Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 01:41 AM EDT

PDB ID	:	8UOQ / pdb_00008uoq
EMDB ID	:	EMD-42437
Title	:	Composite map of PIC_delta_TFIIK form2
Authors	:	Yang, C.; Murakami, K.
Deposited on	:	2023-10-20
Resolution	:	3.80 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 (1)) were used in the production of this report:

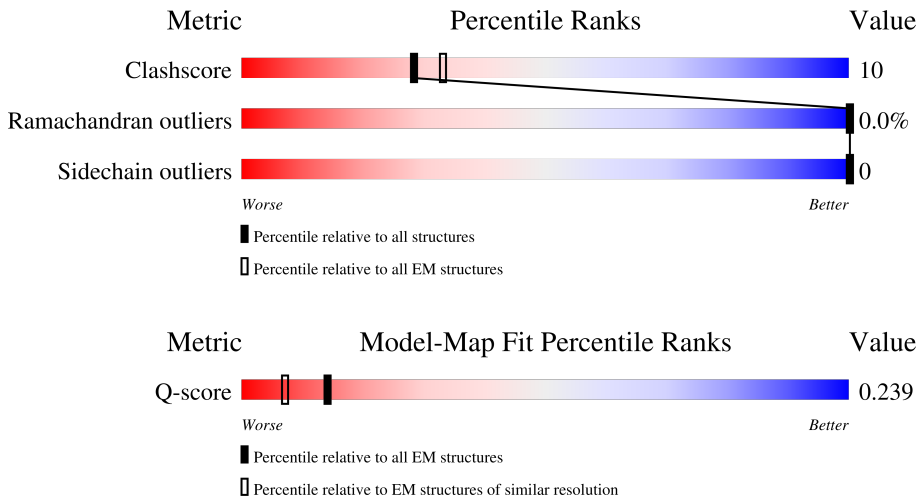
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	M	345	11%; 62%; 17%; •; 19%
2	A	1733	62%; 20%; 18%
3	B	1224	•; 71%; 24%; • 5%
4	C	318	•; 63%; 20%; 17%

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Mol	Chain	Length	Quality of chain
5	E	215	86% 14%
6	F	155	46% 9% 44%
7	H	146	64% 27% 8%
8	I	122	70% 24% 7%
9	J	70	60% 31% 6%
10	K	120	8% 81% 14%
11	L	70	46% 17% 37%
12	Q	735	24% 71%
13	P	400	33% 11% 55%
14	S	309	38% 16% 47%
15	O	240	58% 18% 25%
16	U	286	14% 25% 12% 63%
17	V	122	23% 59% 25% 15%
18	W	482	6% 40% 11% 49%
19	X	328	39% 9% 51%
20	D	221	42% 61% 15% 24%
21	G	171	21% 74% 25%
22	0	778	10% 65% 31%
23	1	642	10% 53% 12% 35%
24	4	338	70% 17% 14%
25	6	461	8% 55% 21% 23%
26	7	843	6% 52% 19% 28%
27	2	513	10% 68% 18% 13%
28	5	72	26% 60% 31% 8%
29	N	64	66% 33%

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Mol	Chain	Length	Quality of chain
30	T	64	77% 22%

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
33	SF4	0	801	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 70481 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 Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M	279	2175	1382	373	403	17	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1425	11167	7036	1948	2121	62	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	1166	9227	5823	1619	1729	56	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	265	2086	1312	347	414	13	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1752	1111	309	321	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	87	705	451	119	132	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	135	1080	679	182	214	5	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	114	927	571	168	178	10	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	66	540	345	94	95	6	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	115	924	593	157	172	2	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	44	352	217	70	61	4	0	0

- Molecule 12 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Q	214	1619	1017	297	299	6	0	0

- Molecule 13 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	179	1484	941	258	279	6	0	0

- Molecule 14 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S	164	1294	809	230	247	8	0	0

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	181	1422	925	243	248	6	0	0

- Molecule 16 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	U	107	885	559	147	176	3	0	0

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	V	104	815	511	136	164	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	W	247	2010	1275	347	381	7	0	0

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	X	160	1288	826	212	245	5	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	D	168	1331	822	237	270	2	0	0

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	171	1335	858	221	248	8	0	0

- Molecule 22 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD/RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	0	752	6091	3882	1029	1142	38	0	0

- Molecule 23 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	1	417	3382	2139	587	640	16	0	0

- Molecule 24 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	4	292	2267	1449	376	428	14	0	0

- Molecule 25 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	6	355	2786	1765	481	512	28	0	0

- Molecule 26 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	7	608	4889	3110	847	906	26	0	0

- Molecule 27 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	2	445	3546	2291	585	654	16	0	0

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	5	66	498	314	89	93	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	N	63	1288	621	225	380	62	0	0

- Molecule 30 is a DNA chain called template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	T	63	1291	619	236	373	63	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-10	DC	DT	conflict	GB 2567904391

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
31	M	1	1	1	0
31	A	2	2	2	0
31	B	1	1	1	0
31	C	1	1	1	0
31	I	2	2	2	0
31	J	1	1	1	0

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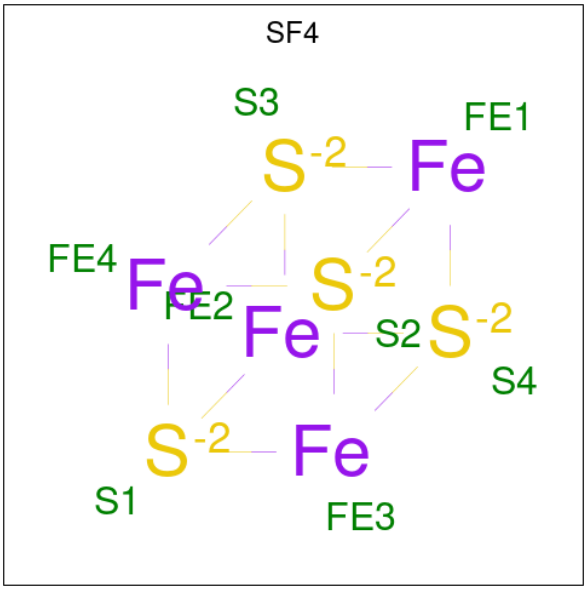
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
31	L	1	1	1	0
			Total	Zn	
31	S	1	1	1	0
			Total	Zn	
31	4	1	1	1	0
			Total	Zn	
31	6	4	4	4	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
32	A	1	1	1	0
			Total	Mg	
32	7	1	1	1	0

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



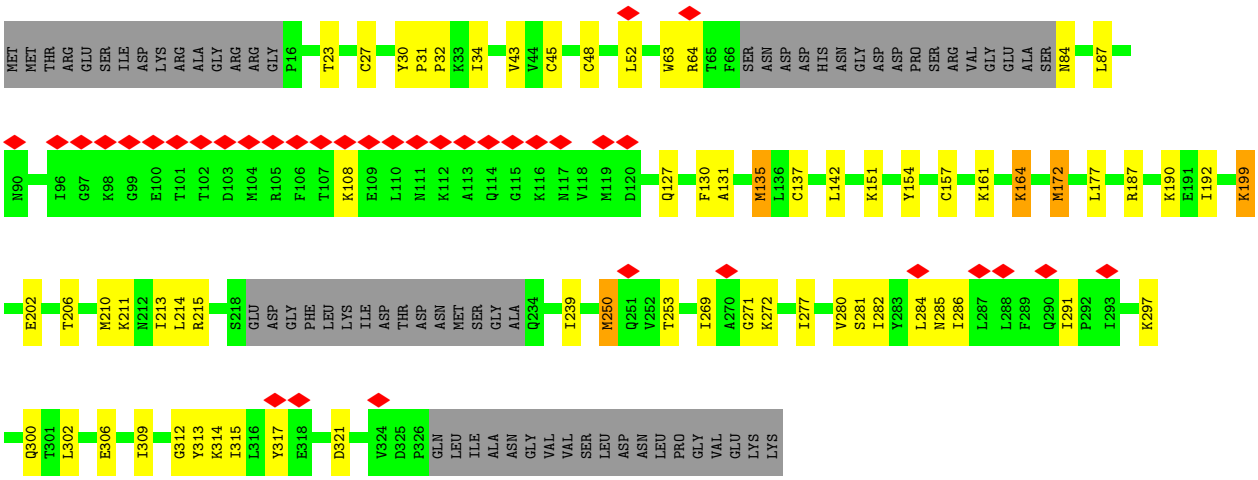
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
33	0	1	8	4	4	0

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.

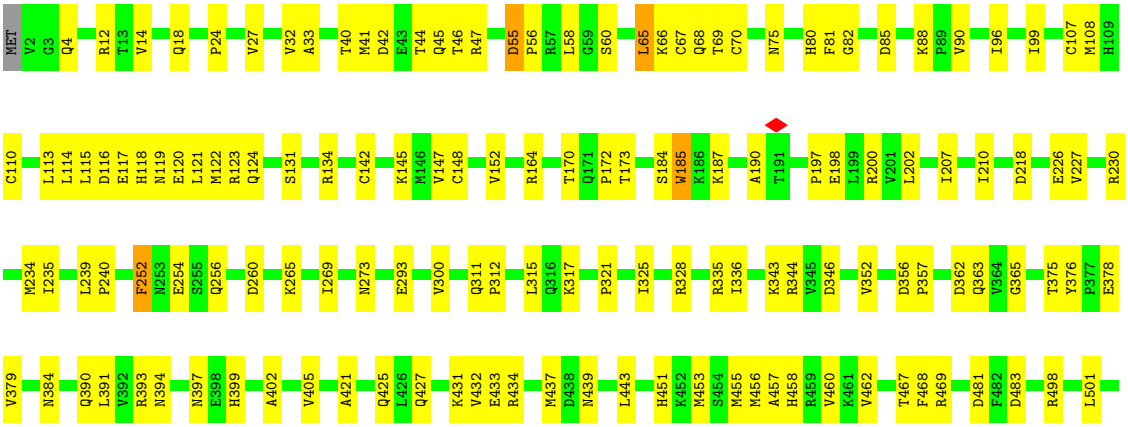
• Molecule 1: Transcription initiation factor IIB

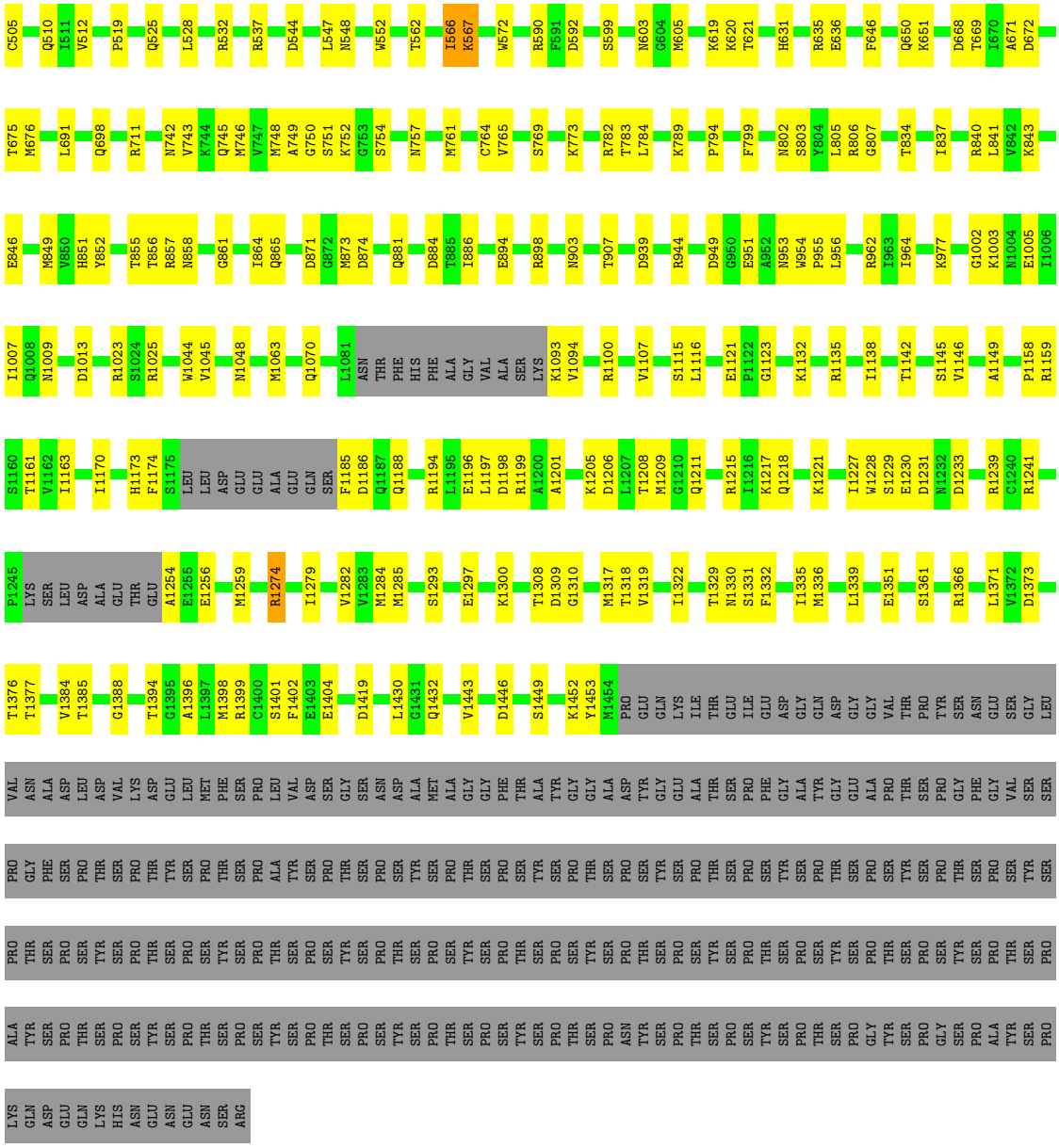
Chain M:



• Molecule 2: DNA-directed RNA polymerase II subunit RPB1

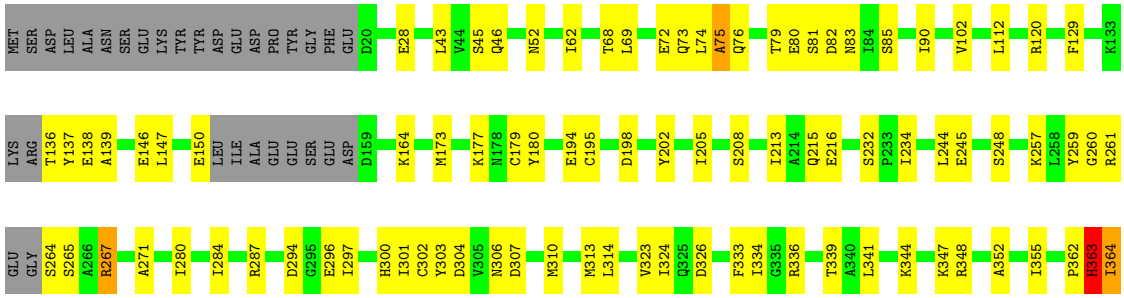
Chain A:

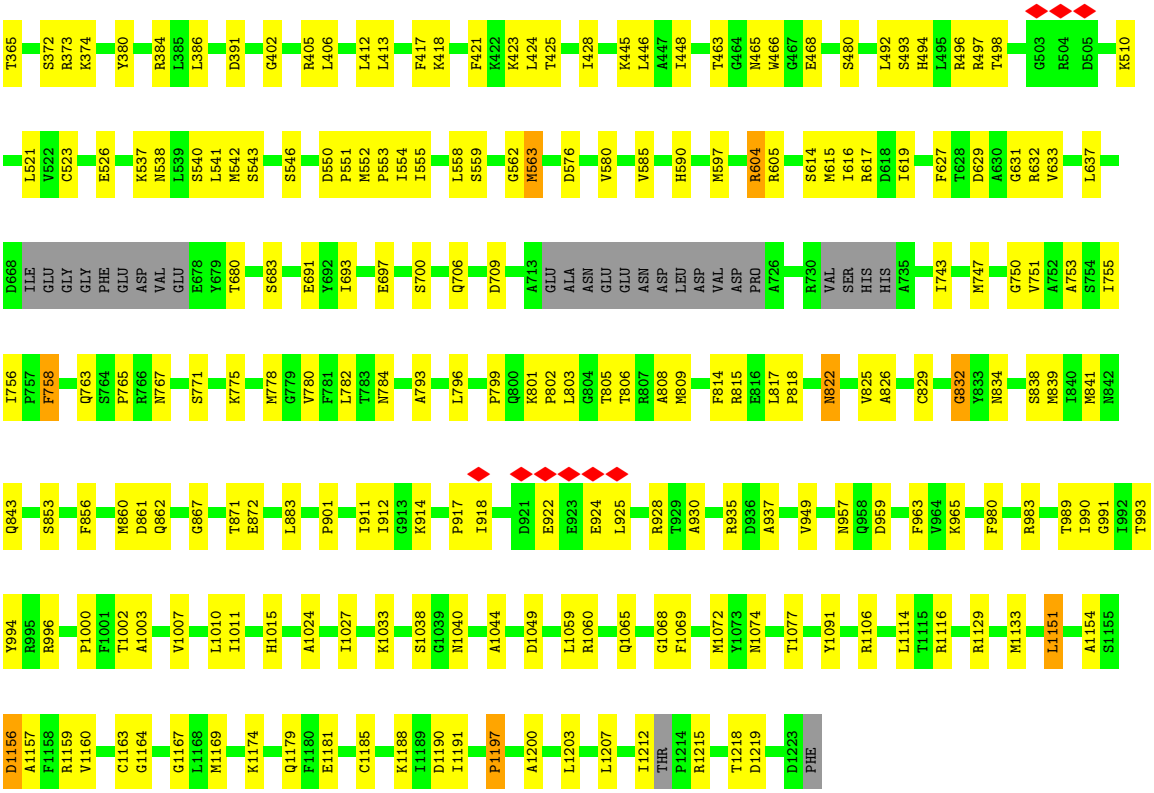




- Molecule 3: DNA-directed RNA polymerase II subunit RPB2

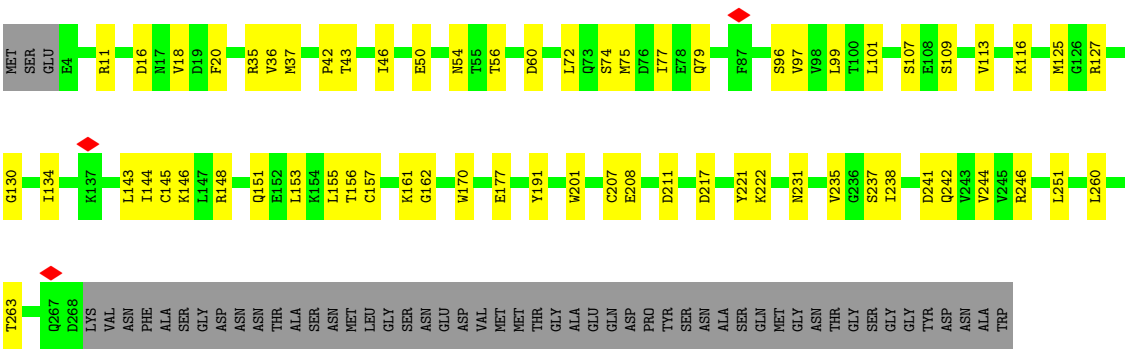
Chain B:





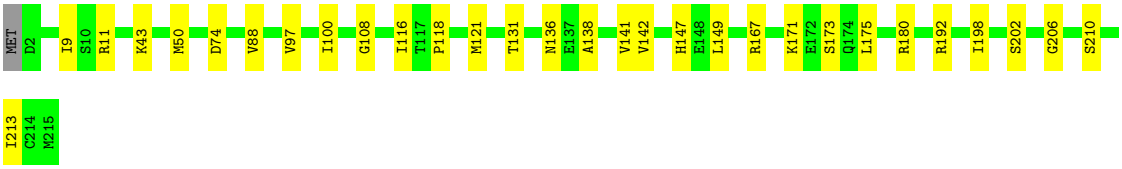
• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

Chain C:



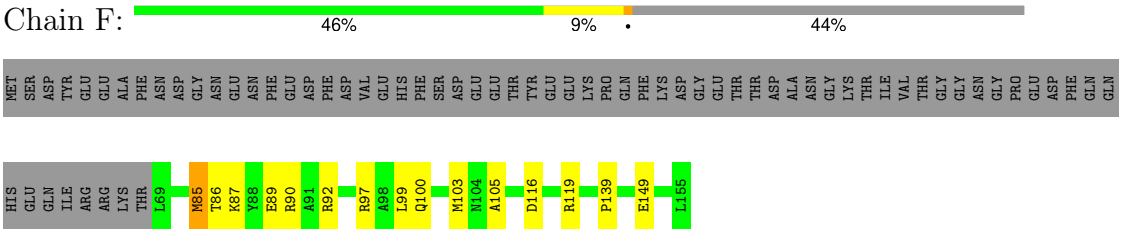
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



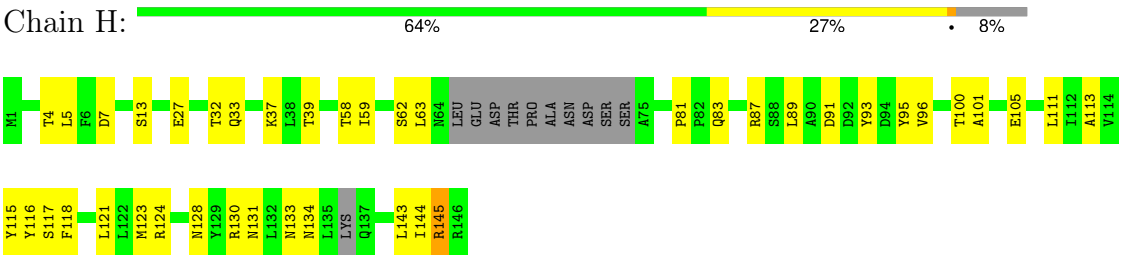
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



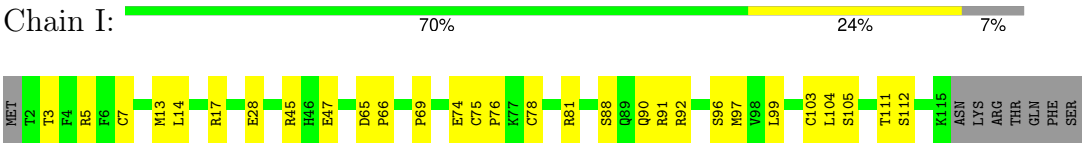
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



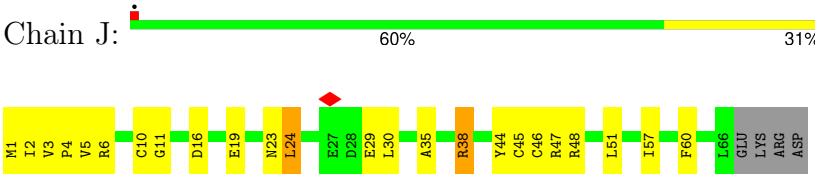
• Molecule 8: DNA-directed RNA polymerase II subunit RPB9

Chain I:



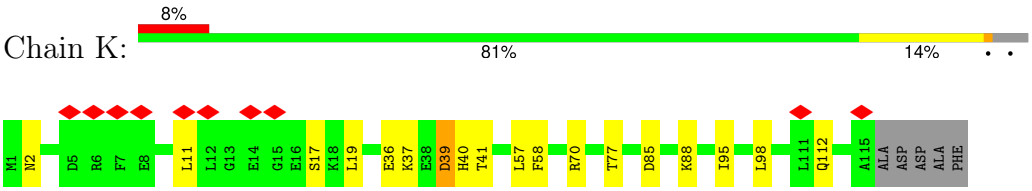
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



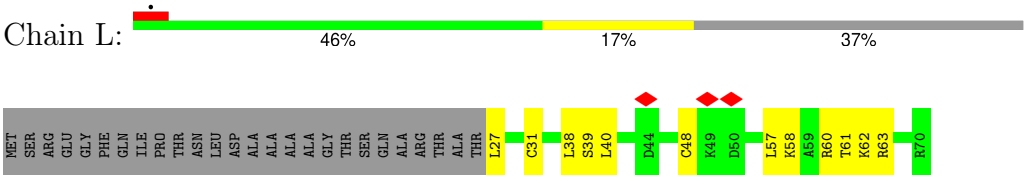
• Molecule 10: DNA-directed RNA polymerase II subunit RPB11

Chain K:



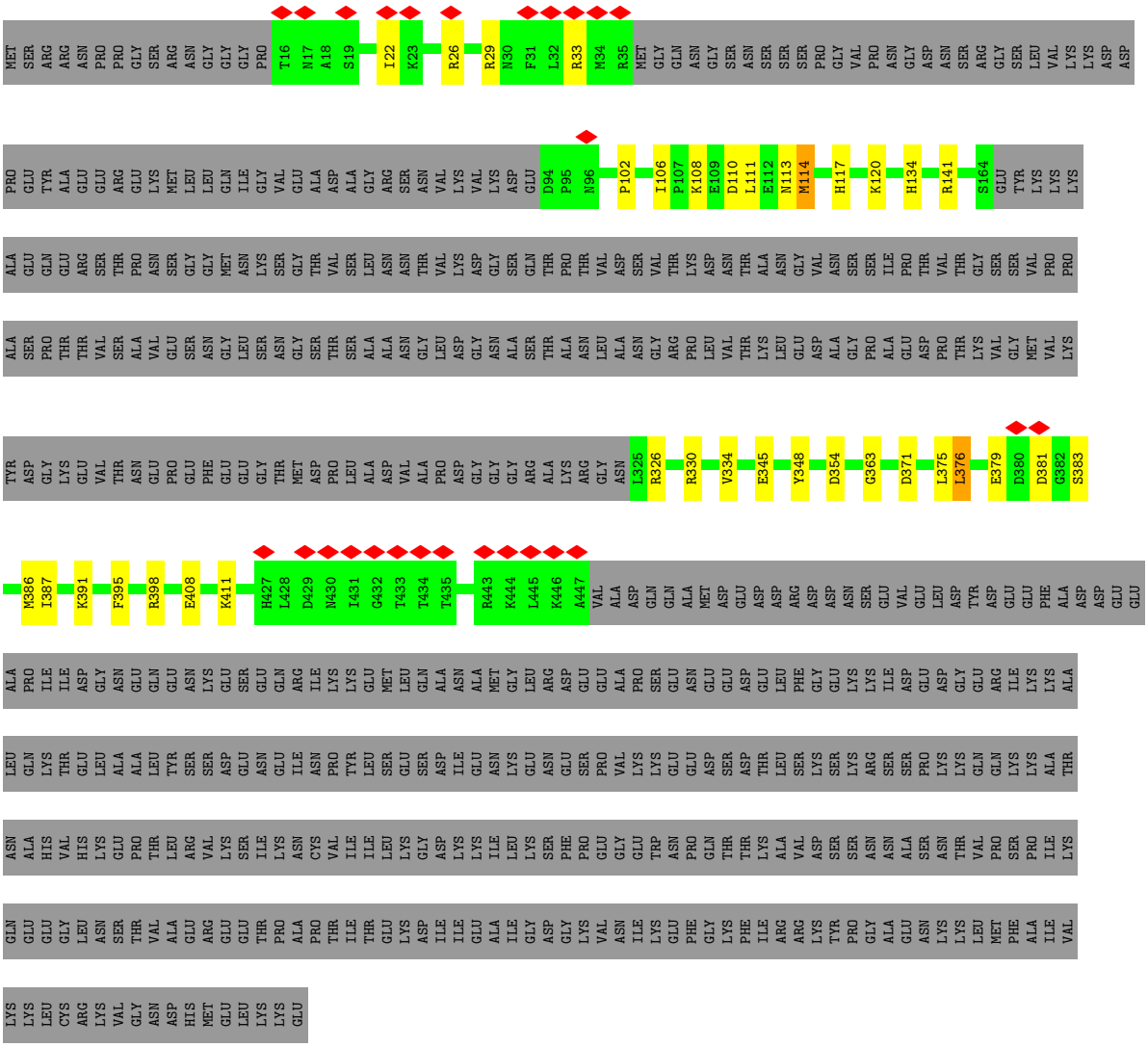
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



