.42
1:A:364:ARG:HD3	1:A:500:GLU:OE1	2.19	0.42
1:A:658:LEU:HD23	1:A:658:LEU:HA	1.88	0.42
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.58	0.42
2:B:56:GLN:OE1	20:T:140:ARG:NH1	2.49	0.42
2:B:333:GLU:HG2	2:B:337:LYS:HE3	2.00	0.42
2:B:758:LEU:HD11	10:J:47:ARG:HB3	2.01	0.42
2:B:881:GLU:C	2:B:883:THR:HG23	2.44	0.42
3:C:136:ASP:C	3:C:138:ASP:N	2.74	0.42
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.54	0.42
13:M:10:LEU:C	13:M:12:ARG:H	2.27	0.42
13:M:178:LYS:HD3	13:M:279:GLY:HA3	2.01	0.42
21:X:41:DT:H2'	21:X:42:DT:O3'	2.19	0.42
1:A:413:TYR:CD1	1:A:414:PRO:HD3	2.54	0.42
1:A:549:THR:O	1:A:589:LYS:NZ	2.44	0.42
1:A:906:LEU:HA	1:A:906:LEU:HD23	1.88	0.42
1:A:914:LYS:O	1:A:918:LYS:HG2	2.19	0.42
2:B:92:TYR:HE1	20:T:141:LEU:CG	2.32	0.42
2:B:275:ALA:O	2:B:314:GLN:NE2	2.48	0.42
9:I:86:CYS:HB3	9:I:89:CYS:SG	2.59	0.42
16:P:208:ARG:NH2	16:P:208:ARG:CG	2.79	0.42
17:Q:19:LYS:O	17:Q:23:ARG:HG3	2.19	0.42
19:S:177:MET:HE2	19:S:177:MET:HB3	1.90	0.42
1:A:126:ILE:HD13	1:A:129:ILE:HD12	2.01	0.42
1:A:322:LEU:HA	1:A:323:PRO:HD3	1.84	0.42
1:A:679:TRP:CZ2	1:A:683:GLU:HG3	2.55	0.42
1:A:959:MET:HE1	1:A:1046:ARG:O	2.19	0.42
2:B:499:ARG:CZ	2:B:522:LEU:HD11	2.49	0.42
2:B:760:THR:OG1	2:B:761:THR:N	2.51	0.42
2:B:776:ILE:HD12	2:B:806:PHE:CD1	2.55	0.42
2:B:861:SER:O	2:B:896:LEU:CD2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1089:MET:HA	2:B:1089:MET:HE3	2.01	0.42
8:H:5:LEU:HD22	8:H:133:HIS:HB3	2.02	0.42
14:N:12:LYS:O	14:N:15:ARG:HB2	2.19	0.42
18:R:214:GLU:O	18:R:216:PHE:N	2.53	0.42
1:A:264:VAL:HB	1:A:272:ASN:HB3	2.00	0.42
1:A:274:ASP:OD2	1:A:276:LEU:N	2.46	0.42
1:A:365:THR:CG2	2:B:1059:ILE:HG22	2.50	0.42
1:A:608:THR:HB	1:A:610:PRO:CD	2.49	0.42
2:B:33:TYR:CE1	2:B:37:LYS:HG3	2.55	0.42
2:B:1040:GLN:N	2:B:1040:GLN:CD	2.77	0.42
2:B:1069:ILE:HD12	2:B:1070:LEU:HD12	2.00	0.42
6:F:69:ARG:NE	6:F:96:GLU:OE2	2.52	0.42
8:H:137:VAL:HG21	8:H:140:ARG:HD2	2.01	0.42
10:J:46:ARG:HH11	10:J:46:ARG:HD3	1.74	0.42
16:P:206:GLU:HB3	16:P:207:PRO:HD2	1.34	0.42
17:Q:70:LYS:NZ	18:R:226:ASP:HA	2.34	0.42
19:S:135:PHE:HD1	19:S:135:PHE:HA	1.71	0.42
1:A:602:CYS:H	1:A:630:VAL:CG1	2.33	0.42
13:M:87:GLY:C	13:M:89:GLY:H	2.28	0.42
13:M:164:LEU:HD12	13:M:164:LEU:HA	1.80	0.42
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.84	0.42
14:N:356:GLY:HA3	14:N:367:PHE:CZ	2.54	0.42
14:N:366:ILE:O	15:O:54:ASN:ND2	2.50	0.42
15:O:3:TYR:HE2	15:O:99:ASP:HA	1.82	0.42
17:Q:113:ARG:NH1	18:R:218:LYS:CA	2.82	0.42
17:Q:154:CYS:SG	17:Q:155:THR:N	2.93	0.42
18:R:118:TRP:HE1	18:R:122:GLU:CD	2.27	0.42
21:X:80:DC:H42	22:Y:14:DG:H1	1.67	0.42
1:A:275:ASP:HA	1:A:278:HIS:HD2	1.84	0.42
1:A:539:GLN:NE2	2:B:791:GLU:OE2	2.52	0.42
1:A:1290:SER:HG	2:B:250:SER:C	2.11	0.42
1:A:1298:LEU:C	1:A:1300:GLY:N	2.77	0.42
1:A:1306:LYS:HB2	1:A:1306:LYS:HE3	1.46	0.42
2:B:47:PHE:O	2:B:50:PHE:HB3	2.20	0.42
2:B:292:PHE:CG	9:I:14:ILE:HD13	2.50	0.42
2:B:570:ASN:OD1	2:B:616:THR:HG22	2.19	0.42
2:B:597:ILE:HB	2:B:600:GLU:HB2	2.02	0.42
2:B:711:ILE:O	2:B:714:PRO:HD3	2.19	0.42
5:E:61:LEU:HD21	5:E:71:GLN:HB2	2.02	0.42
7:G:90:THR:O	7:G:91:GLN:HG3	2.20	0.42
13:M:182:ALA:H	20:T:154:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:151:THR:O	20:T:152:ASN:CG	2.62	0.42
21:X:18:DG:OP2	21:X:18:DG:H2'	2.20	0.42
1:A:485:ASN:O	1:A:486:LEU:C	2.62	0.42
1:A:942:VAL:HG21	1:A:1005:HIS:NE2	2.35	0.42
2:B:76:GLY:O	2:B:77:GLU:HB2	2.18	0.42
2:B:411:LEU:HD11	2:B:435:ILE:HG23	2.01	0.42
2:B:856:PRO:HG2	12:L:46:LYS:O	2.20	0.42
2:B:924:ARG:HH11	3:C:60:HIS:HB2	1.84	0.42
6:F:64:ARG:NH1	7:G:61:PRO:HB3	2.35	0.42
9:I:59:THR:OG1	9:I:60:HIS:N	2.51	0.42
13:M:119:LYS:HD3	22:Y:60:DA:N6	2.34	0.42
17:Q:24:GLY:O	18:R:215:GLU:OE2	2.38	0.42
1:A:53:LYS:HE3	1:A:59:ASP:HB3	2.00	0.42
1:A:375:ILE:HD13	1:A:485:ASN:ND2	2.35	0.42
1:A:378:VAL:HG23	1:A:484:LEU:HD23	2.02	0.42
1:A:926:ASN:OD1	1:A:927:GLU:N	2.52	0.42
2:B:74:ALA:HB2	20:T:201:ASP:HB3	2.00	0.42
2:B:747:LEU:HD23	2:B:747:LEU:C	2.45	0.42
20:T:213:LEU:HA	20:T:213:LEU:HD23	1.78	0.42
1:A:40:GLY:C	1:A:42:LYS:N	2.78	0.42
1:A:521:VAL:HG12	1:A:666:ARG:HH21	1.85	0.42
1:A:912:SER:HB3	1:A:915:ALA:HB3	2.02	0.42
1:A:1162:GLU:HG3	1:A:1306:LYS:O	2.20	0.42
2:B:561:ILE:HD12	2:B:561:ILE:HA	1.86	0.42
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.53	0.42
3:C:44:ILE:HG23	3:C:176:TRP:HD1	1.84	0.42
3:C:220:TYR:CE2	3:C:222:PRO:HB3	2.55	0.42
4:D:110:GLU:HA	7:G:167:TYR:CE2	2.55	0.42
5:E:187:ARG:HG3	5:E:210:GLN:HA	2.02	0.42
7:G:38:CYS:SG	7:G:156:ASP:HA	2.59	0.42
10:J:35:LEU:HA	10:J:35:LEU:HD23	1.86	0.42
14:N:336:VAL:HG23	14:N:357:ILE:HB	2.01	0.42
15:O:63:ASN:HB3	15:O:75:VAL:O	2.20	0.42
17:Q:115:GLU:O	17:Q:119:ARG:N	2.40	0.42
1:A:457:ILE:HD11	2:B:1102:PHE:CE2	2.55	0.41
1:A:458:PHE:HE2	1:A:482:PHE:CE2	2.38	0.41
1:A:531:ASN:ND2	1:A:901:VAL:HG23	2.31	0.41
1:A:609:HIS:O	1:A:609:HIS:CG	2.73	0.41
1:A:689:ILE:HD11	2:B:981:LEU:CB	2.50	0.41
2:B:211:LYS:HE3	21:X:48:DT:H2'	2.02	0.41
2:B:831:LYS:HA	2:B:832:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:75:ASP:HA	9:I:76:PRO:HD2	1.95	0.41
13:M:44:ARG:HD2	13:M:45:VAL:H	1.85	0.41
17:Q:92:TYR:HE2	17:Q:94:ILE:HB	1.84	0.41
17:Q:128:LYS:HB3	17:Q:164:ASP:HA	2.02	0.41
20:T:140:ARG:NE	20:T:140:ARG:CA	2.73	0.41
22:Y:32:DC:H2''	22:Y:33:DT:C6	2.55	0.41
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.02	0.41
1:A:499:ASP:OD1	23:Z:6:C:H4'	2.20	0.41
1:A:1304:ILE:HB	1:A:1307:VAL:HG12	2.02	0.41
2:B:80:GLU:OE1	2:B:134:LYS:HB3	2.20	0.41
2:B:180:ASP:OD1	2:B:181:PRO:HD2	2.20	0.41
2:B:921:ILE:O	2:B:921:ILE:HG13	2.19	0.41
3:C:263:LEU:O	3:C:266:GLU:HB2	2.19	0.41
5:E:82:VAL:HB	5:E:110:MET:SD	2.60	0.41
7:G:148:VAL:HG23	7:G:160:ILE:CD1	2.51	0.41
14:N:14:TYR:CE1	15:O:11:LEU:HD22	2.55	0.41
21:X:1:DG:H2''	21:X:2:DA:C8	2.55	0.41
1:A:367:ILE:HG22	1:A:482:PHE:HB2	2.03	0.41
1:A:505:LEU:HA	1:A:506:PRO:HD2	1.93	0.41
1:A:689:ILE:HD12	1:A:689:ILE:HG23	1.75	0.41
1:A:802:PHE:HE2	1:A:808:PRO:HD3	1.85	0.41
1:A:818:GLU:OE1	1:A:818:GLU:N	2.50	0.41
2:B:56:GLN:CG	20:T:140:ARG:CZ	2.92	0.41
2:B:823:PHE:HA	13:M:140:ASN:HD21	1.86	0.41
5:E:58:LEU:HD23	5:E:76:PHE:CE2	2.55	0.41
8:H:113:SER:HA	8:H:125:LEU:O	2.20	0.41
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.99	0.41
13:M:39:LEU:C	13:M:40:VAL:O	2.62	0.41
15:O:41:ASP:O	15:O:45:ASN:ND2	2.37	0.41
21:X:35:DT:H6	21:X:35:DT:H2'	1.75	0.41
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	0.41
1:A:901:VAL:HB	1:A:978:VAL:CG1	2.51	0.41
2:B:510:CYS:SG	2:B:511:PRO:HD2	2.61	0.41
2:B:767:LEU:C	2:B:769:PHE:N	2.78	0.41
4:D:92:LEU:HD23	4:D:122:PHE:CE2	2.56	0.41
9:I:11:PHE:CE1	9:I:54:TYR:HA	2.55	0.41
9:I:58:ILE:HG22	9:I:58:ILE:O	2.20	0.41
18:R:158:HIS:HA	18:R:161:ARG:HG2	2.02	0.41
1:A:368:THR:HB	1:A:369:PRO:HD2	2.01	0.41
1:A:757:GLN:HG2	1:A:778:LYS:HD2	2.03	0.41
