Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 09:07 pm BST

PDB ID	:	7O75 / pdb_00007o75
EMDB ID	:	EMD-12745
Title	:	Yeast RNA polymerase II transcription pre-initiation complex with open promoter DNA
Authors	:	Schilbach, S.; Aibara, S.; Dienemann, C.; Grabbe, F.; Cramer, P.
Deposited on	:	2021-04-13
Resolution	:	3.20 Å(reported)
Based on initial model	:	5OQJ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

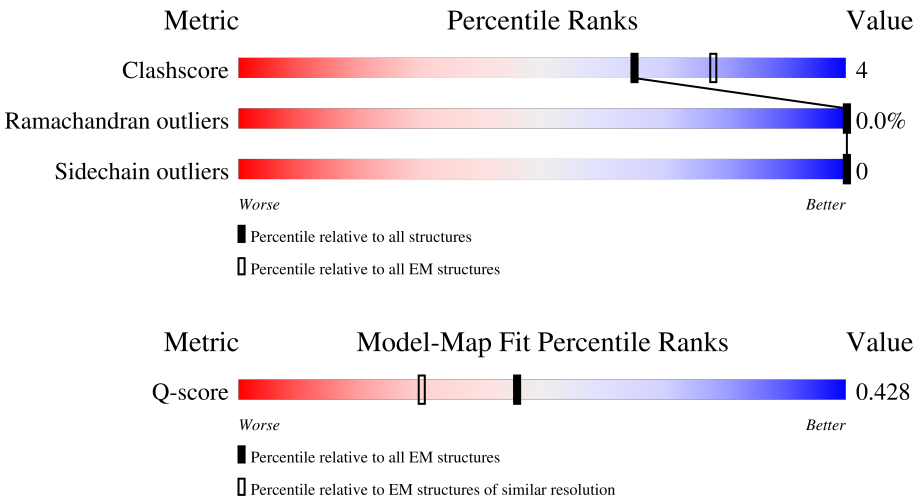
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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	0	778	87% 10% •
2	1	645	6% 75% 6% 19%
3	2	517	20% 75% 11% 14%
4	3	324	36% • 60%

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Mol	Chain	Length	Quality of chain
5	4	341	79% 7% 14%
6	5	76	38% 75% 11% 14%
7	6	464	9% 72% 9% 19%
8	7	843	11% 61% 12% 27%
9	A	1733	76% 7% 17%
10	B	1224	86% 10%
11	C	347	72% 5% 23%
12	D	221	71% 24%
13	E	215	91% 8%
14	F	155	52% 45%
15	G	177	85% 11%
16	H	146	87% 9%
17	I	122	87% 8% 5%
18	J	70	90% 9%
19	K	120	93%
20	L	70	64% 36%
21	M	352	9% 78% 10% 13%
22	N	106	10% 53% 8% 40%
23	O	247	8% 62% 11% 27%
24	Q	738	7% 27% 70%
25	R	400	19% 58% 10% 33%
26	T	106	9% 50% 9% 41%
27	U	286	23% 30% 8% 63%
28	V	129	44% 72% 9% 19%
29	W	492	8% 55% 8% 37%

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Mol	Chain	Length	Quality of chain
30	X	328	23% 55% 8% 37%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 73885 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 General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	752	6091	3882	1029	1142	38	0	0

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	522	4214	2660	734	798	22	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-2	GLY	-	expression tag	UNP P32776
1	-1	GLY	-	expression tag	UNP P32776
1	0	SER	-	expression tag	UNP P32776

- Molecule 3 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	445	3597	2327	591	663	16	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	GLY	-	expression tag	UNP Q02939
2	-2	PRO	-	expression tag	UNP Q02939
2	-1	GLY	-	expression tag	UNP Q02939
2	0	SER	-	expression tag	UNP Q02939

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	131	1089	692	180	209	8	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-2	GLY	-	expression tag	UNP Q03290
3	-1	PRO	-	expression tag	UNP Q03290
3	0	HIS	-	expression tag	UNP Q03290

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	293	2274	1454	377	429	14	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-2	SER	-	expression tag	UNP Q12004
4	-1	ASN	-	expression tag	UNP Q12004
4	0	ALA	-	expression tag	UNP Q12004

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	65	514	326	90	95	3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	-3	GLY	-	expression tag	UNP Q3E7C1
5	-2	PRO	-	expression tag	UNP Q3E7C1
5	-1	GLY	-	expression tag	UNP Q3E7C1
5	0	SER	-	expression tag	UNP Q3E7C1