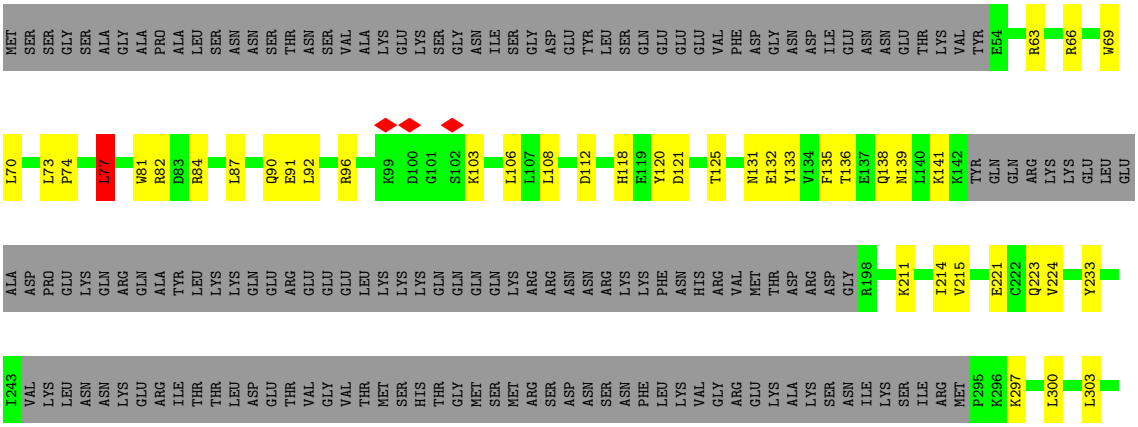
• Molecule 12: Transcription initiation factor IIF subunit alpha

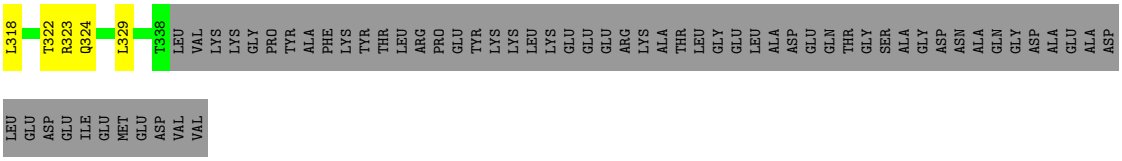
Chain Q:



• Molecule 13: Transcription initiation factor IIF subunit beta

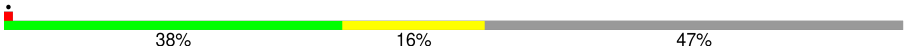
Chain P:

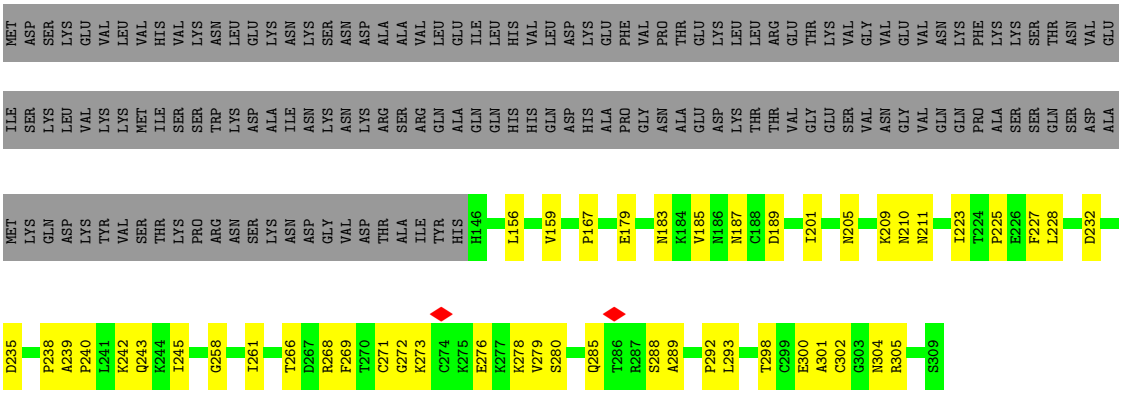




• Molecule 14: Transcription elongation factor S-II

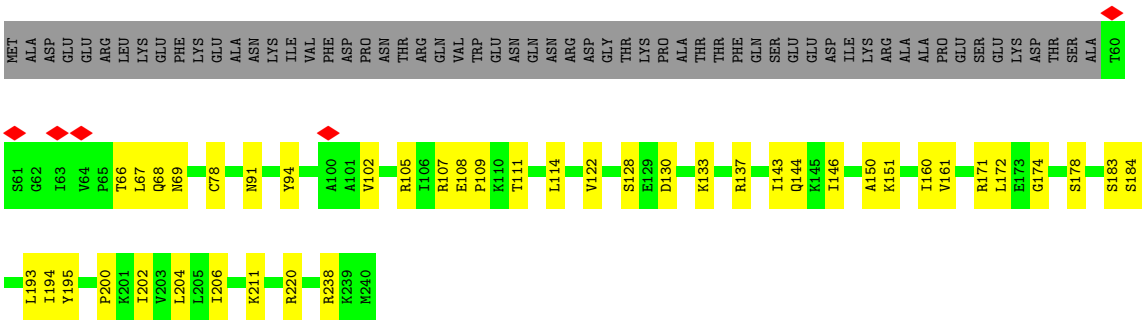
Chain S:





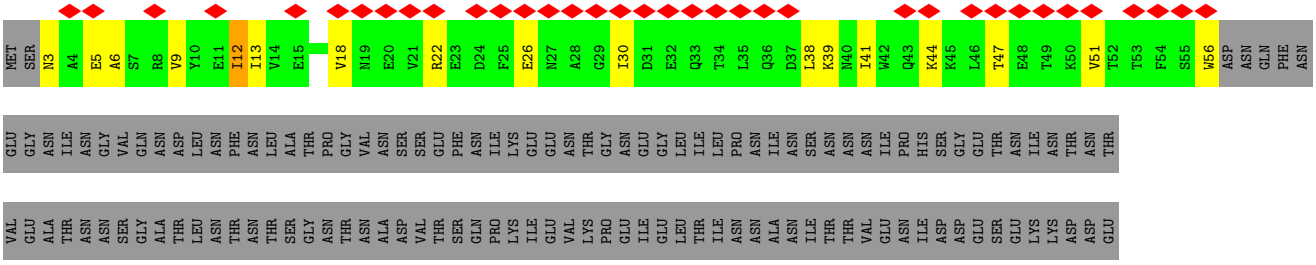
• Molecule 15: TATA-box-binding protein

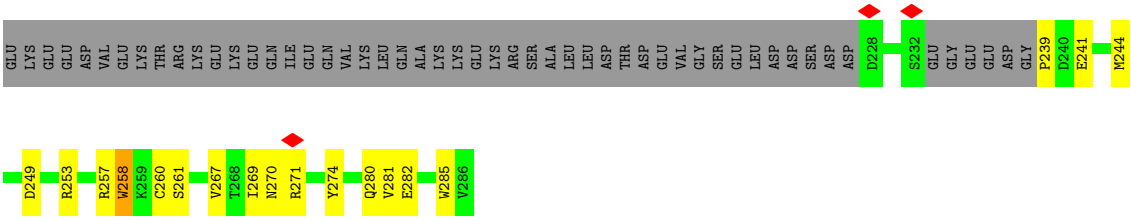
Chain O:



• Molecule 16: Transcription initiation factor IIA large subunit

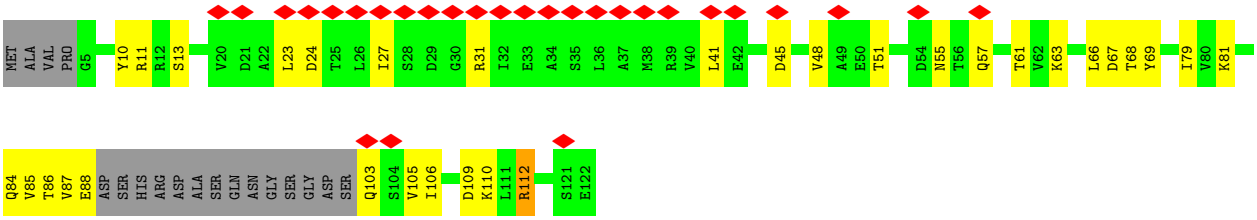
Chain U:





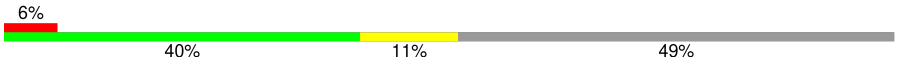
- Molecule 17: Transcription initiation factor IIA subunit 2

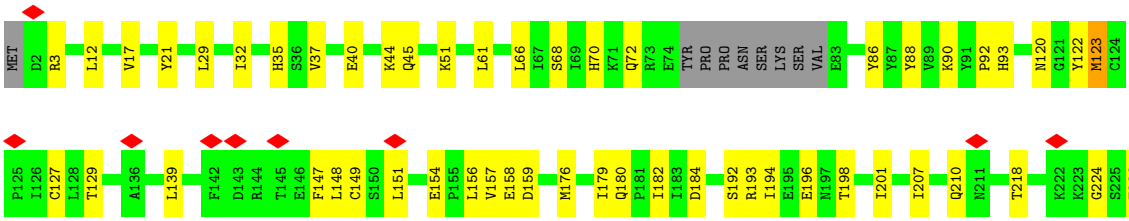
Chain V:

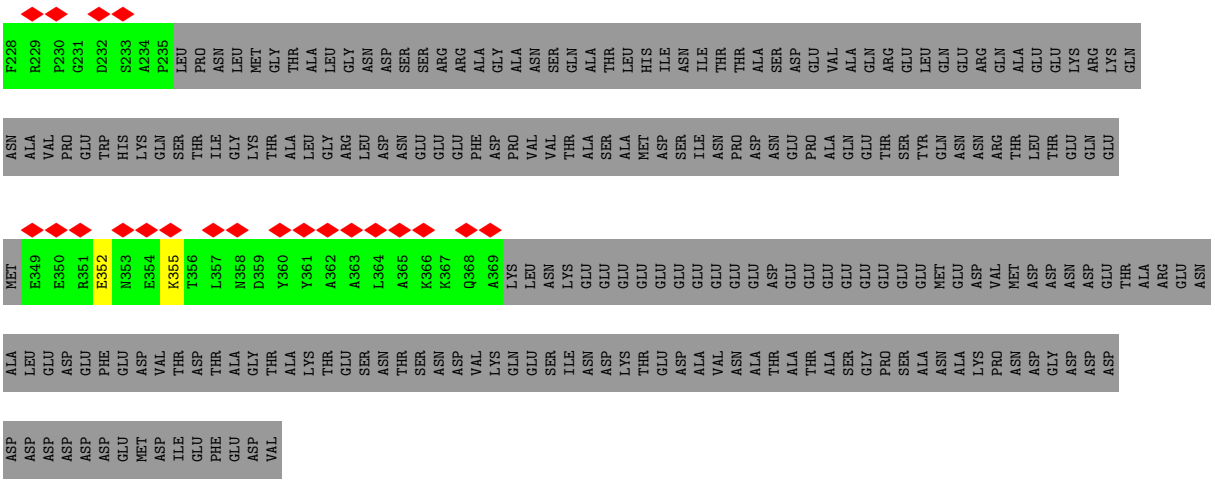


- Molecule 18: Transcription initiation factor IIE subunit alpha

Chain W:

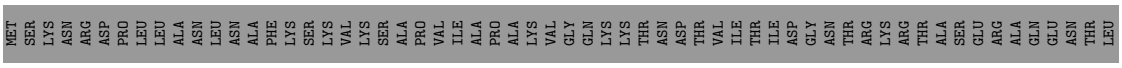


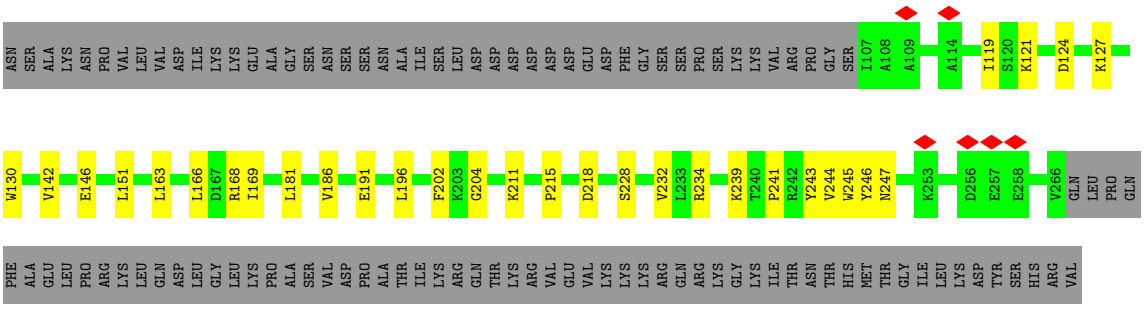




- Molecule 19: Transcription initiation factor IIE subunit beta

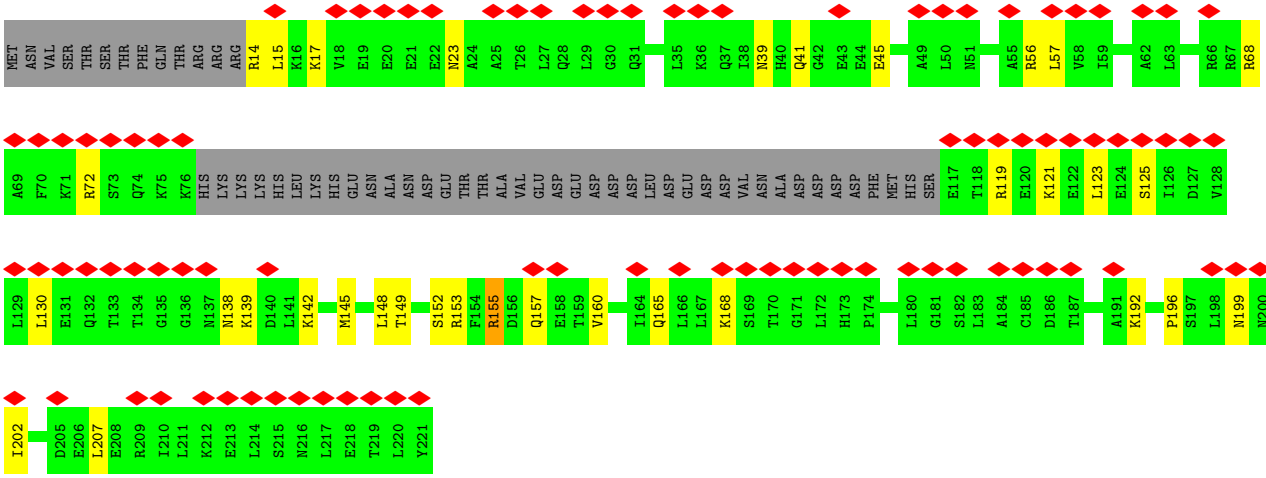
Chain X:





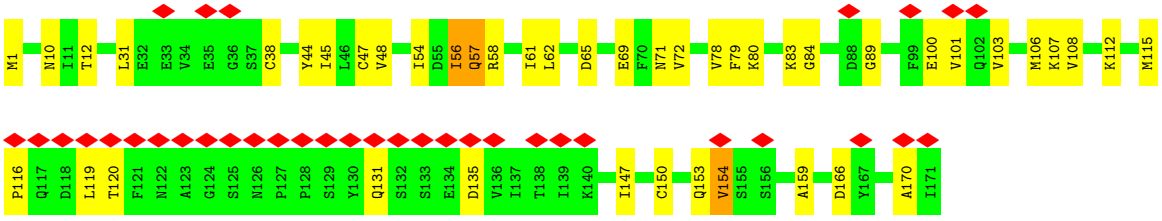
• Molecule 20: DNA-directed RNA polymerase II subunit RPB4

Chain D:



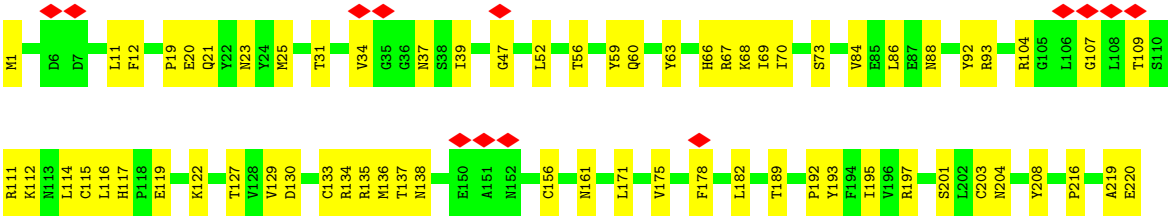
• Molecule 21: DNA-directed RNA polymerase II subunit RPB7

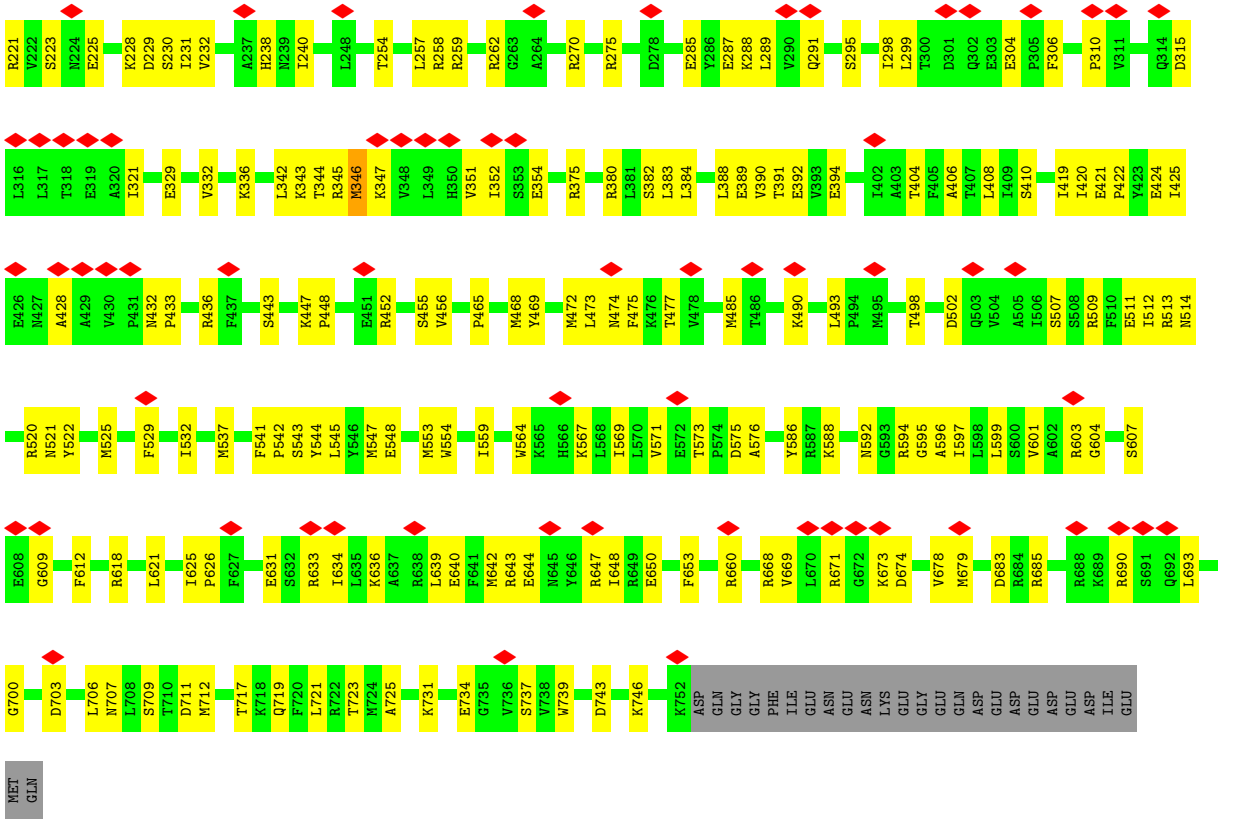
Chain G:



• Molecule 22: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3

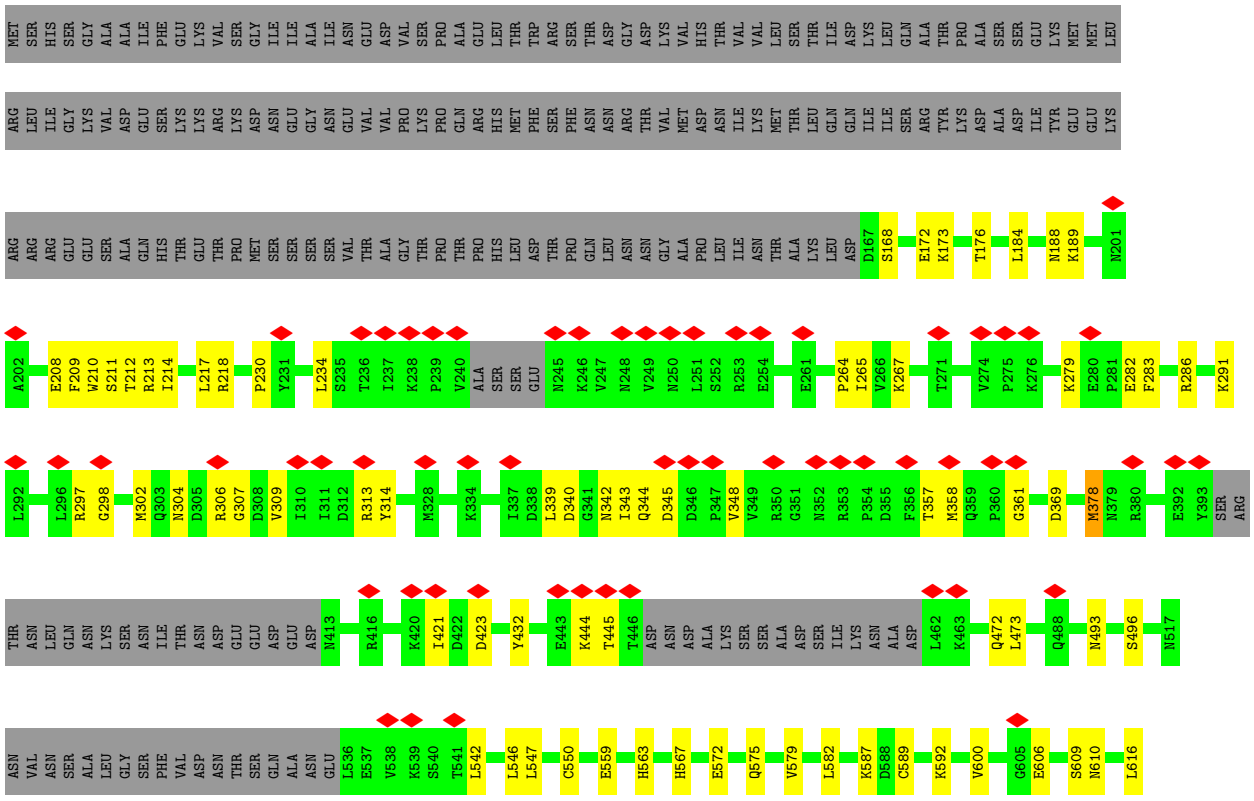
Chain 0:

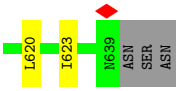




• Molecule 23: General transcription and DNA repair factor IIH subunit TFB1

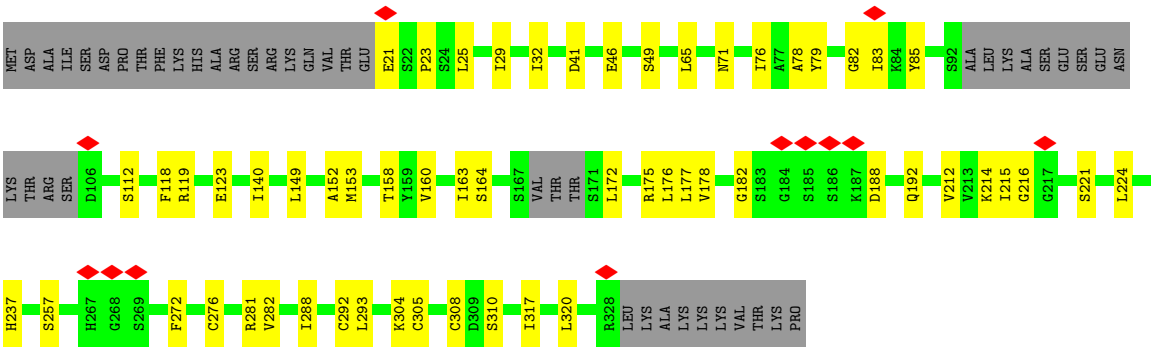
Chain 1:





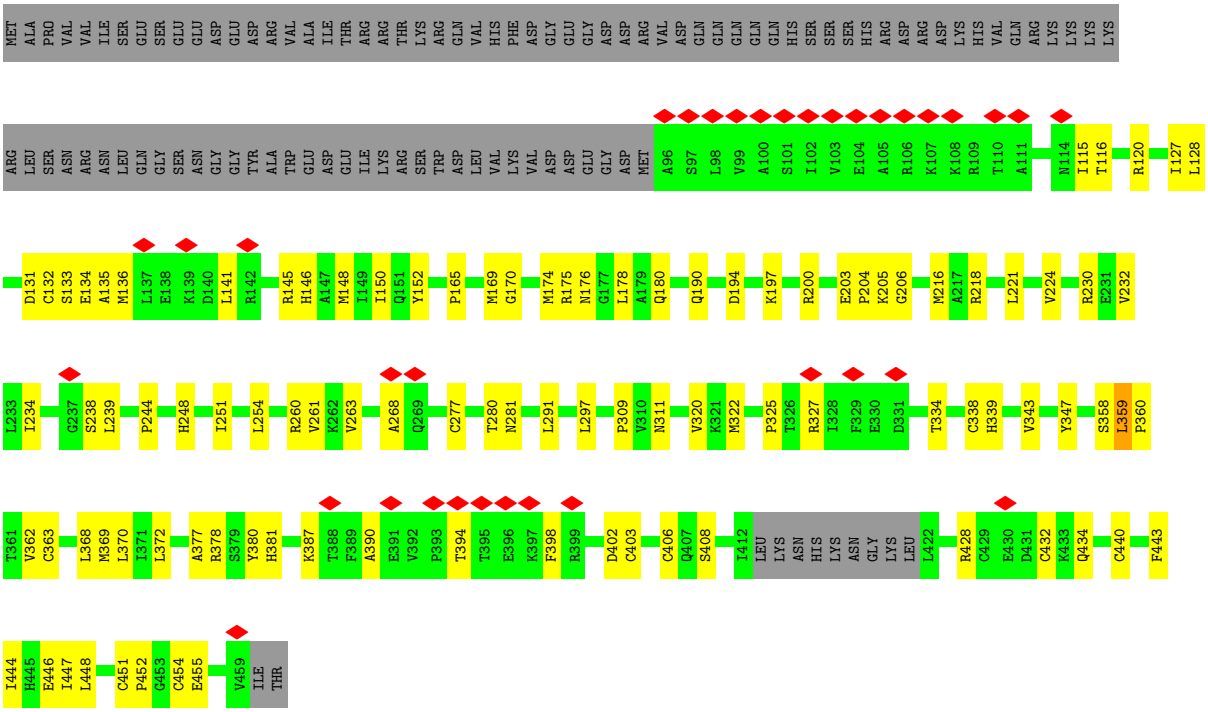
• Molecule 24: General transcription and DNA repair factor IIH subunit TFB4