2:B:506:TRP:O	2:B:506:TRP:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:CYS:HB2	2:B:705:GLY:CA	2.49	0.41
3:C:67:ARG:NH1	3:C:67:ARG:HB3	2.36	0.41
3:C:210:GLU:O	3:C:213:GLU:N	2.54	0.41
9:I:61:GLU:O	9:I:63:ASP:N	2.54	0.41
13:M:30:GLY:CA	13:M:44:ARG:HG2	2.50	0.41
17:Q:23:ARG:NH2	18:R:207:SER:H	2.18	0.41
22:Y:55:DG:H21	22:Y:56:DG:H1	1.67	0.41
1:A:532:ARG:HD2	1:A:647:THR:O	2.20	0.41
1:A:611:ASP:CG	1:A:626:THR:CG2	2.94	0.41
1:A:901:VAL:HB	1:A:978:VAL:HG13	2.01	0.41
1:A:966:LEU:HA	1:A:969:ILE:HD12	2.03	0.41
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	2.02	0.41
2:B:226:GLU:HA	2:B:230:ARG:HG2	2.03	0.41
2:B:711:ILE:HA	2:B:712:PRO:HD3	1.88	0.41
2:B:873:LEU:CB	2:B:874:PRO:CD	2.99	0.41
9:I:23:MET:HE3	9:I:25:TYR:CE1	2.55	0.41
13:M:47:ASP:O	13:M:49:GLY:N	2.54	0.41
17:Q:109:HIS:CG	18:R:225:VAL:HG23	2.55	0.41
21:X:45:DT:H4'	21:X:46:DT:O4'	2.21	0.41
23:Z:3:U:H2'	23:Z:4:C:O4'	2.20	0.41
2:B:246:GLY:HA3	19:S:169:LYS:HD2	2.02	0.41
2:B:262:TYR:O	2:B:263:ILE:HD13	2.20	0.41
8:H:65:TYR:CZ	8:H:70:LEU:HD22	2.56	0.41
9:I:61:GLU:HG3	9:I:103:ARG:HH22	1.86	0.41
16:P:207:PRO:O	16:P:208:ARG:C	2.63	0.41
1:A:1117:VAL:O	1:A:1117:VAL:HG12	2.21	0.41
2:B:215:TYR:CD1	2:B:238:SER:HB3	2.55	0.41
2:B:849:ASP:OD1	2:B:850:ASP:N	2.52	0.41
2:B:1040:GLN:O	2:B:1041:ILE:HD13	2.21	0.41
3:C:49:TRP:CE3	12:L:54:VAL:HG21	2.56	0.41
6:F:104:ILE:O	6:F:120:VAL:HG23	2.21	0.41
7:G:138:GLN:HG2	7:G:139:GLN:N	2.35	0.41
13:M:182:ALA:N	20:T:154:LYS:HB3	2.36	0.41
19:S:46:ARG:NH2	20:T:3:GLU:OE2	2.41	0.41
19:S:144:TYR:CD2	20:T:96:PHE:HZ	2.39	0.41
20:T:153:TYR:CE1	20:T:155:PRO:HG3	2.56	0.41
1:A:514:GLU:CD	2:B:1101:GLN:HE21	2.29	0.41
1:A:811:ILE:HD12	1:A:811:ILE:HA	1.88	0.41
1:A:878:THR:HA	1:A:889:LEU:O	2.20	0.41
1:A:889:LEU:HD23	1:A:889:LEU:HA	1.88	0.41
1:A:1128:ILE:HG23	1:A:1414:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:GLU:HG3	1:A:1304:ILE:HG12	2.02	0.41
2:B:252:ILE:C	2:B:254:GLN:H	2.26	0.41
2:B:554:GLU:OE1	19:S:115:LYS:HG3	2.20	0.41
2:B:576:ILE:HD12	2:B:576:ILE:C	2.46	0.41
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.51	0.41
2:B:1132:THR:HG23	2:B:1133:HIS:ND1	2.36	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.41
3:C:132:SER:HB3	3:C:147:ASP:CB	2.39	0.41
5:E:99:ILE:O	5:E:125:TYR:HE1	2.02	0.41
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.85	0.41
9:I:104:ALA:O	9:I:105:GLU:HB2	2.20	0.41
10:J:2:ILE:HG12	10:J:3:ILE:N	2.36	0.41
13:M:15:CYS:HA	13:M:16:PRO:HD3	1.89	0.41
13:M:62:LYS:HD3	23:Z:1:A:H4'	2.02	0.41
16:P:329:TYR:N	16:P:330:PRO:HD2	2.36	0.41
17:Q:187:ILE:HD13	18:R:211:SER:CA	2.39	0.41
1:A:265:VAL:HG21	13:M:48:VAL:CG2	2.51	0.41
2:B:751:LEU:HD12	2:B:751:LEU:HA	1.90	0.41
7:G:119:PHE:CE2	7:G:121:PRO:HB3	2.56	0.41
15:O:86:GLU:HG3	15:O:87:LEU:H	1.85	0.41
17:Q:187:ILE:O	17:Q:191:LEU:HD13	2.21	0.41
19:S:166:ARG:HH11	19:S:166:ARG:CG	2.32	0.41
19:S:169:LYS:HE3	19:S:169:LYS:HB3	1.83	0.41
21:X:12:DA:C2	21:X:13:DT:C4	3.09	0.41
21:X:59:DC:H2''	21:X:60:DG:O5'	2.21	0.41
22:Y:38:DT:H2''	22:Y:39:DG:O4'	2.20	0.41
7:G:17:TYR:HB3	7:G:25:THR:HG21	2.03	0.40
7:G:97:LEU:N	7:G:108:ILE:O	2.49	0.40
9:I:84:HIS:CG	9:I:85:PRO:CD	2.77	0.40
11:K:3:ALA:HA	11:K:4:PRO:HD3	1.97	0.40
14:N:341:LYS:H	14:N:352:HIS:HB2	1.86	0.40
15:O:9:THR:O	15:O:13:ASN:N	2.48	0.40
16:P:271:GLU:OE1	16:P:271:GLU:N	2.50	0.40
21:X:25:DG:N2	22:Y:70:DC:O2	2.53	0.40
22:Y:84:DG:C2	22:Y:85:DG:C4	3.09	0.40
1:A:909:LEU:HD23	1:A:909:LEU:HA	1.68	0.40
1:A:1324:GLU:H	1:A:1324:GLU:CD	2.28	0.40
2:B:197:GLN:HB2	2:B:394:ASP:HB2	2.04	0.40
2:B:631:GLN:HB3	2:B:685:LYS:HZ1	1.86	0.40
8:H:147:LYS:C	8:H:149:ALA:H	2.29	0.40
10:J:10:CYS:SG	10:J:11:GLY:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:187:ILE:CG2	18:R:211:SER:HA	2.15	0.40
1:A:265:VAL:H	1:A:272:ASN:HB3	1.81	0.40
1:A:520:MET:HG3	1:A:522:PRO:HD2	2.03	0.40
1:A:912:SER:HB3	1:A:915:ALA:CB	2.51	0.40
1:A:966:LEU:HD13	1:A:1043:ILE:HD11	2.03	0.40
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.79	0.40
2:B:873:LEU:HG	2:B:874:PRO:N	2.36	0.40
3:C:256:LEU:HD23	3:C:256:LEU:HA	1.89	0.40
11:K:53:ASP:OD1	11:K:54:PRO:HD2	2.22	0.40
13:M:27:TYR:HA	13:M:44:ARG:HH11	1.86	0.40
13:M:32:MET:SD	13:M:44:ARG:NH2	2.95	0.40
17:Q:14:LEU:HD11	17:Q:103:VAL:HG11	2.04	0.40
18:R:224:THR:HG21	18:R:225:VAL:CG2	2.20	0.40
20:T:154:LYS:HA	20:T:155:PRO:HD3	1.90	0.40
1:A:547:LYS:HE2	1:A:683:GLU:OE1	2.22	0.40
1:A:1005:HIS:HA	1:A:1006:PRO:HD3	1.93	0.40
1:A:1163:HIS:HA	1:A:1300:GLY:HA2	2.04	0.40
2:B:573:TRP:CH2	2:B:576:ILE:HG23	2.56	0.40
3:C:30:VAL:HG22	11:K:45:ILE:HD11	2.02	0.40
3:C:205:LYS:NZ	3:C:217:GLN:OE1	2.54	0.40
5:E:63:ALA:HB1	5:E:64:HIS:H	1.66	0.40
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.57	0.40
8:H:122:LEU:HD23	8:H:122:LEU:HA	1.82	0.40
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.57	0.40
22:Y:89:DC:H2"	22:Y:90:DC:C6	2.56	0.40
1:A:425:ASP:HB2	13:M:39:LEU:CD1	2.52	0.40
1:A:457:ILE:HD13	1:A:457:ILE:HG21	1.75	0.40
1:A:551:ARG:HG2	1:A:551:ARG:NH1	2.37	0.40
1:A:1065:PHE:CZ	1:A:1069:LEU:HD21	2.57	0.40
1:A:1129:ASN:OD1	1:A:1415:THR:HG21	2.22	0.40
1:A:1189:ASP:HA	1:A:1192:TRP:CZ3	2.56	0.40
2:B:95:LYS:HB2	2:B:96:PRO:HD2	2.04	0.40
2:B:218:THR:HG1	2:B:236:TRP:HE3	1.65	0.40
2:B:384:ASP:OD1	2:B:386:ASP:N	2.38	0.40
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.03	0.40
2:B:802:ASP:C	2:B:804:GLY:N	2.80	0.40
3:C:136:ASP:C	3:C:138:ASP:H	2.30	0.40
3:C:210:GLU:O	3:C:213:GLU:CG	2.50	0.40
4:D:30:GLU:O	7:G:3:TYR:HA	2.22	0.40
7:G:18:PHE:HA	7:G:22:LEU:HD13	2.02	0.40
10:J:13:ILE:H	10:J:13:ILE:HG13	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:108:SER:O	13:M:108:SER:OG	2.38	0.40
22:Y:56:DG:C4	22:Y:57:DA:H1'	2.56	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%)	121 (8%)	59 (4%)	2	20
2	B	1163/1174 (99%)	999 (86%)	120 (10%)	44 (4%)	2	21
3	C	273/275 (99%)	241 (88%)	22 (8%)	10 (4%)	2	22
4	D	127/142 (89%)	119 (94%)	8 (6%)	0	100	100
5	E	208/210 (99%)	191 (92%)	11 (5%)	6 (3%)	3	26
6	F	84/127 (66%)	82 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	21	55
8	H	148/150 (99%)	117 (79%)	22 (15%)	9 (6%)	1	15
9	I	123/125 (98%)	90 (73%)	18 (15%)	15 (12%)	0	4
10	J	65/67 (97%)	51 (78%)	8 (12%)	6 (9%)	0	9
11	K	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	7	35
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	2	19
13	M	308/316 (98%)	266 (86%)	31 (10%)	11 (4%)	2	23
14	N	109/376 (29%)	101 (93%)	6 (6%)	2 (2%)	6	34
15	O	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
16	P	183/339 (54%)	172 (94%)	5 (3%)	6 (3%)	3	24
17	Q	176/439 (40%)	158 (90%)	10 (6%)	8 (4%)	2	19
18	R	163/291 (56%)	140 (86%)	15 (9%)	8 (5%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	134/517 (26%)	120 (90%)	10 (8%)	4 (3%)	3	26
20	T	218/249 (88%)	190 (87%)	19 (9%)	9 (4%)	2	20
All	All	5357/7223 (74%)	4702 (88%)	453 (8%)	202 (4%)	4	21