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	374	2946	1870	507	541	28	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	-2	GLY	-	expression tag	UNP Q04673
6	-1	GLY	-	expression tag	UNP Q04673
6	0	SER	-	expression tag	UNP Q04673

- Molecule 8 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		
8	7	615	4954	3153	860	914	27	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	1430	11254	7088	1967	2137	62	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	1180	9404	5946	1643	1760	55	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	266	2092	1315	348	416	13	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	initiating methionine	UNP P16370
C	-27	GLY	-	expression tag	UNP P16370
C	-26	SER	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	HIS	-	expression tag	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	SER	-	expression tag	UNP P16370
C	-18	ASN	-	expression tag	UNP P16370
C	-17	SER	-	expression tag	UNP P16370
C	-16	GLY	-	expression tag	UNP P16370
C	-15	LEU	-	expression tag	UNP P16370
C	-14	ASN	-	expression tag	UNP P16370
C	-13	ASP	-	expression tag	UNP P16370
C	-12	ILE	-	expression tag	UNP P16370
C	-11	PHE	-	expression tag	UNP P16370
C	-10	GLU	-	expression tag	UNP P16370
C	-9	ALA	-	expression tag	UNP P16370
C	-8	GLN	-	expression tag	UNP P16370
C	-7	LYS	-	expression tag	UNP P16370
C	-6	ILE	-	expression tag	UNP P16370
C	-5	GLU	-	expression tag	UNP P16370
C	-4	TRP	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	GLU	-	expression tag	UNP P16370
C	-1	ASP	-	expression tag	UNP P16370
C	0	THR	-	expression tag	UNP P16370
C	1	GLY	-	expression tag	UNP P16370
C	2	SER	-	expression tag	UNP P16370
C	3	SER	-	expression tag	UNP P16370

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	167	1343	829	242	270	2	0	0

- Molecule 13 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		
13	E	214	1752	1111	309	321	11	0	0

- Molecule 14 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		
14	F	86	697	445	118	131	3	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	171	1339	861	222	248	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	HIS	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087

- Molecule 16 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		
16	H	140	1120	704	188	224	4	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	116	944	581	172	181	10	0	0

- Molecule 18 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		
18	J	69	569	362	101	100	6	0	0

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 20 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		
20	L	45	359	221	71	63	4	0	0

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	308	2360	1489	406	447	18	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	346	LYS	-	expression tag	UNP P29055
M	347	HIS	-	expression tag	UNP P29055
M	348	HIS	-	expression tag	UNP P29055
M	349	HIS	-	expression tag	UNP P29055
M	350	HIS	-	expression tag	UNP P29055
M	351	HIS	-	expression tag	UNP P29055
M	352	HIS	-	expression tag	UNP P29055

- Molecule 22 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	N	64	1314	631	239	381	63	0	0

- Molecule 23 is a protein called TATA-box-binding protein.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	241	LYS	-	expression tag	UNP P13393
O	242	HIS	-	expression tag	UNP P13393
O	243	HIS	-	expression tag	UNP P13393
O	244	HIS	-	expression tag	UNP P13393
O	245	HIS	-	expression tag	UNP P13393
O	246	HIS	-	expression tag	UNP P13393
O	247	HIS	-	expression tag	UNP P13393

- Molecule 24 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	218	1849	1167	342	333	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-2	GLY	-	expression tag	UNP P41895
Q	-1	PRO	-	expression tag	UNP P41895
Q	0	GLY	-	expression tag	UNP P41895

- Molecule 25 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	268	2230	1409	392	419	10	0	0

- Molecule 26 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	T	63	1283	617	223	380	63	0	0

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

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

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	123	LYS	-	expression tag	UNP P32774
V	124	HIS	-	expression tag	UNP P32774
V	125	HIS	-	expression tag	UNP P32774

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Chain	Residue	Modelled	Actual	Comment	Reference
V	126	HIS	-	expression tag	UNP P32774
V	127	HIS	-	expression tag	UNP P32774
V	128	HIS	-	expression tag	UNP P32774
V	129	HIS	-	expression tag	UNP P32774

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	312	2532	1595	442	488	7	0	0