Chain 4:



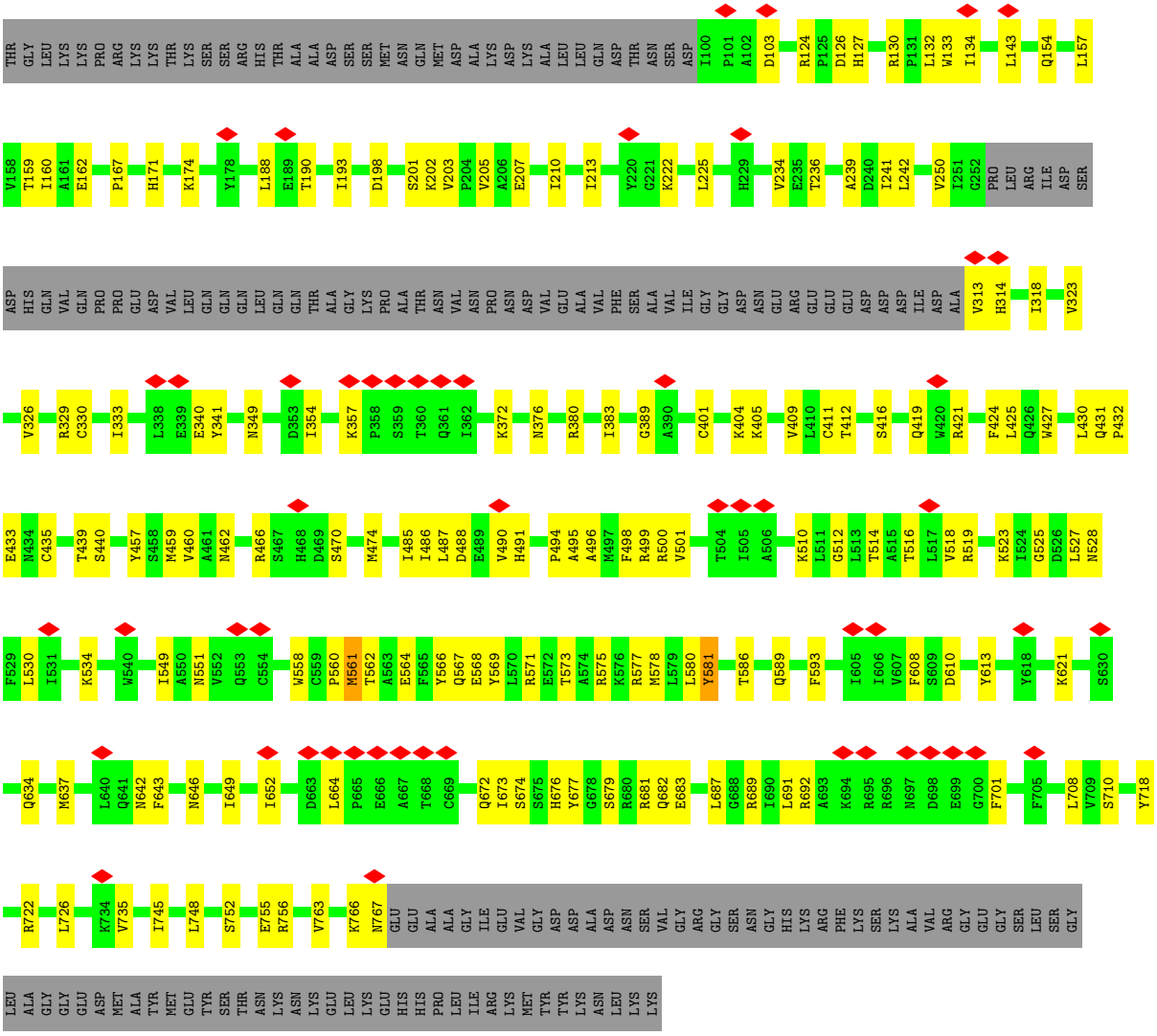
• Molecule 25: General transcription and DNA repair factor IIH subunit SSL1

Chain 6:



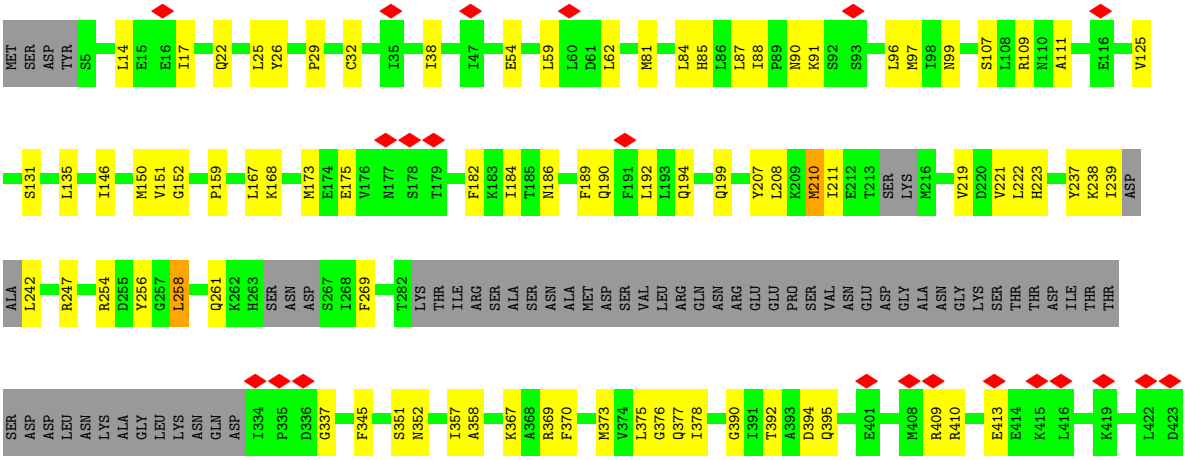
• Molecule 26: General transcription and DNA repair factor IIH helicase subunit XPB

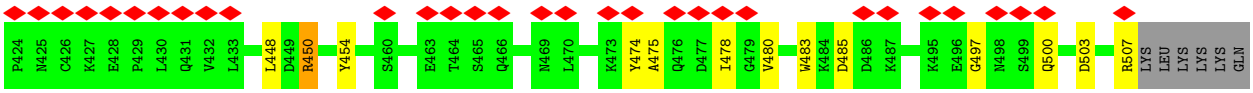
Chain 7:



- Molecule 27: General transcription and DNA repair factor IIH subunit TFB2

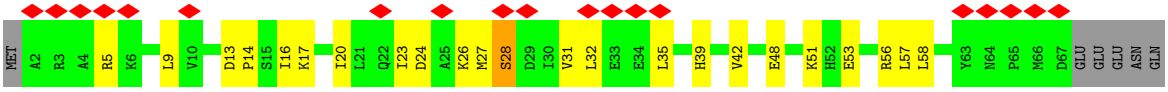
Chain 2:





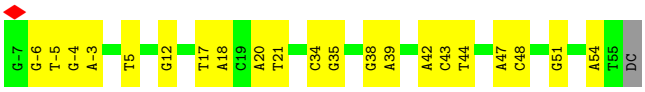
• Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:



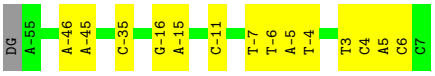
• Molecule 29: non-template strand

Chain N:



• Molecule 30: template strand

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: SF4, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	M	0.46	2/2204 (0.1%)	0.85	8/2963 (0.3%)
2	A	0.44	1/11368 (0.0%)	0.85	15/15383 (0.1%)
3	B	0.49	5/9402 (0.1%)	0.89	26/12680 (0.2%)
4	C	0.43	0/2124	0.80	1/2879 (0.0%)
5	E	0.39	0/1788	0.72	0/2406
6	F	0.43	0/717	0.86	1/967 (0.1%)
7	H	0.56	1/1097 (0.1%)	0.86	0/1484
8	I	0.38	0/945	0.65	1/1273 (0.1%)
9	J	0.89	5/549 (0.9%)	1.41	9/738 (1.2%)
10	K	0.41	0/942	0.76	2/1272 (0.2%)
11	L	0.48	0/354	1.00	0/468
12	Q	0.45	0/1648	0.80	4/2226 (0.2%)
13	P	0.44	1/1511 (0.1%)	0.79	6/2035 (0.3%)
14	S	0.42	0/1317	0.85	2/1778 (0.1%)
15	O	0.36	0/1449	0.66	0/1952
16	U	0.63	2/898 (0.2%)	0.83	0/1212
17	V	0.51	0/822	0.84	0/1109
18	W	0.36	0/2045	0.65	2/2757 (0.1%)
19	X	0.32	0/1312	0.58	0/1767
20	D	0.36	0/1339	0.67	0/1793
21	G	0.42	0/1363	0.80	3/1840 (0.2%)
22	0	0.38	2/6209 (0.0%)	0.67	2/8384 (0.0%)
23	1	0.42	2/3434 (0.1%)	0.72	1/4624 (0.0%)
24	4	0.33	0/2305	0.64	0/3117
25	6	0.41	1/2843 (0.0%)	0.66	3/3845 (0.1%)
26	7	0.39	1/4992 (0.0%)	0.69	4/6754 (0.1%)
27	2	0.42	0/3611	0.72	3/4881 (0.1%)
28	5	0.48	1/502 (0.2%)	0.93	3/677 (0.4%)
29	N	0.39	0/1443	0.63	0/2226
30	T	0.39	0/1449	0.63	0/2233
All	All	0.43	24/71982 (0.0%)	0.78	96/97723 (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	M	0	5
2	A	0	8
3	B	0	6
7	H	0	1
9	J	0	1
10	K	0	1
11	L	0	1
12	Q	0	1
13	P	0	1
14	S	0	2
15	O	0	1
17	V	0	1
20	D	0	1
21	G	0	1
22	0	0	2
27	2	0	1
All	All	0	34

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	758	PHE	C-O	14.17	1.30	1.23
3	B	1156	ASP	CG-OD2	-13.41	0.99	1.25
26	7	575	ARG	CG-CD	-8.96	1.25	1.52
9	J	24	LEU	CB-CG	-8.12	1.37	1.53
16	U	12	ILE	CG1-CD1	-8.01	1.20	1.51
7	H	145	ARG	CB-CG	-7.46	1.30	1.52
22	0	346	MET	SD-CE	-7.28	1.61	1.79
9	J	24	LEU	CG-CD1	6.64	1.74	1.52
1	M	172	MET	SD-CE	-6.32	1.63	1.79
3	B	424	LEU	CG-CD1	-6.32	1.31	1.52
16	U	258	TRP	CE3-CZ3	-6.32	1.19	1.38
23	1	378	MET	SD-CE	-6.26	1.64	1.79
1	M	164	LYS	CD-CE	-6.24	1.33	1.52
25	6	359	LEU	CG-CD1	-5.99	1.32	1.52
13	P	77	LEU	CB-CG	5.96	1.65	1.53
3	B	267	ARG	CZ-NH2	-5.94	1.25	1.33
3	B	822	ASN	CG-ND2	-5.90	1.20	1.33
28	5	58	LEU	CG-CD1	-5.83	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	0	569	ILE	CG1-CD1	-5.76	1.29	1.51
9	J	24	LEU	CA-CB	-5.53	1.45	1.53
9	J	38	ARG	CG-CD	-5.53	1.35	1.52
23	1	234	LEU	CG-CD1	-5.49	1.34	1.52
2	A	325	ILE	CB-CG2	-5.23	1.35	1.52
9	J	24	LEU	CG-CD2	5.06	1.69	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	24	LEU	CB-CG-CD2	-15.31	64.77	110.70
3	B	79	THR	CA-C-N	13.48	145.96	121.70
3	B	79	THR	C-N-CA	13.48	145.96	121.70
2	A	1107	VAL	CA-C-N	12.48	144.17	121.70
2	A	1107	VAL	C-N-CA	12.48	144.17	121.70
3	B	918	ILE	CA-C-N	12.24	143.72	121.70
3	B	918	ILE	C-N-CA	12.24	143.72	121.70
9	J	38	ARG	CA-CB-CG	11.78	137.66	114.10
12	Q	114	MET	CG-SD-CE	-10.81	77.13	100.90
9	J	38	ARG	CG-CD-NE	10.74	135.63	112.00
2	A	44	THR	CA-C-N	9.96	139.63	121.70
2	A	44	THR	C-N-CA	9.96	139.63	121.70
3	B	930	ALA	CA-C-N	9.82	139.37	121.70
3	B	930	ALA	C-N-CA	9.82	139.37	121.70
3	B	867	GLY	CA-C-N	9.46	138.72	121.70
3	B	867	GLY	C-N-CA	9.46	138.72	121.70
1	M	172	MET	CG-SD-CE	-9.45	80.10	100.90
14	S	209	LYS	CA-C-N	9.37	138.56	121.70
14	S	209	LYS	C-N-CA	9.37	138.56	121.70
18	W	227	MET	CG-SD-CE	-9.36	80.30	100.90
9	J	38	ARG	CB-CG-CD	-9.03	90.53	111.30
3	B	82	ASP	CA-C-N	8.97	137.85	121.70
3	B	82	ASP	C-N-CA	8.97	137.85	121.70
3	B	245	GLU	CA-C-N	8.47	136.96	121.70
3	B	245	GLU	C-N-CA	8.47	136.96	121.70
1	M	250	MET	CB-CG-SD	-7.91	88.98	112.70
12	Q	114	MET	CA-CB-CG	-7.65	98.79	114.10
28	5	58	LEU	CD1-CG-CD2	-7.42	94.48	110.80
3	B	1197	PRO	N-CA-C	7.35	122.34	111.03
13	P	77	LEU	CD1-CG-CD2	-7.31	94.71	110.80
26	7	677	TYR	CE1-CZ-OH	-7.16	98.42	119.90
13	P	77	LEU	CA-CB-CG	7.07	141.06	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	29	GLU	CA-CB-CG	7.07	128.24	114.10
26	7	561	MET	CG-SD-CE	-6.92	85.68	100.90
3	B	1151	LEU	CD1-CG-CD2	-6.85	95.73	110.80
3	B	1156	ASP	N-CA-CB	-6.82	98.13	109.72
18	W	123	MET	CG-SD-CE	6.81	115.89	100.90
3	B	81	SER	CA-C-N	6.67	133.71	121.70
3	B	81	SER	C-N-CA	6.67	133.71	121.70
22	0	644	GLU	CG-CD-OE1	6.52	133.39	118.40
9	J	24	LEU	N-CA-CB	-6.45	101.22	110.57
2	A	1209	MET	CG-SD-CE	-6.43	86.75	100.90
26	7	581	TYR	CA-CB-CG	6.38	125.38	113.90
1	M	135	MET	CB-CG-SD	6.33	131.68	112.70
2	A	567	LYS	CA-CB-CG	6.31	126.71	114.10
1	M	164	LYS	CG-CD-CE	6.22	125.60	111.30
12	Q	376	LEU	CD1-CG-CD2	-6.18	97.20	110.80
27	2	210	MET	CG-SD-CE	-6.07	87.55	100.90
2	A	567	LYS	CB-CG-CD	-6.07	97.35	111.30
25	6	358	SER	CA-C-N	5.97	137.30	122.74
25	6	358	SER	C-N-CA	5.97	137.30	122.74
2	A	761	MET	CA-CB-CG	5.96	126.01	114.10
23	1	234	LEU	CB-CG-CD1	-5.92	92.94	110.70
3	B	994	TYR	CA-CB-CG	5.88	124.49	113.90
21	G	56	ILE	CA-C-N	5.80	132.62	121.54
21	G	56	ILE	C-N-CA	5.80	132.62	121.54
3	B	563	MET	CG-SD-CE	-5.69	88.38	100.90
3	B	1156	ASP	N-CA-C	5.66	120.65	111.37
13	P	77	LEU	CB-CG-CD1	5.65	127.66	110.70
3	B	173	MET	CB-CG-SD	-5.65	95.76	112.70
8	I	13	MET	CG-SD-CE	-5.65	88.48	100.90
2	A	185	TRP	CA-CB-CG	5.63	124.30	113.60
2	A	525	GLN	N-CA-C	5.63	117.86	111.11
13	P	73	LEU	CD1-CG-CD2	-5.63	98.42	110.80
28	5	28	SER	CA-C-N	5.63	132.29	121.54
28	5	28	SER	C-N-CA	5.63	132.29	121.54
1	M	210	MET	CG-SD-CE	5.60	113.21	100.90
1	M	199	LYS	CA-C-N	5.52	132.09	121.54
1	M	199	LYS	C-N-CA	5.52	132.09	121.54
3	B	75	ALA	CA-C-N	5.49	132.03	121.54
3	B	75	ALA	C-N-CA	5.49	132.03	121.54
4	C	75	MET	CG-SD-CE	-5.42	88.99	100.90
27	2	258	LEU	CA-CB-CG	5.39	135.15	116.30
22	0	644	GLU	CG-CD-OE2	-5.36	106.08	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	317	LYS	CA-C-N	5.35	131.33	121.70
2	A	317	LYS	C-N-CA	5.35	131.33	121.70
9	J	24	LEU	N-CA-C	5.34	119.35	113.21
3	B	604	ARG	CB-CG-CD	5.32	123.55	111.30
26	7	677	TYR	OH-CZ-CE2	5.25	135.63	119.90
2	A	1259	MET	CG-SD-CE	5.22	112.39	100.90
2	A	65	LEU	CA-CB-CG	5.20	134.51	116.30
9	J	38	ARG	CD-NE-CZ	-5.20	117.12	124.40
27	2	38	ILE	CG1-CB-CG2	-5.17	95.18	110.70
6	F	85	MET	CA-CB-CG	5.17	124.44	114.10
21	G	31	LEU	CB-CG-CD1	5.16	126.19	110.70
1	M	164	LYS	CD-CE-NZ	-5.15	95.41	111.90
2	A	1336	MET	CB-CG-SD	5.12	128.07	112.70
25	6	216	MET	CG-SD-CE	-5.12	89.63	100.90
12	Q	114	MET	N-CA-CB	5.12	118.93	110.69
13	P	233	TYR	CA-C-N	5.11	131.30	121.54
13	P	233	TYR	C-N-CA	5.11	131.30	121.54
9	J	38	ARG	N-CA-C	5.09	117.56	111.71
3	B	1185	CYS	CA-C-N	5.06	131.20	121.54
3	B	1185	CYS	C-N-CA	5.06	131.20	121.54
10	K	39	ASP	CA-C-N	5.02	128.62	120.60
10	K	39	ASP	C-N-CA	5.02	128.62	120.60

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	0	618	ARG	Sidechain
22	0	640	GLU	Mainchain
27	2	450	ARG	Sidechain
2	A	1274	ARG	Sidechain
2	A	1404	GLU	Peptide
2	A	152	VAL	Peptide
2	A	252	PHE	Peptide
2	A	55	ASP	Peptide
2	A	566	ILE	Peptide
2	A	65	LEU	Peptide
2	A	750	GLY	Peptide
3	B	137	TYR	Peptide
3	B	333	PHE	Peptide
3	B	363	HIS	Peptide
3	B	510	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	B	832	GLY	Peptide
3	B	922	GLU	Peptide
20	D	155	ARG	Sidechain
21	G	154	VAL	Peptide
7	H	81	PRO	Peptide
9	J	38	ARG	Sidechain
10	K	112	GLN	Peptide
11	L	58	LYS	Peptide
1	M	269	ILE	Peptide
1	M	271	GLY	Peptide
1	M	272	LYS	Peptide
1	M	30	TYR	Peptide
1	M	31	PRO	Peptide
15	O	107	ARG	Sidechain
13	P	77	LEU	Mainchain
12	Q	110	ASP	Mainchain
14	S	227	PHE	Peptide
14	S	261	ILE	Peptide
17	V	112	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2175	0	2283	37	0
2	A	11167	0	11189	235	0
3	B	9227	0	9200	196	0
4	C	2086	0	2045	37	0
5	E	1752	0	1776	21	0
6	F	705	0	731	10	0
7	H	1080	0	1049	30	0
8	I	927	0	881	19	0
9	J	540	0	553	16	0
10	K	924	0	934	11	0
11	L	352	0	375	9	0
12	Q	1619	0	1452	36	0
13	P	1484	0	1480	31	0
14	S	1294	0	1289	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1422	0	1500	28	0
16	U	885	0	866	27	0
17	V	815	0	822	27	0
18	W	2010	0	2026	38	0
19	X	1288	0	1307	19	0
20	D	1331	0	1345	21	0
21	G	1335	0	1346	28	0
22	0	6091	0	6155	159	0
23	1	3382	0	3436	55	0
24	4	2267	0	2323	38	0
25	6	2786	0	2804	60	0
26	7	4889	0	4876	104	0
27	2	3546	0	3593	63	0
28	5	498	0	506	13	0
29	N	1288	0	719	17	0
30	T	1291	0	713	12	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	S	1	0	0	0	0
32	7	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	2	0
All	All	70481	0	69574	1323	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 10.