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	153	ILE
1	A	154	CYS
1	A	204	HIS
1	A	207	GLU
1	A	208	ASP
1	A	210	GLN
1	A	212	LYS
1	A	264	VAL
1	A	265	VAL
1	A	274	ASP
1	A	531	ASN
1	A	598	GLY
1	A	607	SER
1	A	609	HIS
1	A	610	PRO
1	A	611	ASP
1	A	623	PRO
1	A	625	ASP
1	A	911	PRO
1	A	930	LEU
1	A	931	ARG
1	A	1087	VAL
1	A	1101	GLN
1	A	1116	ASN
1	A	1117	VAL
1	A	1200	PRO
1	A	1275	VAL
1	A	1299	GLN
1	A	1307	VAL
2	B	63	PRO
2	B	74	ALA
2	B	78	VAL
2	B	231	PRO

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Mol	Chain	Res	Type
2	B	251	ALA
2	B	383	ASP
2	B	428	ASP
2	B	876	ASN
2	B	879	GLU
2	B	884	ASN
2	B	958	CYS
2	B	1007	ASN
2	B	1136	GLU
3	C	6	GLN
3	C	7	PRO
5	E	46	ASP
5	E	47	LYS
5	E	48	PRO
5	E	49	SER
9	I	58	ILE
9	I	63	ASP
9	I	85	PRO
9	I	86	CYS
9	I	119	CYS
11	K	112	LYS
13	M	40	VAL
13	M	42	GLY
13	M	43	ASP
13	M	48	VAL
13	M	95	GLU
13	M	101	TYR
14	N	318	ASP
16	P	161	ILE
16	P	162	VAL
16	P	207	PRO
16	P	208	ARG
17	Q	100	VAL
17	Q	172	ASP
18	R	140	LYS
18	R	195	PRO
18	R	196	ASP
18	R	215	GLU
18	R	225	VAL
18	R	228	MET
20	T	124	TYR
20	T	140	ARG