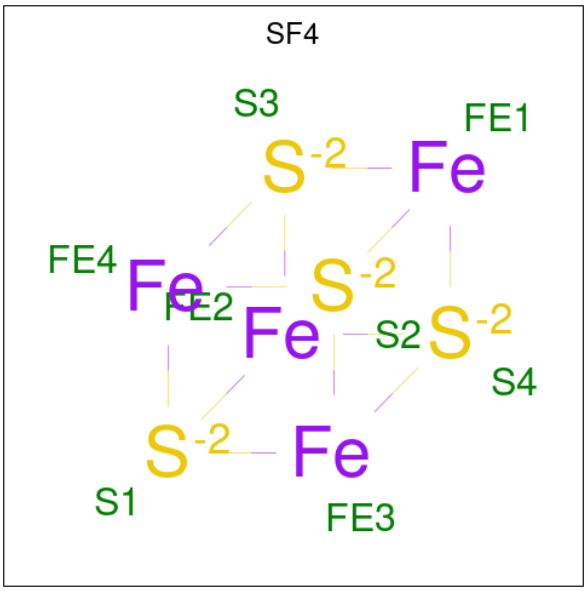
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	483	ALA	-	expression tag	UNP P36100
W	484	ALA	-	expression tag	UNP P36100
W	485	ALA	-	expression tag	UNP P36100
W	486	LEU	-	expression tag	UNP P36100
W	487	GLU	-	expression tag	UNP P36100
W	488	HIS	-	expression tag	UNP P36100
W	489	HIS	-	expression tag	UNP P36100
W	490	HIS	-	expression tag	UNP P36100
W	491	HIS	-	expression tag	UNP P36100
W	492	HIS	-	expression tag	UNP P36100

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	207	1661	1061	281	313	6	0	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

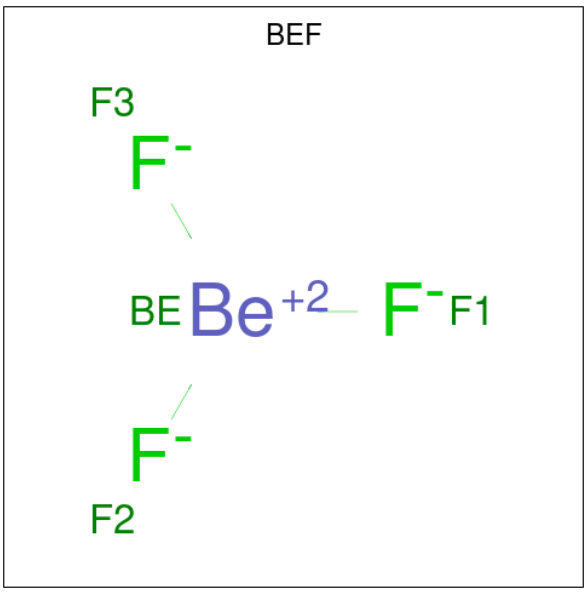


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
31	0	1	8	4	4	0

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
32	3	2	2	2	0
32	4	1	1	1	0
32	6	4	4	4	0
32	A	2	2	2	0
32	B	1	1	1	0
32	C	1	1	1	0
32	I	2	2	2	0
32	J	1	1	1	0
32	L	1	1	1	0
32	M	1	1	1	0
32	W	1	1	1	0

- Molecule 33 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).

