Full wwPDB EM Validation Report (i)

Nov 2, 2022 – 03:59 PM EDT

PDB ID	:	5IYD
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 (i) 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 (i)) were used in the production of this report:

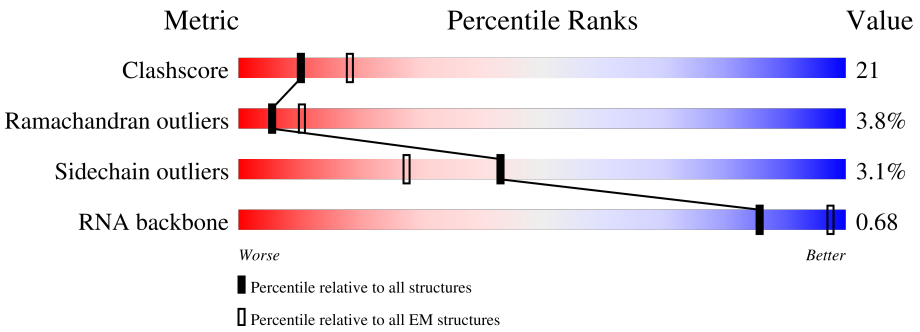
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1970	49% 21% • • 26%
2	B	1174	60% 35% • •
3	C	275	67% 29% • •
4	D	142	5% 76% 14% • 9%
5	E	210	75% 23% •
6	F	127	5% 56% 12% 32%
7	G	172	9% 70% 28% ••

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Mol	Chain	Length	Quality of chain
8	H	150	55% 39%
9	I	125	7% 50% 37% 10%
10	J	67	60% 30% 10%
11	K	117	67% 32%
12	L	58	40% 36% 21%
13	M	316	6% 72% 22% 5%
14	N	376	20% 9% 70%
15	O	109	61% 30% 9%
16	P	339	43% 9% 45%
17	Q	439	10% 21% 18% 59%
18	R	291	15% 37% 15% 43%
19	S	517	18% 8% 73%
20	T	249	9% 57% 28% 11%
21	X	80	19% 48% 50%
22	Y	80	10% 48% 52%
23	Z	6	100%

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 (i)

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
			Total	C	N	O	S		
1	A	1454	11515	7234	2058	2150	73	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	86	689	437	120	127	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1351	875	219	249	8	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a DNA chain called SCP-X.

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

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

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

- Molecule 23 is a RNA chain called RNA.

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

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

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

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

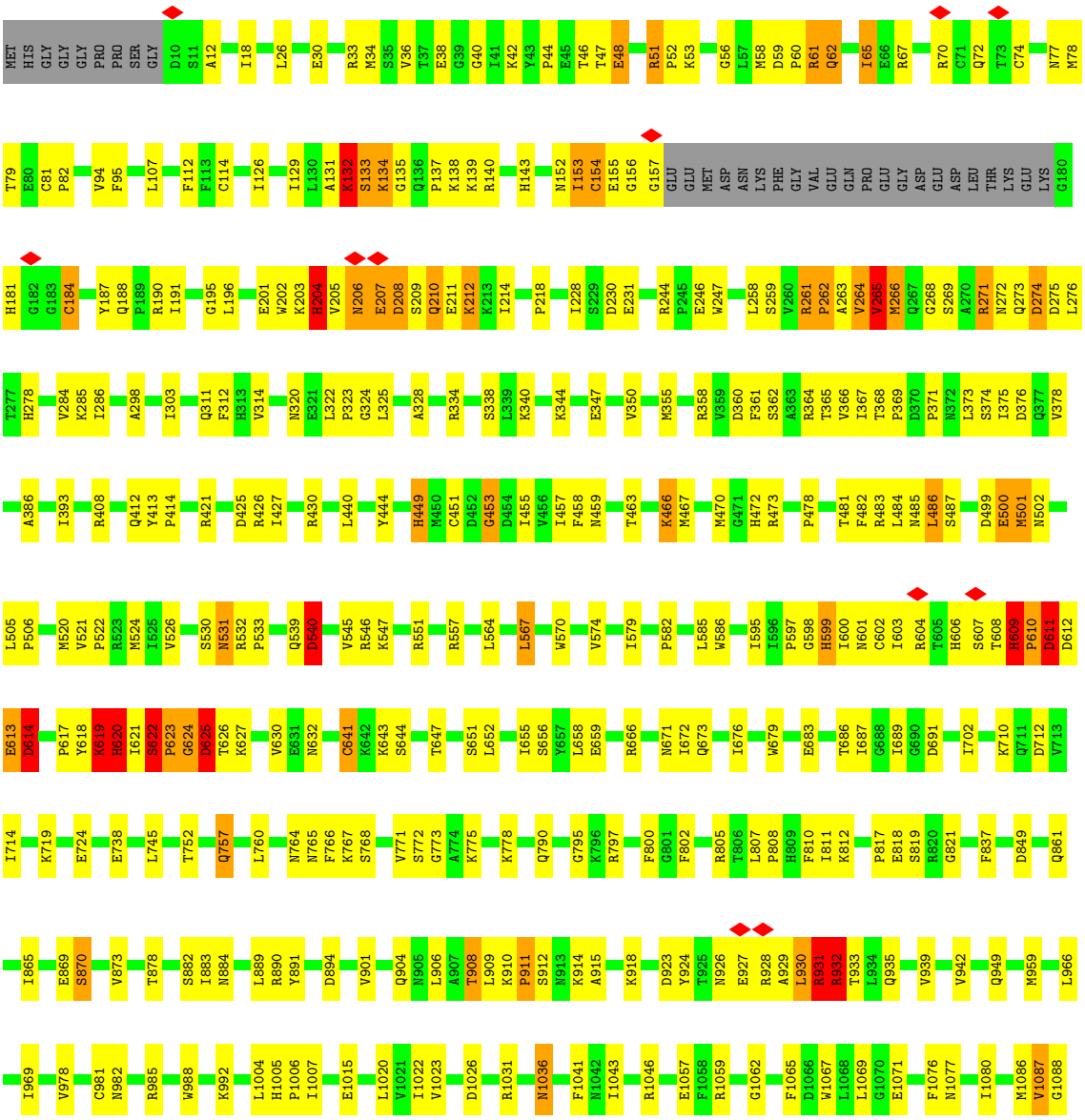
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
25	A	3	3	3	0
25	B	1	1	1	0
25	C	1	1	1	0
25	I	2	2	2	0
25	J	1	1	1	0
25	L	1	1	1	0
25	M	1	1	1	0
25	Q	1	1	1	0

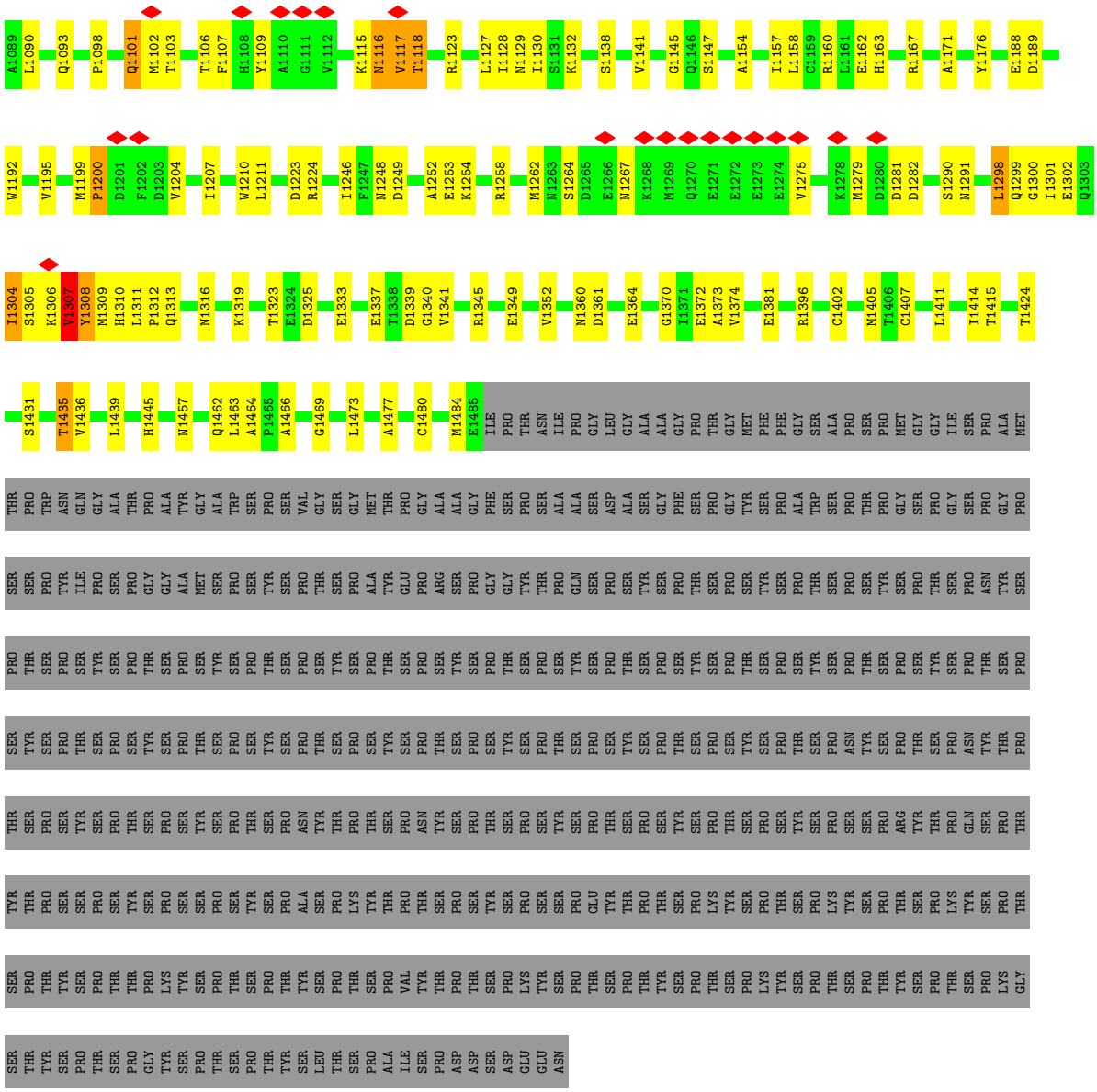
3 Residue-property plots (i)

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

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

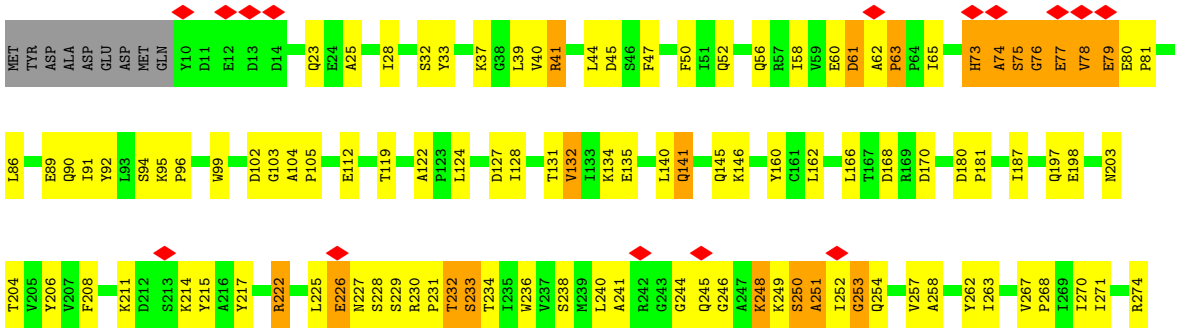
Chain A:

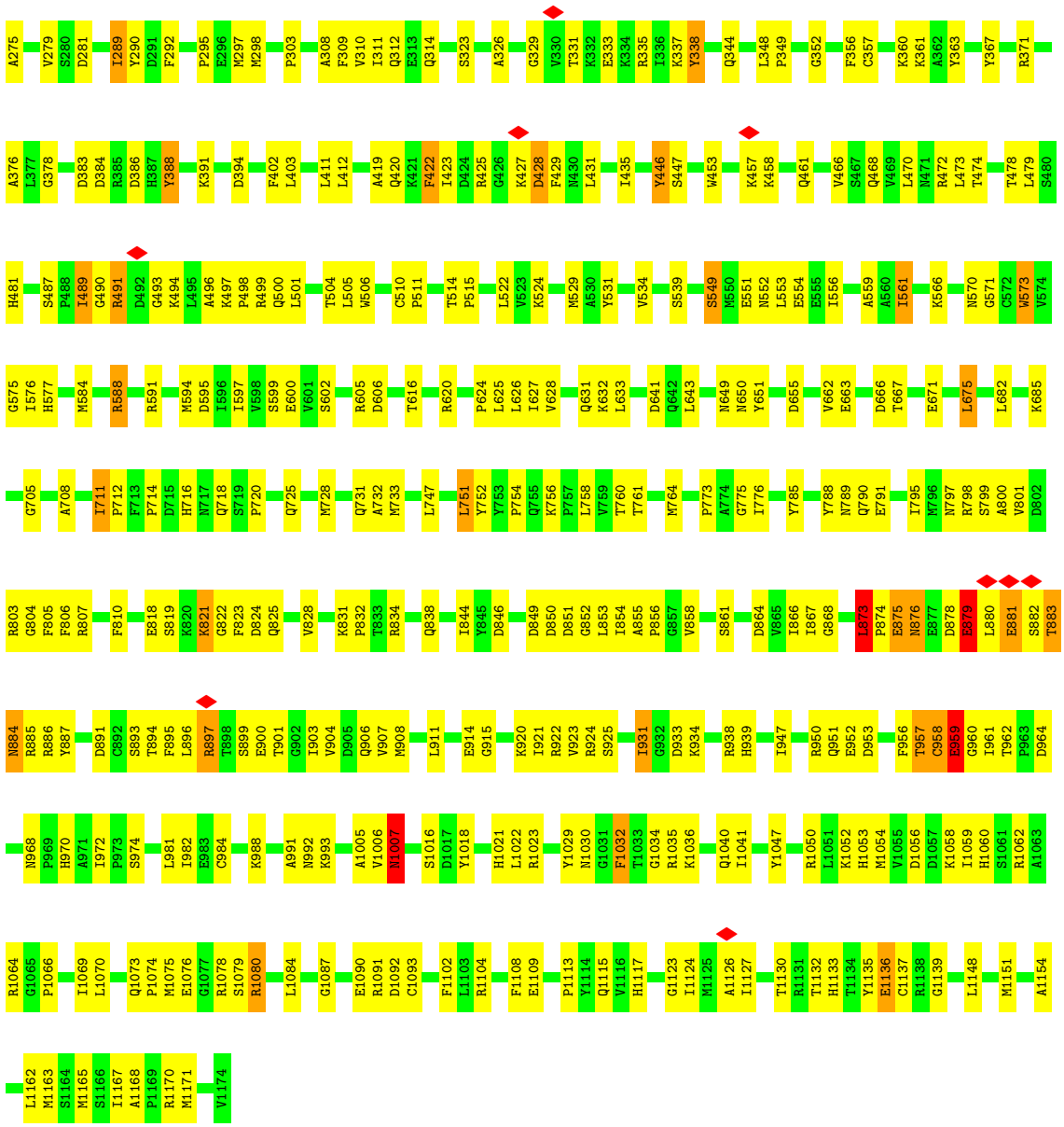




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

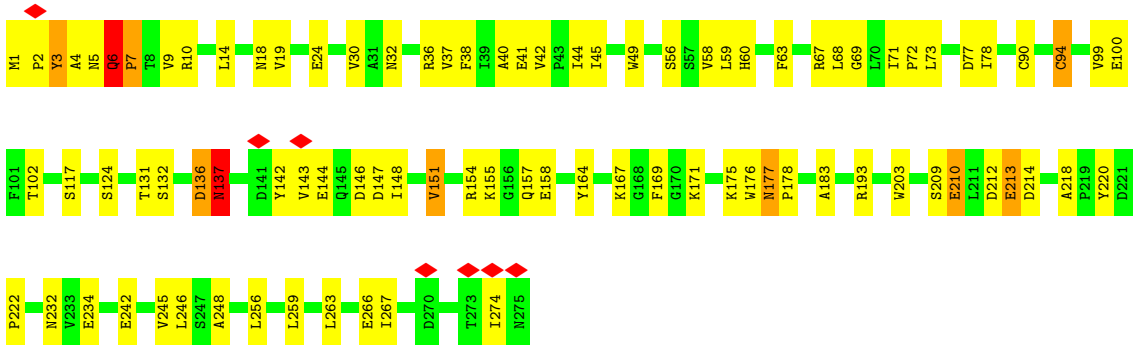
Chain B:





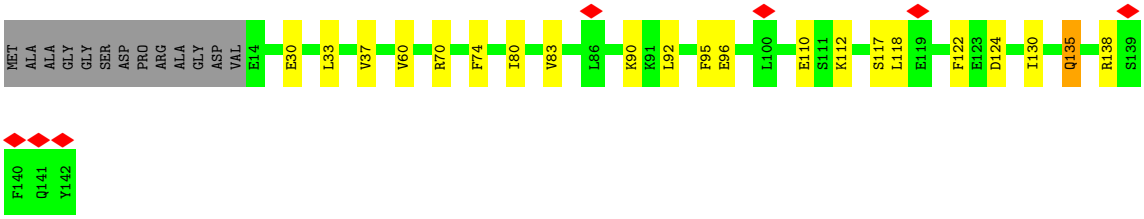
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



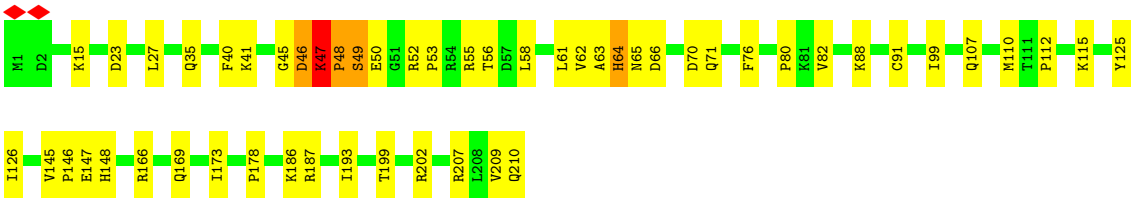
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



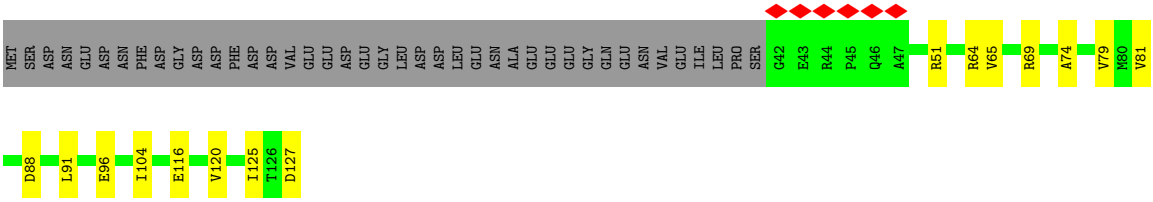
• Molecule 5: DNA-directed RNA polymerase II subunit RPB5

Chain E:



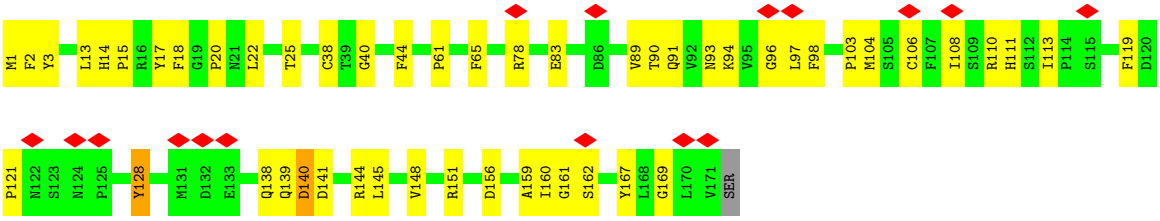
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F:



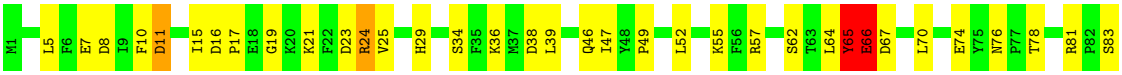
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



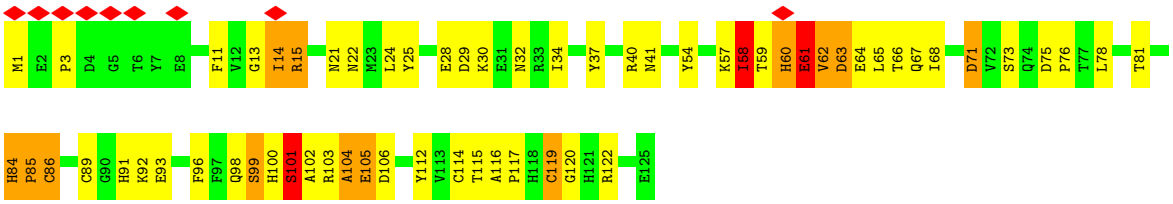
• Molecule 8: DNA-directed RNA polymerase II subunit RPB8

Chain H:



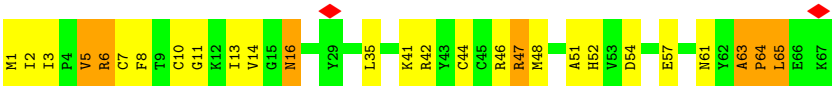
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



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

Chain J:

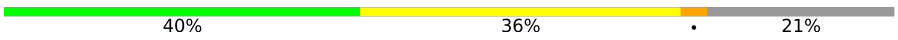


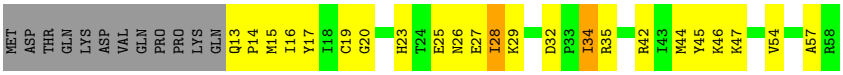
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:

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

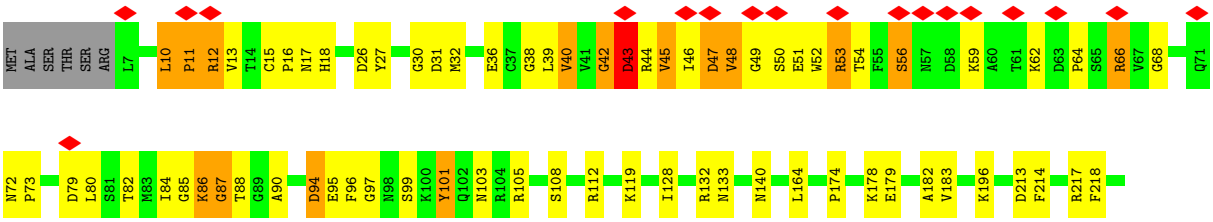
Chain L:





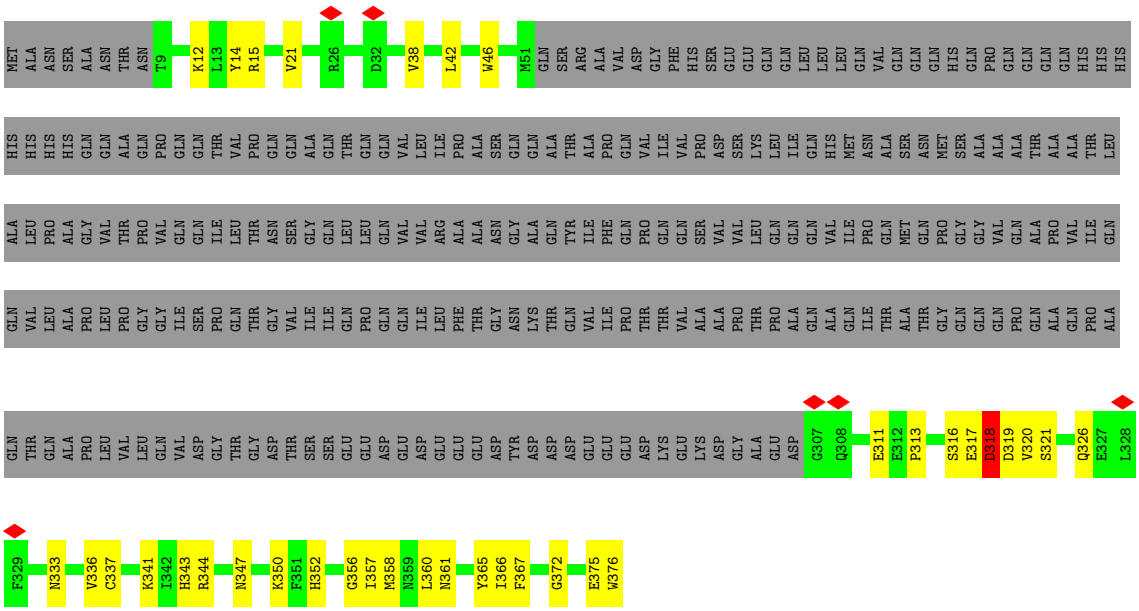
• Molecule 13: Transcription initiation factor IIB

Chain M:



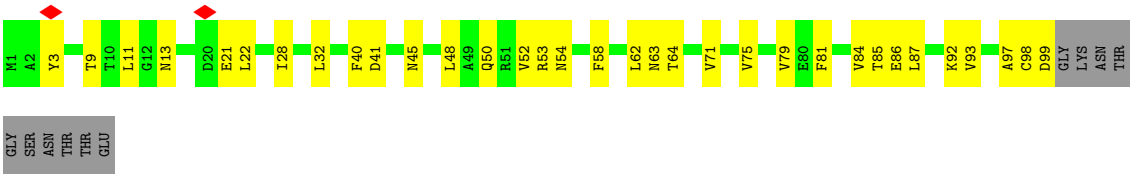
• Molecule 14: Transcription initiation factor IIA subunit 1