All (1323) 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)
9:J:24:LEU:CG	9:J:24:LEU:CD1	1.74	1.56
2:A:107:CYS:HB3	2:A:110:CYS:SG	2.01	1.00
25:6:406:CYS:HB3	25:6:440:CYS:SG	2.04	0.96
22:0:134:ARG:O	22:0:138:ASN:HB2	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1170:ILE:O	2:A:1174:PHE:HB2	1.76	0.85
9:J:24:LEU:CD1	9:J:24:LEU:HG	2.05	0.82
11:L:27:LEU:N	11:L:39:SER:HG	1.75	0.82
11:L:31:CYS:SG	11:L:48:CYS:HB3	2.20	0.80
3:B:597:MET:HE3	3:B:617:ARG:HB2	1.63	0.79
26:7:642:ASN:O	26:7:646:ASN:HB3	1.82	0.79
3:B:259:TYR:O	3:B:267:ARG:NH2	2.17	0.77
12:Q:376:LEU:HD23	12:Q:386:MET:HE1	1.67	0.76
29:N:-6:DG:N2	30:T:6:DC:O2	2.19	0.76
2:A:344:ARG:HH12	3:B:1129:ARG:HH11	1.33	0.76
25:6:338:CYS:SG	25:6:339:HIS:CE1	2.79	0.75
7:H:95:TYR:HB3	7:H:144:ILE:HB	1.66	0.75
3:B:267:ARG:HD3	3:B:313:MET:HE1	1.67	0.74
18:W:122:TYR:HB3	18:W:156:LEU:HB3	1.70	0.73
3:B:364:ILE:HG22	3:B:585:VAL:HG13	1.71	0.73
18:W:123:MET:HE3	18:W:159:ASP:HB2	1.70	0.73
23:1:230:PRO:HD3	25:6:244:PRO:HA	1.70	0.72
2:A:88:LYS:HE2	2:A:293:GLU:HB2	1.70	0.72
9:J:24:LEU:CD1	9:J:24:LEU:CB	2.65	0.72
21:G:89:GLY:HA3	21:G:103:VAL:HG22	1.71	0.71
25:6:169:MET:SD	25:6:169:MET:N	2.63	0.71
2:A:185:TRP:HB2	18:W:227:MET:HE1	1.71	0.70
2:A:1329:THR:HB	2:A:1335:ILE:HD11	1.74	0.70
2:A:1149:ALA:HB3	2:A:1196:GLU:HB2	1.74	0.70
22:0:721:LEU:HD13	25:6:268:ALA:HB2	1.74	0.69
3:B:680:THR:H	3:B:683:SER:HB2	1.58	0.69
11:L:31:CYS:HA	11:L:57:LEU:H	1.57	0.68
13:P:133:TYR:HB3	13:P:214:ILE:HD11	1.76	0.68
22:0:544:TYR:HA	22:0:547:MET:HG3	1.74	0.68
22:0:639:LEU:HA	22:0:642:MET:HE2	1.74	0.68
28:5:24:ASP:O	28:5:28:SER:HA	1.93	0.68
9:J:10:CYS:SG	9:J:11:GLY:N	2.67	0.67
22:0:419:ILE:HB	22:0:436:ARG:HB2	1.76	0.67
3:B:829:CYS:HA	3:B:834:ASN:HD21	1.60	0.67
3:B:323:VAL:HG13	3:B:324:ILE:HG13	1.77	0.66
3:B:883:LEU:HD21	3:B:928:ARG:HD3	1.77	0.66
2:A:108:MET:HA	2:A:210:ILE:HG12	1.77	0.66
24:4:65:LEU:HA	24:4:71:ASN:HD21	1.59	0.66
3:B:1000:PRO:HB2	3:B:1072:MET:HE3	1.76	0.66
26:7:676:HIS:HB3	26:7:679:SER:HB3	1.77	0.66
3:B:287:ARG:NH2	3:B:294:ASP:OD1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:9:LEU:HD21	28:5:39:HIS:HD2	1.58	0.66
26:7:459:MET:SD	26:7:466:ARG:NH2	2.69	0.66
22:0:111:ARG:HH12	22:0:134:ARG:HG3	1.62	0.65
26:7:330:CYS:HA	26:7:333:ILE:HG12	1.77	0.65
2:A:18:GLN:HB3	3:B:1215:ARG:HB2	1.77	0.65
23:1:291:LYS:HG3	23:1:307:GLY:HA3	1.78	0.65
22:0:721:LEU:O	22:0:725:ALA:HB2	1.97	0.65
1:M:27:CYS:SG	1:M:48:CYS:HB3	2.36	0.65
3:B:604:ARG:NH1	3:B:615:MET:SD	2.70	0.65
3:B:806:THR:HG23	3:B:808:ALA:H	1.61	0.65
3:B:336:ARG:NH1	3:B:339:THR:O	2.31	0.64
22:0:289:LEU:HD22	22:0:321:ILE:HG13	1.79	0.64
23:1:297:ARG:HH11	23:1:298:GLY:H	1.45	0.64
2:A:567:LYS:HD3	7:H:95:TYR:HA	1.77	0.64
27:2:190:GLN:HG3	27:2:395:GLN:HE21	1.62	0.64
2:A:1318:THR:HG22	5:E:141:VAL:HG11	1.78	0.64
3:B:73:GLN:HA	12:Q:330:ARG:HH22	1.63	0.64
2:A:1446:ASP:OD1	21:G:58:ARG:NH1	2.30	0.63
22:0:468:MET:SD	22:0:468:MET:N	2.70	0.63
25:6:134:GLU:HG3	25:6:206:GLY:H	1.64	0.63
26:7:132:LEU:HB3	26:7:201:SER:HA	1.81	0.63
3:B:28:GLU:HG3	12:Q:22:ILE:HG21	1.81	0.63
3:B:72:GLU:O	12:Q:330:ARG:NH2	2.32	0.62
22:0:1:MET:N	22:0:92:TYR:OH	2.32	0.62
24:4:305:CYS:HB3	24:4:310:SER:H	1.64	0.62
27:2:207:TYR:HA	27:2:210:MET:HE2	1.80	0.62
13:P:90:GLN:HE21	13:P:92:LEU:HD11	1.64	0.62
16:U:41:ILE:HG13	16:U:44:LYS:HE3	1.80	0.62
1:M:154:TYR:CD1	1:M:172:MET:HE1	2.34	0.62
23:1:444:LYS:NZ	23:1:445:THR:O	2.33	0.62
23:1:559:GLU:O	23:1:563:HIS:ND1	2.32	0.62
2:A:1329:THR:HG22	2:A:1331:SER:H	1.65	0.62
4:C:242:GLN:HB3	4:C:246:ARG:HH12	1.63	0.62
7:H:105:GLU:HB3	7:H:113:ALA:HB3	1.81	0.62
2:A:1443:VAL:HG12	21:G:61:ILE:HD13	1.81	0.62
3:B:80:GLU:HG2	3:B:83:ASN:HB2	1.80	0.62
21:G:112:LYS:HA	21:G:115:MET:HE1	1.82	0.62
22:0:59:TYR:O	22:0:63:TYR:HB2	2.00	0.62
22:0:576:ALA:HB3	23:1:343:ILE:HD13	1.82	0.62
2:A:1398:MET:SD	2:A:1398:MET:N	2.73	0.61
27:2:175:GLU:HA	27:2:182:PHE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:532:ARG:NH2	2:A:748:MET:SD	2.73	0.61
11:L:31:CYS:H	11:L:57:LEU:HB2	1.66	0.61
18:W:45:GLN:OE1	18:W:210:GLN:NE2	2.34	0.61
2:A:202:LEU:HB3	2:A:207:ILE:HD11	1.83	0.61
16:U:257:ARG:HH22	16:U:282:GLU:HA	1.66	0.61
17:V:66:LEU:HD11	17:V:69:TYR:HB3	1.82	0.61
18:W:179:ILE:HG13	18:W:182:ILE:HD12	1.83	0.61
23:1:339:LEU:HD12	23:1:342:ASN:HD22	1.65	0.61
3:B:793:ALA:HB3	3:B:856:PHE:HB2	1.83	0.61
25:6:176:ASN:HD21	25:6:205:LYS:HG3	1.65	0.61
2:A:1173:HIS:NE2	2:A:1228:TRP:O	2.34	0.61
3:B:542:MET:SD	3:B:542:MET:N	2.73	0.61
6:F:100:GLN:HB3	6:F:105:ALA:HB3	1.82	0.60
2:A:328:ARG:HD2	2:A:335:ARG:HH21	1.66	0.60
2:A:107:CYS:SG	2:A:148:CYS:HB2	2.41	0.60
27:2:448:LEU:O	27:2:450:ARG:NH1	2.33	0.60
2:A:856:THR:HB	2:A:865:GLN:H	1.66	0.60
25:6:363:CYS:HB3	25:6:368:LEU:H	1.66	0.60
3:B:771:SER:O	3:B:775:LYS:NZ	2.35	0.60
18:W:17:VAL:HG21	18:W:29:LEU:HD13	1.83	0.60
2:A:173:THR:HG1	2:A:184:SER:HG	1.47	0.60
26:7:589:GLN:HE22	26:7:756:ARG:HH21	1.50	0.60
1:M:284:LEU:HD21	1:M:313:TYR:HA	1.83	0.60
3:B:260:GLY:C	3:B:267:ARG:HH22	2.09	0.60
23:1:210:TRP:HB3	23:1:217:LEU:HD11	1.84	0.60
26:7:527:LEU:HA	26:7:530:LEU:HB2	1.84	0.60
2:A:60:SER:HB3	2:A:67:CYS:H	1.67	0.60
2:A:1229:SER:OG	2:A:1230:GLU:N	2.34	0.60
22:0:545:LEU:HB2	23:1:357:THR:HA	1.84	0.60
3:B:313:MET:HG3	3:B:386:LEU:HD11	1.82	0.60
22:0:127:THR:HG22	23:1:348:VAL:HG12	1.83	0.60
22:0:443:SER:HB3	22:0:473:LEU:HA	1.82	0.60
22:0:548:GLU:OE1	23:1:361:GLY:N	2.34	0.60
8:I:88:SER:O	8:I:91:ARG:NH1	2.35	0.59
23:1:444:LYS:HE2	24:4:282:VAL:HG13	1.84	0.59
7:H:83:GLN:O	7:H:87:ARG:NH1	2.35	0.59
2:A:393:ARG:NH2	2:A:421:ALA:O	2.35	0.59
2:A:874:ASP:O	2:A:1366:ARG:NH1	2.35	0.59
16:U:5:GLU:OE1	17:V:57:GLN:NE2	2.35	0.59
27:2:14:LEU:O	27:2:22:GLN:NE2	2.31	0.59
17:V:63:LYS:HZ1	17:V:86:THR:HG22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:287:ARG:HH21	3:B:297:ILE:HD13	1.68	0.59
18:W:70:HIS:HB3	18:W:86:TYR:HB2	1.84	0.59
26:7:424:PHE:HE2	26:7:430:LEU:HD22	1.67	0.59
1:M:281:SER:O	1:M:285:ASN:ND2	2.34	0.59
2:A:114:LEU:HD12	2:A:142:CYS:HB2	1.85	0.59
2:A:425:GLN:HE22	2:A:427:GLN:HB2	1.67	0.59
2:A:439:ASN:HA	2:A:460:VAL:H	1.68	0.59
22:0:642:MET:HB2	22:0:648:ILE:HD12	1.85	0.59
2:A:42:ASP:O	2:A:45:GLN:NE2	2.35	0.59
2:A:592:ASP:O	2:A:603:ASN:ND2	2.36	0.59
3:B:809:MET:SD	3:B:809:MET:N	2.76	0.59
23:1:606:GLU:HA	23:1:609:SER:HB3	1.84	0.59
3:B:706:GLN:HB2	3:B:709:ASP:HB3	1.84	0.59
22:0:60:GLN:O	22:0:66:HIS:ND1	2.35	0.59
27:2:208:LEU:HD13	27:2:221:VAL:HG11	1.84	0.59
2:A:1199:ARG:NH1	2:A:1231:ASP:O	2.36	0.58
3:B:1174:LYS:HB2	3:B:1179:GLN:HB2	1.84	0.58
2:A:881:GLN:HE21	2:A:956:LEU:HD23	1.69	0.58
2:A:1361:SER:OG	14:S:305:ARG:NH1	2.36	0.58
4:C:37:MET:HE1	4:C:244:VAL:HA	1.85	0.58
4:C:235:VAL:HG13	4:C:237:SER:H	1.68	0.58
10:K:95:ILE:HD12	10:K:98:LEU:HD11	1.85	0.58
27:2:29:PRO:HB3	27:2:111:ALA:HB2	1.84	0.58
2:A:187:LYS:NZ	18:W:226:THR:O	2.36	0.58
2:A:939:ASP:OD2	2:A:1023:ARG:NH1	2.36	0.58
22:0:134:ARG:HH12	22:0:304:GLU:HB2	1.66	0.58
3:B:552:MET:HA	3:B:555:ILE:HG22	1.84	0.58
20:D:139:LYS:HD2	20:D:142:LYS:HD2	1.86	0.58
22:0:1:MET:N	22:0:12:PHE:O	2.36	0.58
1:M:313:TYR:O	1:M:317:TYR:HB2	2.03	0.58
13:P:106:LEU:HB3	13:P:120:TYR:HB2	1.86	0.58
30:T:-46:DA:H2'	30:T:-45:DA:C8	2.38	0.58
2:A:365:GLY:HA3	2:A:469:ARG:HB3	1.85	0.58
3:B:756:ILE:HD13	3:B:767:ASN:HD22	1.67	0.58
11:L:61:THR:HG22	11:L:63:ARG:H	1.68	0.58
2:A:119:ASN:HB3	2:A:122:MET:HG3	1.86	0.57
14:S:280:SER:HB3	14:S:300:GLU:HB2	1.85	0.57
27:2:88:ILE:HB	27:2:99:ASN:HB3	1.85	0.57
27:2:151:VAL:HG11	27:2:358:ALA:HB1	1.85	0.57
7:H:115:TYR:OH	7:H:124:ARG:NH1	2.36	0.57
26:7:354:ILE:HG13	26:7:430:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:805:THR:OG1	3:B:809:MET:SD	2.62	0.57
17:V:11:ARG:NH1	17:V:45:ASP:OD2	2.37	0.57
26:7:188:LEU:HB3	26:7:193:ILE:HD11	1.86	0.57
2:A:405:VAL:HG23	2:A:432:VAL:HG12	1.86	0.57
2:A:1317:MET:HB3	5:E:142:VAL:HG21	1.86	0.57
3:B:310:MET:SD	3:B:310:MET:N	2.76	0.57
18:W:40:GLU:HG2	18:W:44:LYS:HE2	1.87	0.57
22:0:232:VAL:HB	22:0:456:VAL:HA	1.85	0.57
2:A:227:VAL:HA	20:D:15:LEU:HD13	1.87	0.57
3:B:341:LEU:HD22	3:B:344:LYS:HD2	1.87	0.57
3:B:43:LEU:O	3:B:496:ARG:NH2	2.37	0.57
3:B:803:LEU:HD11	3:B:822:ASN:HD22	1.69	0.57
8:I:78:CYS:SG	8:I:105:SER:OG	2.62	0.57
22:0:520:ARG:HH22	22:0:553:MET:HE1	1.70	0.57
4:C:74:SER:HB2	4:C:238:ILE:HB	1.86	0.56
25:6:224:VAL:O	25:6:230:ARG:NH2	2.38	0.56
2:A:745:GLN:O	2:A:749:ALA:HB2	2.04	0.56
2:A:1158:PRO:HB3	2:A:1188:GLN:HE21	1.69	0.56
19:X:232:VAL:HA	19:X:244:VAL:HG12	1.87	0.56
2:A:226:GLU:OE2	2:A:230:ARG:NH2	2.38	0.56
3:B:302:CYS:SG	3:B:303:TYR:N	2.79	0.56
14:S:179:GLU:O	14:S:183:ASN:ND2	2.37	0.56
20:D:196:PRO:HA	20:D:199:ASN:HB2	1.87	0.56
21:G:47:CYS:SG	21:G:48:VAL:N	2.78	0.56
25:6:221:LEU:O	25:6:230:ARG:NH1	2.38	0.56
26:7:236:THR:O	26:7:313:VAL:N	2.38	0.56
27:2:239:ILE:HG12	27:2:247:ARG:HG2	1.87	0.56
22:0:636:LYS:HA	22:0:639:LEU:HD12	1.87	0.56
26:7:676:HIS:O	26:7:722:ARG:NH1	2.39	0.56
22:0:306:PHE:HB3	22:0:382:SER:HA	1.88	0.56
23:1:309:VAL:O	23:1:313:ARG:NH1	2.39	0.56
26:7:491:HIS:O	26:7:519:ARG:NH1	2.39	0.56
1:M:190:LYS:NZ	1:M:302:LEU:O	2.38	0.56
4:C:42:PRO:HB2	4:C:161:LYS:HE2	1.87	0.56
8:I:45:ARG:HH21	8:I:47:GLU:H	1.52	0.56
7:H:62:SER:OG	7:H:63:LEU:N	2.38	0.56
12:Q:371:ASP:O	13:P:82:ARG:NH1	2.38	0.56
17:V:87:VAL:O	17:V:103:GLN:N	2.39	0.56
20:D:165:GLN:HA	20:D:168:LYS:HE3	1.86	0.56
22:0:422:PRO:HA	22:0:433:PRO:HB3	1.88	0.56
23:1:209:PHE:O	23:1:213:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:7:130:ARG:NH1	26:7:198:ASP:O	2.39	0.56
15:O:94:TYR:HB2	15:O:102:VAL:HG23	1.88	0.56
16:U:51:VAL:HG12	16:U:271:ARG:HA	1.87	0.56
24:4:78:ALA:HA	24:4:83:ILE:HA	1.88	0.56
26:7:589:GLN:HB3	26:7:748:LEU:HD22	1.88	0.56
22:0:238:HIS:HB2	22:0:660:ARG:HD2	1.85	0.56
22:0:295:SER:O	22:0:299:LEU:HB2	2.06	0.56
28:5:14:PRO:HA	28:5:17:LYS:HE2	1.87	0.56
12:Q:117:HIS:CE1	12:Q:391:LYS:HB2	2.41	0.56
12:Q:376:LEU:HB2	13:P:69:TRP:HB2	1.88	0.56
27:2:238:LYS:NZ	27:2:239:ILE:O	2.38	0.56
16:U:241:GLU:HG3	17:V:112:ARG:NH2	2.21	0.55
22:0:288:LYS:HE2	22:0:298:ILE:HG12	1.86	0.55
27:2:454:TYR:CZ	27:2:483:TRP:HB2	2.40	0.55
3:B:402:GLY:O	3:B:405:ARG:NH1	2.39	0.55
3:B:841:MET:SD	3:B:990:ILE:HG12	2.46	0.55
2:A:56:PRO:O	2:A:66:LYS:NZ	2.38	0.55
2:A:311:GLN:HG2	2:A:312:PRO:HD3	1.88	0.55
2:A:1159:ARG:NH1	2:A:1186:ASP:OD1	2.39	0.55
7:H:63:LEU:HB3	7:H:89:LEU:HD13	1.88	0.55
26:7:752:SER:HB2	26:7:755:GLU:HB2	1.89	0.55
4:C:54:ASN:ND2	4:C:60:ASP:OD1	2.37	0.55
22:0:11:LEU:HD22	22:0:93:ARG:HG2	1.87	0.55
22:0:588:LYS:O	22:0:592:ASN:ND2	2.39	0.55
25:6:327:ARG:HD2	25:6:347:TYR:HE1	1.72	0.55
2:A:75:ASN:HA	3:B:1116:ARG:HH22	1.72	0.55
2:A:840:ARG:NH1	2:A:1384:VAL:O	2.40	0.55
3:B:825:VAL:HG23	3:B:1010:LEU:HG	1.89	0.55
3:B:839:MET:HE3	3:B:980:PHE:HB2	1.89	0.55
3:B:1156:ASP:OD2	3:B:1197:PRO:HA	2.07	0.55
12:Q:408:GLU:HA	12:Q:411:LYS:HE2	1.88	0.55
2:A:802:ASN:ND2	2:A:807:GLY:O	2.40	0.55
4:C:241:ASP:N	4:C:241:ASP:OD1	2.39	0.55
3:B:1133:MET:SD	3:B:1133:MET:N	2.79	0.55
9:J:5:VAL:HG12	9:J:6:ARG:HG2	1.89	0.55
1:M:84:ASN:OD1	1:M:151:LYS:NZ	2.40	0.55
3:B:806:THR:HG22	3:B:809:MET:HE1	1.89	0.55
16:U:257:ARG:NH1	16:U:258:TRP:O	2.38	0.55
24:4:292:CYS:HB3	24:4:308:CYS:SG	2.47	0.55
27:2:81:MET:HG3	27:2:87:LEU:HB2	1.88	0.55
1:M:63:TRP:HD1	1:M:64:ARG:HH12	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:0:25:MET:HE1	22:0:52:LEU:HD23	1.88	0.55
23:1:265:ILE:HD11	23:1:314:TYR:HB3	1.89	0.55
27:2:392:THR:HG22	27:2:394:ASP:H	1.71	0.55
3:B:799:PRO:HB2	3:B:818:PRO:HG2	1.89	0.54
22:0:135:ARG:NH1	22:0:392:GLU:OE2	2.40	0.54
1:M:215:ARG:NH1	15:O:183:SER:O	2.39	0.54
3:B:1060:ARG:O	3:B:1060:ARG:NH1	2.38	0.54
22:0:542:PRO:HB3	22:0:626:PRO:HA	1.88	0.54
26:7:127:HIS:O	26:7:202:LYS:NZ	2.38	0.54
14:S:271:CYS:SG	14:S:272:GLY:N	2.80	0.54
22:0:287:GLU:OE1	22:0:291:GLN:NE2	2.41	0.54
15:O:91:ASN:ND2	15:O:105:ARG:O	2.41	0.54
29:N:17:DT:H2"	29:N:18:DA:H5"	1.89	0.54
3:B:194:GLU:HA	3:B:784:ASN:HD22	1.73	0.54
14:S:271:CYS:HB3	14:S:276:GLU:H	1.72	0.54
22:0:465:PRO:HG2	22:0:468:MET:HE1	1.89	0.54
22:0:509:ARG:NH1	22:0:511:GLU:OE1	2.41	0.54
2:A:116:ASP:O	2:A:118:HIS:ND1	2.40	0.54
2:A:335:ARG:HH22	3:B:1114:LEU:HD21	1.73	0.54
2:A:745:GLN:O	2:A:749:ALA:CB	2.56	0.54
3:B:136:THR:N	3:B:138:GLU:OE2	2.41	0.54
3:B:296:GLU:O	3:B:300:HIS:ND1	2.31	0.54
26:7:487:LEU:HB2	26:7:512:GLY:HA2	1.88	0.54
26:7:573:THR:OG1	29:N:54:DA:O5'	2.26	0.54
3:B:74:LEU:HA	3:B:85:SER:HA	1.90	0.54
14:S:156:LEU:HA	14:S:159:VAL:HG22	1.90	0.54
2:A:1373:ASP:HA	2:A:1376:THR:HG22	1.90	0.54
25:6:347:TYR:CE2	25:6:359:LEU:HD13	2.42	0.54
2:A:184:SER:HB2	2:A:197:PRO:HB2	1.89	0.54
26:7:340:GLU:OE2	26:7:380:ARG:NH1	2.40	0.54
26:7:672:GLN:NE2	26:7:683:GLU:OE2	2.41	0.54
4:C:143:LEU:HD21	4:C:146:LYS:HE3	1.90	0.53
14:S:185:VAL:O	14:S:189:ASP:N	2.38	0.53
2:A:512:VAL:HA	2:A:519:PRO:HA	1.90	0.53
2:A:1115:SER:OG	2:A:1330:ASN:ND2	2.40	0.53
4:C:16:ASP:OD1	4:C:16:ASP:N	2.41	0.53
5:E:88:VAL:HB	5:E:116:ILE:HG23	1.90	0.53
22:0:509:ARG:HB2	22:0:512:ILE:HG12	1.89	0.53
22:0:545:LEU:N	23:1:357:THR:O	2.41	0.53
26:7:159:THR:HB	26:7:160:ILE:HD12	1.90	0.53
3:B:924:GLU:HG2	3:B:925:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:141:ARG:NH1	12:Q:345:GLU:O	2.41	0.53
13:P:87:LEU:H	13:P:90:GLN:HE22	1.55	0.53
8:I:3:THR:O	8:I:5:ARG:NH1	2.42	0.53
16:U:22:ARG:HE	16:U:26:GLU:HG2	1.74	0.53
22:0:223:SER:O	22:0:452:ARG:NH2	2.41	0.53
22:0:507:SER:OG	22:0:685:ARG:NH2	2.42	0.53
4:C:177:GLU:OE2	4:C:231:ASN:ND2	2.42	0.53
18:W:120:ASN:HD22	18:W:158:GLU:HG2	1.73	0.53
22:0:522:TYR:HA	22:0:525:MET:HE2	1.91	0.53
23:1:563:HIS:O	23:1:567:HIS:ND1	2.32	0.53
2:A:894:GLU:O	2:A:898:ARG:HB3	2.08	0.53
3:B:326:ASP:OD1	12:Q:398:ARG:NH1	2.39	0.53
3:B:546:SER:OG	3:B:631:GLY:N	2.40	0.53
4:C:101:LEU:HB3	4:C:155:LEU:HB2	1.91	0.53
14:S:273:LYS:H	14:S:304:ASN:HD22	1.55	0.53
25:6:135:ALA:O	25:6:145:ARG:NH1	2.41	0.53
26:7:222:LYS:HB3	26:7:241:ILE:HG12	1.89	0.53
2:A:1199:ARG:NH2	2:A:1233:ASP:O	2.42	0.53
3:B:334:ILE:HA	3:B:347:LYS:HG3	1.90	0.53
10:K:11:LEU:O	10:K:37:LYS:NZ	2.36	0.53
19:X:228:SER:O	19:X:247:ASN:ND2	2.40	0.53
22:0:315:ASP:O	22:0:375:ARG:NH2	2.42	0.53
26:7:239:ALA:HA	26:7:242:LEU:HD23	1.91	0.53
22:0:270:ARG:NH2	22:0:389:GLU:O	2.41	0.53
2:A:40:THR:OG1	2:A:41:MET:N	2.42	0.53
9:J:19:GLU:O	9:J:23:ASN:ND2	2.41	0.53
14:S:266:THR:HG23	14:S:268:ARG:H	1.74	0.53
19:X:163:LEU:HG	19:X:169:ILE:HG21	1.91	0.53
22:0:136:MET:HE1	22:0:156:CYS:HB2	1.91	0.53
24:4:317:ILE:HA	24:4:320:LEU:HD12	1.91	0.53
26:7:549:ILE:HD12	26:7:691:LEU:HD11	1.91	0.53
26:7:610:ASP:H	26:7:674:SER:HB3	1.74	0.53
27:2:186:ASN:ND2	27:2:390:GLY:O	2.42	0.53
3:B:911:ILE:HG13	3:B:912:ILE:HG12	1.89	0.53
20:D:39:ASN:ND2	20:D:41:GLN:OE1	2.42	0.53
22:0:310:PRO:HB3	22:0:404:THR:HG23	1.91	0.53
25:6:377:ALA:HA	25:6:380:TYR:CE2	2.44	0.53
2:A:252:PHE:HB3	2:A:256:GLN:HB2	1.91	0.52
3:B:146:GLU:HG2	3:B:147:LEU:H	1.74	0.52
3:B:352:ALA:HA	3:B:355:ILE:HD12	1.91	0.52
7:H:5:LEU:H	7:H:59:ILE:HB	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:67:LEU:HD21	15:O:220:ARG:HH12	1.73	0.52
22:0:111:ARG:O	22:0:115:CYS:N	2.42	0.52
25:6:120:ARG:HA	25:6:309:PRO:HA	1.91	0.52
22:0:310:PRO:HB2	22:0:408:LEU:HG	1.90	0.52
24:4:29:ILE:HB	24:4:178:VAL:HA	1.89	0.52
2:A:70:CYS:SG	2:A:80:HIS:CE1	3.02	0.52
2:A:1100:ARG:NH2	2:A:1351:GLU:OE2	2.42	0.52
3:B:1002:THR:OG1	3:B:1003:ALA:N	2.41	0.52
16:U:47:THR:HB	16:U:56:TRP:HD1	1.73	0.52
25:6:234:ILE:HB	25:6:263:VAL:HA	1.91	0.52
4:C:145:CYS:SG	4:C:146:LYS:N	2.82	0.52
3:B:232:SER:O	3:B:261:ARG:NH1	2.43	0.52
4:C:148:ARG:O	4:C:151:GLN:NE2	2.39	0.52
11:L:38:LEU:HB3	11:L:40:LEU:HD23	1.90	0.52
22:0:601:VAL:HG12	22:0:603:ARG:H	1.75	0.52
26:7:687:LEU:HG	26:7:726:LEU:HD21	1.90	0.52
2:A:14:VAL:HG21	2:A:1430:LEU:HD12	1.92	0.52
2:A:1446:ASP:OD2	2:A:1449:SER:N	2.39	0.52
22:0:447:LYS:NZ	22:0:474:ASN:O	2.43	0.52
2:A:1285:MET:HE1	14:S:258:GLY:HA3	1.92	0.52
18:W:3:ARG:NH2	18:W:192:SER:OG	2.39	0.52
3:B:364:ILE:HD11	3:B:374:LYS:HD3	1.92	0.52
3:B:540:SER:OG	3:B:541:LEU:N	2.43	0.52
2:A:379:VAL:O	2:A:384:ASN:ND2	2.43	0.52
2:A:802:ASN:HD21	2:A:806:ARG:HB2	1.75	0.52
3:B:755:ILE:O	3:B:983:ARG:NH2	2.40	0.52
16:U:244:MET:HB3	16:U:267:VAL:HG23	1.92	0.52
22:0:56:THR:HB	22:0:69:ILE:HD13	1.91	0.52
22:0:68:LYS:NZ	22:0:203:CYS:O	2.43	0.52
22:0:84:VAL:O	22:0:88:ASN:ND2	2.43	0.52
22:0:285:GLU:OE2	22:0:380:ARG:NH1	2.42	0.52
25:6:238:SER:OG	25:6:239:LEU:N	2.43	0.52
25:6:444:ILE:HG12	25:6:448:LEU:HD12	1.91	0.52
2:A:108:MET:SD	2:A:108:MET:N	2.83	0.52
2:A:802:ASN:ND2	2:A:803:SER:O	2.43	0.52
3:B:989:THR:OG1	3:B:990:ILE:N	2.42	0.52
7:H:13:SER:OG	7:H:27:GLU:OE2	2.28	0.52
22:0:114:LEU:HD13	22:0:193:TYR:HA	1.92	0.52
22:0:116:LEU:HD21	22:0:182:LEU:HD22	1.91	0.52
24:4:76:ILE:HG12	24:4:85:TYR:HA	1.91	0.52
25:6:260:ARG:HH21	25:6:281:ASN:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:7:132:LEU:HD23	26:7:201:SER:HB2	1.91	0.52
2:A:528:LEU:HD11	2:A:619:LYS:HB3	1.91	0.51
4:C:79:GLN:HB3	4:C:127:ARG:HH11	1.75	0.51
5:E:74:ASP:N	5:E:74:ASP:OD1	2.42	0.51
20:D:68:ARG:HD2	20:D:72:ARG:HH12	1.75	0.51
22:0:573:THR:OG1	22:0:575:ASP:O	2.26	0.51
2:A:117:GLU:H	2:A:122:MET:HE1	1.74	0.51
3:B:778:MET:HE1	3:B:853:SER:HB2	1.91	0.51
4:C:72:LEU:HB3	4:C:130:GLY:HA2	1.91	0.51
22:0:20:GLU:HG2	22:0:485:MET:HA	1.92	0.51
22:0:571:VAL:HG13	22:0:599:LEU:HB2	1.92	0.51
25:6:175:ARG:NH1	25:6:203:GLU:O	2.38	0.51
3:B:216:GLU:HB3	3:B:406:LEU:HD13	1.91	0.51
3:B:1033:LYS:HD2	3:B:1059:LEU:HD11	1.92	0.51
7:H:100:THR:O	7:H:117:SER:N	2.44	0.51
18:W:180:GLN:NE2	18:W:184:ASP:OD1	2.40	0.51
20:D:130:LEU:HB3	20:D:138:ASN:HD21	1.75	0.51
21:G:79:PHE:HE2	21:G:106:MET:HE1	1.75	0.51
23:1:473:LEU:HD22	24:4:140:ILE:HD13	1.93	0.51
25:6:320:VAL:HB	25:6:322:MET:HE3	1.92	0.51
27:2:167:LEU:HD22	27:2:173:MET:HB2	1.91	0.51
2:A:1205:LYS:HZ1	2:A:1274:ARG:HB3	1.74	0.51
12:Q:29:ARG:HB3	12:Q:33:ARG:HH12	1.74	0.51
19:X:119:ILE:HG13	19:X:127:LYS:HE3	1.93	0.51
1:M:211:LYS:NZ	15:O:184:SER:OG	2.42	0.51
2:A:783:THR:OG1	2:A:784:LEU:N	2.44	0.51
16:U:249:ASP:N	16:U:261:SER:O	2.43	0.51
17:V:48:VAL:HA	17:V:51:THR:HG22	1.93	0.51
22:0:674:ASP:N	22:0:674:ASP:OD1	2.43	0.51
2:A:1300:LYS:HZ3	14:S:302:CYS:HA	1.75	0.51
3:B:637:LEU:HD12	3:B:693:ILE:HG13	1.92	0.51
18:W:72:GLN:NE2	18:W:218:THR:O	2.43	0.51
22:0:541:PHE:HB2	22:0:547:MET:HE2	1.91	0.51
26:7:357:LYS:NZ	26:7:427:TRP:O	2.43	0.51
26:7:460:VAL:HB	26:7:501:VAL:HG12	1.92	0.51
27:2:194:GLN:O	27:2:199:GLN:NE2	2.44	0.51
2:A:453:MET:HE1	2:A:510:GLN:HB3	1.92	0.51
2:A:537:ARG:NH2	2:A:599:SER:OG	2.43	0.51
2:A:711:ARG:HG2	8:I:97:MET:HE3	1.91	0.51
14:S:201:ILE:O	14:S:205:ASN:ND2	2.42	0.51
14:S:239:ALA:HA	14:S:242:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:7:421:ARG:NH1	26:7:435:CYS:SG	2.83	0.51
2:A:782:ARG:HD3	2:A:789:LYS:HD3	1.91	0.51
14:S:232:ASP:HB3	14:S:235:ASP:HB3	1.92	0.51
18:W:127:CYS:SG	18:W:129:THR:OG1	2.68	0.51
22:0:259:ARG:NH2	22:0:394:GLU:O	2.43	0.51
25:6:190:GLN:NE2	25:6:194:ASP:OD1	2.43	0.51
27:2:25:LEU:HD22	27:2:222:LEU:HD13	1.93	0.51
2:A:949:ASP:OD1	2:A:949:ASP:N	2.41	0.51
2:A:1002:GLY:HA3	2:A:1007:ILE:HG21	1.93	0.51
3:B:996:ARG:HD3	3:B:1007:VAL:HG21	1.91	0.51
4:C:99:LEU:HB2	4:C:157:CYS:HB2	1.93	0.51
21:G:1:MET:SD	21:G:1:MET:N	2.82	0.51
25:6:394:THR:HA	25:6:398:PHE:HZ	1.76	0.51
26:7:425:LEU:HD13	26:7:432:PRO:HG3	1.93	0.51
3:B:120:ARG:NH2	3:B:957:ASN:O	2.44	0.51
16:U:258:TRP:CZ3	16:U:285:TRP:HB2	2.46	0.51
17:V:51:THR:O	17:V:55:ASN:CB	2.59	0.51
18:W:147:PHE:HB2	18:W:156:LEU:HB2	1.93	0.51
23:1:282:GLU:OE2	23:1:286:ARG:NH2	2.41	0.51
26:7:416:SER:HA	26:7:419:GLN:HG2	1.93	0.51
26:7:608:PHE:HB2	26:7:672:GLN:HG2	1.92	0.51
27:2:54:GLU:OE2	27:2:109:ARG:NH2	2.44	0.51
2:A:378:GLU:CD	2:A:434:ARG:HE	2.18	0.50
5:E:118:PRO:HA	5:E:121:MET:HB2	1.93	0.50
24:4:119:ARG:NH1	24:4:123:GLU:OE1	2.44	0.50
24:4:160:VAL:HG21	24:4:176:LEU:HD21	1.92	0.50
28:5:31:VAL:HG22	28:5:42:VAL:HG23	1.93	0.50
2:A:849:MET:HG2	2:A:1063:MET:HE1	1.92	0.50
2:A:852:TYR:OH	6:F:89:GLU:OE2	2.29	0.50
2:A:873:MET:O	2:A:1366:ARG:NH1	2.44	0.50
2:A:1161:THR:HG22	2:A:1163:ILE:H	1.76	0.50
3:B:62:ILE:HD11	3:B:418:LYS:HB2	1.93	0.50
3:B:542:MET:HE3	3:B:743:ILE:HD11	1.93	0.50
12:Q:111:LEU:HA	12:Q:114:MET:HE1	1.93	0.50
14:S:185:VAL:HB	14:S:189:ASP:HA	1.92	0.50
24:4:46:GLU:HB3	24:4:49:SER:HB3	1.93	0.50
27:2:409:ARG:HE	27:2:413:GLU:HG2	1.76	0.50
1:M:34:ILE:HG22	1:M:45:CYS:HA	1.94	0.50
2:A:131:SER:O	2:A:134:ARG:NH2	2.45	0.50
2:A:871:ASP:OD2	2:A:1366:ARG:NH2	2.44	0.50
13:P:70:LEU:HB3	13:P:221:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:115:ILE:O	25:6:387:LYS:NZ	2.45	0.50
26:7:496:ALA:O	26:7:500:ARG:NH1	2.35	0.50
27:2:150:MET:SD	27:2:173:MET:HG3	2.50	0.50
7:H:58:THR:HB	7:H:143:LEU:HB2	1.93	0.50
18:W:120:ASN:ND2	18:W:159:ASP:O	2.44	0.50
21:G:38:CYS:HA	21:G:44:TYR:HA	1.93	0.50
23:1:212:THR:OG1	23:1:213:ARG:NH1	2.44	0.50
2:A:1430:LEU:HB3	2:A:1432:GLN:HE22	1.76	0.50
3:B:248:SER:H	3:B:418:LYS:HZ1	1.60	0.50
3:B:862:GLN:HB3	3:B:963:PHE:HD1	1.76	0.50
19:X:163:LEU:HD12	19:X:166:LEU:HD12	1.94	0.50
2:A:457:ALA:N	2:A:505:CYS:O	2.44	0.50
2:A:519:PRO:HG3	2:A:631:HIS:HB2	1.93	0.50
3:B:304:ASP:OD1	3:B:306:ASN:ND2	2.42	0.50
3:B:576:ASP:OD1	3:B:576:ASP:N	2.43	0.50
20:D:192:LYS:O	20:D:199:ASN:ND2	2.45	0.50
22:0:37:ASN:HB2	22:0:477:THR:HA	1.94	0.50
22:0:67:ARG:NE	22:0:229:ASP:O	2.39	0.50
23:1:340:ASP:HA	23:1:343:ILE:HG12	1.93	0.50
26:7:411:CYS:HB2	26:7:488:ASP:HB2	1.93	0.50
29:N:38:DG:H2"	29:N:39:DA:C8	2.46	0.50
3:B:69:LEU:HD23	3:B:90:ILE:HD11	1.93	0.50
10:K:17:SER:OG	10:K:19:LEU:O	2.30	0.50
21:G:153:GLN:HG3	21:G:154:VAL:HG22	1.93	0.50
25:6:338:CYS:SG	25:6:339:HIS:N	2.85	0.50
26:7:551:ASN:H	26:7:701:PHE:HE2	1.58	0.50
15:O:144:GLN:NE2	15:O:150:ALA:O	2.44	0.50
17:V:87:VAL:HG12	17:V:88:GLU:HG3	1.92	0.50
18:W:198:THR:H	18:W:201:ILE:HB	1.77	0.50
26:7:401:CYS:O	26:7:404:LYS:NZ	2.38	0.50
3:B:445:LYS:HG3	3:B:446:LEU:HD22	1.94	0.50
23:1:567:HIS:HB3	23:1:579:VAL:HG22	1.92	0.50
2:A:451:HIS:HA	2:A:1070:GLN:HB3	1.93	0.49
2:A:855:THR:OG1	2:A:857:ARG:NH1	2.44	0.49
2:A:1293:SER:HB3	2:A:1297:GLU:H	1.76	0.49
3:B:616:ILE:HG12	3:B:697:GLU:HA	1.94	0.49
5:E:11:ARG:HH22	5:E:138:ALA:HB2	1.77	0.49
5:E:108:GLY:N	5:E:131:THR:O	2.37	0.49
26:7:679:SER:O	26:7:683:GLU:HB2	2.11	0.49
2:A:46:THR:O	2:A:47:ARG:NE	2.45	0.49
3:B:1219:ASP:OD1	3:B:1219:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:36:VAL:HG21	4:C:251:LEU:HD12	1.95	0.49
7:H:4:THR:HG21	7:H:7:ASP:HB2	1.94	0.49
22:0:86:LEU:HD22	22:0:175:VAL:HG11	1.94	0.49
22:0:112:LYS:HD3	22:0:129:VAL:HG21	1.94	0.49
27:2:503:ASP:OD1	27:2:507:ARG:NH1	2.45	0.49
3:B:76:GLN:HB2	12:Q:326:ARG:HE	1.77	0.49
3:B:1197:PRO:HB2	3:B:1200:ALA:H	1.76	0.49
5:E:97:VAL:HA	5:E:100:ILE:HD12	1.94	0.49
12:Q:371:ASP:OD1	12:Q:371:ASP:N	2.45	0.49
22:0:469:TYR:HA	22:0:472:MET:HG2	1.94	0.49
23:1:279:LYS:O	23:1:283:PHE:HB2	2.12	0.49
24:4:29:ILE:N	24:4:177:LEU:O	2.41	0.49
25:6:362:VAL:HA	25:6:369:MET:HA	1.95	0.49
3:B:391:ASP:O	8:I:90:GLN:NE2	2.45	0.49
3:B:914:LYS:HD2	3:B:937:ALA:HB3	1.95	0.49
12:Q:375:LEU:HD12	12:Q:387:ILE:HB	1.94	0.49
14:S:223:ILE:HG13	14:S:225:PRO:HD2	1.94	0.49
28:5:53:GLU:HA	28:5:56:ARG:HG2	1.93	0.49
2:A:346:ASP:H	3:B:1154:ALA:HB1	1.78	0.49
2:A:751:SER:OG	2:A:752:LYS:N	2.45	0.49
2:A:964:ILE:HG22	2:A:1045:VAL:HG21	1.94	0.49
3:B:271:ALA:O	3:B:280:ILE:N	2.44	0.49
12:Q:134:HIS:ND1	12:Q:354:ASP:OD2	2.42	0.49
14:S:240:PRO:O	14:S:243:GLN:NE2	2.45	0.49
23:1:572:GLU:OE1	23:1:575:GLN:NE2	2.43	0.49
26:7:613:TYR:CZ	26:7:766:LYS:HE3	2.48	0.49
27:2:17:ILE:O	27:2:22:GLN:NE2	2.46	0.49
30:T:-46:DA:H2'	30:T:-45:DA:H8	1.75	0.49
2:A:363:GLN:O	2:A:458:HIS:ND1	2.46	0.49
2:A:1132:LYS:HA	2:A:1135:ARG:HG2	1.93	0.49
2:A:1208:THR:OG1	2:A:1211:GLN:OE1	2.29	0.49
3:B:179:CYS:SG	3:B:180:TYR:N	2.85	0.49
3:B:901:PRO:HA	3:B:949:VAL:HG13	1.94	0.49
18:W:139:LEU:O	18:W:148:LEU:N	2.45	0.49
19:X:119:ILE:HG12	19:X:151:LEU:HB2	1.95	0.49
22:0:197:ARG:HH22	22:0:221:ARG:HB3	1.78	0.49
25:6:403:CYS:HB3	25:6:408:SER:H	1.78	0.49
26:7:134:ILE:HD13	26:7:205:VAL:HG13	1.95	0.49
26:7:340:GLU:OE1	26:7:376:ASN:ND2	2.45	0.49
26:7:431:GLN:NE2	26:7:433:GLU:OE1	2.46	0.49
30:T:-16:DG:H2'	30:T:-15:DA:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:843:LYS:HG2	2:A:1402:PHE:CD1	2.47	0.49
2:A:1158:PRO:O	2:A:1241:ARG:NH1	2.39	0.49
18:W:68:SER:N	18:W:88:TYR:O	2.46	0.49
19:X:211:LYS:NZ	19:X:215:PRO:O	2.46	0.49
22:0:275:ARG:NH1	22:0:329:GLU:OE2	2.46	0.49
25:6:178:LEU:O	25:6:180:GLN:NE2	2.45	0.49
26:7:578:MET:HA	26:7:581:TYR:CE1	2.48	0.49
1:M:239:ILE:HG23	1:M:282:ILE:HD11	1.94	0.49
2:A:147:VAL:HA	2:A:170:THR:HA	1.95	0.49
2:A:1142:THR:O	2:A:1145:SER:OG	2.28	0.49
22:0:472:MET:HG3	22:0:473:LEU:HG	1.94	0.49
2:A:335:ARG:HH12	3:B:1114:LEU:HG	1.77	0.49
2:A:1005:GLU:OE2	2:A:1009:ASN:ND2	2.45	0.49
7:H:123:MET:SD	7:H:123:MET:N	2.86	0.49
13:P:318:LEU:HG	13:P:329:LEU:HD21	1.93	0.49
22:0:228:LYS:HZ3	22:0:452:ARG:HH11	1.61	0.49
26:7:167:PRO:HD2	26:7:171:HIS:HA	1.94	0.49
27:2:125:VAL:H	27:2:237:TYR:HA	1.77	0.49
22:0:238:HIS:O	22:0:660:ARG:NH1	2.46	0.49
24:4:78:ALA:HB2	24:4:152:ALA:HB2	1.95	0.49
28:5:13:ASP:HB3	28:5:16:ILE:HG12	1.95	0.49
5:E:141:VAL:HG13	5:E:142:VAL:HG23	1.95	0.48
24:4:158:THR:HG22	25:6:443:PHE:HE2	1.77	0.48
26:7:494:PRO:HG2	26:7:523:LYS:HE3	1.95	0.48
3:B:301:ILE:HG21	3:B:314:LEU:HD11	1.95	0.48
6:F:99:LEU:HD12	6:F:103:MET:HE1	1.95	0.48
22:0:352:ILE:HB	22:0:420:ILE:HB	1.95	0.48
22:0:544:TYR:HB3	23:1:358:MET:HA	1.95	0.48
23:1:214:ILE:HG22	23:1:218:ARG:HH12	1.78	0.48
27:2:168:LYS:HD2	27:2:175:GLU:HB2	1.94	0.48
14:S:298:THR:HA	14:S:305:ARG:HA	1.94	0.48
22:0:607:SER:O	22:0:668:ARG:NH2	2.47	0.48
27:2:337:GLY:H	27:2:351:SER:HB3	1.79	0.48
2:A:362:ASP:N	2:A:362:ASP:OD1	2.46	0.48
15:O:160:ILE:HG21	15:O:220:ARG:NH2	2.29	0.48
22:0:135:ARG:NH1	22:0:391:THR:OG1	2.46	0.48
26:7:349:ASN:O	26:7:405:LYS:NZ	2.47	0.48
2:A:390:GLN:NE2	2:A:394:ASN:OD1	2.44	0.48
2:A:1146:VAL:HG23	2:A:1197:LEU:HD22	1.95	0.48
3:B:758:PHE:H	3:B:1044:ALA:HB1	1.78	0.48
15:O:114:LEU:HB2	15:O:122:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:145:MET:HA	20:D:148:LEU:HD12	1.95	0.48
20:D:152:SER:HB2	20:D:155:ARG:NH2	2.28	0.48
22:0:406:ALA:O	22:0:410:SER:OG	2.29	0.48
22:0:498:THR:OG1	22:0:707:ASN:OD1	2.31	0.48
23:1:589:CYS:HA	23:1:592:LYS:HE3	1.96	0.48
27:2:152:GLY:HA2	27:2:182:PHE:HE1	1.78	0.48
2:A:1385:THR:OG1	2:A:1388:GLY:N	2.41	0.48
3:B:558:LEU:HD21	3:B:580:VAL:HG11	1.94	0.48
5:E:9:ILE:HG21	5:E:43:LYS:HD3	1.95	0.48
8:I:96:SER:OG	8:I:97:MET:N	2.47	0.48
22:0:114:LEU:HD22	22:0:192:PRO:HB2	1.96	0.48
22:0:192:PRO:HA	22:0:195:ILE:HB	1.95	0.48
24:4:182:GLY:N	24:4:215:ILE:O	2.47	0.48
24:4:188:ASP:O	24:4:192:GLN:NE2	2.46	0.48
26:7:642:ASN:HB3	26:7:649:ILE:HG13	1.94	0.48
27:2:352:ASN:ND2	27:2:370:PHE:O	2.47	0.48
27:2:497:GLY:HA2	27:2:500:GLN:HE21	1.78	0.48
1:M:43:VAL:HG23	1:M:52:LEU:HB3	1.96	0.48
12:Q:102:PRO:HB2	13:P:91:GLU:HB3	1.95	0.48
23:1:279:LYS:O	23:1:283:PHE:CB	2.61	0.48
25:6:363:CYS:N	25:6:368:LEU:O	2.43	0.48
26:7:234:VAL:HG21	26:7:318:ILE:HD12	1.95	0.48
26:7:763:VAL:O	26:7:767:ASN:ND2	2.46	0.48
17:V:85:VAL:O	17:V:106:ILE:N	2.44	0.48
27:2:90:ASN:O	27:2:97:MET:N	2.47	0.48
27:2:186:ASN:HD21	27:2:392:THR:HG1	1.58	0.48
3:B:198:ASP:OD2	3:B:202:TYR:OH	2.31	0.48
3:B:801:LYS:HD3	3:B:815:ARG:HG3	1.96	0.48
13:P:322:THR:O	13:P:324:GLN:HG3	2.14	0.48
26:7:124:ARG:NH2	26:7:203:VAL:O	2.47	0.48
26:7:133:TRP:CH2	26:7:202:LYS:HE3	2.48	0.48
27:2:131:SER:HA	27:2:135:LEU:HD13	1.96	0.48
2:A:668:ASP:OD2	2:A:743:VAL:N	2.47	0.48
15:O:108:GLU:HG2	15:O:109:PRO:HD3	1.96	0.48
15:O:128:SER:OG	15:O:130:ASP:OD1	2.28	0.48
21:G:56:ILE:HG22	21:G:72:VAL:HG22	1.96	0.48
26:7:143:LEU:HB3	26:7:171:HIS:HB2	1.95	0.48
26:7:564:GLU:O	26:7:567:GLN:NE2	2.46	0.48
2:A:260:ASP:OD1	2:A:260:ASP:N	2.43	0.47
3:B:1065:GLN:OE1	3:B:1069:PHE:N	2.41	0.47
20:D:119:ARG:HH21	20:D:149:THR:HG23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:123:LEU:HD11	20:D:149:THR:HG21	1.96	0.47
2:A:68:GLN:HE21	2:A:80:HIS:CE1	2.32	0.47
2:A:646:PHE:O	2:A:650:GLN:HB2	2.14	0.47
3:B:553:PRO:HG2	3:B:554:ILE:HD12	1.96	0.47
3:B:809:MET:HB2	3:B:814:PHE:HB3	1.97	0.47
3:B:861:ASP:OD1	3:B:914:LYS:NZ	2.41	0.47
4:C:11:ARG:HG3	4:C:20:PHE:HA	1.95	0.47
7:H:32:THR:OG1	7:H:33:GLN:OE1	2.32	0.47
14:S:285:GLN:HB3	14:S:293:LEU:HD23	1.96	0.47
22:0:104:ARG:O	22:0:204:ASN:N	2.47	0.47
25:6:146:HIS:CG	25:6:204:PRO:HG3	2.49	0.47
26:7:372:LYS:HA	26:7:372:LYS:HD3	1.76	0.47
2:A:1394:THR:HB	2:A:1399:ARG:HD3	1.96	0.47
13:P:96:ARG:NH2	13:P:103:LYS:O	2.47	0.47
21:G:62:LEU:HD23	21:G:65:ASP:HB2	1.96	0.47
3:B:521:LEU:HD22	3:B:633:VAL:HG12	1.95	0.47
3:B:983:ARG:HD2	3:B:1091:TYR:HB3	1.95	0.47
22:0:625:ILE:HD11	22:0:685:ARG:HB2	1.96	0.47
13:P:66:ARG:HD3	13:P:66:ARG:HA	1.74	0.47
22:0:117:HIS:N	33:0:801:SF4:S3	2.85	0.47
25:6:131:ASP:HA	25:6:174:MET:HB3	1.96	0.47
26:7:409:VAL:HG22	26:7:486:ILE:HD13	1.95	0.47
26:7:462:ASN:O	26:7:466:ARG:NH1	2.40	0.47
26:7:634:GLN:NE2	29:N:42:DA:OP2	2.47	0.47
2:A:399:HIS:CE1	2:A:462:VAL:HG21	2.50	0.47
2:A:1132:LYS:NZ	2:A:1206:ASP:OD2	2.48	0.47
3:B:425:THR:HA	3:B:428:ILE:HD12	1.96	0.47
4:C:35:ARG:HH21	10:K:41:THR:HG23	1.80	0.47
4:C:221:TYR:CD1	4:C:222:LYS:HG3	2.50	0.47
8:I:17:ARG:HE	8:I:28:GLU:CD	2.23	0.47
12:Q:108:LYS:HE2	13:P:84:ARG:HE	1.79	0.47
21:G:150:CYS:HA	21:G:159:ALA:HA	1.96	0.47
22:0:731:LYS:HA	22:0:734:GLU:HB2	1.97	0.47
22:0:743:ASP:OD1	22:0:746:LYS:NZ	2.43	0.47
26:7:341:TYR:OH	26:7:349:ASN:OD1	2.32	0.47
1:M:277:ILE:HA	1:M:280:VAL:HG22	1.97	0.47
2:A:33:ALA:HB3	2:A:82:GLY:HA3	1.96	0.47
2:A:402:ALA:HA	2:A:434:ARG:HA	1.97	0.47
2:A:1159:ARG:NH2	2:A:1185:PHE:O	2.45	0.47
3:B:838:SER:OG	3:B:839:MET:N	2.46	0.47
3:B:1074:ASN:ND2	3:B:1077:THR:OG1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:26:ARG:HA	12:Q:29:ARG:HH21	1.79	0.47
14:S:269:PHE:HB2	14:S:279:VAL:HG21	1.97	0.47
15:O:195:TYR:HB3	15:O:204:LEU:HB2	1.95	0.47
20:D:153:ARG:HH22	20:D:160:VAL:HA	1.79	0.47
22:0:161:ASN:ND2	22:0:189:THR:O	2.48	0.47
22:0:513:ARG:NH1	22:0:514:ASN:OD1	2.47	0.47
24:4:308:CYS:SG	24:4:310:SER:OG	2.68	0.47
26:7:383:ILE:HB	26:7:534:LYS:HA	1.96	0.47
26:7:634:GLN:HA	26:7:637:MET:HG3	1.97	0.47
28:5:20:ILE:HA	28:5:23:ILE:HD12	1.97	0.47
7:H:101:ALA:HA	7:H:116:TYR:HA	1.96	0.47
22:0:669:VAL:HG21	22:0:679:MET:HE1	1.96	0.47
26:7:718:TYR:HB3	26:7:722:ARG:HH12	1.79	0.47
28:5:26:LYS:HE2	28:5:27:MET:HE1	1.96	0.47
3:B:480:SER:O	3:B:480:SER:OG	2.29	0.47
10:K:36:GLU:HA	10:K:70:ARG:HA	1.97	0.47
22:0:380:ARG:HH22	22:0:384:LEU:HD13	1.80	0.47
22:0:719:GLN:O	22:0:723:THR:OG1	2.26	0.47