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Mol	Chain	Res	Type
20	T	143	GLN
20	T	145	LEU
1	A	12	ALA
1	A	466	LYS
1	A	624	GLY
1	A	932	ARG
1	A	1118	THR
1	A	1145	GLY
1	A	1435	THR
2	B	77	GLU
2	B	141	GLN
2	B	226	GLU
2	B	229	SER
2	B	253	GLY
2	B	491	ARG
2	B	785	TYR
2	B	900	GLU
3	C	143	VAL
5	E	70	ASP
8	H	21	LYS
8	H	65	TYR
9	I	61	GLU
9	I	67	GLN
9	I	99	SER
9	I	106	ASP
10	J	5	VAL
10	J	6	ARG
13	M	53	ARG
16	P	299	ARG
17	Q	126	SER
17	Q	158	HIS
1	A	61	ARG
1	A	70	ARG
1	A	184	CYS
1	A	262	PRO
1	A	599	HIS
1	A	613	GLU
1	A	614	ASP
1	A	1109	TYR
2	B	61	ASP
2	B	75	SER
2	B	233	SER

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Mol	Chain	Res	Type
2	B	245	GLN
2	B	458	LYS
2	B	549	SER
2	B	873	LEU
2	B	875	GLU
3	C	3	TYR
3	C	210	GLU
3	C	213	GLU
5	E	65	ASN
7	G	140	ASP
8	H	66	GLU
8	H	111	ARG
9	I	15	ARG
9	I	105	GLU
12	L	17	TYR
16	P	298	PRO
17	Q	125	ALA
17	Q	133	SER
18	R	163	LEU
19	S	160	ALA
20	T	139	VAL
20	T	141	LEU
20	T	142	SER
1	A	38	GLU
1	A	51	ARG
1	A	62	GLN
1	A	134	LYS
1	A	266	MET
1	A	622	SER
2	B	427	LYS
2	B	559	ALA
2	B	821	LYS
2	B	1032	PHE
8	H	100	GLU
8	H	128	ASP
9	I	73	SER
9	I	101	SER
9	I	117	PRO
10	J	16	ASN
10	J	41	LYS
11	K	29	ASN
13	M	56	SER

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Mol	Chain	Res	Type
13	M	87	GLY
19	S	156	THR
19	S	170	VAL
20	T	155	PRO
1	A	619	LYS
1	A	620	HIS
1	A	981	CYS
2	B	457	LYS
2	B	515	PRO
8	H	24	ARG
12	L	34	ILE
13	M	45	VAL
13	M	66	ARG
14	N	320	VAL
17	Q	25	PHE
20	T	152	ASN
1	A	195	GLY
1	A	453	GLY
2	B	76	GLY
3	C	2	PRO
8	H	109	ALA
10	J	64	PRO
19	S	154	THR
1	A	1304	ILE
2	B	493	GLY
2	B	1006	VAL
2	B	1113	PRO
9	I	62	VAL
17	Q	102	VAL
18	R	194	ARG
3	C	58	VAL
3	C	78	ILE
2	B	561	ILE
2	B	931	ILE
3	C	151	VAL
8	H	49	PRO
1	A	56	GLY
2	B	289	ILE
2	B	1034	GLY
10	J	14	VAL
1	A	1312	PRO
2	B	489	ILE

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%)	1232 (96%)	47 (4%)	30	53
2	B	1020/1028 (99%)	976 (96%)	44 (4%)	26	49
3	C	252/252 (100%)	245 (97%)	7 (3%)	38	59
4	D	119/126 (94%)	118 (99%)	1 (1%)	73	77
5	E	192/192 (100%)	187 (97%)	5 (3%)	40	60
6	F	74/111 (67%)	74 (100%)	0	100	100
7	G	152/153 (99%)	151 (99%)	1 (1%)	76	78
8	H	131/131 (100%)	126 (96%)	5 (4%)	29	52
9	I	112/112 (100%)	108 (96%)	4 (4%)	31	54
10	J	56/56 (100%)	54 (96%)	2 (4%)	31	54
11	K	106/106 (100%)	105 (99%)	1 (1%)	70	75
12	L	43/55 (78%)	40 (93%)	3 (7%)	14	40
13	M	263/268 (98%)	256 (97%)	7 (3%)	39	60
14	N	105/324 (32%)	104 (99%)	1 (1%)	68	75
15	O	90/98 (92%)	89 (99%)	1 (1%)	65	74
16	P	159/293 (54%)	157 (99%)	2 (1%)	61	71
17	Q	164/373 (44%)	159 (97%)	5 (3%)	36	57
18	R	150/261 (58%)	140 (93%)	10 (7%)	15	41
19	S	121/448 (27%)	118 (98%)	3 (2%)	42	62
20	T	196/218 (90%)	188 (96%)	8 (4%)	27	51
All	All	4784/6353 (75%)	4627 (97%)	157 (3%)	34	56

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	65	ILE
1	A	132	LYS

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Mol	Chain	Res	Type
1	A	204	HIS
1	A	205	VAL
1	A	226	LYS
1	A	259	SER
1	A	261	ARG
1	A	264	VAL
1	A	265	VAL
1	A	271	ARG
1	A	286	ILE
1	A	303	ILE
1	A	305	GLU
1	A	463	THR
1	A	502	ASN
1	A	540	ASP
1	A	567	LEU
1	A	611	ASP
1	A	614	ASP
1	A	619	LYS
1	A	620	HIS
1	A	625	ASP
1	A	652	LEU
1	A	712	ASP
1	A	757	GLN
1	A	771	VAL
1	A	849	ASP
1	A	870	SER
1	A	873	VAL
1	A	908	THR
1	A	1036	ASN
1	A	1101	GLN
1	A	1102	MET
1	A	1119	LEU
1	A	1167	ARG
1	A	1279	MET
1	A	1282	ASP
1	A	1298	LEU
1	A	1306	LYS
1	A	1307	VAL
1	A	1309	MET
1	A	1311	LEU
1	A	1337	GLU
1	A	1341	VAL

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Mol	Chain	Res	Type
1	A	1385	VAL
1	A	1407	CYS
2	B	40	VAL
2	B	41	ARG
2	B	73	HIS
2	B	78	VAL
2	B	79	GLU
2	B	131	THR
2	B	132	VAL
2	B	140	LEU
2	B	156	LEU
2	B	168	ASP
2	B	222	ARG
2	B	232	THR
2	B	248	LYS
2	B	249	LYS
2	B	250	SER
2	B	256	ILE
2	B	289	ILE
2	B	388	TYR
2	B	412	LEU
2	B	422	PHE
2	B	446	TYR
2	B	491	ARG
2	B	509	VAL
2	B	539	SER
2	B	573	TRP
2	B	588	ARG
2	B	606	ASP
2	B	641	ASP
2	B	666	ASP
2	B	667	THR
2	B	675	LEU
2	B	711	ILE
2	B	737	ILE
2	B	879	GLU
2	B	880	LEU
2	B	897	ARG
2	B	957	THR
2	B	959	GLU
2	B	961	ILE
2	B	1007	ASN

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Mol	Chain	Res	Type
2	B	1056	ASP
2	B	1080	ARG
2	B	1090	GLU
2	B	1092	ASP
3	C	77	ASP
3	C	94	CYS
3	C	102	THR
3	C	136	ASP
3	C	137	ASN
3	C	177	ASN
3	C	242	GLU
4	D	135	GLN
5	E	23	ASP
5	E	47	LYS
5	E	64	HIS
5	E	147	GLU
5	E	199	THR
7	G	128	TYR
8	H	11	ASP
8	H	65	TYR
8	H	66	GLU
8	H	107	GLU
8	H	116	VAL
9	I	14	ILE
9	I	58	ILE
9	I	61	GLU
9	I	95	VAL
10	J	47	ARG
10	J	65	LEU
11	K	48	SER
12	L	27	GLU
12	L	28	ILE
12	L	43	ILE
13	M	10	LEU
13	M	12	ARG
13	M	31	ASP
13	M	46	ILE
13	M	47	ASP
13	M	86	LYS
13	M	133	ASN
14	N	318	ASP
15	O	21	GLU

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Mol	Chain	Res	Type
16	P	206	GLU
16	P	297	LYS
17	Q	38	ILE
17	Q	102	VAL
17	Q	128	LYS
17	Q	135	THR
17	Q	191	LEU
18	R	100	ASP
18	R	152	LEU
18	R	163	LEU
18	R	175	LEU
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
18	R	223	VAL
18	R	225	VAL
19	S	135	PHE
19	S	166	ARG
19	S	177	MET
20	T	140	ARG
20	T	141	LEU
20	T	145	LEU
20	T	147	LYS
20	T	153	TYR
20	T	154	LYS
20	T	160	GLN
20	T	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	122	ASN
1	A	188	GLN
1	A	272	ASN
1	A	278	HIS
1	A	403	GLN
1	A	410	ASN
1	A	449	HIS
1	A	465	HIS
1	A	516	GLN