Chain N:



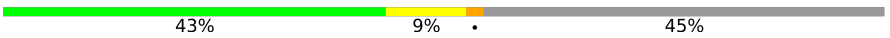
• Molecule 15: Transcription initiation factor IIA subunit 2

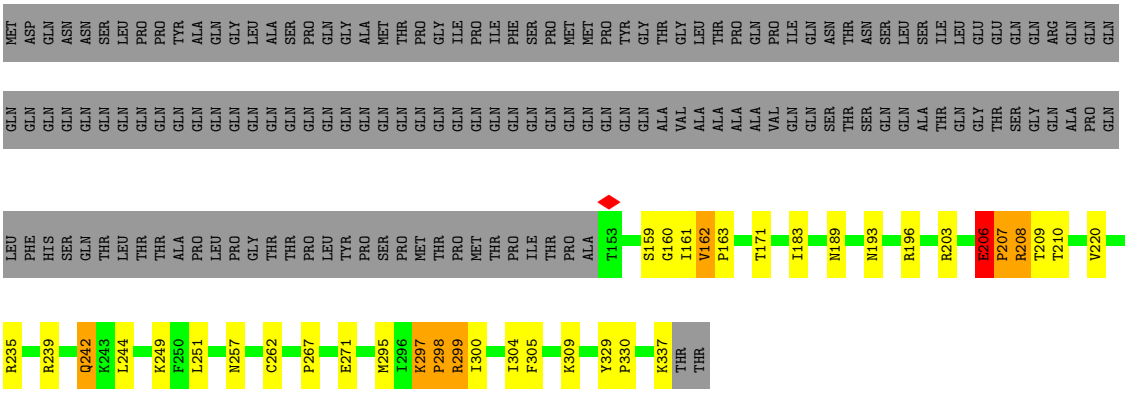
Chain O:



• Molecule 16: TATA-box-binding protein

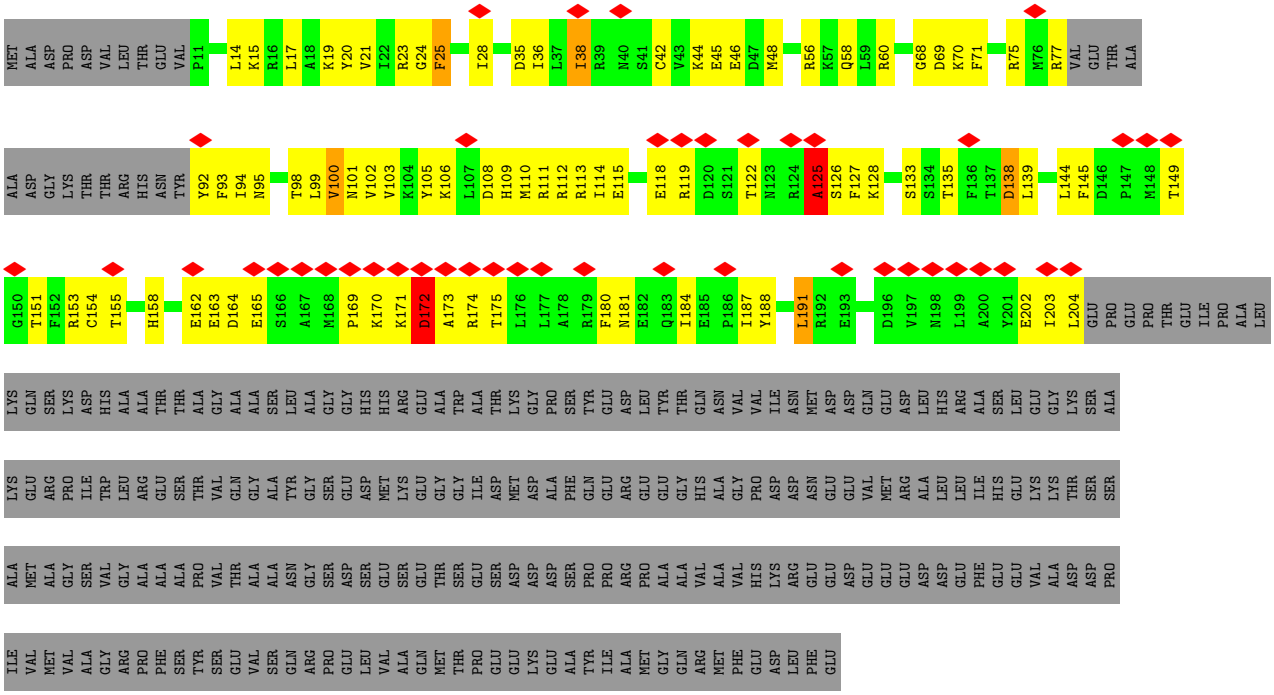
Chain P:





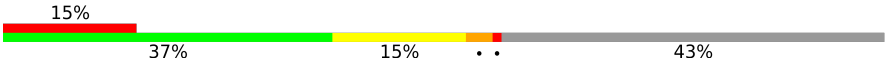
• Molecule 17: General transcription factor IIE subunit 1

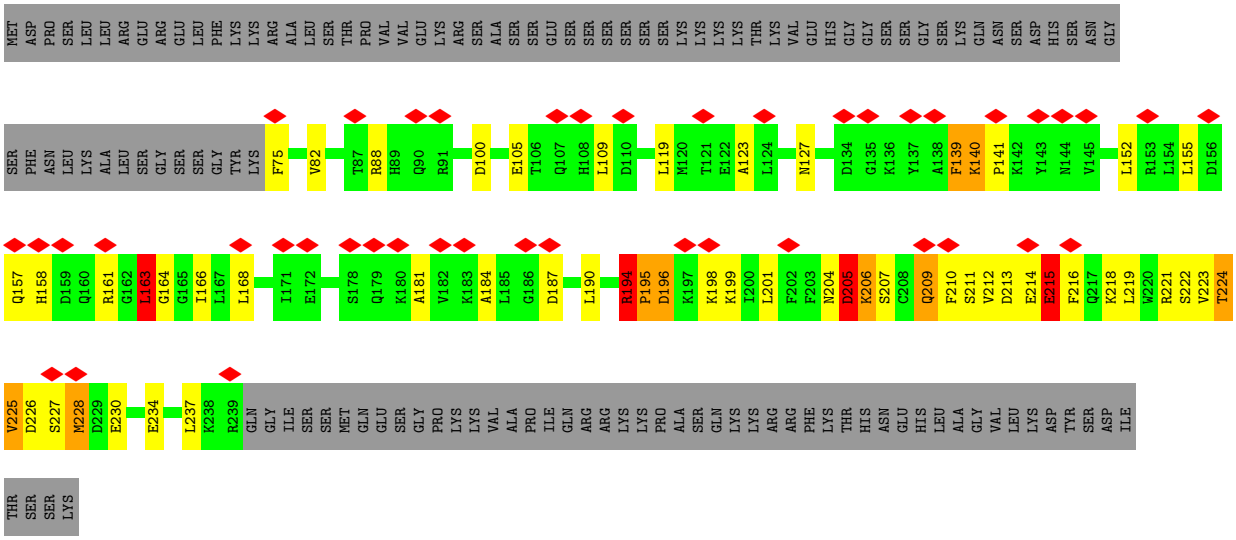
Chain Q:



• Molecule 18: Transcription initiation factor IIE subunit beta

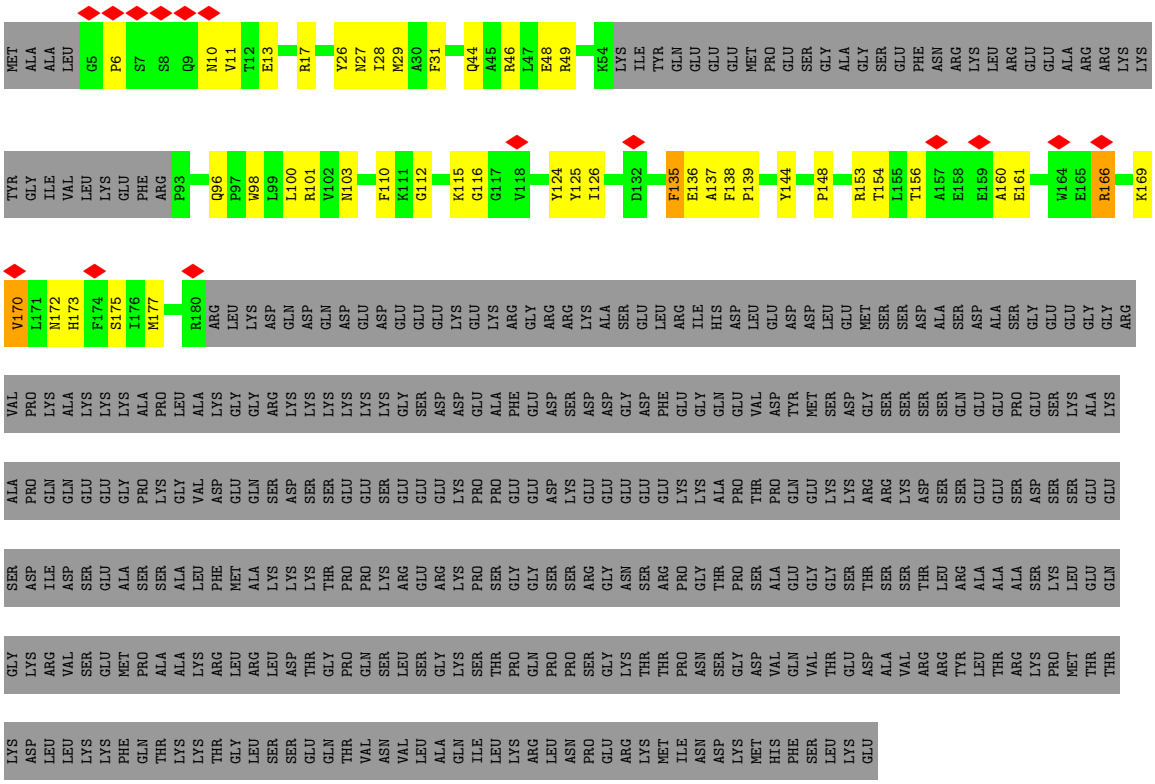
Chain R:





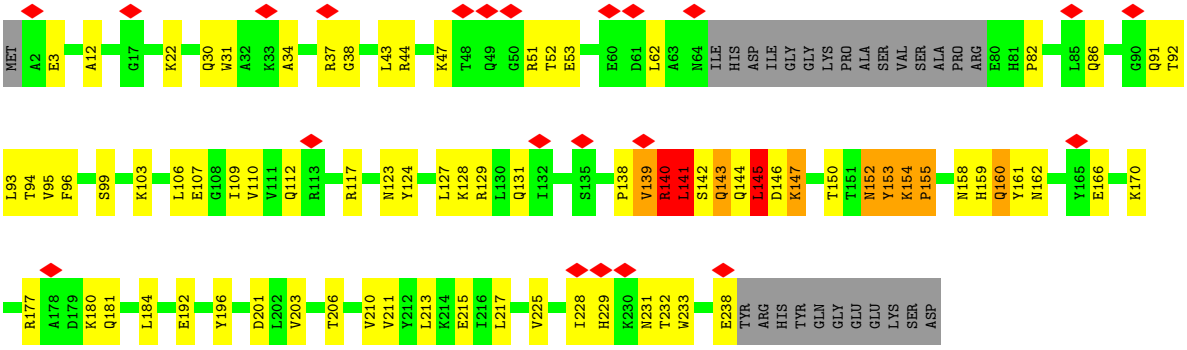
• Molecule 19: General transcription factor IIF subunit 1

Chain S:



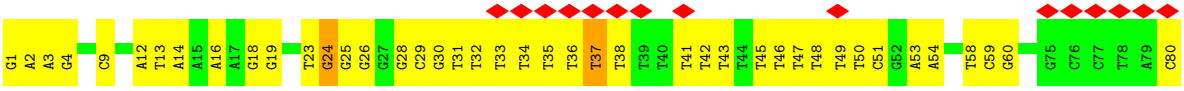
- Molecule 20: General transcription factor IIF subunit 2

Chain T:



- Molecule 21: SCP-X

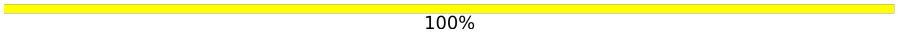
Chain X:

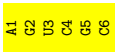


- Molecule 22: SCP-Y

Chain Y:

- Molecule 23: RNA

Chain Z: 