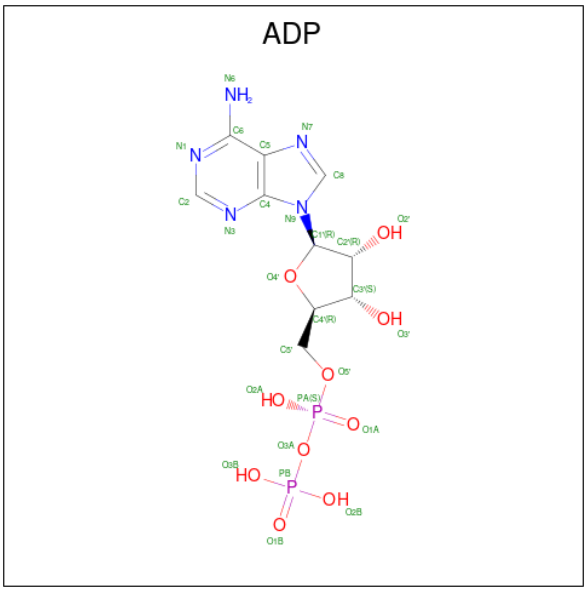


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
33	7	1	4	1	3	0

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	7	1	1	1	0
34	A	1	1	1	0

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



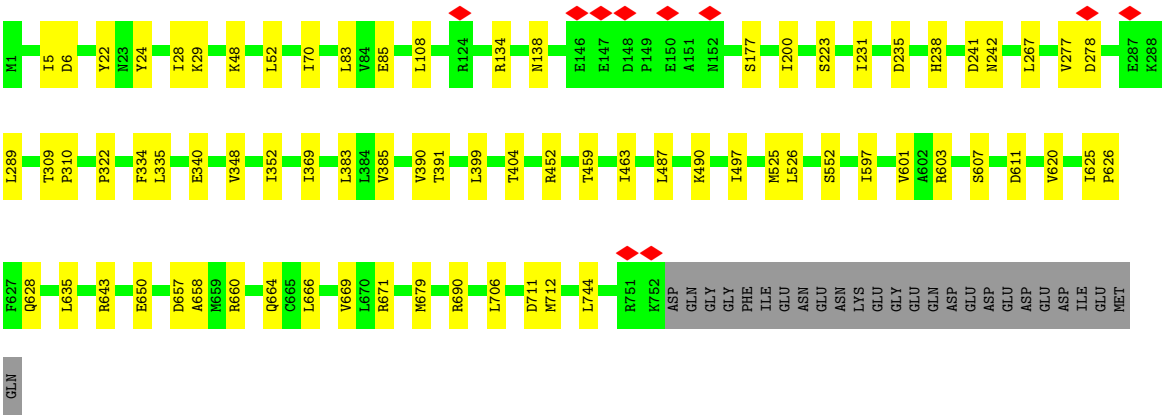
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	7	1	27	10	5	10	2	0

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.

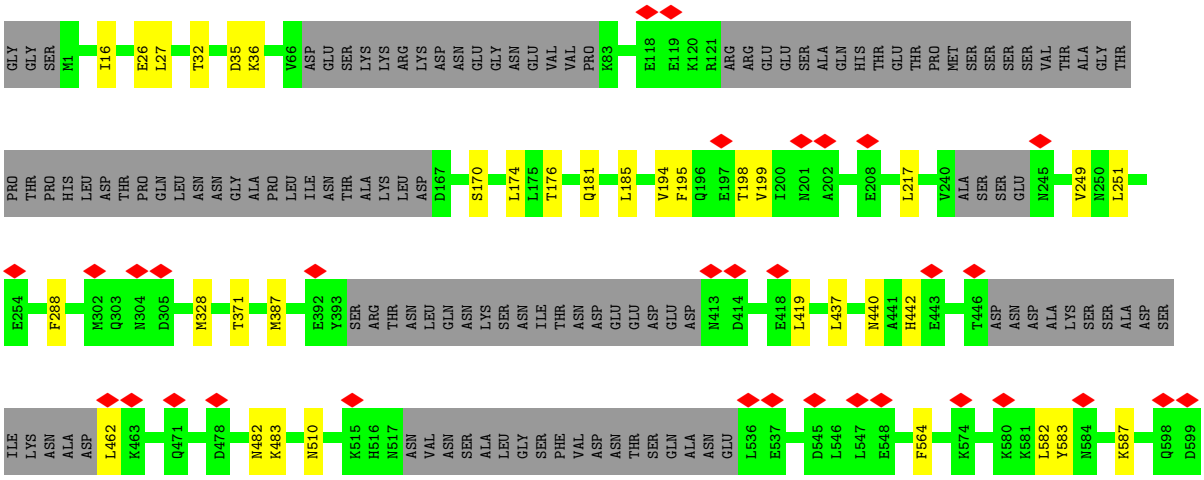
• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD

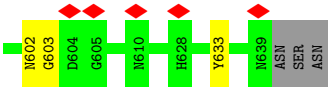
Chain 0:



• Molecule 2: General transcription and DNA repair factor IIH subunit TFB1

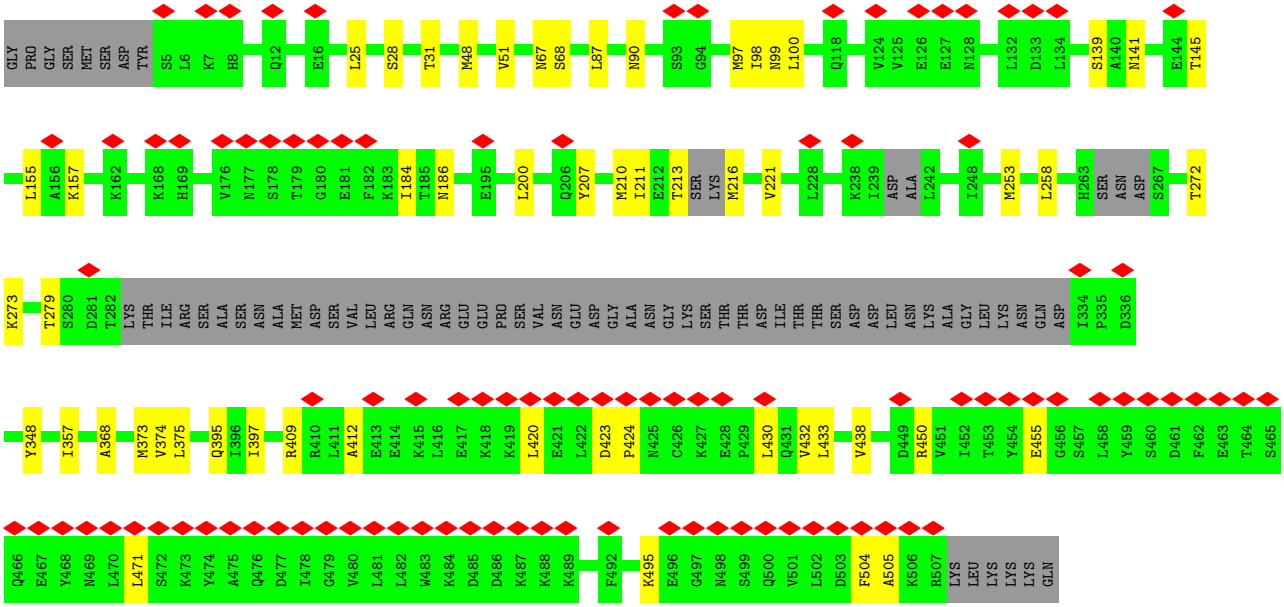
Chain 1:





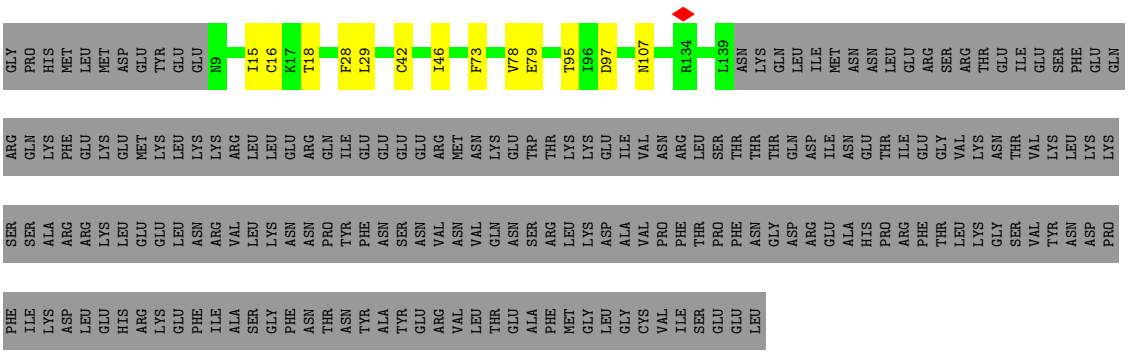
• Molecule 3: General transcription and DNA repair factor IIH subunit TFB2

Chain 2:



• Molecule 4: RNA polymerase II transcription factor B subunit 3

Chain 3:

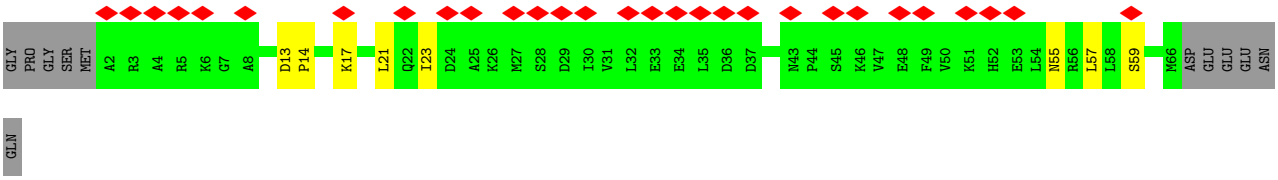


• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

Chain 4:

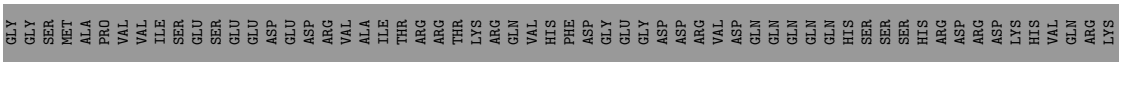
• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