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Mol	Chain	Res	Type
1	A	590	GLN
1	A	711	GLN
1	A	740	GLN
1	A	746	ASN
1	A	757	GLN
1	A	790	GLN
1	A	947	HIS
1	A	1044	HIS
1	A	1077	ASN
1	A	1105	ASN
1	A	1116	ASN
1	A	1190	GLN
1	A	1310	HIS
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	203	ASN
2	B	654	GLN
2	B	695	HIS
2	B	716	HIS
2	B	948	GLN
2	B	1053	HIS
2	B	1073	GLN
2	B	1097	HIS
2	B	1101	GLN
3	C	134	ASN
3	C	137	ASN
3	C	145	GLN
4	D	19	GLN
7	G	24	ASN
7	G	28	GLN
9	I	87	GLN
9	I	121	HIS
10	J	52	HIS
11	K	84	GLN
13	M	229	GLN
14	N	338	GLN
15	O	35	GLN
15	O	57	ASN
16	P	193	ASN
16	P	277	HIS
17	Q	95	ASN

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Mol	Chain	Res	Type
18	R	117	GLN
19	S	96	GLN
19	S	121	ASN
19	S	142	ASN
20	T	86	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	Z	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

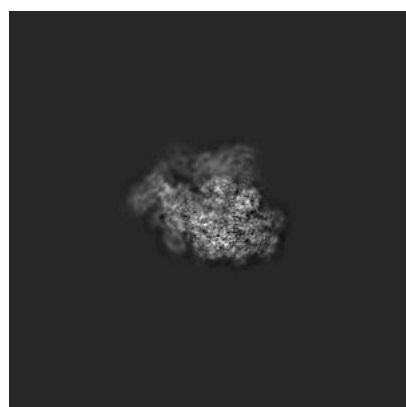
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8138. These allow visual inspection of the internal detail of the map and identification of artifacts.

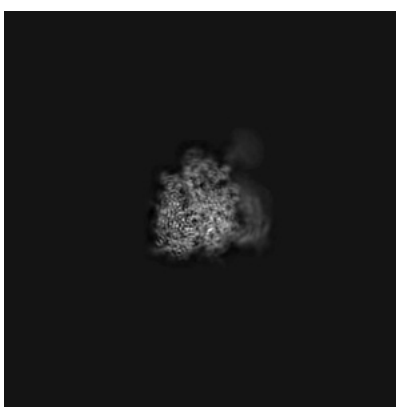
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

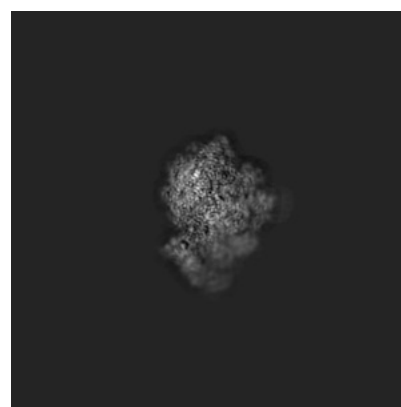
6.1.1 Primary map



X



Y

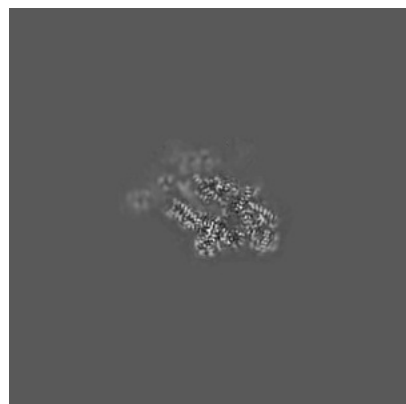


Z

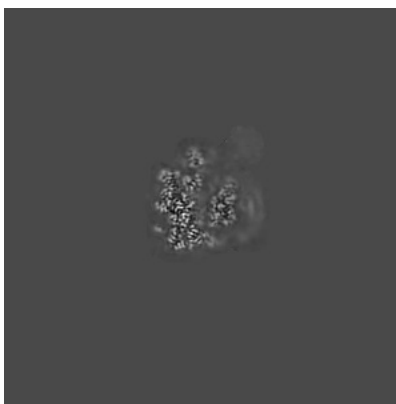
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

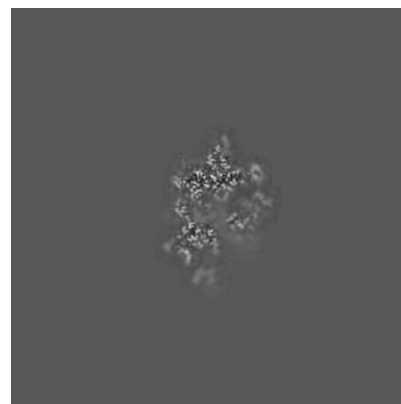
6.2.1 Primary map



X Index: 192



Y Index: 192

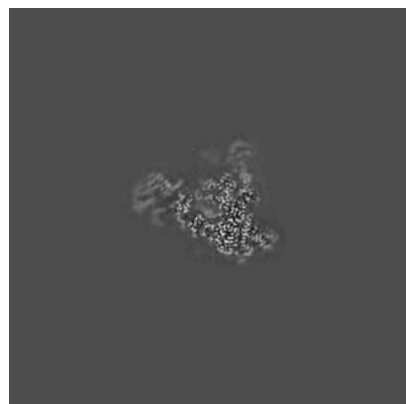


Z Index: 192

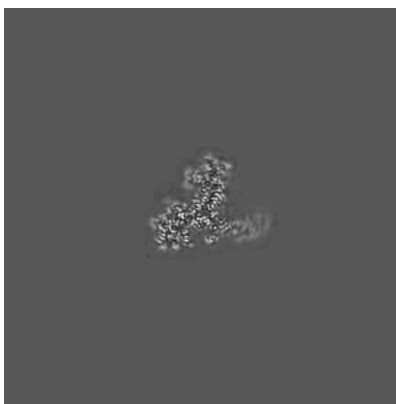
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

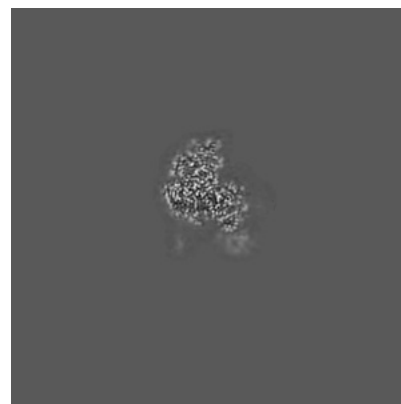
6.3.1 Primary map



X Index: 178



Y Index: 224

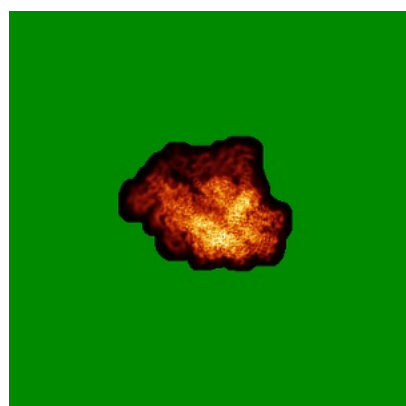


Z Index: 166

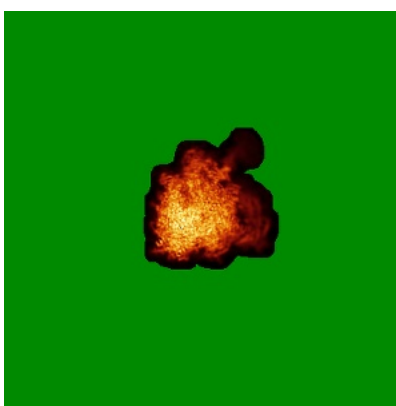
The images above show the largest variance slices of the map in three orthogonal directions.