2:A:376:TYR:OH	2:A:498:ARG:NH1	2.48	0.47
2:A:698:GLN:HG2	8:I:99:LEU:HD21	1.96	0.47
3:B:546:SER:OG	3:B:632:ARG:N	2.42	0.47
5:E:175:LEU:HD22	5:E:213:ILE:HB	1.96	0.47
8:I:74:GLU:HB3	8:I:81:ARG:HD3	1.96	0.47
17:V:67:ASP:HB3	17:V:79:ILE:HG22	1.96	0.47
17:V:109:ASP:OD2	17:V:110:LYS:N	2.47	0.47
23:1:208:GLU:HA	23:1:211:SER:HB3	1.96	0.47
25:6:402:ASP:OD1	25:6:402:ASP:N	2.48	0.47
27:2:208:LEU:HA	27:2:211:ILE:HG22	1.96	0.47
30:T:4:DC:N3	30:T:5:DA:N6	2.63	0.47
2:A:352:VAL:O	2:A:467:THR:OG1	2.33	0.46
3:B:363:HIS:O	3:B:365:THR:N	2.48	0.46
3:B:494:HIS:HA	3:B:497:ARG:HE	1.80	0.46
3:B:629:ASP:N	3:B:629:ASP:OD1	2.46	0.46
12:Q:106:ILE:HG12	12:Q:111:LEU:HD13	1.96	0.46
26:7:567:GLN:HB2	26:7:571:ARG:HH21	1.80	0.46
27:2:256:TYR:HB3	27:2:258:LEU:HD23	1.96	0.46
16:U:30:ILE:HD11	17:V:31:ARG:NH1	2.31	0.46
22:0:133:CYS:O	22:0:137:THR:OG1	2.25	0.46
3:B:871:THR:OG1	3:B:872:GLU:N	2.47	0.46
4:C:125:MET:SD	4:C:127:ARG:NE	2.86	0.46
20:D:23:ASN:H	21:G:83:LYS:HZ3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:10:ASN:HA	21:G:71:ASN:HA	1.97	0.46
24:4:221:SER:HB3	24:4:224:LEU:HD13	1.97	0.46
2:A:4:GLN:O	3:B:1159:ARG:NH2	2.45	0.46
2:A:24:PRO:HA	2:A:27:VAL:HG12	1.97	0.46
2:A:116:ASP:HB3	2:A:164:ARG:HD3	1.97	0.46
2:A:1335:ILE:O	2:A:1339:LEU:HB2	2.15	0.46
3:B:363:HIS:HD2	3:B:364:ILE:HG23	1.81	0.46
3:B:796:LEU:HA	3:B:853:SER:HA	1.97	0.46
12:Q:113:ASN:HD21	13:P:139:ASN:HB2	1.80	0.46
1:M:161:LYS:O	1:M:164:LYS:HE2	2.14	0.46
2:A:544:ASP:O	2:A:548:ASN:ND2	2.36	0.46
2:A:843:LYS:NZ	2:A:1401:SER:O	2.47	0.46
2:A:1217:LYS:HE3	2:A:1221:LYS:HE2	1.97	0.46
3:B:76:GLN:OE1	12:Q:326:ARG:NH2	2.47	0.46
3:B:822:ASN:HD21	9:J:48:ARG:HD3	1.79	0.46
9:J:16:ASP:OD1	9:J:16:ASP:N	2.48	0.46
14:S:187:ASN:HB2	14:S:228:LEU:HD11	1.96	0.46
18:W:192:SER:OG	18:W:193:ARG:N	2.46	0.46
22:0:119:GLU:HA	22:0:122:LYS:HE2	1.97	0.46
22:0:436:ARG:HD3	22:0:634:ILE:HD11	1.96	0.46
22:0:612:PHE:O	22:0:671:ARG:NH1	2.48	0.46
22:0:690:ARG:HD2	22:0:706:LEU:HD11	1.97	0.46
23:1:542:LEU:HB2	23:1:547:LEU:HD12	1.96	0.46
1:M:84:ASN:HB3	1:M:87:LEU:HD12	1.97	0.46
1:M:321:ASP:OD1	1:M:321:ASP:N	2.46	0.46
2:A:562:THR:O	2:A:572:TRP:NE1	2.39	0.46
2:A:864:ILE:HD12	2:A:1377:THR:HG21	1.98	0.46
2:A:903:ASN:O	2:A:907:THR:OG1	2.32	0.46
12:Q:326:ARG:HH12	12:Q:330:ARG:HB3	1.80	0.46
19:X:234:ARG:HD3	19:X:239:LYS:HB3	1.97	0.46
24:4:288:ILE:HB	24:4:293:LEU:HA	1.98	0.46
25:6:261:VAL:HB	25:6:280:THR:HG21	1.97	0.46
26:7:642:ASN:O	26:7:646:ASN:CB	2.58	0.46
1:M:177:LEU:HD13	1:M:192:ILE:HD11	1.98	0.46
2:A:443:LEU:HD22	2:A:501:LEU:HD11	1.96	0.46
2:A:1279:ILE:HA	2:A:1310:GLY:HA3	1.97	0.46
4:C:96:SER:OG	4:C:97:VAL:N	2.49	0.46
16:U:253:ARG:HB3	16:U:258:TRP:CD1	2.51	0.46
17:V:51:THR:O	17:V:55:ASN:HB3	2.15	0.46
22:0:388:LEU:HB3	22:0:390:VAL:HG13	1.98	0.46
22:0:490:LYS:NZ	22:0:700:GLY:O	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1:172:GLU:O	23:1:176:THR:OG1	2.26	0.46
26:7:154:GLN:HA	26:7:157:LEU:HB2	1.97	0.46
3:B:822:ASN:ND2	9:J:48:ARG:HD3	2.31	0.46
4:C:43:THR:HA	4:C:77:ILE:HG12	1.98	0.46
17:V:11:ARG:HD2	17:V:41:LEU:HD12	1.96	0.46
2:A:746:MET:HE1	3:B:1015:HIS:NE2	2.31	0.46
2:A:1198:ASP:HB3	2:A:1201:ALA:HB3	1.98	0.46
2:A:1229:SER:OG	2:A:1233:ASP:OD2	2.30	0.46
3:B:872:GLU:HG2	3:B:917:PRO:HD3	1.98	0.46
4:C:107:SER:OG	4:C:109:SER:O	2.33	0.46
17:V:68:THR:HB	17:V:79:ILE:HB	1.98	0.46
17:V:81:LYS:HA	17:V:110:LYS:HA	1.98	0.46
22:0:332:VAL:HG12	22:0:336:LYS:HE2	1.98	0.46
22:0:673:LYS:NZ	22:0:737:SER:O	2.47	0.46
22:0:683:ASP:OD2	22:0:685:ARG:NH2	2.40	0.46
24:4:216:GLY:O	24:4:237:HIS:NE2	2.43	0.46
26:7:323:VAL:HA	26:7:326:VAL:HG22	1.98	0.46
3:B:413:LEU:O	3:B:417:PHE:HB2	2.16	0.46
3:B:493:SER:HA	3:B:751:VAL:HG21	1.98	0.46
3:B:1160:VAL:HG11	3:B:1169:MET:HE1	1.97	0.46
13:P:297:LYS:HE2	19:X:130:TRP:CZ2	2.51	0.46
18:W:149:CYS:HB3	18:W:154:GLU:H	1.81	0.46
22:0:67:ARG:NH2	22:0:455:SER:OG	2.49	0.46
22:0:201:SER:HB3	22:0:225:GLU:HB3	1.98	0.46
25:6:248:HIS:HA	25:6:251:ILE:HD12	1.98	0.46
2:A:841:LEU:HD11	2:A:1371:LEU:HD11	1.98	0.45
12:Q:117:HIS:ND1	12:Q:391:LYS:HB2	2.32	0.45
22:0:703:ASP:N	22:0:703:ASP:OD1	2.49	0.45
25:6:334:THR:N	25:6:343:VAL:O	2.47	0.45
27:2:367:LYS:HZ1	27:2:377:GLN:HB2	1.81	0.45
3:B:1163:CYS:O	3:B:1167:GLY:N	2.39	0.45
19:X:186:VAL:HG13	19:X:191:GLU:HB2	1.98	0.45
26:7:207:GLU:HA	26:7:210:ILE:HB	1.98	0.45
26:7:679:SER:HB2	26:7:682:GLN:HB3	1.97	0.45
2:A:636:GLU:HB2	2:A:962:ARG:HH21	1.81	0.45
2:A:754:SER:H	2:A:757:ASN:HB2	1.80	0.45
5:E:136:ASN:HD21	5:E:138:ALA:HB3	1.82	0.45
9:J:1:MET:SD	9:J:2:ILE:N	2.71	0.45
15:O:143:ILE:HA	15:O:146:ILE:HD12	1.98	0.45
21:G:166:ASP:N	21:G:166:ASP:OD1	2.49	0.45
2:A:1135:ARG:HE	2:A:1282:VAL:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1254:ALA:N	2:A:1256:GLU:OE2	2.49	0.45
3:B:213:ILE:O	3:B:215:GLN:NE2	2.49	0.45
3:B:1049:ASP:OD1	3:B:1049:ASP:N	2.42	0.45
3:B:1065:GLN:OE1	3:B:1068:GLY:N	2.49	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.81	0.45
7:H:128:ASN:OD1	7:H:131:ASN:ND2	2.49	0.45
12:Q:120:LYS:HD3	13:P:132:GLU:HG2	1.98	0.45
19:X:196:LEU:HB3	19:X:246:TYR:HB2	1.98	0.45
22:0:67:ARG:NH2	22:0:230:SER:O	2.50	0.45
23:1:184:LEU:HD21	23:1:217:LEU:HD23	1.98	0.45
23:1:302:MET:HG3	23:1:304:ASN:H	1.80	0.45
26:7:103:ASP:OD1	26:7:103:ASP:N	2.49	0.45
26:7:225:LEU:HD12	26:7:234:VAL:HG22	1.98	0.45
29:N:-4:DG:H1'	29:N:-3:DA:H5'	1.98	0.45
2:A:769:SER:OG	2:A:773:LYS:O	2.29	0.45
2:A:951:GLU:OE2	2:A:953:ASN:N	2.46	0.45
3:B:43:LEU:HD22	3:B:492:LEU:HD12	1.99	0.45
3:B:860:MET:HE1	3:B:965:LYS:HE3	1.98	0.45
7:H:117:SER:OG	7:H:118:PHE:N	2.49	0.45
11:L:60:ARG:HE	11:L:61:THR:H	1.63	0.45
13:P:125:THR:OG1	13:P:221:GLU:OE1	2.34	0.45
15:O:171:ARG:NH2	15:O:238:ARG:O	2.48	0.45
17:V:61:THR:O	17:V:63:LYS:NZ	2.46	0.45
23:1:291:LYS:NZ	23:1:306:ARG:O	2.49	0.45
2:A:884:ASP:OD2	2:A:1025:ARG:NE	2.41	0.45
2:A:1194:ARG:NE	2:A:1196:GLU:OE2	2.50	0.45
5:E:202:SER:N	5:E:206:GLY:O	2.41	0.45
10:K:36:GLU:HG2	10:K:37:LYS:HG2	1.97	0.45
16:U:282:GLU:HB3	17:V:63:LYS:HG3	1.97	0.45
22:0:270:ARG:HG2	22:0:390:VAL:HG12	1.99	0.45
22:0:586:TYR:HD1	22:0:596:ALA:HB3	1.81	0.45
23:1:214:ILE:HA	23:1:217:LEU:HD12	1.98	0.45
24:4:21:GLU:OE1	24:4:257:SER:OG	2.33	0.45
26:7:470:SER:HB3	26:7:474:MET:HE1	1.98	0.45
30:T:3:DT:H2'	30:T:4:DC:C2	2.52	0.45
2:A:55:ASP:HA	2:A:58:LEU:HD23	1.98	0.45
2:A:567:LYS:HG2	7:H:96:VAL:H	1.81	0.45
2:A:1121:GLU:HG3	2:A:1123:GLY:H	1.80	0.45
2:A:1308:THR:OG1	2:A:1309:ASP:N	2.49	0.45
3:B:448:ILE:HD12	3:B:448:ILE:HA	1.78	0.45
13:P:112:ASP:OD1	13:P:118:HIS:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:32:CYS:HG	27:2:107:SER:HG	1.54	0.45
1:M:239:ILE:HD12	1:M:282:ILE:HD11	1.99	0.45
2:A:99:ILE:HG12	2:A:234:MET:HE1	1.98	0.45
4:C:116:LYS:HB3	4:C:134:ILE:HD11	1.99	0.45
7:H:145:ARG:HH11	7:H:145:ARG:HD2	1.68	0.45
13:P:138:GLN:HB2	13:P:211:LYS:HB3	1.97	0.45
22:0:721:LEU:O	22:0:725:ALA:CB	2.65	0.45
23:1:493:ASN:HA	23:1:496:SER:HB3	1.98	0.45
25:6:150:ILE:HG21	25:6:200:ARG:HB2	1.98	0.45
26:7:485:ILE:HD11	26:7:510:LYS:HD2	1.99	0.45
26:7:560:PRO:HG2	26:7:586:THR:HG21	1.98	0.45
27:2:357:ILE:HD11	27:2:369:ARG:HD3	1.98	0.45
1:M:23:THR:HA	1:M:32:PRO:HG3	1.98	0.45
4:C:50:GLU:HB2	4:C:156:THR:HB	1.99	0.45
22:0:537:MET:HB3	22:0:597:ILE:HD12	1.99	0.45
23:1:587:LYS:HA	23:1:587:LYS:HD3	1.82	0.45
24:4:112:SER:HA	24:4:119:ARG:HE	1.82	0.45
25:6:325:PRO:HD3	25:6:370:LEU:HB3	1.97	0.45
27:2:146:ILE:HD13	27:2:159:PRO:HB3	1.99	0.45
2:A:1453:TYR:CZ	6:F:149:GLU:HG3	2.52	0.45
6:F:86:THR:OG1	6:F:87:LYS:N	2.45	0.45
12:Q:141:ARG:NH1	12:Q:348:TYR:O	2.48	0.45
12:Q:379:GLU:HB2	12:Q:383:SER:HB2	1.99	0.45
22:0:21:GLN:NE2	22:0:47:GLY:O	2.50	0.45
22:0:351:VAL:HG13	22:0:421:GLU:HG2	1.99	0.45
22:0:678:VAL:HG11	22:0:717:THR:HG22	1.99	0.45
23:1:606:GLU:OE2	23:1:610:ASN:ND2	2.50	0.45
25:6:127:ILE:HB	25:6:232:VAL:HG22	1.98	0.45
26:7:389:GLY:HA3	26:7:692:ARG:HB3	1.97	0.45
29:N:42:DA:H2"	29:N:43:DC:H5"	1.99	0.45
3:B:102:VAL:H	3:B:112:LEU:HD23	1.82	0.44
3:B:463:THR:HG22	3:B:465:ASN:H	1.82	0.44
17:V:10:TYR:O	17:V:13:SER:OG	2.35	0.44
21:G:12:THR:HA	21:G:69:GLU:HA	1.99	0.44
22:0:116:LEU:N	33:0:801:SF4:S3	2.90	0.44
25:6:165:PRO:HB2	25:6:360:PRO:HG3	1.99	0.44
25:6:446:GLU:HG3	25:6:447:ILE:HG12	2.00	0.44
27:2:173:MET:HE1	27:2:184:ILE:HG23	1.99	0.44
2:A:254:GLU:O	3:B:935:ARG:NH1	2.50	0.44
3:B:412:LEU:HB3	3:B:466:TRP:HZ2	1.81	0.44
11:L:27:LEU:HD21	11:L:62:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:175:ARG:HE	24:4:177:LEU:HD21	1.83	0.44
2:A:121:LEU:O	2:A:124:GLN:NE2	2.50	0.44
4:C:191:TYR:HD2	4:C:201:TRP:CE2	2.35	0.44
5:E:198:ILE:O	5:E:210:SER:OG	2.33	0.44
15:O:68:GLN:HB2	15:O:161:VAL:HG12	1.99	0.44
21:G:115:MET:SD	21:G:115:MET:N	2.90	0.44
21:G:120:THR:OG1	21:G:131:GLN:O	2.35	0.44
22:0:567:LYS:HE3	22:0:595:GLY:HA3	2.00	0.44
1:M:312:GLY:HA2	1:M:315:ILE:HG22	2.00	0.44
2:A:190:ALA:HB2	18:W:224:GLY:HA2	1.99	0.44
3:B:627:PHE:O	3:B:632:ARG:NH1	2.50	0.44
3:B:883:LEU:HB2	3:B:935:ARG:HA	1.99	0.44
14:S:210:ASN:HA	14:S:211:ASN:HA	1.64	0.44
22:0:220:GLU:HA	22:0:223:SER:HB3	1.99	0.44
22:0:424:GLU:HB3	22:0:432:ASN:HB3	1.99	0.44
25:6:132:CYS:HB2	25:6:175:ARG:HB2	1.99	0.44
26:7:643:PHE:HB2	26:7:652:ILE:HD11	1.99	0.44
1:M:314:LYS:HE2	1:M:314:LYS:HB2	1.84	0.44
3:B:195:CYS:HB3	3:B:782:LEU:HD12	1.99	0.44
5:E:147:HIS:HE1	5:E:149:LEU:HD13	1.83	0.44
9:J:57:ILE:HA	9:J:60:PHE:HB2	1.99	0.44
14:S:235:ASP:HA	14:S:242:LYS:HD3	1.99	0.44
18:W:17:VAL:HA	18:W:21:TYR:HD2	1.82	0.44
19:X:204:GLY:HA3	19:X:243:TYR:HB3	1.99	0.44
20:D:14:ARG:HE	20:D:17:LYS:HD2	1.81	0.44
22:0:39:ILE:HD11	22:0:475:PHE:HZ	1.81	0.44
24:4:149:LEU:HG	24:4:153:MET:HE1	2.00	0.44
24:4:276:CYS:N	24:4:281:ARG:O	2.50	0.44
27:2:480:VAL:HG11	27:2:500:GLN:NE2	2.32	0.44
2:A:12:ARG:NH2	3:B:1218:THR:OG1	2.50	0.44
2:A:18:GLN:O	3:B:1215:ARG:N	2.51	0.44
2:A:1205:LYS:O	2:A:1274:ARG:NH2	2.50	0.44
3:B:52:ASN:OD1	3:B:177:LYS:N	2.51	0.44
3:B:304:ASP:OD2	3:B:307:ASP:N	2.45	0.44
15:O:133:LYS:HB3	15:O:137:ARG:HH12	1.82	0.44
15:O:174:GLY:O	15:O:178:SER:OG	2.33	0.44
27:2:17:ILE:HG22	27:2:22:GLN:HG3	1.99	0.44
27:2:478:ILE:HD12	27:2:500:GLN:CD	2.42	0.44
2:A:590:ARG:NH1	2:A:620:LYS:O	2.44	0.44
3:B:344:LYS:HD3	3:B:348:ARG:H	1.82	0.44
3:B:843:GLN:HB2	3:B:993:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:113:VAL:HG12	4:C:144:ILE:HD13	2.00	0.44
15:O:69:ASN:HB2	30:T:-6:DT:H1'	2.00	0.44
15:O:184:SER:N	15:O:194:ILE:O	2.51	0.44
22:0:107:GLY:HA3	22:0:178:PHE:HZ	1.82	0.44
25:6:128:LEU:N	25:6:170:GLY:O	2.46	0.44
27:2:32:CYS:SG	27:2:107:SER:OG	2.61	0.44
2:A:170:THR:HG21	2:A:187:LYS:HA	2.00	0.44
7:H:37:LYS:HD2	7:H:37:LYS:HA	1.82	0.44
7:H:118:PHE:HB2	7:H:121:LEU:HB2	1.99	0.44
25:6:451:CYS:HB3	25:6:454:CYS:SG	2.57	0.44
27:2:239:ILE:HG23	27:2:247:ARG:HD3	1.99	0.44
27:2:254:ARG:NH2	27:2:261:GLN:O	2.47	0.44
27:2:261:GLN:HA	27:2:269:PHE:HA	2.00	0.44
2:A:672:ASP:O	2:A:675:THR:OG1	2.29	0.44
2:A:1332:PHE:HA	2:A:1335:ILE:HD13	2.00	0.44
3:B:763:GLN:HG2	3:B:765:PRO:HD2	2.00	0.44
12:Q:379:GLU:HA	13:P:63:ARG:HH22	1.82	0.44
18:W:92:PRO:HB3	18:W:194:ILE:HD11	1.98	0.44
22:0:31:THR:HA	22:0:34:VAL:HG12	2.00	0.44
24:4:212:VAL:HG21	24:4:224:LEU:HB3	2.00	0.44
2:A:794:PRO:O	2:A:799:PHE:N	2.51	0.43
3:B:69:LEU:HB3	3:B:90:ILE:HG13	1.99	0.43
3:B:809:MET:HE3	3:B:809:MET:HB3	1.71	0.43
4:C:46:ILE:HD13	4:C:46:ILE:HG21	1.85	0.43
14:S:288:SER:OG	14:S:289:ALA:N	2.51	0.43
20:D:121:LYS:O	20:D:125:SER:HB3	2.18	0.43
22:0:258:ARG:HD2	22:0:262:ARG:HH21	1.83	0.43
22:0:345:ARG:NH2	22:0:354:GLU:OE2	2.51	0.43
22:0:448:PRO:O	22:0:452:ARG:HB2	2.17	0.43
2:A:455:MET:C	2:A:456:MET:HE2	2.44	0.43
2:A:1284:MET:C	2:A:1285:MET:HE2	2.43	0.43
3:B:45:SER:OG	3:B:46:GLN:NE2	2.51	0.43
3:B:523:CYS:SG	3:B:526:GLU:HG3	2.59	0.43
3:B:780:VAL:HG21	3:B:817:LEU:HD12	2.00	0.43
10:K:85:ASP:HA	10:K:88:LYS:HG2	1.99	0.43
20:D:57:LEU:HD22	20:D:157:GLN:HB3	2.00	0.43
22:0:502:ASP:OD2	22:0:521:ASN:ND2	2.51	0.43
26:7:562:THR:O	26:7:566:TYR:HB2	2.18	0.43
28:5:5:ARG:HH12	28:5:32:LEU:HD13	1.82	0.43
28:5:35:LEU:HB2	28:5:39:HIS:HB2	2.00	0.43
2:A:605:MET:HG2	2:A:621:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:858:ASN:OD1	2:A:861:GLY:N	2.51	0.43
3:B:363:HIS:CD2	3:B:364:ILE:H	2.36	0.43
5:E:171:LYS:O	5:E:173:SER:N	2.51	0.43
16:U:12:ILE:HG13	16:U:13:ILE:N	2.33	0.43
24:4:25:LEU:HD13	24:4:163:ILE:HG21	2.00	0.43
26:7:593:PHE:HB2	26:7:745:ILE:HG21	2.01	0.43
27:2:475:ALA:HA	27:2:478:ILE:HD11	2.00	0.43
2:A:742:ASN:O	2:A:746:MET:HG2	2.18	0.43
3:B:244:LEU:HD23	3:B:362:PRO:HB2	1.99	0.43
3:B:1156:ASP:OD1	3:B:1157:ALA:N	2.45	0.43
9:J:45:CYS:SG	9:J:46:CYS:N	2.92	0.43
15:O:68:GLN:HE21	30:T:-5:DA:H4'	1.83	0.43
16:U:22:ARG:NH2	16:U:26:GLU:OE2	2.52	0.43
21:G:54:ILE:HD12	21:G:54:ILE:HA	1.90	0.43
22:0:295:SER:HA	22:0:383:LEU:HD21	2.00	0.43
2:A:451:HIS:CD2	2:A:453:MET:HB2	2.54	0.43
3:B:139:ALA:N	3:B:150:GLU:O	2.51	0.43
3:B:445:LYS:HE2	3:B:445:LYS:HB2	1.86	0.43
19:X:168:ARG:O	19:X:181:LEU:N	2.52	0.43
21:G:84:GLY:N	21:G:147:ILE:O	2.41	0.43
21:G:135:ASP:HB3	21:G:170:ALA:HA	2.00	0.43
22:0:424:GLU:OE1	22:0:432:ASN:ND2	2.51	0.43
29:N:43:DC:H2"	29:N:44:DT:H5"	2.01	0.43
2:A:669:THR:HG22	2:A:805:LEU:HD22	2.01	0.43
2:A:843:LYS:HD3	2:A:846:GLU:OE2	2.18	0.43
2:A:1319:VAL:HG23	2:A:1322:ILE:HG13	2.01	0.43
3:B:750:GLY:H	3:B:753:ALA:HB3	1.82	0.43
9:J:44:TYR:HA	9:J:47:ARG:HB2	2.01	0.43
13:P:322:THR:O	13:P:323:ARG:HD3	2.18	0.43
14:S:242:LYS:O	14:S:245:ILE:N	2.52	0.43
15:O:66:THR:OG1	15:O:67:LEU:N	2.52	0.43
16:U:44:LYS:HA	16:U:47:THR:HG22	2.01	0.43
18:W:176:MET:HA	18:W:179:ILE:HG22	2.00	0.43
23:1:620:LEU:HA	23:1:623:ILE:HD12	1.99	0.43
24:4:65:LEU:HB2	24:4:118:PHE:HE1	1.83	0.43
27:2:189:PHE:HA	27:2:192:LEU:HD12	2.01	0.43
1:M:202:GLU:O	1:M:206:THR:OG1	2.28	0.43
2:A:481:ASP:OD1	2:A:481:ASP:N	2.49	0.43
2:A:1135:ARG:HA	2:A:1138:ILE:HG22	2.00	0.43
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.89	0.43
7:H:58:THR:HG21	7:H:143:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:193:LEU:HB3	15:O:206:ILE:HB	2.01	0.43
22:0:633:ARG:HH21	22:0:636:LYS:HE2	1.83	0.43
23:1:472:GLN:NE2	24:4:41:ASP:OD2	2.52	0.43
27:2:345:PHE:HD2	27:2:378:ILE:HB	1.84	0.43
3:B:391:ASP:OD2	8:I:92:ARG:HG2	2.19	0.43
3:B:805:THR:O	3:B:1044:ALA:N	2.51	0.43
18:W:37:VAL:HG12	18:W:88:TYR:HB3	2.00	0.43
18:W:44:LYS:HD3	18:W:51:LYS:HG3	2.01	0.43
19:X:124:ASP:OD1	19:X:124:ASP:N	2.52	0.43
19:X:202:PHE:O	19:X:245:TRP:NE1	2.47	0.43
23:1:264:PRO:HA	23:1:267:LYS:HB3	2.01	0.43
26:7:621:LYS:HA	26:7:621:LYS:HD2	1.87	0.43
27:2:367:LYS:HG3	27:2:376:GLY:HA2	2.00	0.43
27:2:373:MET:SD	27:2:375:LEU:HB3	2.58	0.43
27:2:410:ARG:HE	27:2:410:ARG:HB2	1.67	0.43
2:A:346:ASP:OD2	3:B:1106:ARG:NH1	2.51	0.43
2:A:711:ARG:NH1	8:I:97:MET:HE1	2.33	0.43
2:A:1227:ILE:HB	2:A:1239:ARG:HB2	2.00	0.43
3:B:428:ILE:HA	3:B:445:LYS:HE3	1.99	0.43
8:I:7:CYS:HB2	8:I:14:LEU:HD21	2.00	0.43
18:W:12:LEU:HD11	18:W:182:ILE:HG23	2.00	0.43
21:G:116:PRO:HD2	21:G:119:LEU:HD22	2.00	0.43
22:0:73:SER:OG	22:0:208:TYR:O	2.32	0.43
25:6:277:CYS:O	25:6:281:ASN:HB2	2.19	0.43
26:7:494:PRO:HA	26:7:499:ARG:HD2	2.01	0.43
26:7:673:ILE:HG22	26:7:708:LEU:HB2	2.01	0.43
2:A:547:LEU:HG	10:K:58:PHE:CE1	2.54	0.43
18:W:29:LEU:HA	18:W:32:ILE:HG12	1.99	0.43
19:X:168:ARG:HA	19:X:181:LEU:HB3	2.01	0.43
19:X:218:ASP:HB3	19:X:241:PRO:HG3	2.01	0.43
22:0:19:PRO:O	22:0:23:ASN:ND2	2.36	0.43
22:0:254:THR:OG1	22:0:432:ASN:OD1	2.29	0.43
22:0:257:LEU:HD13	22:0:343:LYS:HG2	2.00	0.43
25:6:141:LEU:HD13	25:6:145:ARG:HG2	2.01	0.43
25:6:390:ALA:N	25:6:428:ARG:O	2.39	0.43
3:B:68:THR:HG21	12:Q:334:VAL:HG21	2.01	0.42
3:B:559:SER:HA	3:B:563:MET:SD	2.58	0.42
21:G:58:ARG:HD3	21:G:58:ARG:HA	1.73	0.42
22:0:529:PHE:CD2	22:0:621:LEU:HD21	2.53	0.42
22:0:642:MET:HE1	22:0:653:PHE:CD2	2.54	0.42
27:2:91:LYS:HA	27:2:96:LEU:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:127:GLN:HA	1:M:130:PHE:HB2	2.01	0.42
2:A:590:ARG:NH1	2:A:621:THR:OG1	2.52	0.42
3:B:1181:GLU:HA	3:B:1188:LYS:HE3	2.00	0.42
12:Q:117:HIS:HB2	13:P:135:PHE:CE1	2.55	0.42
20:D:148:LEU:O	20:D:152:SER:OG	2.29	0.42
21:G:100:GLU:HB3	21:G:107:LYS:HD2	2.00	0.42
25:6:169:MET:HE3	25:6:169:MET:HB3	1.96	0.42
25:6:291:LEU:HD13	25:6:297:LEU:HD13	2.01	0.42
27:2:474:TYR:O	27:2:478:ILE:HG12	2.19	0.42
2:A:69:THR:HG21	18:W:151:LEU:HD22	2.01	0.42
2:A:1044:TRP:O	2:A:1048:ASN:ND2	2.39	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.83	0.42
7:H:130:ARG:O	7:H:133:ASN:N	2.53	0.42
16:U:260:CYS:HB3	16:U:281:VAL:HB	2.02	0.42
19:X:142:VAL:HB	19:X:146:GLU:HG3	2.01	0.42
22:0:631:GLU:HB3	22:0:633:ARG:HH22	1.84	0.42
23:1:546:LEU:HD11	23:1:600:VAL:HG13	2.01	0.42
26:7:664:LEU:HB2	26:7:689:ARG:HD2	2.01	0.42
1:M:45:CYS:HB3	1:M:48:CYS:SG	2.59	0.42
1:M:187:ARG:HA	1:M:187:ARG:HD3	1.74	0.42
1:M:306:GLU:HA	1:M:309:ILE:HD12	2.01	0.42
2:A:552:TRP:CD1	2:A:651:LYS:HB3	2.55	0.42
4:C:217:ASP:OD1	4:C:217:ASP:N	2.49	0.42
8:I:103:CYS:SG	8:I:104:LEU:N	2.92	0.42
12:Q:114:MET:HB2	12:Q:114:MET:HE2	1.69	0.42
22:0:604:GLY:O	22:0:607:SER:OG	2.37	0.42
22:0:690:ARG:HA	22:0:693:LEU:HD12	2.01	0.42
22:0:711:ASP:OD1	22:0:712:MET:N	2.51	0.42
24:4:23:PRO:HB2	24:4:172:LEU:HD22	2.01	0.42
24:4:164:SER:HA	24:4:172:LEU:HD12	2.02	0.42
27:2:242:LEU:O	27:2:247:ARG:NH2	2.52	0.42
28:5:9:LEU:HD11	28:5:39:HIS:HB3	2.01	0.42
2:A:834:THR:HA	2:A:837:ILE:HG22	2.01	0.42
3:B:614:SER:OG	3:B:632:ARG:NH1	2.52	0.42
3:B:983:ARG:HD2	3:B:1091:TYR:HD2	1.85	0.42
13:P:108:LEU:HB3	13:P:118:HIS:HA	2.00	0.42
15:O:172:LEU:HD22	15:O:193:LEU:HD13	2.01	0.42
17:V:68:THR:O	17:V:79:ILE:N	2.45	0.42
20:D:56:ARG:HH22	20:D:155:ARG:HH21	1.67	0.42
23:1:550:CYS:HB2	23:1:616:LEU:HD11	2.00	0.42
24:4:79:TYR:N	24:4:82:GLY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:483:ASP:N	2:A:483:ASP:OD1	2.52	0.42
2:A:746:MET:HE3	2:A:746:MET:HB3	1.85	0.42
2:A:1003:LYS:HA	2:A:1003:LYS:HD3	1.85	0.42
14:S:278:LYS:HD2	14:S:301:ALA:HB2	2.00	0.42
15:O:130:ASP:OD1	15:O:130:ASP:N	2.53	0.42
18:W:90:LYS:HB3	18:W:93:HIS:HB2	2.01	0.42
18:W:90:LYS:HD2	18:W:196:GLU:HG3	2.02	0.42
25:6:116:THR:O	25:6:120:ARG:NH2	2.53	0.42
29:N:20:DA:C8	29:N:21:DT:H72	2.55	0.42
2:A:764:CYS:SG	2:A:765:VAL:N	2.93	0.42
5:E:202:SER:OG	5:E:206:GLY:N	2.53	0.42
7:H:134:ASN:OD1	7:H:134:ASN:N	2.51	0.42
11:L:27:LEU:N	11:L:39:SER:OG	2.47	0.42
22:0:543:SER:HB2	23:1:357:THR:HB	2.01	0.42
23:1:421:ILE:HG22	23:1:423:ASP:H	1.84	0.42
26:7:412:THR:HB	26:7:457:TYR:HB2	2.01	0.42
26:7:439:THR:OG1	26:7:440:SER:N	2.51	0.42
26:7:518:VAL:HG13	26:7:681:ARG:HB2	2.00	0.42
1:M:87:LEU:HD13	1:M:151:LYS:HD3	2.01	0.42
2:A:671:ALA:HB3	2:A:676:MET:HE3	2.02	0.42
2:A:954:TRP:HE3	2:A:955:PRO:HD2	1.84	0.42
3:B:380:TYR:CZ	3:B:384:ARG:HD2	2.55	0.42
3:B:542:MET:HE1	3:B:747:MET:HB3	2.01	0.42
3:B:1074:ASN:ND2	3:B:1077:THR:H	2.18	0.42
5:E:50:MET:SD	5:E:50:MET:N	2.93	0.42
12:Q:29:ARG:HB3	12:Q:33:ARG:NH1	2.33	0.42
16:U:258:TRP:HH2	16:U:285:TRP:CD1	2.38	0.42
22:0:529:PHE:HD2	22:0:621:LEU:HD21	1.85	0.42
25:6:432:CYS:O	25:6:434:GLN:NE2	2.47	0.42
2:A:566:ILE:HB	7:H:96:VAL:HG13	2.01	0.42
2:A:1339:LEU:HD21	5:E:147:HIS:CD2	2.54	0.42
3:B:1038:SER:OG	3:B:1040:ASN:N	2.52	0.42
4:C:260:LEU:HA	4:C:263:THR:HG22	2.02	0.42
8:I:111:THR:OG1	8:I:112:SER:N	2.51	0.42
12:Q:363:GLY:HA2	12:Q:395:PHE:HA	2.02	0.42
18:W:352:GLU:HA	18:W:355:LYS:HE2	2.01	0.42
22:0:643:ARG:HH11	22:0:647:ARG:HH12	1.68	0.42
25:6:148:MET:O	25:6:152:TYR:HB2	2.20	0.42
25:6:218:ARG:HB2	25:6:254:LEU:HD21	2.02	0.42
26:7:495:ALA:HB3	26:7:498:PHE:HD2	1.84	0.42
27:2:22:GLN:OE1	27:2:85:HIS:ND1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:87:LEU:HD12	27:2:87:LEU:HA	1.85	0.42
1:M:108:LYS:HD3	1:M:108:LYS:HA	1.78	0.42
2:A:691:LEU:HD23	2:A:691:LEU:HA	1.88	0.42
2:A:1093:LYS:HB3	2:A:1094:VAL:H	1.66	0.42
3:B:617:ARG:HE	3:B:619:ILE:HD13	1.85	0.42
4:C:207:CYS:SG	4:C:208:GLU:N	2.92	0.42
6:F:92:ARG:HD2	6:F:92:ARG:HA	1.80	0.42
9:J:3:VAL:HA	9:J:4:PRO:HD3	1.88	0.42
22:0:380:ARG:NH1	22:0:380:ARG:O	2.52	0.42
22:0:639:LEU:HB3	22:0:650:GLU:HG3	2.00	0.42
22:0:709:SER:HB3	22:0:712:MET:HE1	2.02	0.42
23:1:188:ASN:OD1	23:1:189:LYS:N	2.51	0.42
26:7:561:MET:HE1	26:7:581:TYR:HB2	2.00	0.42
27:2:483:TRP:CZ2	27:2:485:ASP:HB2	2.55	0.42
2:A:336:ILE:HD11	3:B:1203:LEU:HD13	2.02	0.41
2:A:431:LYS:HE2	2:A:431:LYS:HB2	1.90	0.41
22:0:216:PRO:HA	22:0:219:ALA:HB3	2.01	0.41
22:0:342:LEU:O	22:0:346:MET:HB2	2.19	0.41
23:1:369:ASP:OD1	23:1:369:ASP:N	2.53	0.41
26:7:354:ILE:HG21	26:7:430:LEU:HB2	2.02	0.41
27:2:59:LEU:HB2	27:2:96:LEU:HB3	2.01	0.41
29:N:-5:DT:H6	29:N:-5:DT:H2'	1.65	0.41
2:A:467:THR:OG1	2:A:468:PHE:N	2.53	0.41
2:A:857:ARG:HB3	2:A:861:GLY:HA2	2.02	0.41
3:B:341:LEU:HB3	3:B:344:LYS:HG3	2.02	0.41
3:B:839:MET:O	3:B:991:GLY:N	2.43	0.41
12:Q:120:LYS:HE3	13:P:131:ASN:HB2	2.01	0.41
16:U:9:VAL:HA	16:U:12:ILE:HG12	2.02	0.41
21:G:1:MET:N	21:G:80:LYS:O	2.44	0.41
21:G:56:ILE:HG13	21:G:57:GLN:H	1.85	0.41
22:0:564:TRP:HH2	23:1:378:MET:HE2	1.84	0.41
25:6:452:PRO:HA	25:6:455:GLU:HG2	2.02	0.41
26:7:326:VAL:HA	26:7:329:ARG:HB3	2.02	0.41
26:7:490:VAL:HG12	26:7:514:THR:HB	2.03	0.41
2:A:120:GLU:OE1	2:A:123:ARG:NH1	2.54	0.41
2:A:375:THR:OG1	2:A:433:GLU:OE1	2.28	0.41
2:A:397:ASN:HB3	10:K:2:ASN:ND2	2.35	0.41
2:A:789:LYS:HB2	8:I:69:PRO:HD3	2.01	0.41
2:A:1396:ALA:N	2:A:1419:ASP:OD2	2.53	0.41
7:H:111:LEU:HA	7:H:128:ASN:HB2	2.02	0.41
15:O:109:PRO:HB2	15:O:111:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:PRO:HG2	15:O:202:ILE:HD12	2.02	0.41
22:0:109:THR:OG1	23:1:345:ASP:OD1	2.37	0.41
26:7:573:THR:O	26:7:577:ARG:HG3	2.20	0.41
2:A:265:LYS:O	2:A:269:ILE:HG12	2.20	0.41
2:A:528:LEU:HD22	2:A:751:SER:HB3	2.02	0.41
2:A:886:ILE:O	2:A:944:ARG:NH2	2.53	0.41
15:O:69:ASN:ND2	30:T:-7:DT:H2"	2.35	0.41
15:O:211:LYS:HB3	30:T:-4:DT:H4'	2.02	0.41
16:U:18:VAL:HG11	16:U:39:LYS:HD3	2.02	0.41
24:4:272:PHE:HB2	25:6:372:LEU:HD22	2.02	0.41
24:4:304:LYS:HE2	24:4:304:LYS:HB3	1.90	0.41
25:6:194:ASP:HA	25:6:197:LYS:HE3	2.02	0.41
26:7:126:ASP:OD2	26:7:130:ARG:NE	2.53	0.41
26:7:766:LYS:HB2	26:7:766:LYS:HE2	1.89	0.41
2:A:32:VAL:N	2:A:81:PHE:O	2.51	0.41
2:A:239:LEU:HD12	2:A:240:PRO:HD2	2.03	0.41
2:A:603:ASN:OD1	2:A:603:ASN:N	2.50	0.41
3:B:521:LEU:O	3:B:540:SER:N	2.50	0.41
3:B:526:GLU:O	3:B:538:ASN:ND2	2.54	0.41
6:F:116:ASP:OD2	6:F:119:ARG:N	2.50	0.41
9:J:30:LEU:HG	9:J:35:ALA:HB2	2.03	0.41
10:K:57:LEU:HG	10:K:77:THR:HA	2.03	0.41
13:P:121:ASP:OD1	13:P:121:ASP:N	2.52	0.41
14:S:238:PRO:HB2	14:S:240:PRO:HD2	2.02	0.41
18:W:90:LYS:HG3	18:W:92:PRO:HD2	2.03	0.41
23:1:432:TYR:HD1	25:6:311:ASN:HA	1.86	0.41
24:4:32:ILE:HG13	24:4:79:TYR:HA	2.02	0.41
26:7:525:GLY:O	26:7:528:ASN:ND2	2.47	0.41
29:N:12:DG:N2	30:T:-11:DC:O2	2.53	0.41
2:A:115:LEU:HD21	2:A:145:LYS:HD3	2.01	0.41
2:A:198:GLU:HB2	18:W:227:MET:HE3	2.02	0.41
3:B:284:ILE:H	3:B:284:ILE:HG13	1.63	0.41
3:B:550:ASP:HA	3:B:551:PRO:HD3	1.82	0.41
3:B:605:ARG:NH2	3:B:691:GLU:OE1	2.53	0.41
4:C:162:GLY:HA3	4:C:170:TRP:CE2	2.55	0.41
10:K:39:ASP:CG	10:K:40:HIS:H	2.29	0.41
16:U:3:ASN:HB3	16:U:6:ALA:HB3	2.01	0.41
18:W:35:HIS:HA	18:W:207:ILE:HB	2.03	0.41
20:D:202:ILE:HD13	20:D:207:LEU:HD13	2.02	0.41
22:0:104:ARG:NH2	22:0:171:LEU:O	2.54	0.41
22:0:564:TRP:CH2	23:1:378:MET:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:0:609:GLY:H	22:0:668:ARG:NH1	2.18	0.41
26:7:568:GLU:HG3	26:7:580:LEU:HD21	2.01	0.41
27:2:59:LEU:HA	27:2:62:LEU:HD12	2.01	0.41
2:A:66:LYS:HE2	2:A:68:GLN:HA	2.03	0.41
2:A:185:TRP:HZ3	2:A:200:ARG:HB3	1.86	0.41
3:B:498:THR:OG1	3:B:537:LYS:O	2.36	0.41
3:B:563:MET:HB3	3:B:563:MET:HE3	1.64	0.41
3:B:957:ASN:ND2	3:B:959:ASP:OD1	2.50	0.41
4:C:43:THR:HG23	4:C:170:TRP:HD1	1.85	0.41
17:V:63:LYS:N	17:V:84:GLN:O	2.51	0.41
24:4:71:ASN:OD1	24:4:71:ASN:N	2.52	0.41
26:7:569:TYR:CE1	26:7:577:ARG:HB3	2.56	0.41
1:M:157:CYS:HB3	1:M:213:ILE:HG21	2.02	0.41
2:A:96:ILE:HD13	2:A:99:ILE:HD12	2.03	0.41
2:A:113:LEU:HD21	2:A:218:ASP:HB3	2.02	0.41
3:B:423:LYS:NZ	3:B:468:GLU:OE1	2.49	0.41
3:B:1024:ALA:HA	3:B:1027:ILE:HG22	2.01	0.41
7:H:4:THR:HG23	7:H:58:THR:HG23	2.03	0.41
7:H:93:TYR:HD2	7:H:143:LEU:HB3	1.86	0.41
12:Q:381:ASP:OD1	12:Q:381:ASP:N	2.53	0.41
18:W:61:LEU:HD23	18:W:66:LEU:HD12	2.02	0.41
21:G:45:ILE:HA	21:G:78:VAL:HG12	2.03	0.41
21:G:101:VAL:HB	21:G:108:VAL:HG13	2.03	0.41
23:1:168:SER:HA	23:1:173:LYS:HG3	2.02	0.41
24:4:214:LYS:HD3	24:4:237:HIS:HB2	2.02	0.41
28:5:48:GLU:HA	28:5:51:LYS:HB2	2.03	0.41
28:5:57:LEU:HD23	28:5:57:LEU:HA	1.96	0.41
29:N:35:DG:H22	30:T:-35:DC:H42	1.68	0.41
1:M:137:CYS:HB2	1:M:142:LEU:HB2	2.01	0.41
1:M:250:MET:O	1:M:253:THR:OG1	2.30	0.41
2:A:85:ASP:O	2:A:273:ASN:ND2	2.54	0.41
2:A:172:PRO:HB3	2:A:185:TRP:CD2	2.55	0.41
2:A:1116:LEU:HG	2:A:1308:THR:HG21	2.03	0.41
3:B:205:ILE:O	3:B:208:SER:OG	2.32	0.41
3:B:562:GLY:O	3:B:590:HIS:ND1	2.53	0.41
3:B:700:SER:O	3:B:700:SER:OG	2.35	0.41
3:B:802:PRO:HB3	3:B:1091:TYR:CG	2.56	0.41
3:B:826:ALA:HB3	3:B:1011:ILE:HG13	2.03	0.41
7:H:91:ASP:OD1	7:H:91:ASP:N	2.52	0.41
8:I:65:ASP:HA	8:I:66:PRO:HD3	1.91	0.41
13:P:74:PRO:HD2	13:P:77:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:239:PRO:O	16:U:270:ASN:N	2.54	0.41
16:U:274:TYR:HD2	17:V:87:VAL:HG11	1.85	0.41
17:V:86:THR:HB	17:V:105:VAL:HG12	2.03	0.41
18:W:123:MET:N	18:W:157:VAL:O	2.39	0.41
19:X:119:ILE:HA	19:X:121:LYS:HE3	2.03	0.41
22:0:70:ILE:N	22:0:231:ILE:O	2.38	0.41
22:0:111:ARG:NH1	22:0:130:ASP:O	2.54	0.41
22:0:567:LYS:HA	22:0:594:ARG:HE	1.86	0.41
27:2:26:TYR:OH	27:2:84:LEU:O	2.27	0.41
27:2:219:VAL:O	27:2:223:HIS:ND1	2.39	0.41
29:N:5:DT:H6	29:N:5:DT:H2'	1.63	0.41
29:N:47:DA:H2"	29:N:48:DC:H5'	2.03	0.41
2:A:635:ARG:HD3	2:A:635:ARG:HA	1.81	0.41
3:B:1164:GLY:N	3:B:1190:ASP:OD2	2.54	0.41
12:Q:114:MET:N	12:Q:114:MET:SD	2.94	0.41
15:O:78:CYS:SG	15:O:151:LYS:NZ	2.94	0.41
22:0:240:ILE:HD12	22:0:240:ILE:HA	1.95	0.41
22:0:344:THR:HA	22:0:347:LYS:HE2	2.03	0.41
22:0:493:LEU:HB3	22:0:678:VAL:HG12	2.03	0.41
26:7:561:MET:HE2	26:7:710:SER:HB3	2.03	0.41
29:N:34:DC:H2"	29:N:35:DG:N7	2.36	0.41
1:M:131:ALA:O	1:M:135:MET:HG2	2.21	0.40
1:M:199:LYS:HE3	1:M:202:GLU:HB2	2.03	0.40
2:A:315:LEU:HB2	2:A:321:PRO:HA	2.03	0.40
2:A:343:LYS:NZ	3:B:1151:LEU:HD12	2.35	0.40
2:A:356:ASP:HB2	2:A:469:ARG:HD2	2.03	0.40
2:A:357:PRO:HG3	3:B:832:GLY:HA2	2.02	0.40
2:A:1009:ASN:O	2:A:1013:ASP:HB2	2.21	0.40
3:B:1207:LEU:HD22	3:B:1212:ILE:HG13	2.02	0.40
4:C:18:VAL:HG12	4:C:20:PHE:HD1	1.86	0.40
4:C:211:ASP:OD1	4:C:211:ASP:N	2.53	0.40
6:F:85:MET:HE1	6:F:90:ARG:HB2	2.03	0.40
13:P:136:THR:HG23	13:P:215:VAL:HG21	2.03	0.40
22:0:425:ILE:HB	22:0:428:ALA:HB2	2.03	0.40
25:6:133:SER:HB2	25:6:136:MET:HE1	2.03	0.40
25:6:378:ARG:O	25:6:381:HIS:NE2	2.54	0.40
26:7:162:GLU:N	26:7:174:LYS:O	2.45	0.40
26:7:190:THR:HG23	26:7:213:ILE:HG22	2.02	0.40
26:7:568:GLU:HA	26:7:571:ARG:HG2	2.03	0.40
2:A:391:LEU:HD23	2:A:402:ALA:HB2	2.04	0.40
9:J:51:LEU:HA	9:J:51:LEU:HD12	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:141:LYS:HE2	13:P:141:LYS:HB3	1.91	0.40
16:U:280:GLN:HB2	17:V:61:THR:HG22	2.03	0.40
17:V:23:LEU:HD23	17:V:23:LEU:HA	1.91	0.40
22:0:554:TRP:HZ3	22:0:559:ILE:HD12	1.86	0.40
26:7:250:VAL:HG21	26:7:329:ARG:HD3	2.04	0.40
27:2:131:SER:HB2	27:2:135:LEU:HD22	2.02	0.40
1:M:214:LEU:HD12	1:M:215:ARG:HG3	2.04	0.40
1:M:297:LYS:HD2	1:M:300:GLN:HE21	1.85	0.40
2:A:90:VAL:HG21	2:A:300:VAL:HG11	2.04	0.40
2:A:235:ILE:HD13	2:A:235:ILE:HA	1.93	0.40
2:A:977:LYS:HA	2:A:977:LYS:HD3	1.81	0.40
2:A:1215:ARG:O	2:A:1218:GLN:NE2	2.47	0.40
2:A:1398:MET:HB2	2:A:1398:MET:HE2	1.85	0.40
3:B:234:ILE:HG21	3:B:257:LYS:HD2	2.03	0.40
3:B:417:PHE:O	3:B:421:PHE:HB2	2.21	0.40
3:B:540:SER:O	3:B:543:SER:OG	2.37	0.40
7:H:27:GLU:HA	7:H:39:THR:HA	2.02	0.40
13:P:77:LEU:O	13:P:81:TRP:HE3	2.04	0.40
17:V:24:ASP:HA	17:V:27:ILE:HB	2.02	0.40
22:0:19:PRO:HG3	22:0:739:TRP:CE2	2.57	0.40
23:1:567:HIS:CE1	23:1:582:LEU:HG	2.56	0.40
26:7:516:THR:HB	26:7:518:VAL:HG12	2.03	0.40
29:N:38:DG:H2"	29:N:39:DA:N7	2.37	0.40
1:M:286:ILE:HD11	1:M:291:ILE:HB	2.03	0.40
2:A:757:ASN:HD21	14:S:292:PRO:HB3	1.86	0.40
3:B:129:PHE:CD2	3:B:164:LYS:HB2	2.57	0.40
3:B:372:SER:OG	3:B:373:ARG:NH1	2.54	0.40
3:B:1191:ILE:HD12	3:B:1191:ILE:HA	1.89	0.40
8:I:81:ARG:HD3	8:I:81:ARG:HA	1.84	0.40
13:P:223:GLN:NE2	13:P:224:VAL:O	2.54	0.40
16:U:38:LEU:HA	16:U:41:ILE:HG22	2.03	0.40
20:D:39:ASN:HB2	20:D:45:GLU:HB2	2.02	0.40
22:0:259:ARG:HG2	22:0:262:ARG:HH12	1.86	0.40
26:7:558:TRP:HZ3	26:7:735:VAL:HA	1.86	0.40
26:7:676:HIS:NE2	29:N:51:DG:H3'	2.37	0.40
2:A:437:MET:HE2	2:A:437:MET:HB3	1.86	0.40
2:A:851:HIS:ND1	6:F:139:PRO:HG3	2.36	0.40
2:A:1452:LYS:HE3	2:A:1452:LYS:HB3	1.89	0.40
3:B:75:ALA:HB2	3:B:83:ASN:H	1.87	0.40
3:B:264:SER:OG	3:B:265:SER:N	2.54	0.40
4:C:56:THR:HG23	4:C:153:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:75:CYS:HA	8:I:76:PRO:HD3	1.95	0.40
13:P:300:LEU:HD23	13:P:303:LEU:HD21	2.03	0.40
16:U:267:VAL:HG22	16:U:269:ILE:HG23	2.02	0.40
22:0:112:LYS:HG2	23:1:344:GLN:OE1	2.21	0.40
22:0:529:PHE:HA	22:0:532:ILE:HG12	2.03	0.40
25:6:347:TYR:HE2	25:6:359:LEU:HD13	1.87	0.40
26:7:242:LEU:HD21	26:7:314:HIS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	273/345 (79%)	238 (87%)	35 (13%)	0	100	100
2	A	1417/1733 (82%)	1249 (88%)	168 (12%)	0	100	100
3	B	1150/1224 (94%)	1000 (87%)	148 (13%)	2 (0%)	43	73
4	C	263/318 (83%)	231 (88%)	32 (12%)	0	100	100
5	E	212/215 (99%)	193 (91%)	19 (9%)	0	100	100
6	F	85/155 (55%)	78 (92%)	7 (8%)	0	100	100
7	H	129/146 (88%)	109 (84%)	20 (16%)	0	100	100
8	I	112/122 (92%)	98 (88%)	14 (12%)	0	100	100
9	J	64/70 (91%)	55 (86%)	9 (14%)	0	100	100
10	K	113/120 (94%)	107 (95%)	6 (5%)	0	100	100
11	L	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
12	Q	208/735 (28%)	198 (95%)	10 (5%)	0	100	100
13	P	173/400 (43%)	161 (93%)	12 (7%)	0	100	100
14	S	162/309 (52%)	143 (88%)	18 (11%)	1 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
16	U	101/286 (35%)	96 (95%)	5 (5%)	0	100	100
17	V	100/122 (82%)	97 (97%)	3 (3%)	0	100	100
18	W	241/482 (50%)	230 (95%)	11 (5%)	0	100	100
19	X	158/328 (48%)	145 (92%)	13 (8%)	0	100	100
20	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
21	G	169/171 (99%)	154 (91%)	14 (8%)	1 (1%)	21	54
22	0	750/778 (96%)	715 (95%)	35 (5%)	0	100	100
23	1	407/642 (63%)	394 (97%)	13 (3%)	0	100	100
24	4	286/338 (85%)	276 (96%)	10 (4%)	0	100	100
25	6	351/461 (76%)	334 (95%)	17 (5%)	0	100	100
26	7	604/843 (72%)	564 (93%)	40 (7%)	0	100	100
27	2	435/513 (85%)	417 (96%)	18 (4%)	0	100	100
28	5	64/72 (89%)	55 (86%)	9 (14%)	0	100	100
All	All	8412/11459 (73%)	7694 (92%)	714 (8%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	364	ILE
3	B	363	HIS
21	G	57	GLN
14	S	167	PRO