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.56	1/11727 (0.0%)	0.81	19/15833 (0.1%)
2	B	0.66	3/9503 (0.0%)	0.86	7/12831 (0.1%)
3	C	0.54	0/2259	0.95	3/3073 (0.1%)
4	D	0.27	0/1077	0.52	0/1446
5	E	0.43	0/1753	0.79	1/2368 (0.0%)
6	F	0.43	0/700	0.69	0/946
7	G	0.32	0/1382	0.58	0/1874
8	H	0.45	0/1227	0.74	3/1654 (0.2%)
9	I	0.38	0/1038	0.97	3/1407 (0.2%)
10	J	0.66	1/542 (0.2%)	0.91	1/730 (0.1%)
11	K	0.50	0/956	0.72	1/1294 (0.1%)
12	L	0.56	0/394	0.69	0/524
13	M	0.41	0/2429	0.71	4/3281 (0.1%)
14	N	0.23	0/945	0.51	0/1274
15	O	0.25	0/816	0.48	0/1105
16	P	0.29	0/1489	0.72	1/2005 (0.0%)
17	Q	0.28	0/1507	0.62	2/2023 (0.1%)
18	R	0.57	0/1380	1.10	6/1854 (0.3%)
19	S	0.26	0/1167	0.54	0/1576
20	T	0.27	0/1817	0.59	0/2445
21	X	0.68	0/1843	1.05	3/2847 (0.1%)
22	Y	0.62	0/1817	0.96	0/2800
23	Z	0.37	0/139	0.84	0/215
All	All	0.53	5/47907 (0.0%)	0.81	54/65405 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	44	CYS	CB-SG	-6.57	1.71	1.82
1	A	500	GLU	CG-CD	6.11	1.61	1.51
2	B	984	CYS	CB-SG	-5.70	1.72	1.81
2	B	959	GLU	CG-CD	5.59	1.60	1.51
2	B	112	GLU	CD-OE2	5.17	1.31	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	6	GLN	C-N-CD	-31.36	51.61	120.60
9	I	84	HIS	C-N-CD	-25.23	65.08	120.60
18	R	194	ARG	C-N-CD	-21.76	72.73	120.60
16	P	206	GLU	C-N-CD	-21.58	73.12	120.60
5	E	47	LYS	C-N-CD	-17.54	82.01	120.60
1	A	622	SER	N-CA-C	-9.24	86.06	111.00
1	A	622	SER	C-N-CD	-9.14	100.49	120.60
2	B	112	GLU	OE1-CD-OE2	-8.36	113.27	123.30
1	A	609	HIS	C-N-CD	-8.09	102.80	120.60
1	A	501	MET	CA-CB-CG	8.05	126.99	113.30
3	C	137	ASN	N-CA-C	-8.00	89.41	111.00
13	M	94	ASP	N-CA-C	-7.62	90.44	111.00
18	R	224	THR	N-CA-C	7.18	130.38	111.00
2	B	479	LEU	CB-CG-CD2	-7.00	99.11	111.00
9	I	104	ALA	N-CA-C	-6.90	92.38	111.00
1	A	614	ASP	N-CA-C	6.90	129.62	111.00
1	A	1307	VAL	N-CA-C	6.80	129.36	111.00
21	X	37	DT	O4'-C1'-N1	6.79	112.75	108.00
13	M	43	ASP	N-CA-C	-6.63	93.09	111.00
8	H	148	LEU	CA-CB-CG	6.43	130.10	115.30
18	R	88	ARG	NE-CZ-NH1	6.40	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	63	ALA	C-N-CD	-6.00	107.40	120.60
1	A	641	CYS	CA-CB-SG	-6.00	103.21	114.00
3	C	6	GLN	N-CA-C	5.98	127.14	111.00
18	R	163	LEU	C-N-CA	-5.97	109.76	122.30
2	B	883	THR	C-N-CA	-5.92	106.91	121.70
9	I	84	HIS	N-CA-C	5.91	126.96	111.00
1	A	932	ARG	C-N-CA	-5.90	106.94	121.70
1	A	620	HIS	N-CA-C	5.83	126.74	111.00
2	B	79	GLU	C-N-CA	-5.75	107.33	121.70
13	M	11	PRO	N-CA-C	-5.62	97.48	112.10
1	A	1396	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	540	ASP	CB-CG-OD2	-5.58	113.28	118.30
13	M	42	GLY	N-CA-C	5.55	126.97	113.10
2	B	388	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	1090	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	1402	CYS	CA-CB-SG	-5.41	104.27	114.00
8	H	85	ALA	N-CA-C	-5.31	96.67	111.00
8	H	66	GLU	N-CA-C	5.30	125.31	111.00
18	R	224	THR	CA-C-N	-5.29	105.56	117.20
1	A	206	ASN	C-N-CA	-5.26	108.54	121.70
18	R	205	ASP	N-CA-C	5.24	125.16	111.00
11	K	67	LEU	CA-CB-CG	-5.21	103.31	115.30
1	A	807	LEU	CB-CG-CD2	-5.19	102.18	111.00
21	X	37	DT	C1'-O4'-C4'	-5.18	104.92	110.10
1	A	133	SER	N-CA-C	5.14	124.87	111.00
17	Q	172	ASP	N-CA-C	5.14	124.87	111.00
2	B	751	LEU	CB-CG-CD1	-5.12	102.30	111.00
17	Q	100	VAL	N-CA-C	5.11	124.80	111.00
1	A	486	LEU	CA-CB-CG	-5.07	103.64	115.30
1	A	894	ASP	CB-CG-OD1	5.06	122.86	118.30
21	X	24	DG	O4'-C4'-C3'	-5.05	102.48	104.50
2	B	922	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	655	ILE	CG1-CB-CG2	-5.01	100.38	111.40

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

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11615	527	0
2	B	9317	0	9312	463	0
3	C	2213	0	2157	99	0
4	D	1062	0	1042	14	0
5	E	1723	0	1745	49	0
6	F	689	0	715	11	0
7	G	1351	0	1358	43	0
8	H	1205	0	1168	64	0
9	I	1013	0	939	80	0
10	J	533	0	557	43	0
11	K	937	0	959	27	0
12	L	388	0	397	24	0
13	M	2391	0	2413	160	0
14	N	930	0	888	32	0
15	O	806	0	818	27	0
16	P	1462	0	1548	49	0
17	Q	1484	0	1501	231	0
18	R	1357	0	1381	229	0
19	S	1138	0	1103	42	0
20	T	1788	0	1817	153	0
21	X	1645	0	908	53	0
22	Y	1624	0	899	48	0
23	Z	125	0	67	10	0
24	A	2	0	0	0	0
25	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1937	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 21.