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

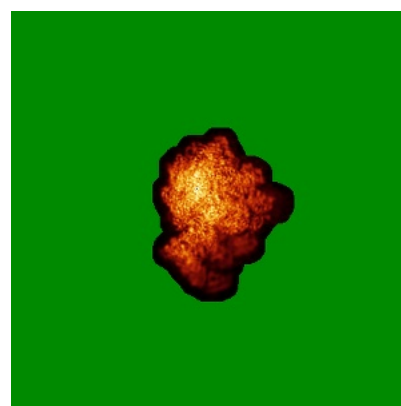
6.4.1 Primary map



X



Y

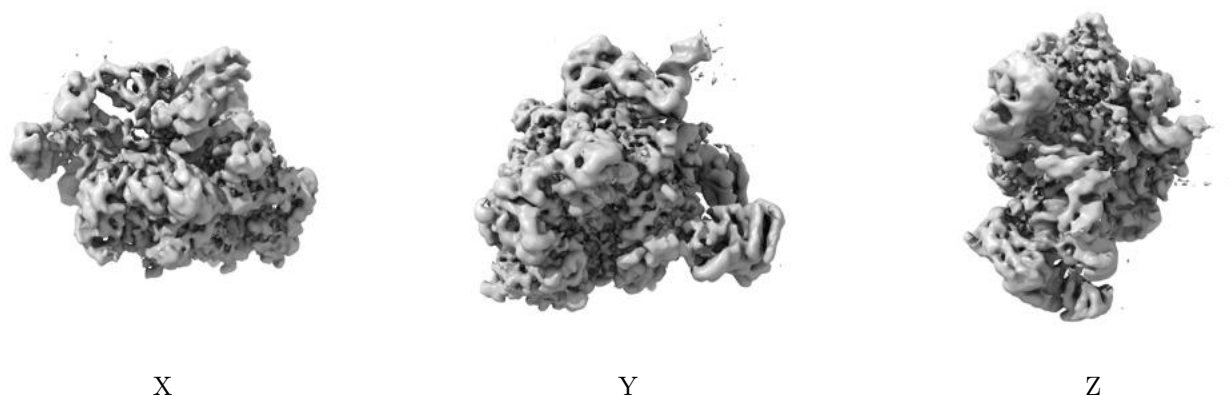


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

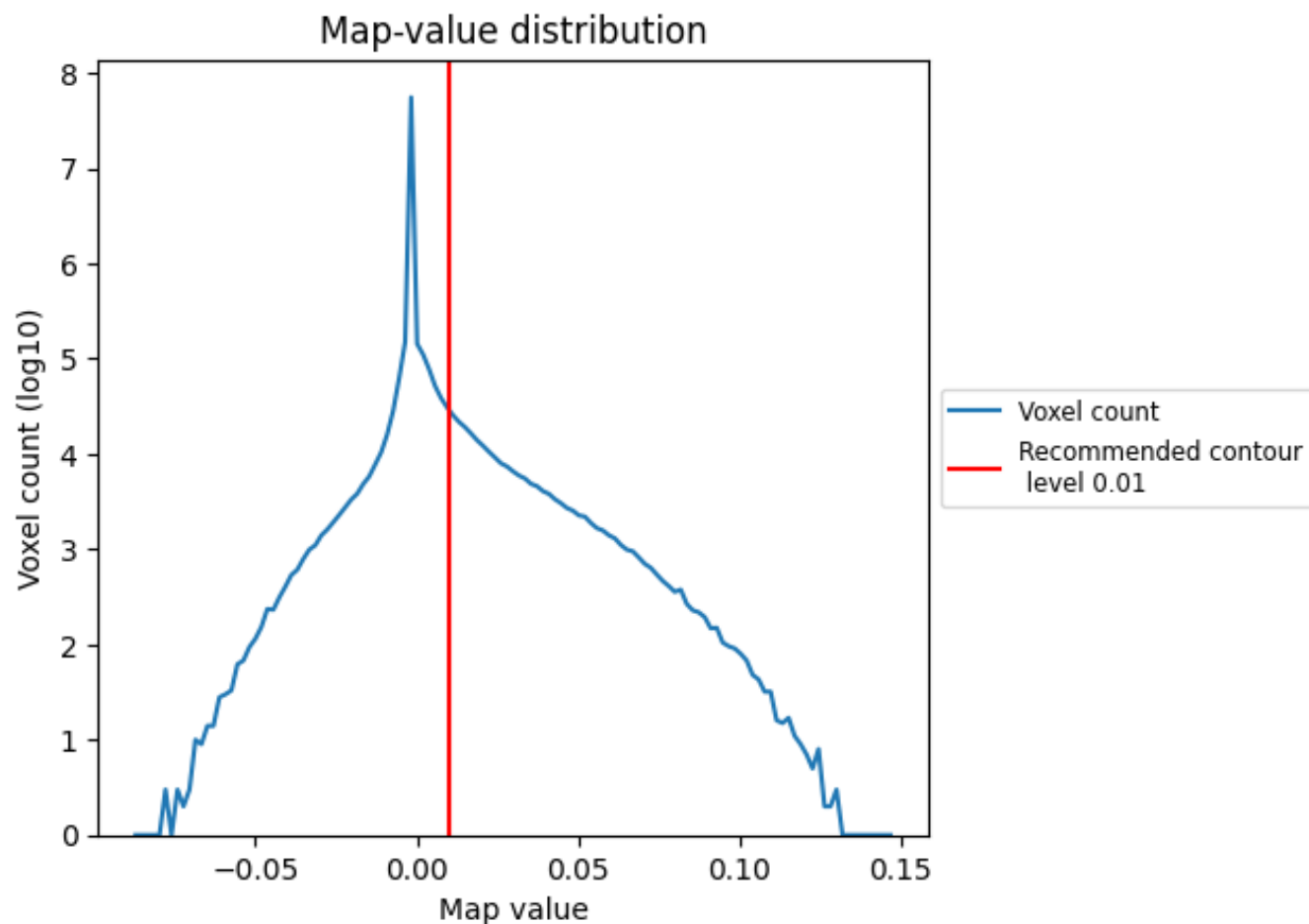
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

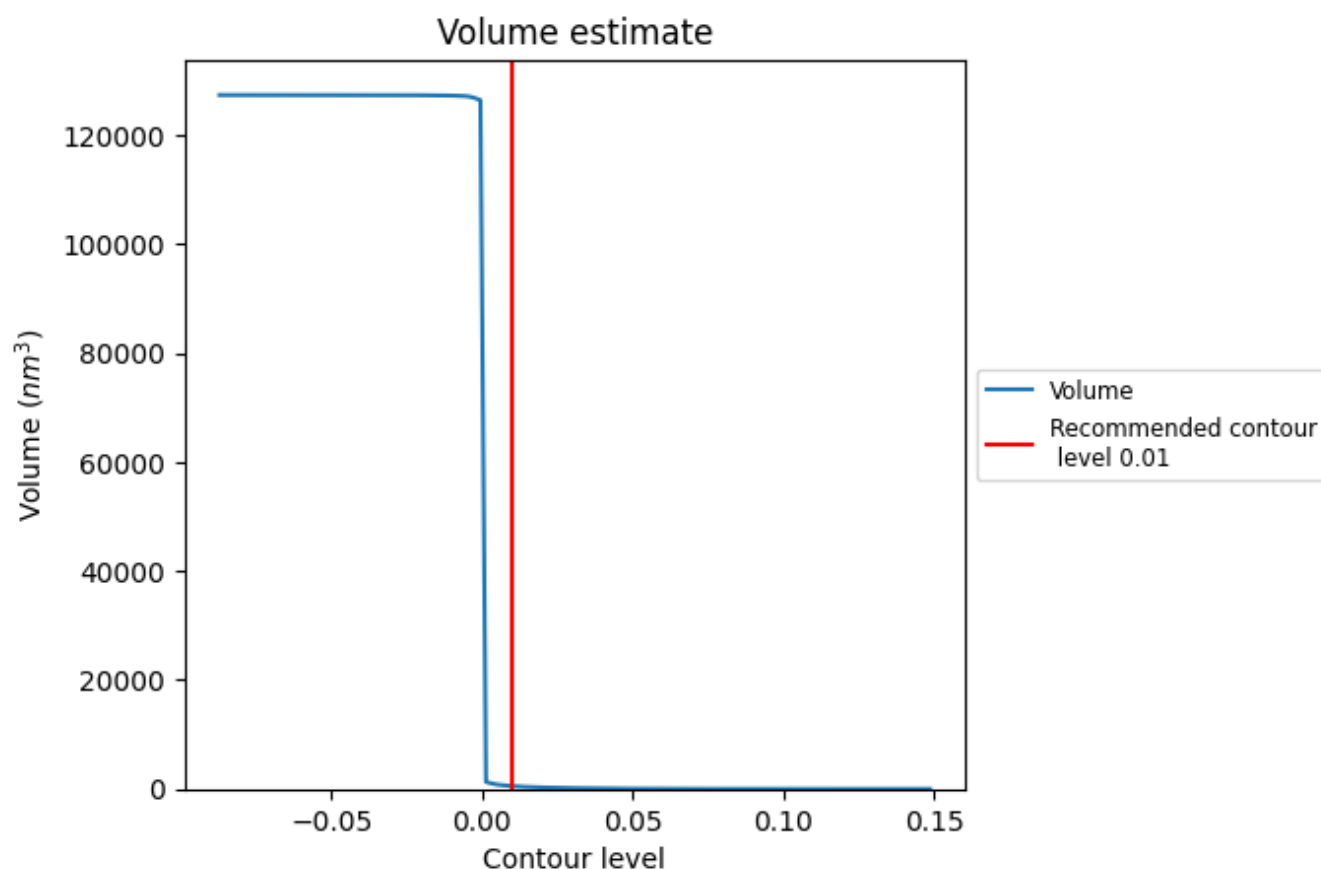
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