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	M	245/299 (82%)	245 (100%)	0	100	100
2	A	1235/1520 (81%)	1235 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	1000/1061 (94%)	1000 (100%)	0	100	100
4	C	233/274 (85%)	233 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	H	118/128 (92%)	118 (100%)	0	100	100
8	I	108/116 (93%)	108 (100%)	0	100	100
9	J	61/65 (94%)	61 (100%)	0	100	100
10	K	99/102 (97%)	99 (100%)	0	100	100
11	L	39/57 (68%)	39 (100%)	0	100	100
12	Q	147/641 (23%)	147 (100%)	0	100	100
13	P	166/363 (46%)	166 (100%)	0	100	100
14	S	141/274 (52%)	141 (100%)	0	100	100
15	O	153/205 (75%)	153 (100%)	0	100	100
16	U	99/260 (38%)	99 (100%)	0	100	100
17	V	94/108 (87%)	94 (100%)	0	100	100
18	W	224/429 (52%)	224 (100%)	0	100	100
19	X	144/295 (49%)	144 (100%)	0	100	100
20	D	146/200 (73%)	146 (100%)	0	100	100
21	G	151/152 (99%)	151 (100%)	0	100	100
22	0	684/707 (97%)	684 (100%)	0	100	100
23	1	389/589 (66%)	389 (100%)	0	100	100
24	4	259/300 (86%)	259 (100%)	0	100	100
25	6	322/418 (77%)	322 (100%)	0	100	100
26	7	540/737 (73%)	540 (100%)	0	100	100
27	2	394/468 (84%)	394 (100%)	0	100	100
28	5	53/66 (80%)	53 (100%)	0	100	100
All	All	7517/10168 (74%)	7517 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	235	ASN
2	A	45	GLN
2	A	273	ASN
2	A	313	GLN
2	A	339	ASN
2	A	425	GLN
2	A	447	GLN
2	A	451	HIS
2	A	479	ASN
2	A	488	ASN
2	A	545	GLN
2	A	626	ASN
2	A	854	ASN
2	A	935	GLN
2	A	965	GLN
2	A	966	ASN
2	A	969	GLN
2	A	996	ASN
2	A	1188	GLN
2	A	1258	HIS
2	A	1270	ASN
2	A	1378	GLN
3	B	325	GLN
3	B	363	HIS
3	B	484	ASN
3	B	686	ASN
3	B	770	GLN
3	B	784	ASN
3	B	986	GLN
3	B	1040	ASN
3	B	1062	HIS
3	B	1161	HIS
4	C	7	GLN
4	C	203	GLN
4	C	214	ASN
4	C	264	GLN
5	E	101	GLN
5	E	174	GLN
7	H	3	ASN
8	I	22	ASN
8	I	23	ASN
9	J	23	ASN
10	K	2	ASN