All (1937) 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
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
8:H:65:TYR:CE2	8:H:70:LEU:HB3	1.51	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
1:A:608:THR:C	1:A:610:PRO:HD2	1.41	1.37
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:184:ILE:HD11	18:R:213:ASP:CG	1.42	1.37
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
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
17:Q:113:ARG:HD3	18:R:221:ARG:C	1.50	1.31
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:GLN:CD	10:J:65:LEU:HB3	1.52	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
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
1:A:264:VAL:C	1:A:272:ASN:HD22	1.40	1.25
9:I:62:VAL:O	9:I:64:GLU:N	1.71	1.23
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
17:Q:113:ARG:CD	18:R:221:ARG:C	2.06	1.22
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
18:R:224:THR:HG22	18:R:225:VAL:N	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
9:I:85:PRO:O	9:I:86:CYS:C	1.89	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
1:A:608:THR:C	1:A:610:PRO:CD	2.22	1.08
17:Q:110:MET:HG2	18:R:222:SER:HB2	1.08	1.08
2:B:883:THR:O	2:B:884:ASN:C	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:LYS:CB	5:E:48:PRO:CD	2.13	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
1:A:264:VAL:HB	1:A:272:ASN:CG	1.75	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:264:VAL:C	1:A:272:ASN:ND2	2.08	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
17:Q:23:ARG:NH1	18:R:206:LYS:HG2	1.70	1.03
17:Q:188:TYR:CE1	18:R:211:SER:HB3	1.93	1.02
2:B:292:PHE:CD2	9:I:14:ILE:HD13	1.94	1.01
1:A:425:ASP:CG	13:M:39:LEU:HD11	1.79	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
1:A:1290:SER:OG	2:B:250:SER:O	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:5:ASN:C	3:C:7:PRO:HD3	1.73	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
2:B:56:GLN:CD	20:T:140:ARG:NH1	2.17	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
1:A:156:GLY:CA	1:A:181:HIS:ND1	2.28	0.96
3:C:157:GLN:CD	10:J:65:LEU:CB	2.32	0.95
17:Q:184:ILE:CD1	18:R:213:ASP:CG	2.27	0.95
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
1:A:1117:VAL:O	1:A:1118:THR:C	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:ALA:CB	25:I:202:ZN:ZN	1.46	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
1:A:264:VAL:O	1:A:272:ASN:ND2	2.03	0.91
17:Q:113:ARG:HD2	18:R:221:ARG:C	1.90	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
9:I:57:LYS:C	9:I:58:ILE:HG12	1.92	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: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
5:E:48:PRO:O	5:E:50:GLU:N	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
17:Q:184:ILE:CD1	18:R:213:ASP:OD1	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:GLN:HE21	10:J:65:LEU:HB3	1.03	0.83
17:Q:21:VAL:C	18:R:210:PHE:CE2	2.52	0.83
1:A:133:SER:C	1:A:135:GLY:H	1.80	0.82
13:M:178:LYS:C	20:T:154:LYS:HB2	1.99	0.82
1:A:623:PRO:O	1:A:625:ASP:N	2.12	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
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
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
20:T:139:VAL:C	20:T:141:LEU:H	1.83	0.81
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.63	0.81
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
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
17:Q:101:ASN:C	17:Q:103:VAL:H	1.80	0.81
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.13	0.80
16:P:159:SER:CB	16:P:329:TYR:CG	2.64	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
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
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.61	0.79
17:Q:23:ARG:HH22	18:R:206:LYS:HB3	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
18:R:213:ASP:C	18:R:215:GLU:H	1.82	0.78
1:A:608:THR:OG1	1:A:610:PRO:HG2	1.84	0.78
2:B:56:GLN:CD	20:T:140:ARG:HH11	1.85	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
1:A:129:ILE:O	1:A:132:LYS:HB2	1.84	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
20:T:141:LEU:C	20:T:143:GLN:OE1	2.23	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:225:LEU:O	2:B:226:GLU:C	2.22	0.76
17:Q:184:ILE:HD12	18:R:218:LYS:HZ3	1.50	0.76
18:R:194:ARG:C	18:R:196:ASP:H	1.88	0.76
9:I:103:ARG:C	9:I:105:GLU:N	2.34	0.76
13:M:44:ARG:HE	13:M:46:ILE:HG23	1.50	0.76
14:N:343:HIS:NE2	21:X:9:DC:OP1	2.19	0.76
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
5:E:64:HIS:C	5:E:66:ASP:H	1.89	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:103:ARG:C	9:I:105:GLU:H	1.92	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
7:G:97:LEU:HB2	7:G:108:ILE:HB	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
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:612:ASP:C	1:A:614:ASP:H	1.91	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
1:A:622:SER:C	1:A:624:GLY:H	1.93	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
13:M:179:GLU:HA	20:T:154:LYS:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:O	1:A:154:CYS:C	2.28	0.71
1:A:926:ASN:ND2	1:A:932:ARG:HG2	2.06	0.71
17:Q:24:GLY:HA2	18:R:209:GLN:CD	2.11	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
2:B:56:GLN:CG	20:T:140:ARG:NH1	2.54	0.70
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
13:M:94:ASP:CG	13:M:97:GLY:O	2.30	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:101:ASN:C	17:Q:103:VAL:N	2.43	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
9:I:119:CYS:SG	9:I:120:GLY:N	2.64	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
18:R:213:ASP:C	18:R:215:GLU:N	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:686:THR:OG1	1:A:687:ILE:N	2.26	0.68
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
1:A:1086:MET:O	1:A:1088:GLY:N	2.27	0.68
1:A:1116:ASN:C	1:A:1118:THR:H	1.97	0.68
17:Q:188:TYR:CZ	18:R:210:PHE:CE1	2.65	0.68
9:I:85:PRO:C	9:I:86:CYS:O	2.31	0.68
3:C:157:GLN:HG3	10:J:65:LEU:HB2	1.73	0.68
2:B:92:TYR:CB	20:T:145:LEU:CD1	2.59	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
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
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
1:A:207:GLU:O	1:A:209:SER:N	2.27	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
17:Q:187:ILE:CG2	18:R:210:PHE:C	2.62	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:264:VAL:C	1:A:272:ASN:CB	2.64	0.66
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.59	0.66
1:A:775:LYS:HB3	2:B:974:SER:OG	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:ASP:O	11:K:113:GLN:N	2.28	0.66
17:Q:112:ARG:NH2	18:R:237:LEU:CB	2.58	0.66
1:A:929:ALA:C	1:A:931:ARG:H	2.00	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
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
2:B:834:ARG:O	2:B:885:ARG:NH1	2.24	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
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
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
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:622:SER:C	1:A:624:GLY:N	2.50	0.65
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.12	0.65
18:R:227:SER:O	18:R:228:MET:O	2.14	0.65
1:A:608:THR:O	1:A:610:PRO:HD2	1.94	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
3:C:212:ASP:C	3:C:214:ASP:N	2.50	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
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
1:A:67:ARG:H	1:A:78:MET:HE1	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
20:T:141:LEU:C	20:T:141:LEU:HD22	2.18	0.63
1:A:618:TYR:C	1:A:620:HIS:H	2.01	0.63
2:B:73:HIS:C	2:B:75:SER:H	2.01	0.63
2:B:298:MET:SD	9:I:13:GLY:C	2.77	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
14:N:319:ASP:C	14:N:321:SER:H	2.01	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
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:152:ASN:C	1:A:153:ILE:HG12	2.16	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
8:H:23:ASP:O	8:H:25:VAL:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:375:ILE:HB	1:A:666:ARG:HD2	1.80	0.62
6:F:125:ILE:HG22	6:F:127:ASP:H	1.63	0.62
9:I:14:ILE:HG23	9:I:14:ILE:O	1.99	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
1:A:265:VAL:C	1:A:272:ASN:ND2	2.52	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
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:225:LEU:C	2:B:227:ASN:N	2.52	0.61
2:B:461:GLN:NE2	21:X:43:DT:O2	2.34	0.61
9:I:116:ALA:HB2	25:I:202:ZN:ZN	1.26	0.61
18:R:194:ARG:C	18:R:196:ASP:N	2.54	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:610:PRO:C	1:A:626:THR:HG21	2.20	0.61
17:Q:42:CYS:C	17:Q:95:ASN:HD21	2.04	0.61
1:A:153:ILE:O	1:A:153:ILE:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:SER:HB2	2:B:250:SER:HB2	1.79	0.61
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
1:A:265:VAL:N	1:A:272:ASN:HD22	1.95	0.61
1:A:486:LEU:HD22	2:B:790:GLN:CD	2.22	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: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
2:B:1005:ALA:C	2:B:1007:ASN:H	2.04	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
3:C:212:ASP:C	3:C:214:ASP:H	2.03	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
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:930:LEU:O	1:A:931:ARG:O	2.20	0.60
8:H:64:LEU:C	8:H:66:GLU:H	2.05	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
18:R:166:ILE:HG22	18:R:168:LEU:H	1.66	0.60
2:B:553:LEU:HD13	2:B:573:TRP:CZ3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:621:ILE:HG22	1:A:621:ILE:O	2.01	0.59
17:Q:113:ARG:CD	18:R:222:SER:CA	2.77	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
22:Y:49:DG:H2'	22:Y:50:DA:C8	2.37	0.58
1:A:355:MET:HE1	1:A:1431:SER:HB2	1.84	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
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
5:E:64:HIS:C	5:E:66:ASP:N	2.56	0.58
17:Q:184:ILE:CD1	18:R:218:LYS:HZ2	2.14	0.58
2:B:74:ALA:C	2:B:75:SER:OG	2.40	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:619:LYS:C	1:A:620:HIS:CG	2.76	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
13:M:44:ARG:CZ	13:M:46:ILE:CG2	2.80	0.58
1:A:1307:VAL:HG21	1:A:1339:ASP:N	2.18	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
13:M:39:LEU:C	13:M:40:VAL:HG22	2.24	0.58
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
2:B:422:PHE:CD1	2:B:422:PHE:C	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1116:ASN:C	1:A:1118:THR:N	2.57	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: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:133:SER:C	1:A:135:GLY:N	2.46	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: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
2:B:94:SER:O	2:B:122:ALA:HB1	2.05	0.56
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:425:ASP:HB2	13:M:39:LEU:CG	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.87	0.56
18:R:163:LEU:O	18:R:164:GLY:C	2.42	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:263:ALA:C	1:A:265:VAL:H	2.09	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
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
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:65:ILE:HA	1:A:78:MET:HE2	1.88	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
13:M:72:ASN:HB2	22:Y:58:DC:H42	1.70	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:187:ILE:HG21	18:R:210:PHE:C	2.27	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: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
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	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
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: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
8:H:106:THR:O	8:H:108:ALA:N	2.37	0.54
9:I:61:GLU:C	9:I:63:ASP:H	2.08	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:285:LYS:HD2	13:M:80:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:Q:113:ARG:NH1	18:R:218:LYS:C	2.59	0.54
22:Y:64:DC:H2"	22:Y:65:DG:H5'	1.89	0.54
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.89	0.54
2:B:1162:LEU:HD23	2:B:1165:MET:HE3	1.90	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
17:Q:21:VAL:CA	18:R:210:PHE:CE2	2.91	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: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
17:Q:112:ARG:NH2	18:R:237:LEU:HD22	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:C:56:SER:HG	3:C:158:GLU:H	1.55	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: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
7:G:104:MET:HE2	7:G:159:ALA:HB2	1.91	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:132:VAL:HG21	2:B:141:GLN:CD	2.29	0.52
2:B:800:ALA:O	2:B:805:PHE:HB2	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1098:PRO:O	1:A:1101:GLN:CD	2.48	0.52
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.35	0.52
2:B:822:GLY:HA3	2:B:825:GLN:HG2	1.92	0.52
3:C:4:ALA:HA	11:K:52:LYS:HZ1	1.74	0.52
6:F:64:ARG:HH12	7:G:61:PRO:HB3	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1053:HIS:CE1	2:B:1058:LYS:HE3	2.45	0.51
8:H:17:PRO:C	8:H:19:GLY:H	2.13	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
2:B:214:LYS:O	2:B:240:LEU:HD12	2.11	0.51
9:I:91:HIS:ND1	9:I:92:LYS:O	2.43	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
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:266:MET:HG2	1:A:272:ASN:CG	2.29	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
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
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1151:MET:HE1	2:B:1171:MET:SD	2.50	0.51
14:N:347:ASN:O	14:N:375:GLU:HA	2.11	0.51
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.41	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
3:C:157:GLN:CD	10:J:65:LEU:CG	2.79	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:930:LEU:O	1:A:931:ARG:C	2.49	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:S:172:ASN:OD1	19:S:173:HIS:N	2.45	0.50
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
9:I:57:LYS:C	9:I:58:ILE:CG1	2.75	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
2:B:225:LEU:O	2:B:227:ASN:C	2.51	0.50
3:C:142:TYR:O	3:C:144:GLU:N	2.45	0.50
3:C:212:ASP:O	3:C:213:GLU:C	2.50	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
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:273:GLN:O	1:A:274:ASP:C	2.49	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:612:ASP:C	1:A:614:ASP:N	2.62	0.49
17:Q:70:LYS:NZ	18:R:230:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1473:LEU:HD13	6:F:104:ILE:HD12	1.94	0.49
15:O:48:LEU:HD23	15:O:52:VAL:HG21	1.93	0.49
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:883:ILE:HG21	1:A:1424:THR:HA	1.93	0.49
13:M:52:TRP:C	13:M:54:THR:H	2.16	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:131:ALA:C	1:A:133:SER:N	2.56	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
1:A:358:ARG:HE	2:B:1076:GLU:CD	2.16	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: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
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:1290:SER:OG	2:B:250:SER:C	2.48	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
2:B:1080:ARG:NH1	13:M:53:ARG:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:266:MET:HE2	13:M:52:TRP:CE2	2.49	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:312:PHE:HB2	13:M:101:TYR:OH	2.14	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
18:R:161:ARG:HG3	18:R:161:ARG:O	2.13	0.48
20:T:217:LEU:HB3	20:T:233:TRP:CE3	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
1:A:930:LEU:C	1:A:931:ARG:O	2.50	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:540:ASP:HB3	2:B:790:GLN:HG2	1.96	0.48
1:A:623:PRO:C	1:A:625:ASP:N	2.67	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
12:L:13:GLN:C	12:L:15:MET:H	2.17	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
17:Q:106:LYS:NZ	18:R:223:VAL:O	2.33	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
2:B:1075:MET:HE3	13:M:51:GLU:HG2	1.96	0.47
5:E:173:ILE:CG2	5:E:209:VAL:HG22	2.44	0.47
14:N:317:GLU:C	14:N:318:ASP:O	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:485:ASN:C	1:A:485:ASN:OD1	2.52	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:8:PHE:H	10:J:48:MET:HE1	1.80	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
1:A:360:ASP:CG	2:B:1064:ARG:H	2.17	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
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.40	0.47
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
2:B:896:LEU:C	2:B:897:ARG:HG3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:N:333:ASN:CG	14:N:361:ASN:H	2.19	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
1:A:926:ASN:CG	1:A:931:ARG:HB3	2.35	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: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
13:M:196:LYS:NZ	21:X:13:DT:OP1	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.54	0.46
1:A:687:ILE:HG13	1:A:691:ASP:OD2	2.16	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
8:H:64:LEU:C	8:H:66:GLU:N	2.69	0.46
9:I:61:GLU:C	9:I:63:ASP:N	2.69	0.46
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.15	0.46
17:Q:184:ILE:CD1	18:R:218:LYS:HZ3	2.18	0.46
20:T:211:VAL:O	20:T:215:GLU:HG2	2.15	0.46
1:A:265:VAL:C	1:A:272:ASN:HD22	2.19	0.46
2:B:203:ASN:O	2:B:204:THR:OG1	2.27	0.46
9:I:84:HIS:ND1	9:I:85:PRO:CD	2.77	0.46
16:P:298:PRO:O	16:P:299:ARG:C	2.53	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:74:ALA:HB2	20:T:201:ASP:CG	2.35	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:N	3:C:136:ASP:OD1	2.49	0.46
11:K:49:GLN:HG3	11:K:94:LEU:HB2	1.97	0.46
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:264:VAL:C	1:A:272:ASN:CG	2.70	0.46
1:A:795:GLY:HA3	1:A:1107:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:157:GLN:CD	10:J:65:LEU:HG	2.36	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
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: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
13:M:94:ASP:HB3	13:M:99:SER:C	2.36	0.46
14:N:376:TRP:HD1	15:O:62:LEU:O	1.98	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
3:C:131:THR:HB	3:C:147:ASP:OD1	2.15	0.45
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
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
8:H:108:ALA:O	8:H:109:ALA:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:M:10:LEU:C	13:M:12:ARG:N	2.69	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
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
1:A:959:MET:HE1	1:A:1046:ARG:O	2.17	0.45
1:A:1484:MET:SD	7:G:20:PRO:HA	2.57	0.45
2:B:73:HIS:C	2:B:75:SER:N	2.66	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
17:Q:105:TYR:OH	18:R:234:GLU:CD	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
1:A:622:SER:O	1:A:623:PRO:C	2.48	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
1:A:1160:ARG:NH1	1:A:1349:GLU:OE2	2.50	0.44
2:B:899:SER:C	2:B:901:THR:H	2.21	0.44
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.82	0.44
12:L:26:ASN:HB2	12:L:44:MET:HE1	1.98	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:374:SER:C	1:A:485:ASN:HD22	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:N:317:GLU:O	14:N:318:ASP:C	2.56	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
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:878:ASP:C	2:B:879:GLU:O	2.55	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
20:T:141:LEU:C	20:T:141:LEU:CD2	2.86	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: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
9:I:59:THR:OG1	9:I:60:HIS:N	2.51	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
16:P:171:THR:HG21	21:X:16:DA:H4'	1.99	0.44
17:Q:70:LYS:HZ2	18:R:226:ASP:HA	1.83	0.44
17:Q:98:THR:H	17:Q:98:THR:HG1	1.58	0.44
22:Y:70:DC:H2"	22:Y:71:DA:H8	1.82	0.44
1:A:152:ASN:C	1:A:153:ILE:CG1	2.79	0.44
1:A:278:HIS:HB3	13:M:82:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:139:VAL:C	20:T:141:LEU:N	2.50	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
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
2:B:1079:SER:C	2:B:1080:ARG:HD2	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:LEU:C	1:A:1300:GLY:H	2.21	0.43
3:C:45:ILE:HG22	3:C:73:LEU:HD12	2.00	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:264:VAL:C	1:A:272:ASN:HB3	2.37	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
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: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
17:Q:127:PHE:HA	17:Q:163:GLU:C	2.39	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
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:231:GLU:H	1:A:231:GLU:CD	2.19	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
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
1:A:459:ASN:C	1:A:459:ASN:OD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:I:62:VAL:O	9:I:63:ASP:C	2.45	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:546:ARG:HG2	1:A:546:ARG:O	2.18	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
20:T:141:LEU:C	20:T:143:GLN:N	2.72	0.43
20:T:150:THR:C	20:T:152:ASN:H	2.22	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:375:ILE:HG13	1:A:666:ARG:NH1	2.34	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
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: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:878:ASP:O	2:B:879:GLU:C	2.56	0.42
2:B:993:LYS:HA	2:B:1018:TYR:OH	2.19	0.42
20:T:154:LYS:H	20:T:154:LYS:CD	2.31	0.42
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.54	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:882:SER:C	1:A:884:ASN:H	2.22	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
20:T:143:GLN:O	20:T:144:GLN:C	2.58	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:CYS:H	1:A:630:VAL:CG1	2.33	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:105:TYR:CE1	18:R:234:GLU:CD	2.93	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
21:X:80:DC:H42	22:Y:14:DG:H1	1.67	0.42
1:A:266:MET:HE3	13:M:68:GLY:O	2.19	0.42
1:A:275:ASP:HA	1:A:278:HIS:HD2	1.84	0.42
1:A:344:LYS:HZ1	22:Y:43:DG:H5”	1.83	0.42
1:A:539:GLN:NE2	2:B:791:GLU:OE2	2.52	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
2:B:908:MET:CE	2:B:920:LYS:HB2	2.50	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
21:X:18:DG:OP2	21:X:18:DG:H2’	2.20	0.42
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	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
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:486:LEU:O	1:A:486:LEU:HG	2.19	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
20:T:213:LEU:HA	20:T:213:LEU:HD23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:Q:184:ILE:HG13	18:R:218:LYS:HZ2	1.85	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
8:H:81:ARG:C	8:H:83:SER:H	2.23	0.41
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:128:LYS:NZ	20:T:131:GLN:OE1	2.52	0.41
20:T:140:ARG:NE	20:T:140:ARG:CA	2.73	0.41
20:T:153:TYR:CD1	20:T:153:TYR:C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ASN:CG	19:S:153:ARG:HD2	2.40	0.41
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.99	0.41
15:O:41:ASP:O	15:O:45:ASN:ND2	2.37	0.41
17:Q:108:ASP:CG	18:R:237:LEU:HD22	2.39	0.41
21:X:35:DT:H6	21:X:35:DT:H2'	1.75	0.41
1:A:155:GLU:O	1:A:181:HIS:ND1	2.54	0.41
1:A:618:TYR:C	1:A:620:HIS:N	2.71	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
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
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
9:I:62:VAL:C	9:I:64:GLU:N	2.57	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:800:PHE:HD1	1:A:805:ARG:C	2.23	0.41
1:A:901:VAL:HB	1:A:978:VAL:HG13	2.01	0.41
1:A:908:THR:C	1:A:910:LYS:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
17:Q:202:GLU:C	17:Q:204:LEU:H	2.23	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: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
1:A:1302:GLU:HG3	1:A:1304:ILE:HG12	2.02	0.41
2:B:554:GLU:OE1	19:S:115:LYS:HG3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:MET:HE3	2:B:624:PRO:HD2	2.03	0.41
2:B:751:LEU:HD12	2:B:751:LEU:HA	1.90	0.41
3:C:10:ARG:HH21	3:C:24:GLU:CD	2.23	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
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
2:B:1054:MET:HE3	2:B:1054:MET:HB2	1.78	0.40
10:J:10:CYS:SG	10:J:11:GLY:N	2.94	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:108:ALA:O	8:H:110:THR:OG1	2.35	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:384:ASP:OD1	2:B:386:ASP:N	2.38	0.40
2:B:402:PHE:CD1	2:B:402:PHE:C	2.95	0.40
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.03	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
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%)	3 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1163/1174 (99%)	999 (86%)	120 (10%)	44 (4%)	3	28
3	C	273/275 (99%)	241 (88%)	22 (8%)	10 (4%)	3	29
4	D	127/142 (89%)	119 (94%)	8 (6%)	0	100	100
5	E	208/210 (99%)	191 (92%)	11 (5%)	6 (3%)	4	33
6	F	84/127 (66%)	82 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	25	63
8	H	148/150 (99%)	117 (79%)	22 (15%)	9 (6%)	1	20
9	I	123/125 (98%)	90 (73%)	18 (15%)	15 (12%)	0	6
10	J	65/67 (97%)	51 (78%)	8 (12%)	6 (9%)	1	12
11	K	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	9	43
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	2	25
13	M	308/316 (98%)	266 (86%)	31 (10%)	11 (4%)	3	29
14	N	109/376 (29%)	101 (93%)	6 (6%)	2 (2%)	8	42
15	O	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
16	P	183/339 (54%)	172 (94%)	5 (3%)	6 (3%)	4	31
17	Q	176/439 (40%)	158 (90%)	10 (6%)	8 (4%)	2	25
18	R	163/291 (56%)	140 (86%)	15 (9%)	8 (5%)	2	24
19	S	134/517 (26%)	120 (90%)	10 (8%)	4 (3%)	4	33
20	T	218/249 (88%)	190 (87%)	19 (9%)	9 (4%)	3	27
All	All	5357/7223 (74%)	4702 (88%)	453 (8%)	202 (4%)	5	28