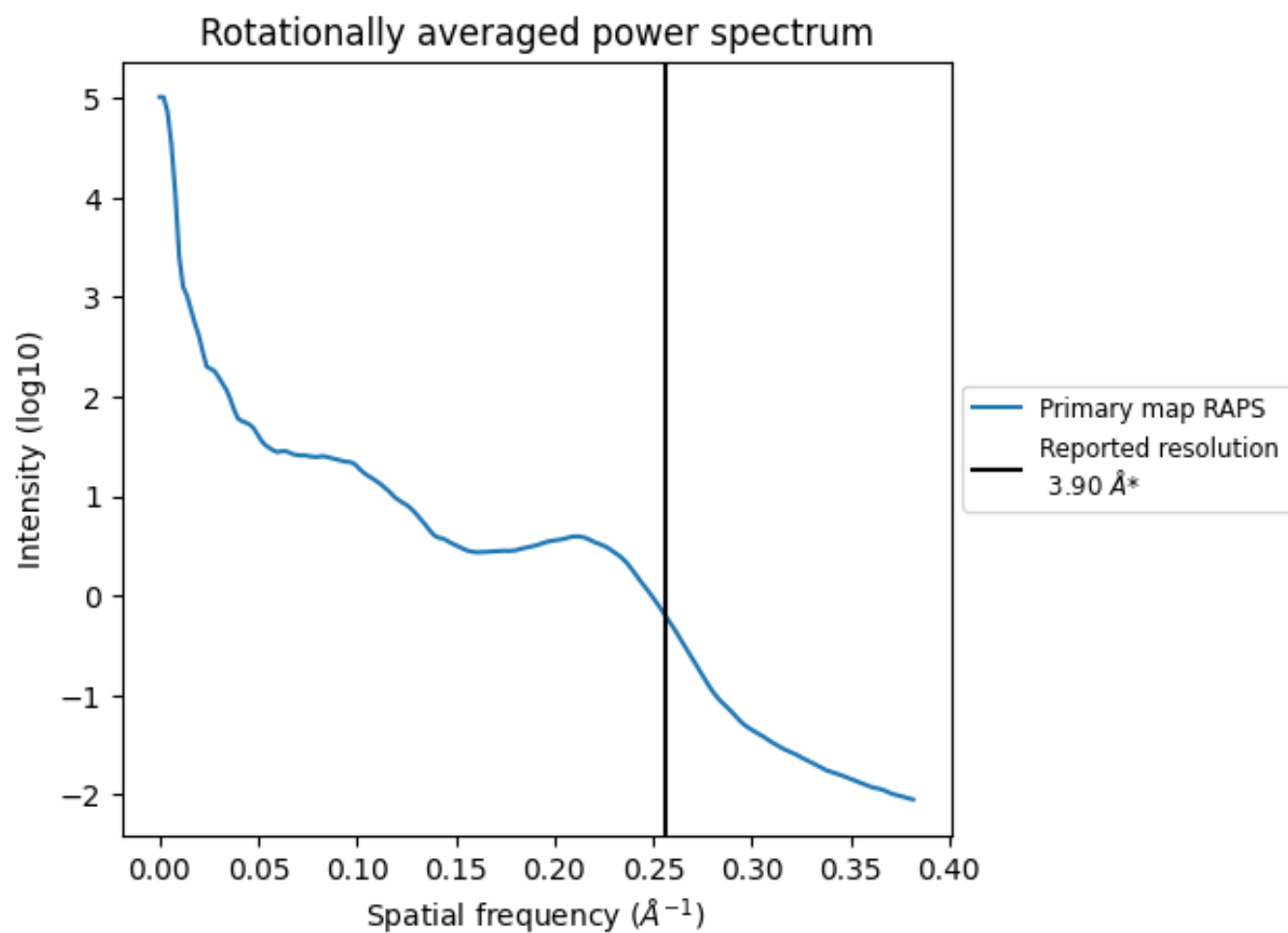
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm³; this corresponds to an approximate mass of 475 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 ⓘ

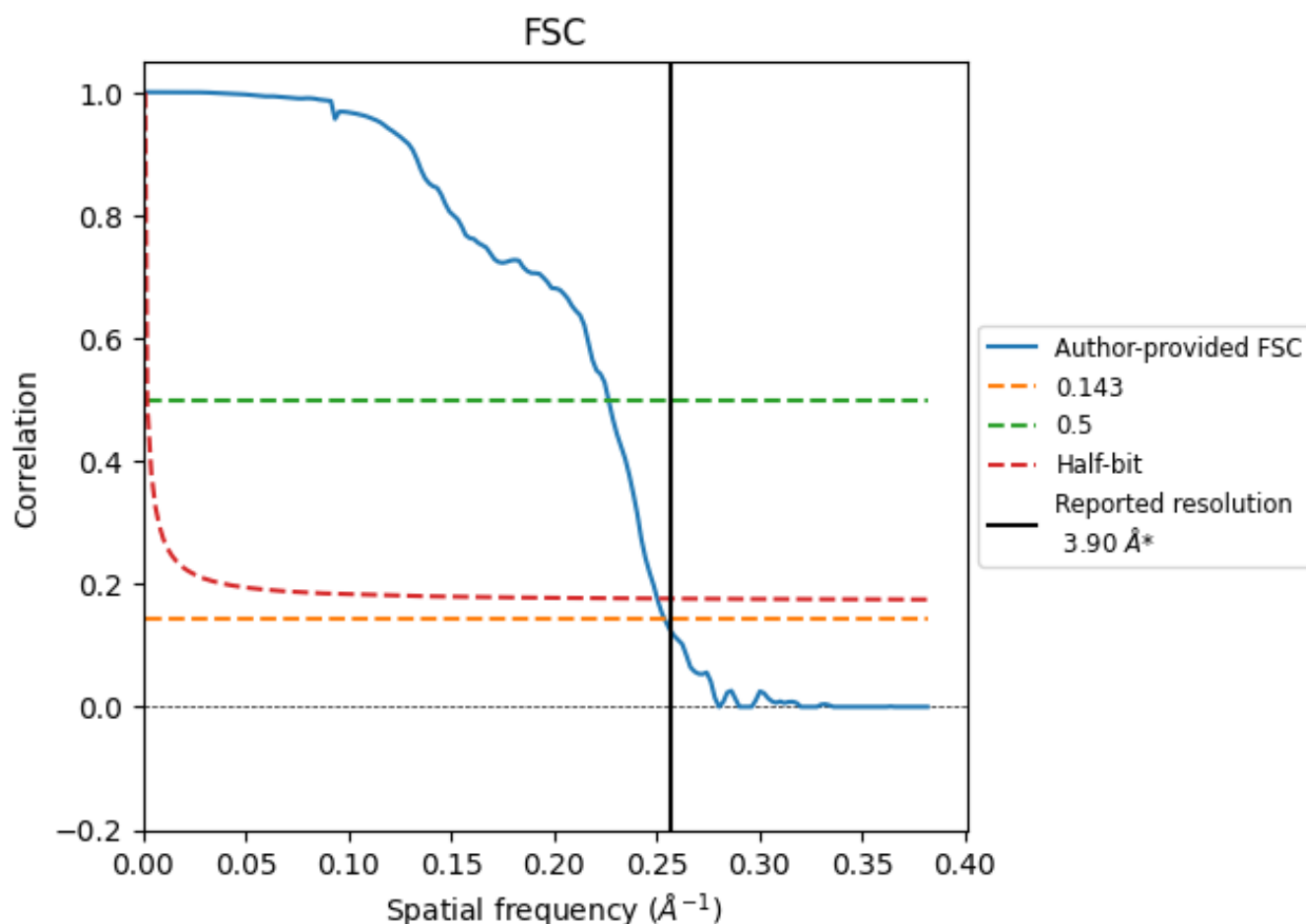


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

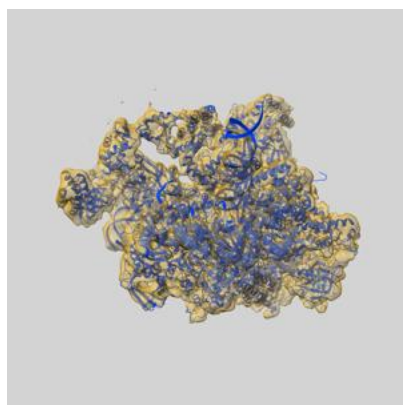
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.41	4.00
Unmasked-calculated*	-	-	-

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

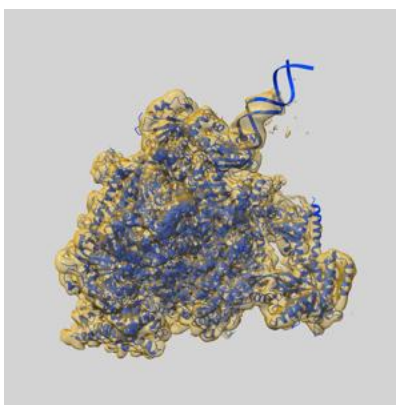
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8138 and PDB model 5IYD. Per-residue inclusion information can be found in section [3](#) on page [8](#).