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Mol	Chain	Res	Type
11	L	66	GLN
12	Q	117	HIS
12	Q	122	GLN
13	P	90	GLN
13	P	139	ASN
14	S	173	HIS
14	S	220	ASN
14	S	251	GLN
14	S	255	ASN
15	O	225	GLN
16	U	40	ASN
18	W	50	ASN
18	W	165	ASN
19	X	123	HIS
19	X	136	GLN
19	X	216	GLN
20	D	28	GLN
20	D	138	ASN
21	G	153	GLN
22	0	521	ASN
22	0	577	GLN
22	0	592	ASN
22	0	645	ASN
23	1	277	ASN
23	1	342	ASN
23	1	352	ASN
23	1	554	HIS
23	1	602	ASN
23	1	610	ASN
23	1	621	ASN
23	1	628	HIS
23	1	639	ASN
24	4	71	ASN
24	4	143	ASN
25	6	146	HIS
25	6	163	GLN
25	6	227	HIS
25	6	351	ASN
26	7	431	GLN
26	7	447	GLN
26	7	545	GLN
26	7	584	ASN

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Mol	Chain	Res	Type
26	7	589	GLN
26	7	648	GLN
26	7	672	GLN
26	7	740	HIS
26	7	747	ASN
27	2	75	GLN
27	2	76	ASN
27	2	110	ASN
27	2	118	GLN
27	2	148	HIS
27	2	186	ASN
27	2	194	GLN
27	2	206	GLN
27	2	251	GLN
27	2	352	ASN
27	2	500	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	SF4	0	801	22	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SF4	0	801	22	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	2	0

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.