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1279/1748 (73%)	1234 (96%)	45 (4%)	36	62
2	B	1020/1028 (99%)	980 (96%)	40 (4%)	32	59
3	C	252/252 (100%)	245 (97%)	7 (3%)	43	66
4	D	119/126 (94%)	118 (99%)	1 (1%)	81	89
5	E	192/192 (100%)	187 (97%)	5 (3%)	46	68
6	F	74/111 (67%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	152/153 (99%)	151 (99%)	1 (1%)	84	90
8	H	131/131 (100%)	126 (96%)	5 (4%)	33	59
9	I	112/112 (100%)	107 (96%)	5 (4%)	27	56
10	J	56/56 (100%)	53 (95%)	3 (5%)	22	52
11	K	106/106 (100%)	105 (99%)	1 (1%)	78	87
12	L	43/55 (78%)	41 (95%)	2 (5%)	26	55
13	M	263/268 (98%)	257 (98%)	6 (2%)	50	71
14	N	105/324 (32%)	104 (99%)	1 (1%)	76	86
15	O	90/98 (92%)	89 (99%)	1 (1%)	73	84
16	P	159/293 (54%)	157 (99%)	2 (1%)	69	82
17	Q	164/373 (44%)	159 (97%)	5 (3%)	41	64
18	R	150/261 (58%)	143 (95%)	7 (5%)	26	55
19	S	121/448 (27%)	118 (98%)	3 (2%)	47	69
20	T	196/218 (90%)	188 (96%)	8 (4%)	30	58
All	All	4784/6353 (75%)	4636 (97%)	148 (3%)	43	64

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	65	ILE
1	A	74	CYS
1	A	132	LYS
1	A	204	HIS
1	A	205	VAL
1	A	259	SER
1	A	261	ARG
1	A	265	VAL
1	A	271	ARG
1	A	286	ILE
1	A	303	ILE
1	A	449	HIS
1	A	463	THR
1	A	502	ASN
1	A	540	ASP
1	A	567	LEU
1	A	611	ASP

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Mol	Chain	Res	Type
1	A	614	ASP
1	A	619	LYS
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	928	ARG
1	A	931	ARG
1	A	1015	GLU
1	A	1036	ASN
1	A	1077	ASN
1	A	1102	MET
1	A	1167	ARG
1	A	1279	MET
1	A	1282	ASP
1	A	1298	LEU
1	A	1307	VAL
1	A	1309	MET
1	A	1311	LEU
1	A	1337	GLU
1	A	1341	VAL
1	A	1407	CYS
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	168	ASP
2	B	222	ARG
2	B	232	THR
2	B	248	LYS
2	B	249	LYS
2	B	250	SER
2	B	338	TYR
2	B	388	TYR

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Mol	Chain	Res	Type
2	B	412	LEU
2	B	422	PHE
2	B	446	TYR
2	B	472	ARG
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	879	GLU
2	B	880	LEU
2	B	881	GLU
2	B	897	ARG
2	B	957	THR
2	B	959	GLU
2	B	1007	ASN
2	B	1056	ASP
2	B	1080	ARG
2	B	1090	GLU
2	B	1091	ARG
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	29	HIS
8	H	65	TYR

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Mol	Chain	Res	Type
8	H	66	GLU
8	H	107	GLU
9	I	14	ILE
9	I	58	ILE
9	I	60	HIS
9	I	61	GLU
9	I	71	ASP
10	J	7	CYS
10	J	47	ARG
10	J	65	LEU
11	K	48	SER
12	L	27	GLU
12	L	28	ILE
13	M	10	LEU
13	M	12	ARG
13	M	31	ASP
13	M	47	ASP
13	M	86	LYS
13	M	133	ASN
14	N	318	ASP
15	O	21	GLU
16	P	206	GLU
16	P	297	LYS
17	Q	38	ILE
17	Q	45	GLU
17	Q	138	ASP
17	Q	172	ASP
17	Q	191	LEU
18	R	100	ASP
18	R	105	GLU
18	R	152	LEU
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
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

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Mol	Chain	Res	Type
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	122	ASN
1	A	272	ASN
1	A	449	HIS
1	A	601	ASN
1	A	1077	ASN
1	A	1116	ASN
1	A	1310	HIS
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	390	ASN
2	B	716	HIS
2	B	1053	HIS
2	B	1097	HIS
3	C	137	ASN
8	H	126	GLN
11	K	84	GLN
17	Q	95	ASN

5.3.3 RNA (i)

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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

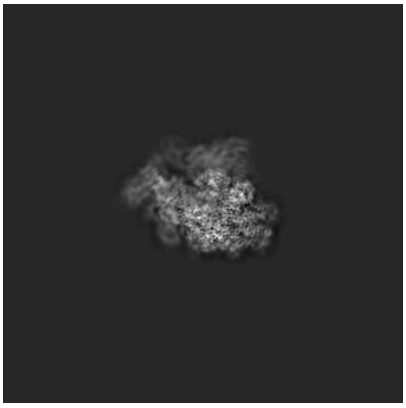
6 Map visualisation (i)

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

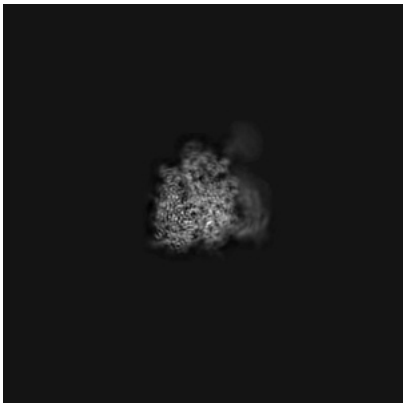
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

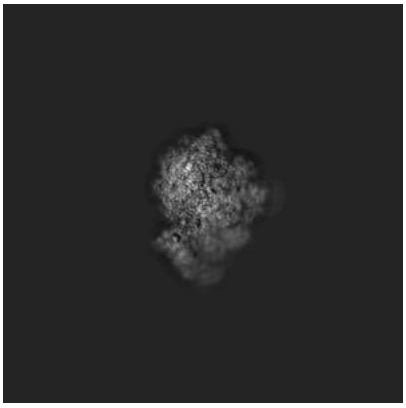
6.1.1 Primary map



X



Y



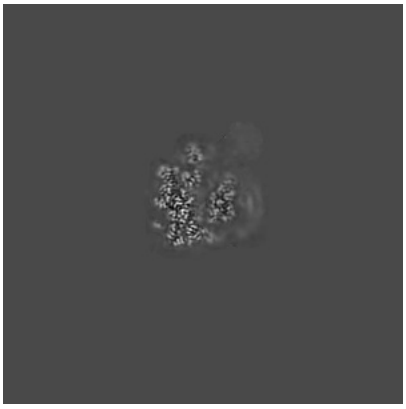
Z

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

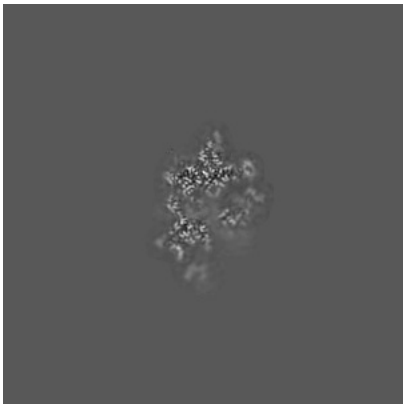
6.2 Central slices (i)

6.2.1 Primary map

X Index: 192



Y Index: 192

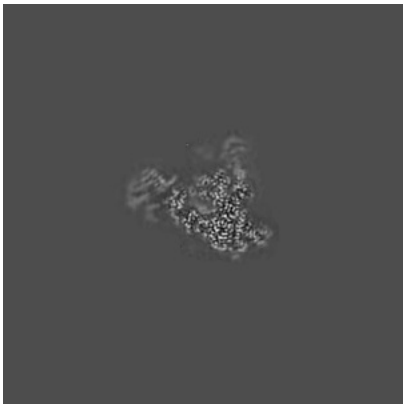


Z Index: 192

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

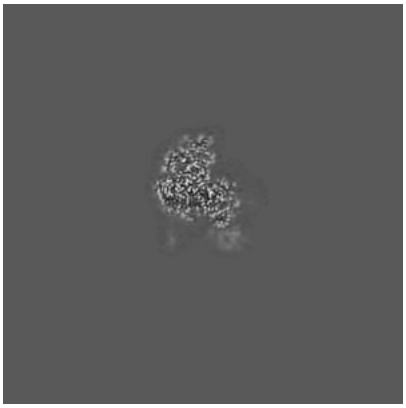
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 178