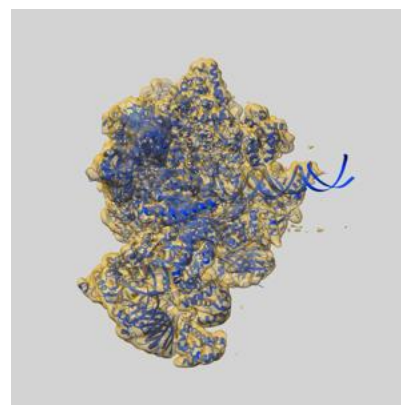
9.1 Map-model overlay [i](#)



X



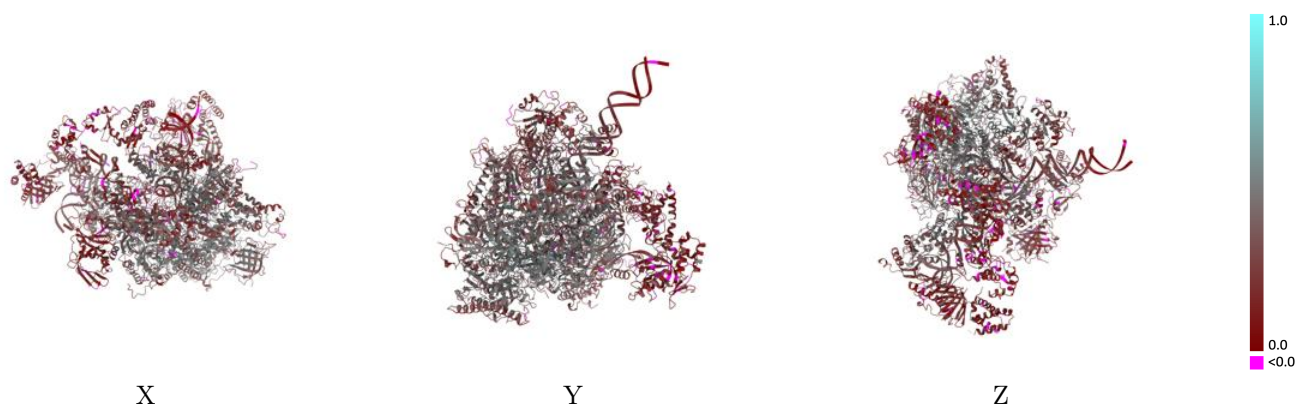
Y



Z

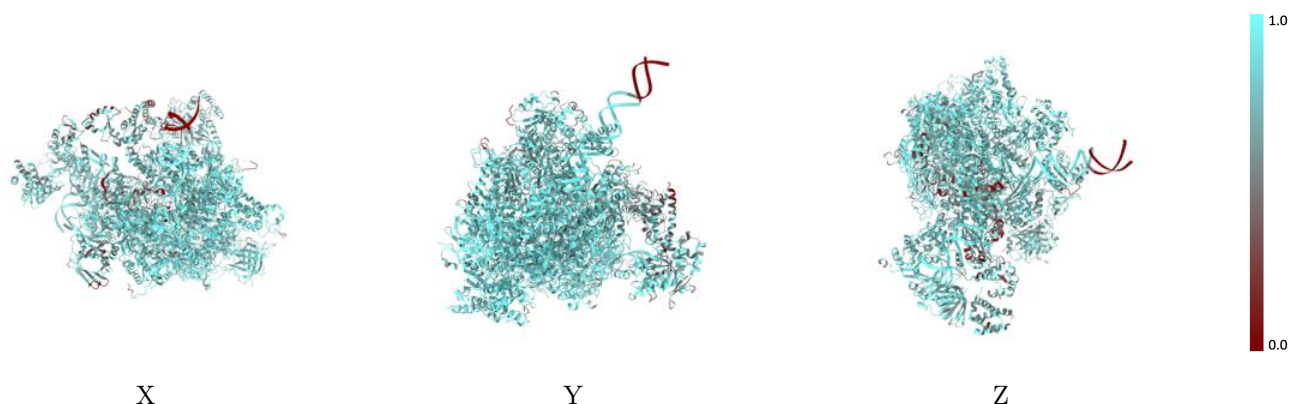
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



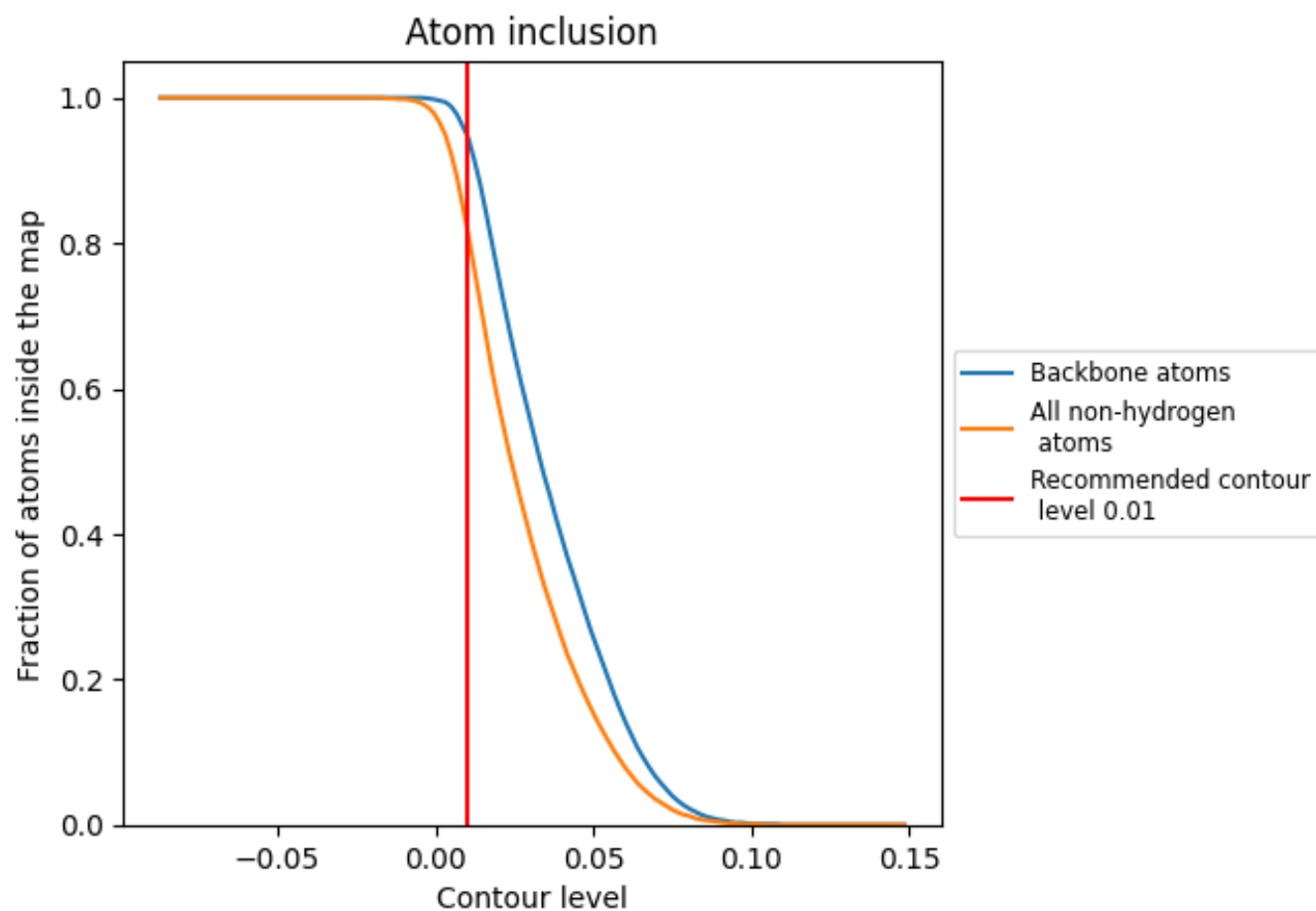
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 82% 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	 0.8210	 0.3220
A	 0.8650	 0.3830
B	 0.8720	 0.4120
C	 0.8820	 0.3920
D	 0.7390	 0.1730
E	 0.8470	 0.3370
F	 0.8380	 0.3990
G	 0.7660	 0.2110
H	 0.8560	 0.3470
I	 0.8210	 0.2770
J	 0.8700	 0.4020
K	 0.8920	 0.3920
L	 0.8820	 0.3750
M	 0.8200	 0.3220
N	 0.7470	 0.1670
O	 0.7680	 0.1840
P	 0.8400	 0.2540
Q	 0.6160	 0.1490
R	 0.5720	 0.1220
S	 0.7120	 0.1650
T	 0.7010	 0.1810
X	 0.7440	 0.2230
Y	 0.8390	 0.2580
Z	 0.8560	 0.3090