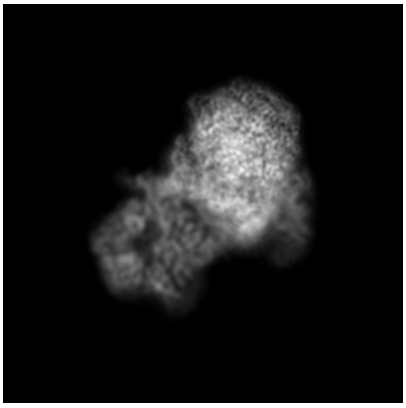
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-42437. These allow visual inspection of the internal detail of the map and identification of artifacts.

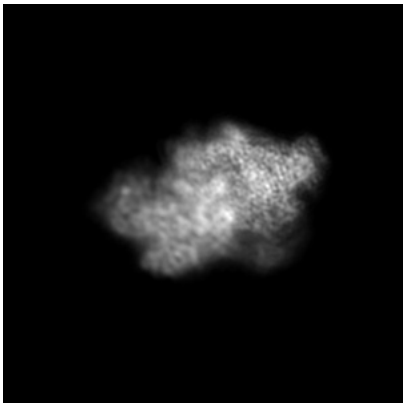
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

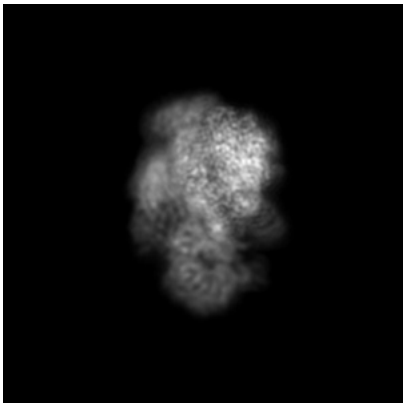
6.1.1 Primary map



X



Y



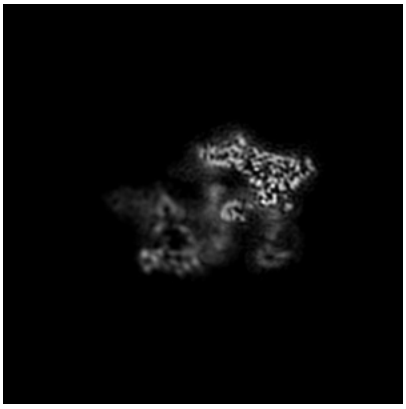
Z

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

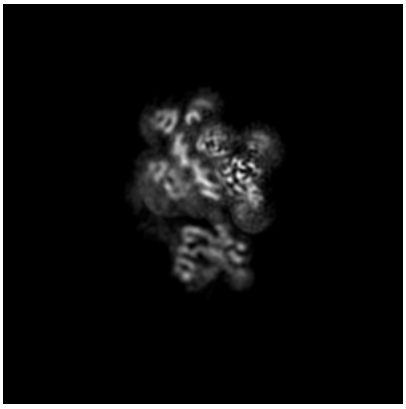
6.2 Central slices (i)

6.2.1 Primary map

X Index: 192



Y Index: 192

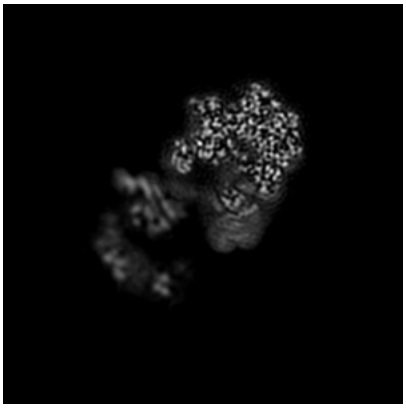


Z Index: 192

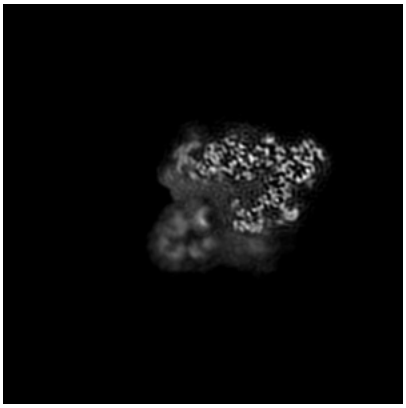
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 216



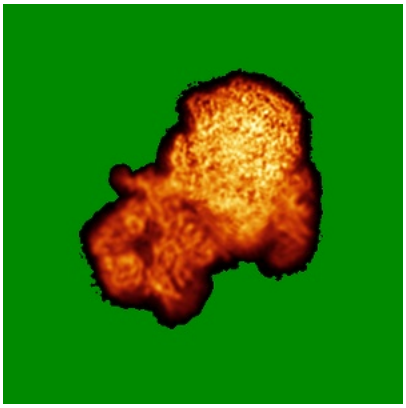
Y Index: 232

Z Index: 210

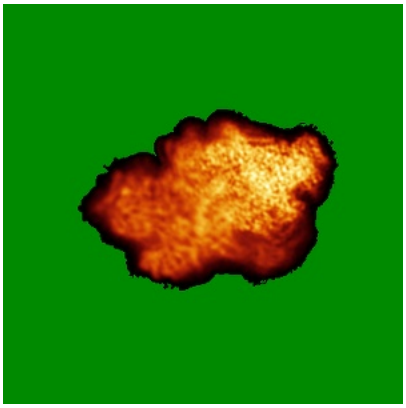
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

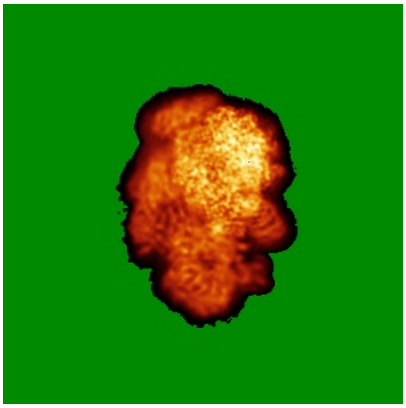
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

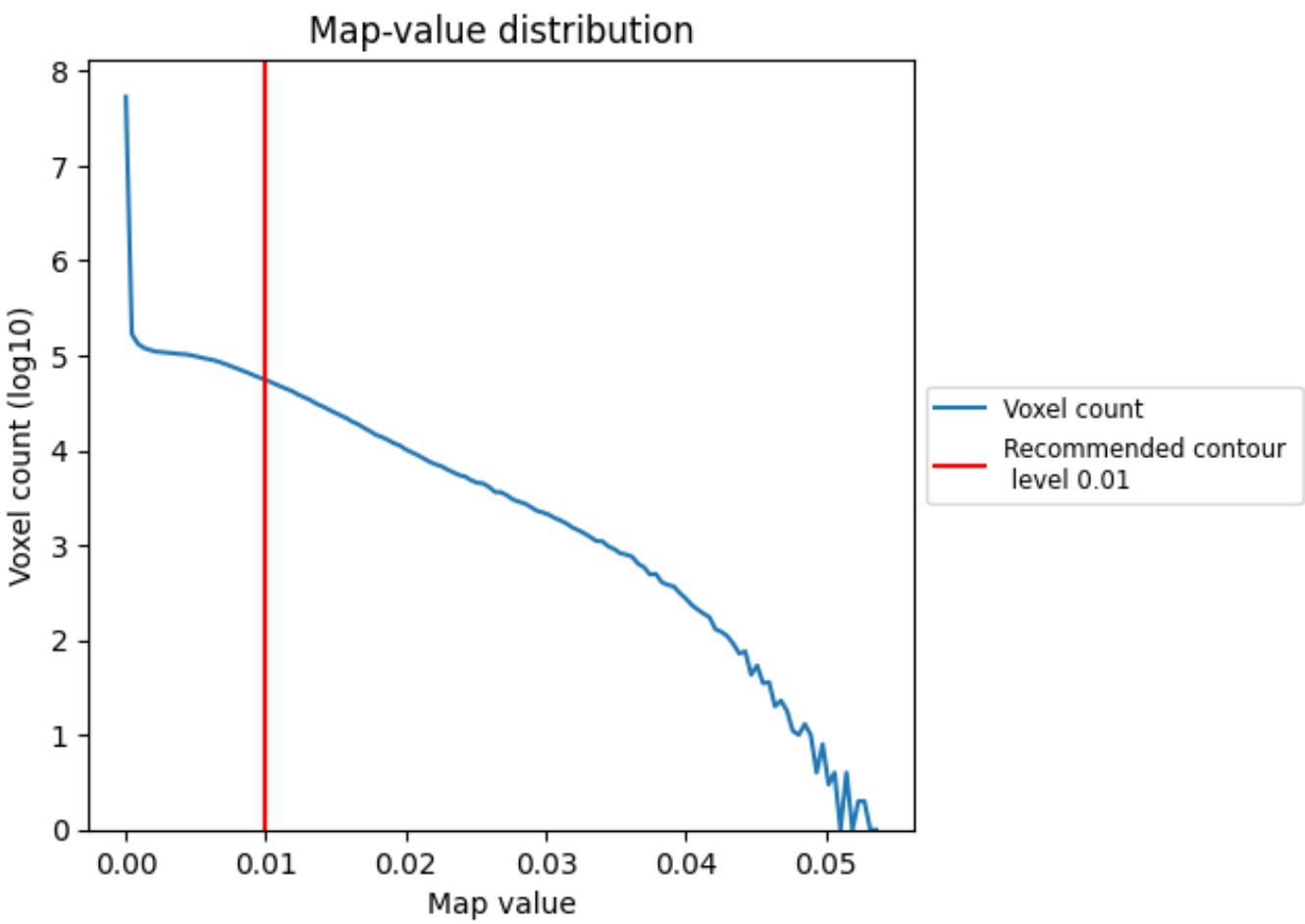
6.6 Mask visualisation (i)

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

7 Map analysis (i)

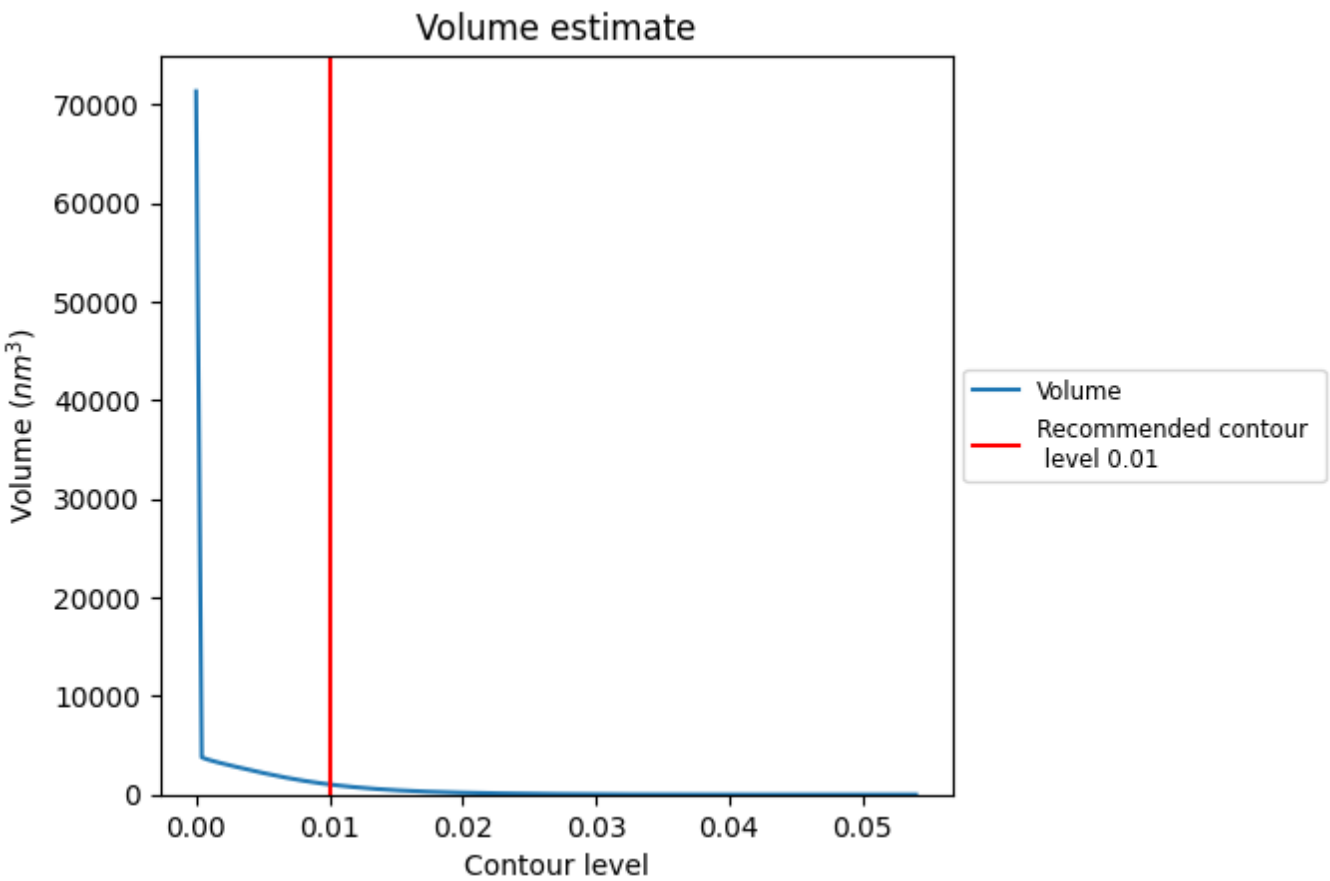
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

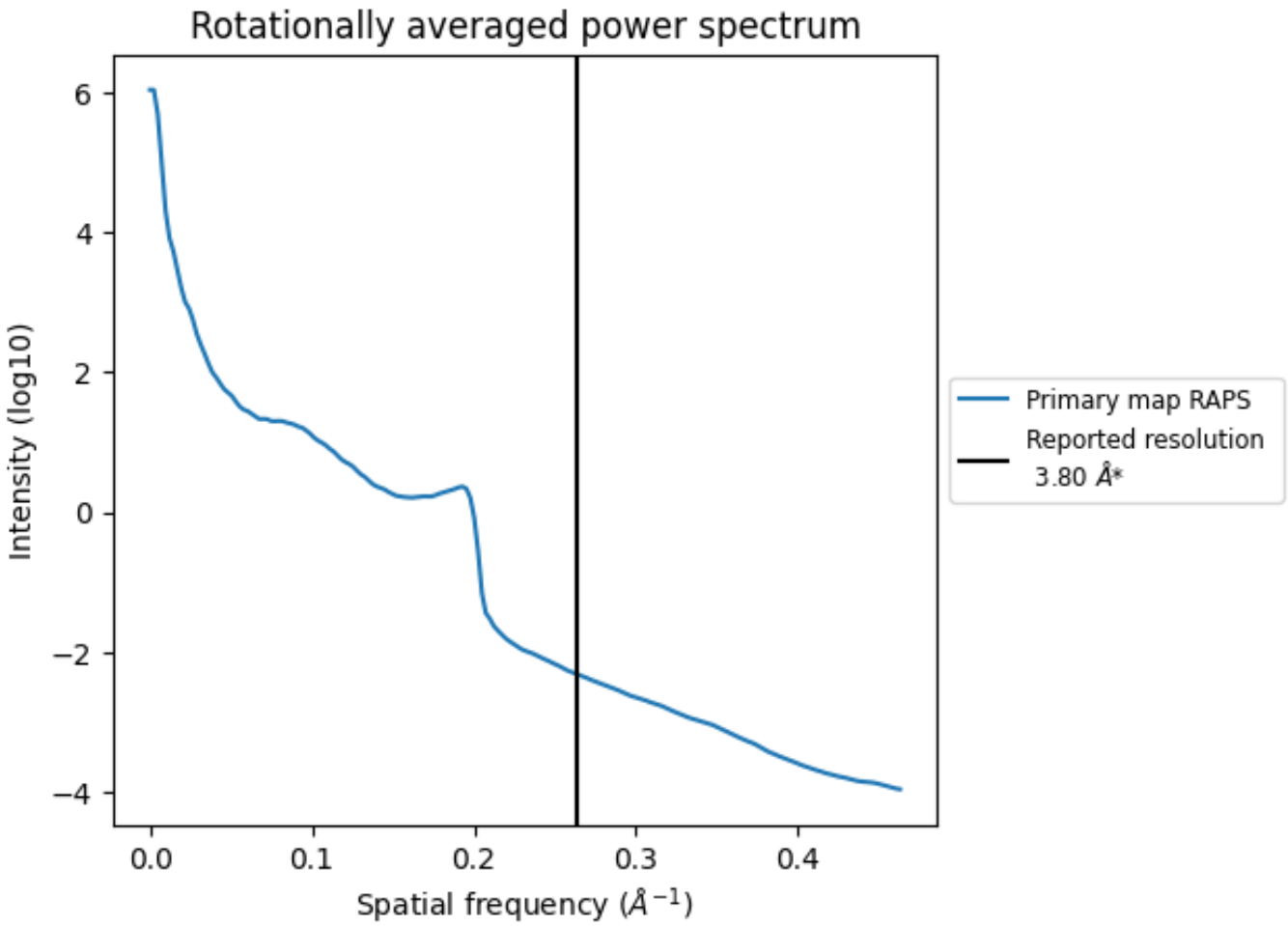
7.2 Volume estimate (i)



The volume at the recommended contour level is 1031 nm^3; this corresponds to an approximate mass of 932 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 0.263 Å^{-1}

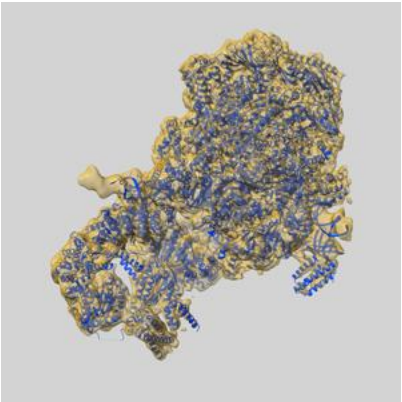
8 Fourier-Shell correlation (i)

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

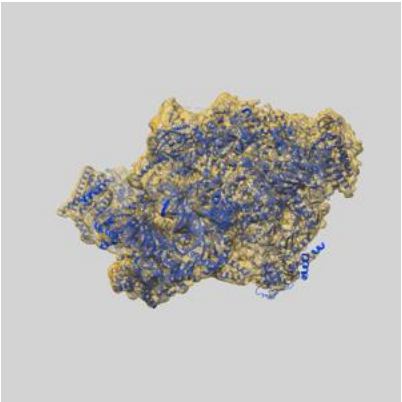
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42437 and PDB model 8UOQ. Per-residue inclusion information can be found in section 3 on page 11.

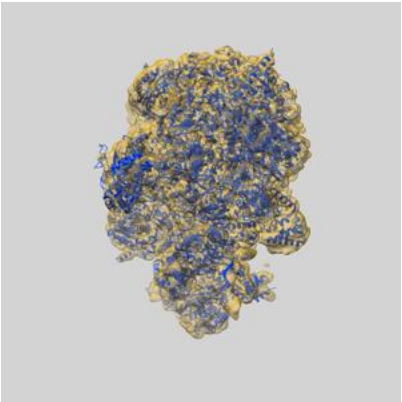
9.1 Map-model overlay (i)



X



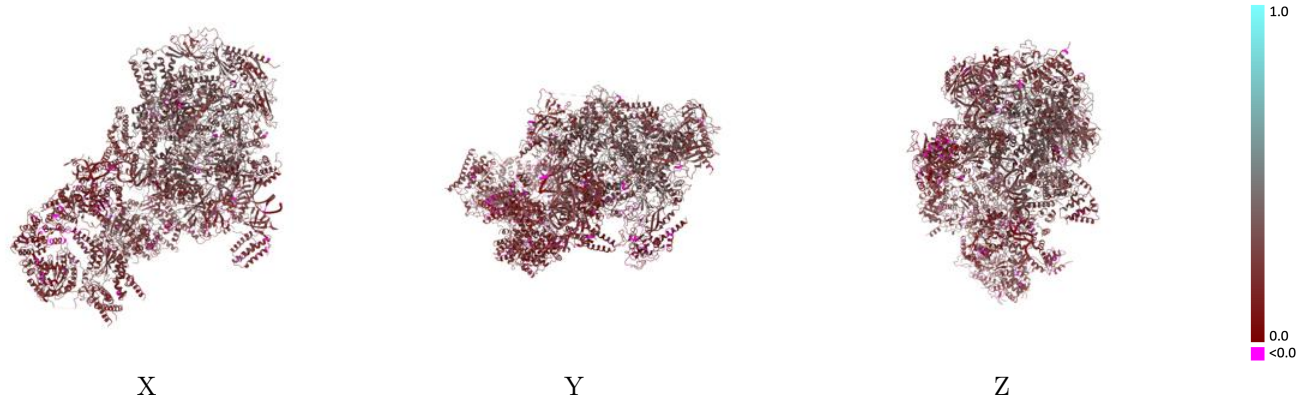
Y



Z

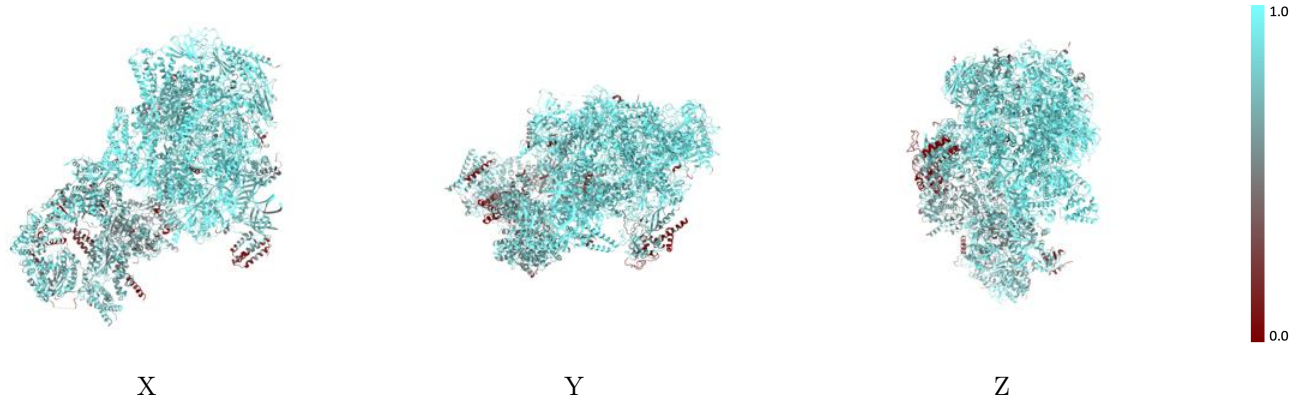
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



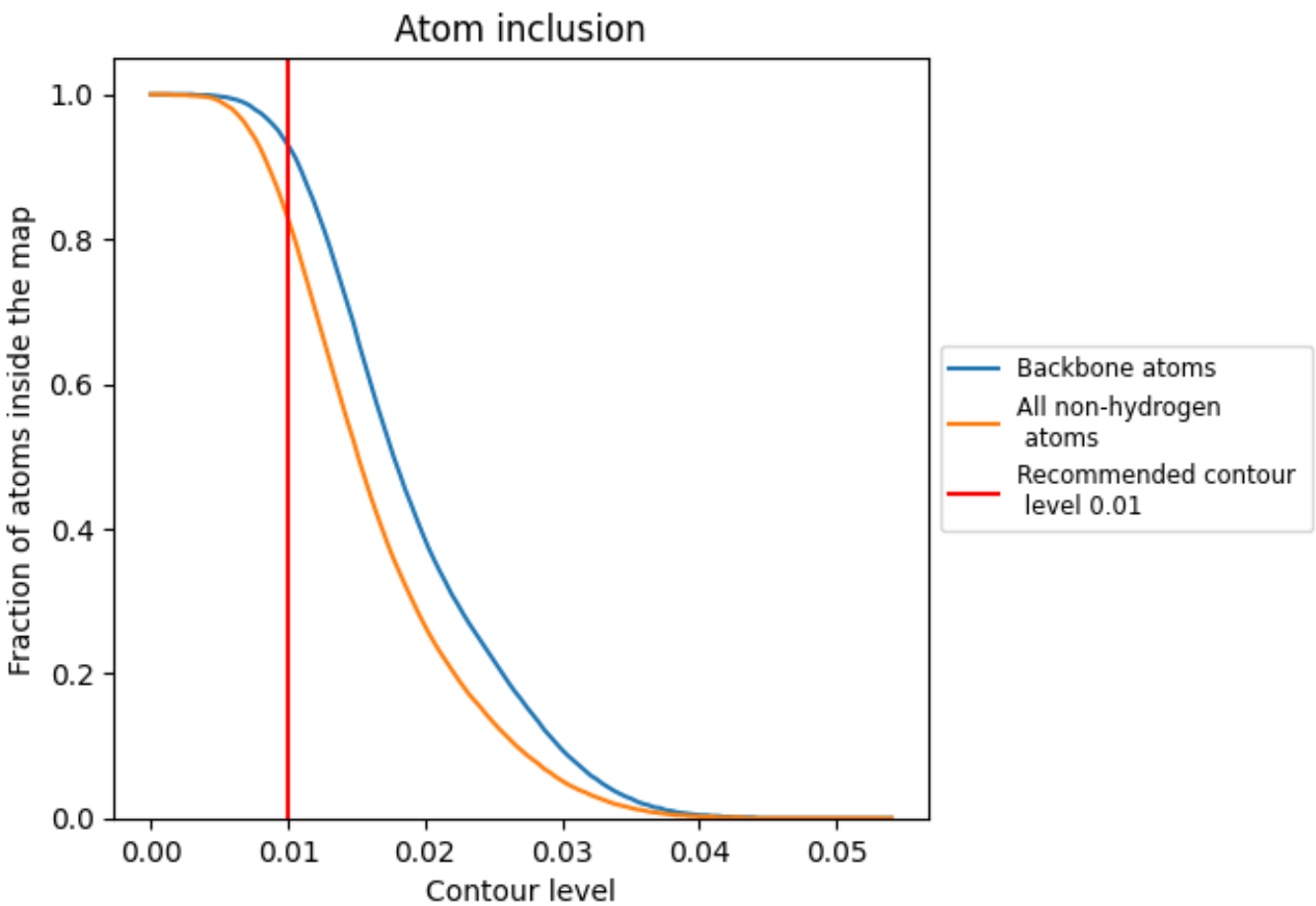
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 83% 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	0.8280	0.2390
0	0.6950	0.1780
1	0.6570	0.1870
2	0.7450	0.1480
4	0.7750	0.1900
5	0.6180	0.1540
6	0.7370	0.1850
7	0.7490	0.1710
A	0.9580	0.3280
B	0.9520	0.3380
C	0.9020	0.2690
D	0.3700	0.1540
E	0.9640	0.3190
F	0.9300	0.3100
G	0.6530	0.1970
H	0.9270	0.3000
I	0.9470	0.3070
J	0.9010	0.2700
K	0.8330	0.2730
L	0.7940	0.1800
M	0.7590	0.2010
N	0.9490	0.2210
O	0.9000	0.1860
P	0.9170	0.2080
Q	0.8310	0.2520
S	0.9020	0.1940
T	0.9480	0.2290
U	0.5180	0.1400
V	0.6040	0.1810
W	0.8160	0.1690
X	0.8750	0.1570