Y Index: 224

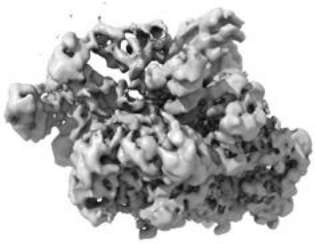


Z Index: 166

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

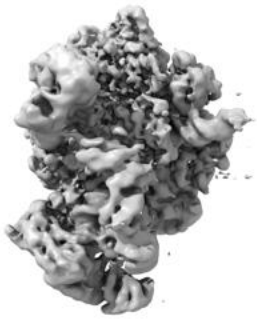
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

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

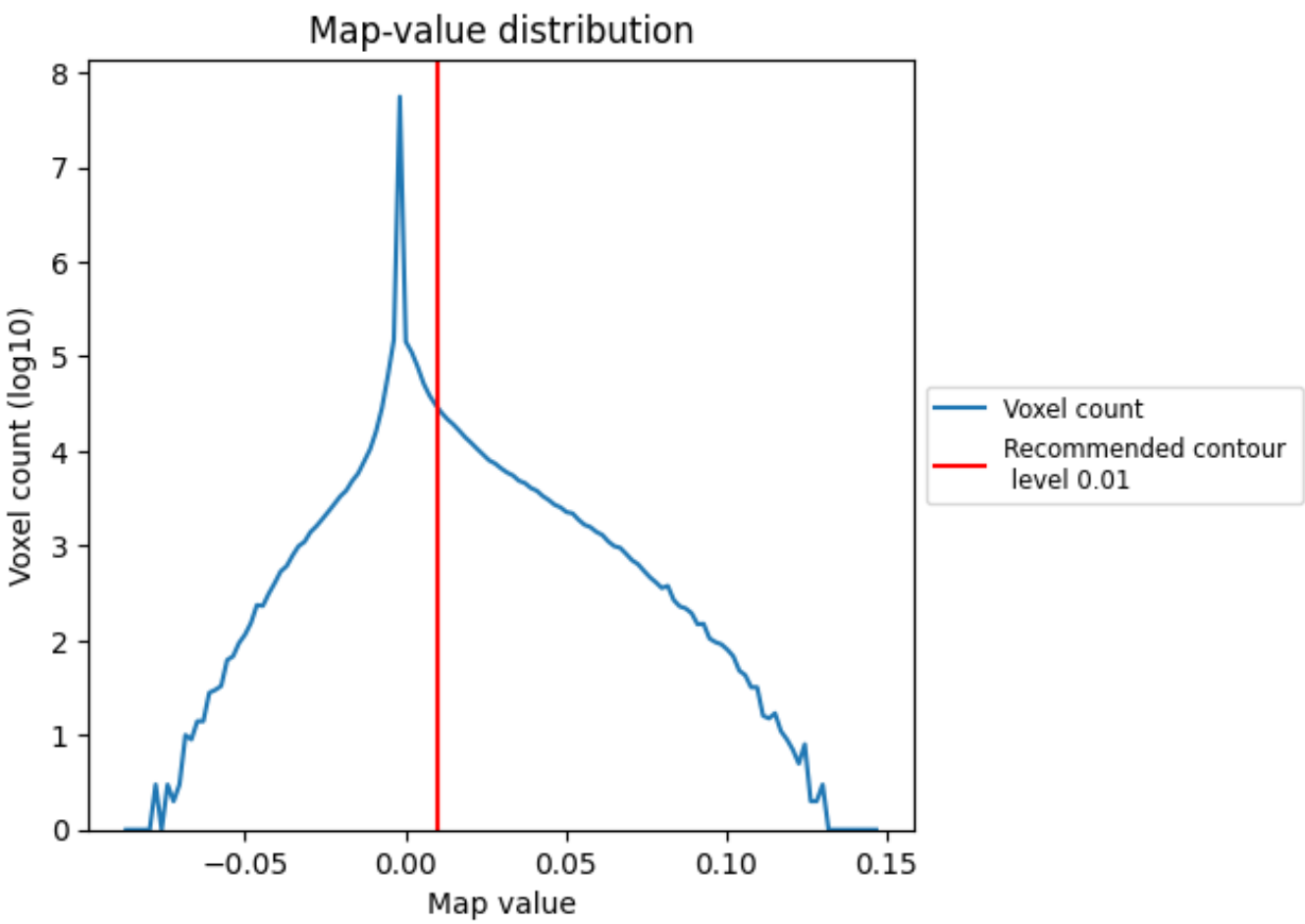
6.5 Mask visualisation (i)

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

7 Map analysis (i)

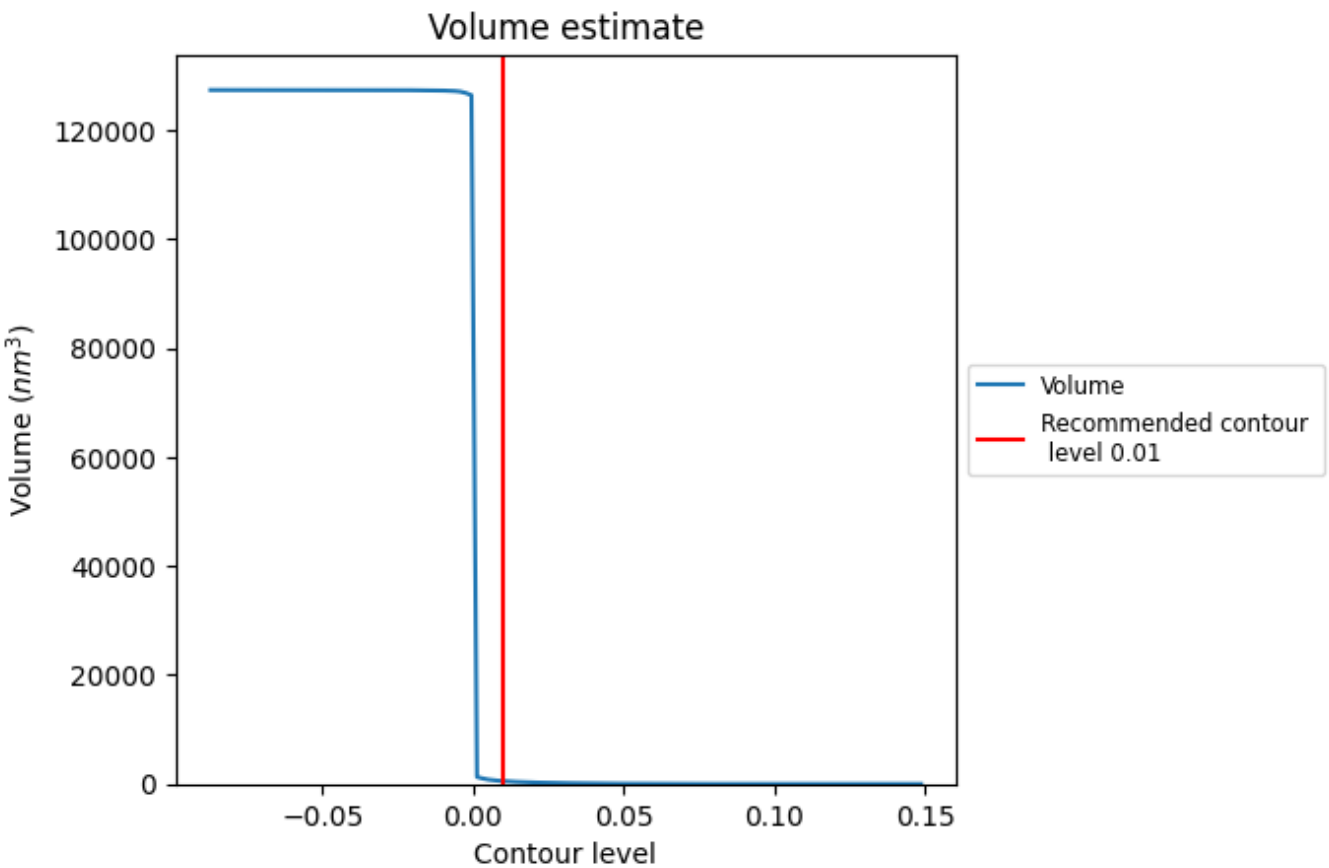
This section contains the results of statistical analysis of the map.

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.

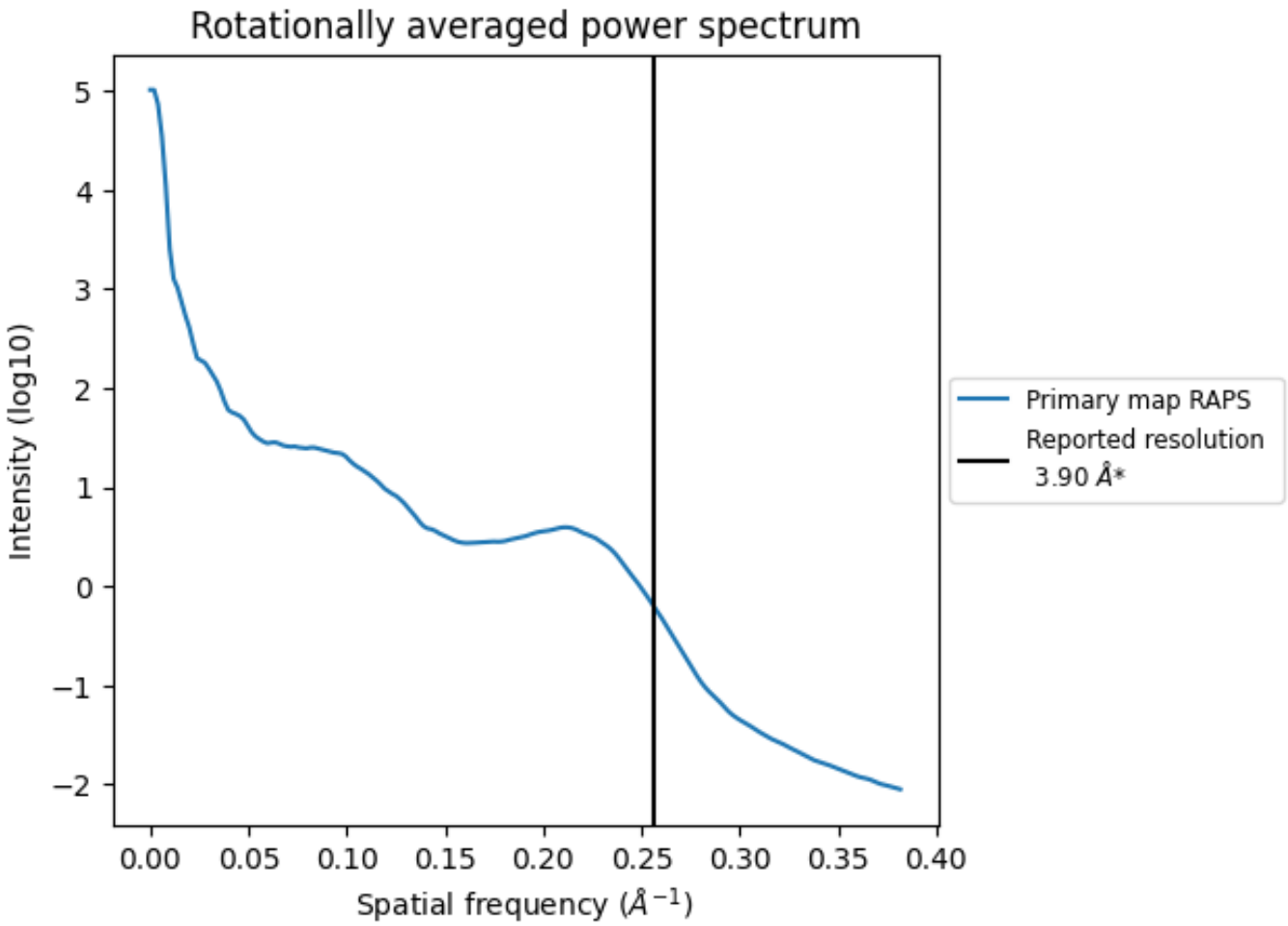
7.2 Volume estimate (i)



The volume at the recommended contour level is 526 nm^3; 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 (i)

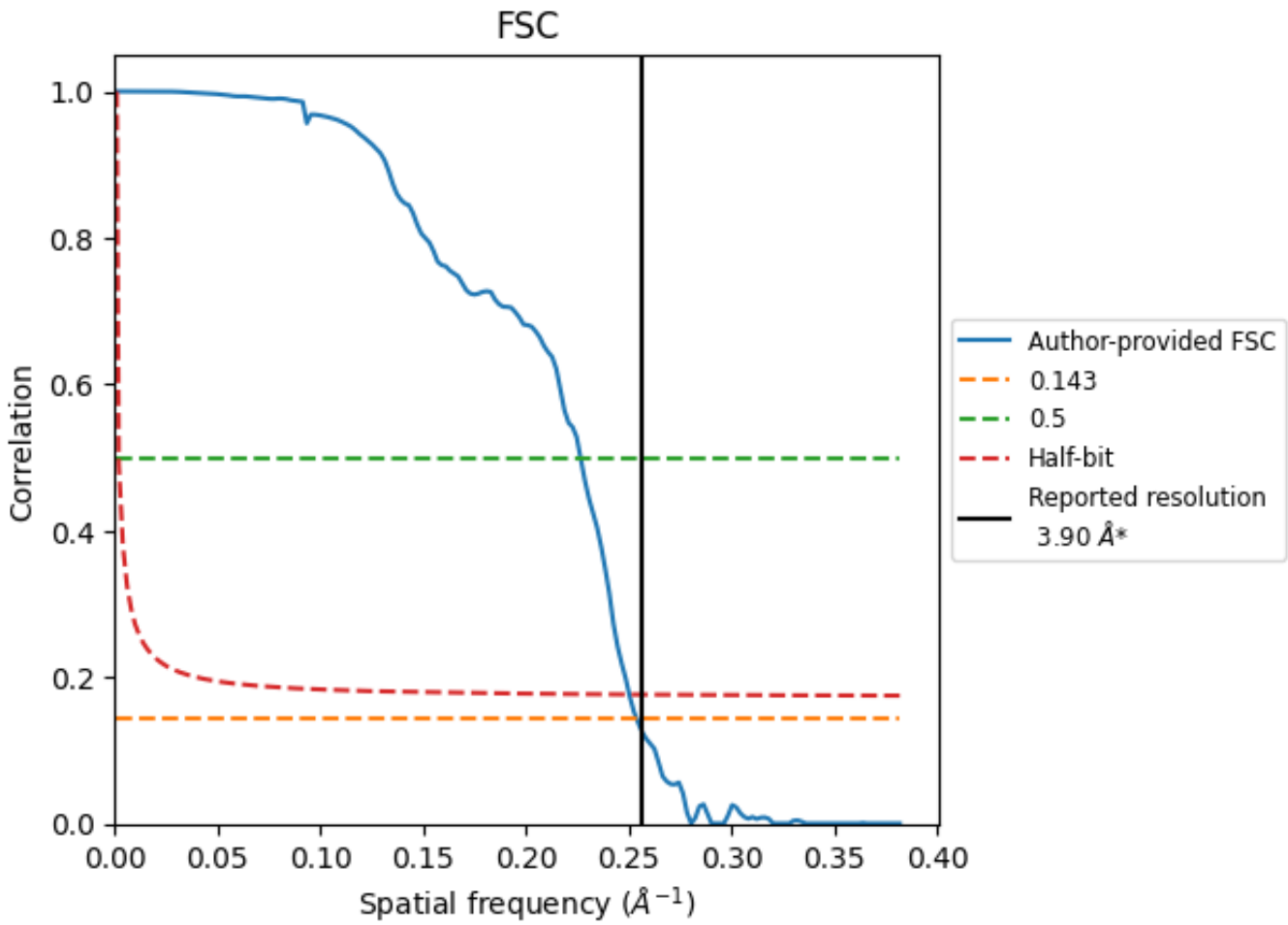


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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)

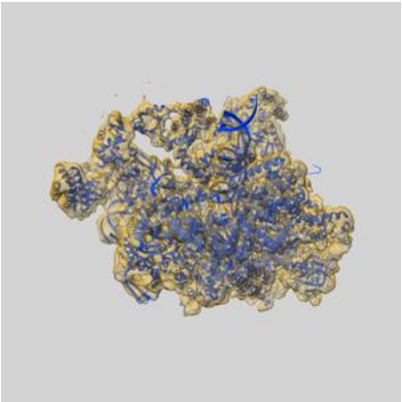
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.41	4.00
Unmasked-calculated*	-	-	-

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

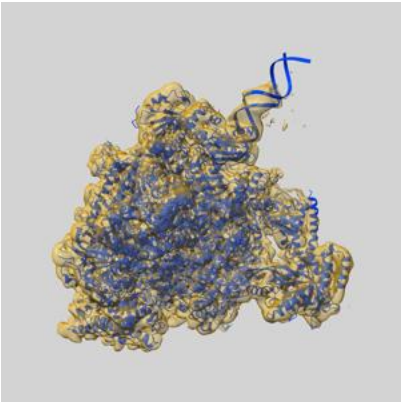
9 Map-model fit (i)

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.

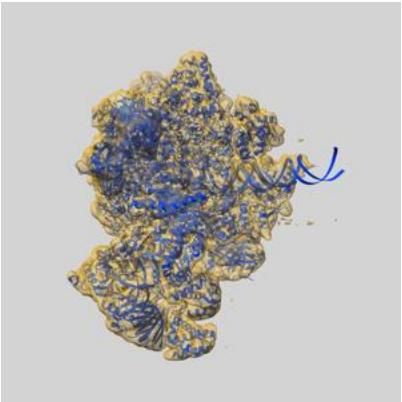
9.1 Map-model overlay (i)



X



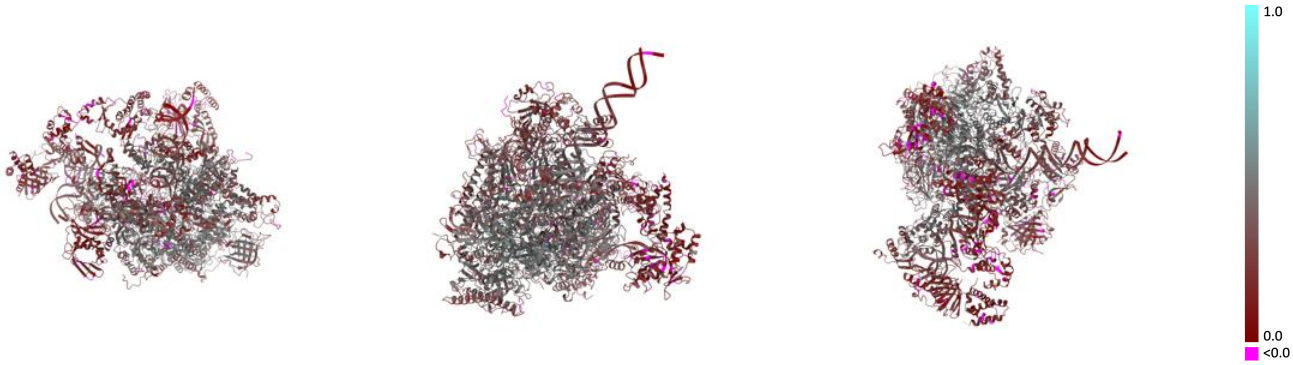
Y



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.

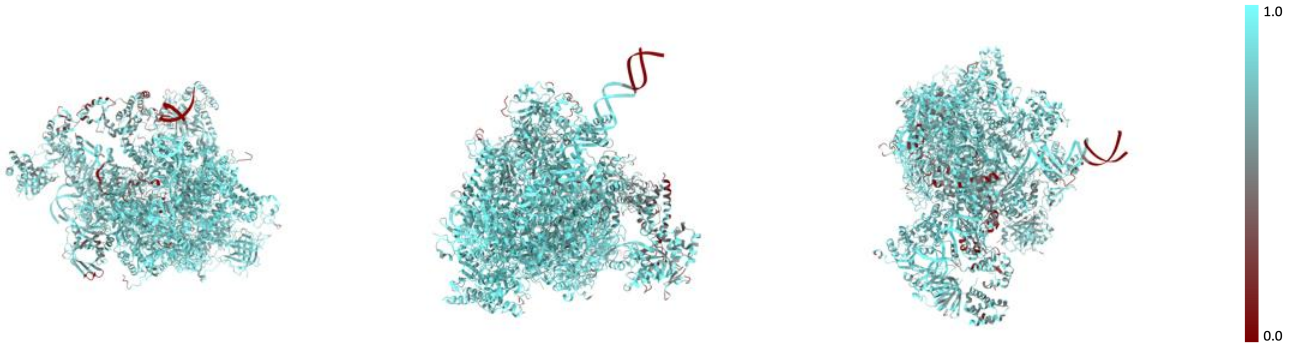
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

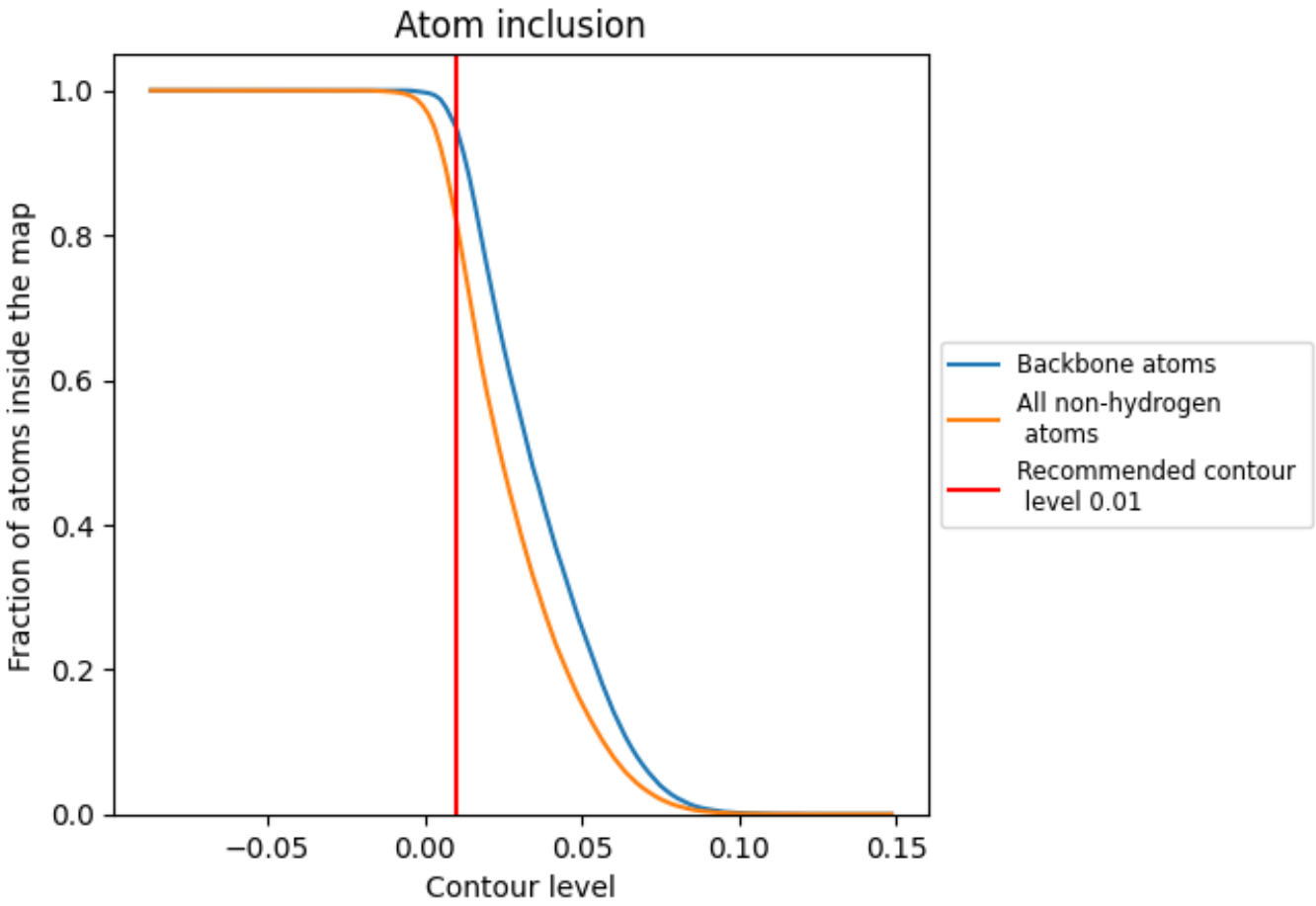
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

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 (i)

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	0.8211	0.3220
A	0.8645	0.3830
B	0.8724	0.4120
C	0.8819	0.3920
D	0.7390	0.1730
E	0.8472	0.3370
F	0.8383	0.3990
G	0.7658	0.2110
H	0.8557	0.3470
I	0.8207	0.2770
J	0.8695	0.4020
K	0.8924	0.3920
L	0.8817	0.3750
M	0.8199	0.3220
N	0.7467	0.1670
O	0.7678	0.1840
P	0.8403	0.2540
Q	0.6157	0.1490
R	0.5723	0.1220
S	0.7115	0.1650
T	0.7011	0.1810
X	0.7441	0.2230
Y	0.8387	0.2580
Z	0.8560	0.3090