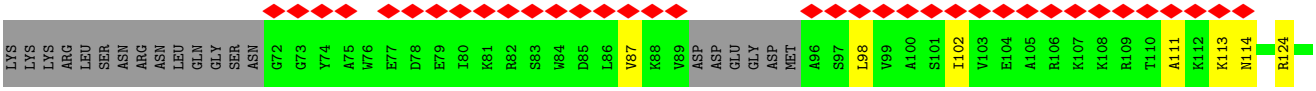
Chain 5:

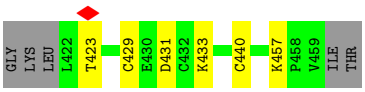


• Molecule 7: General transcription and DNA repair factor IIH subunit SSL1

Chain 6:

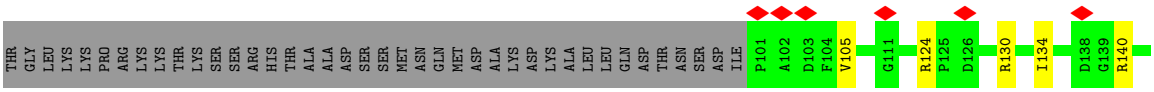


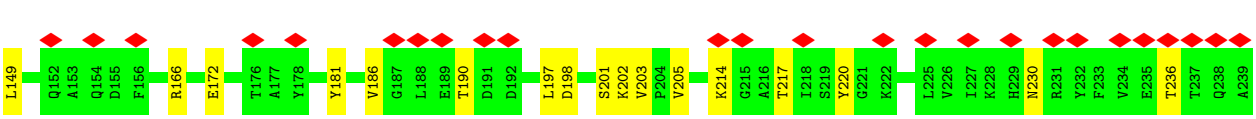


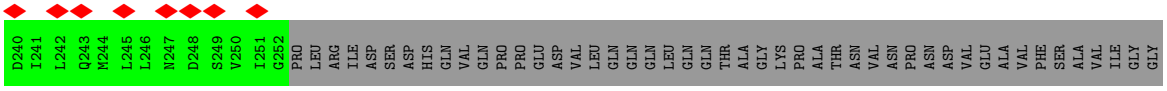


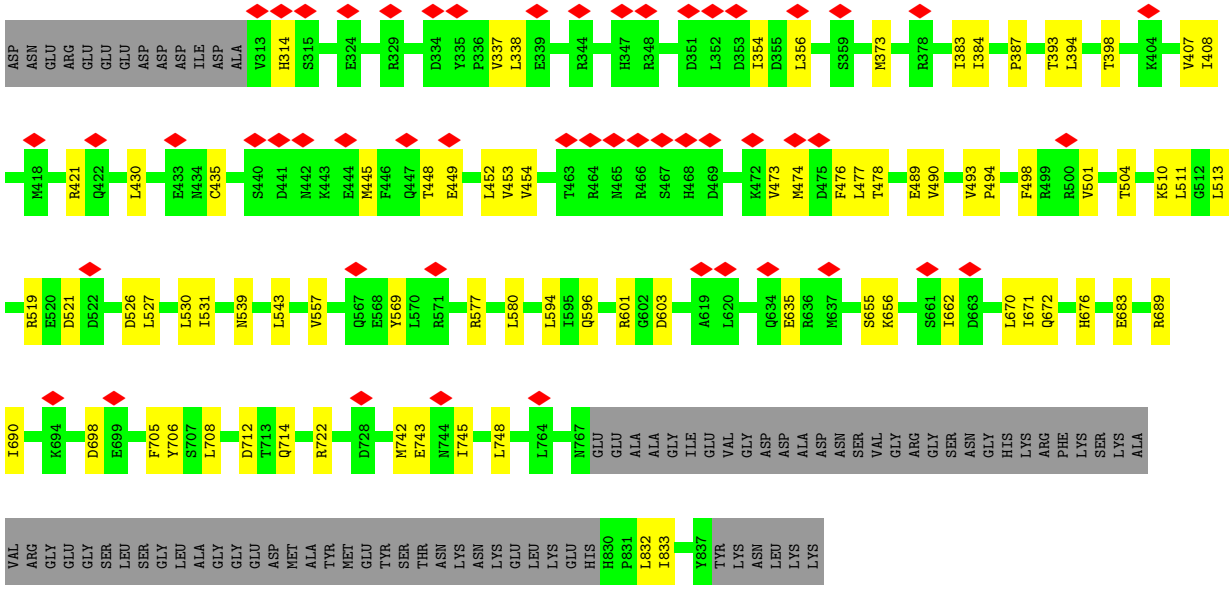
• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:



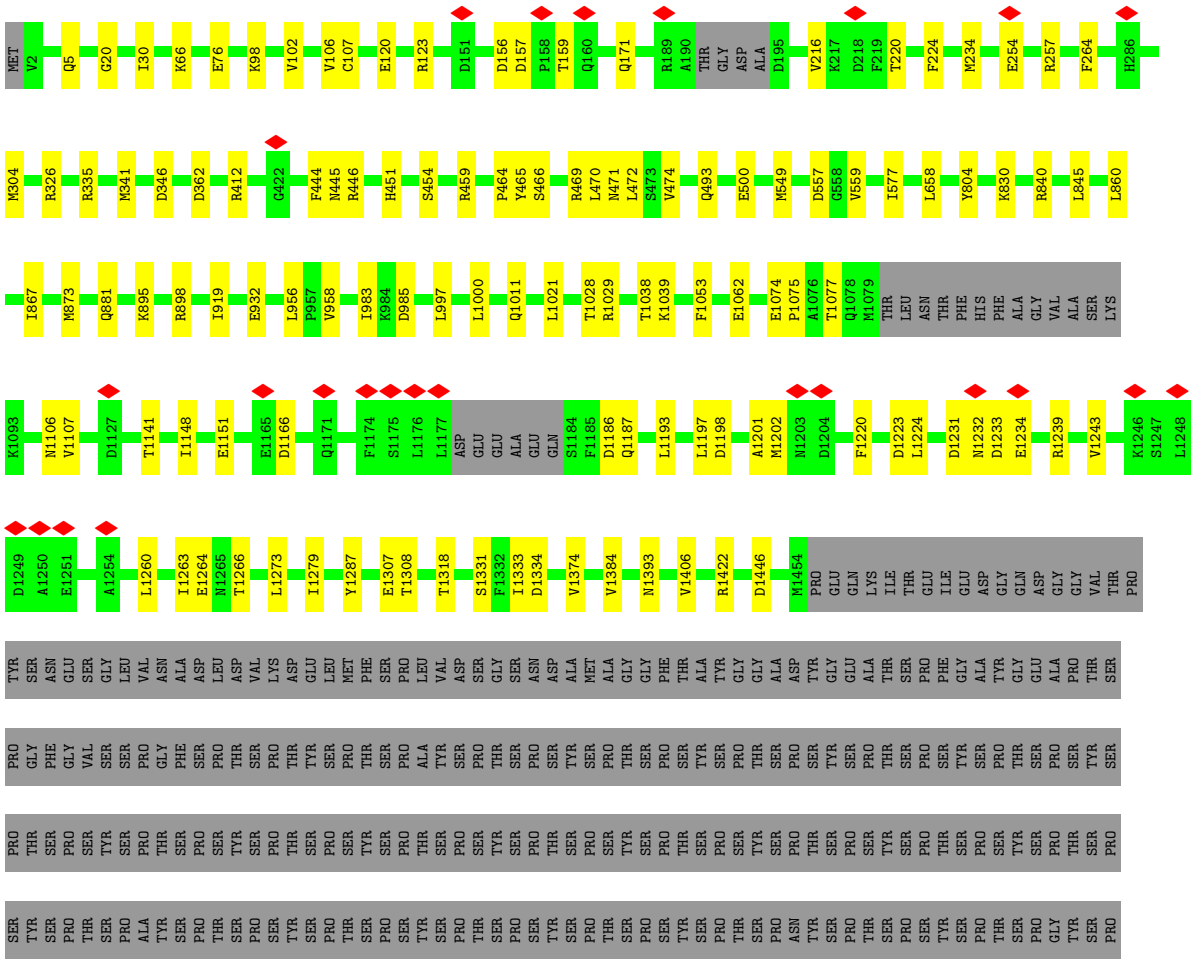


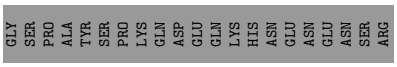




• Molecule 9: DNA-directed RNA polymerase II subunit RPB1

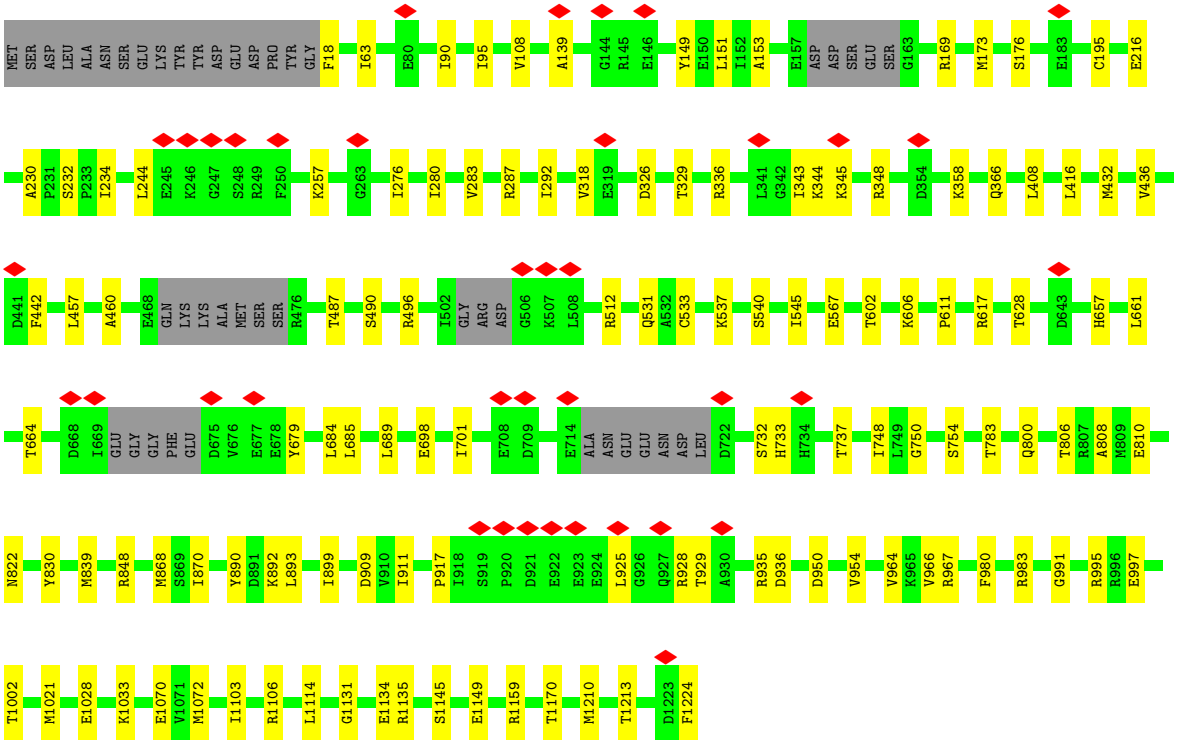
Chain A: 76% 7% 17%





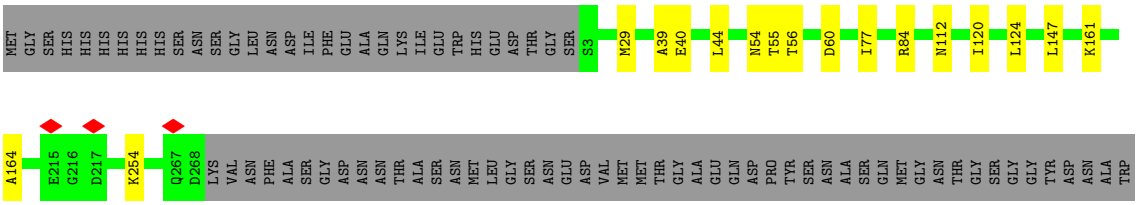
• Molecule 10: DNA-directed RNA polymerase II subunit RPB2

Chain B:



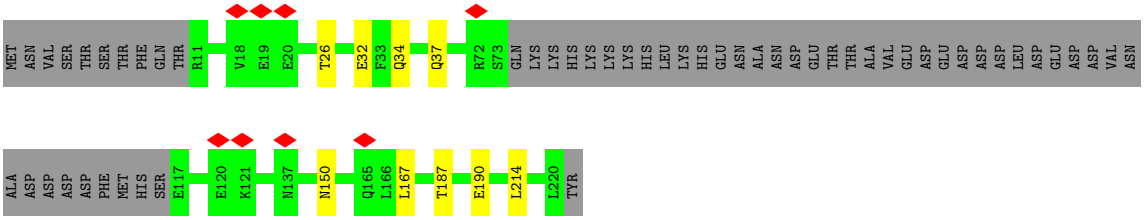
• Molecule 11: DNA-directed RNA polymerase II subunit RPB3

Chain C:



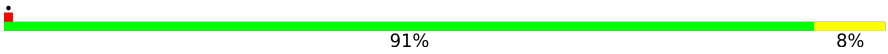
• Molecule 12: DNA-directed RNA polymerase II subunit RPB4

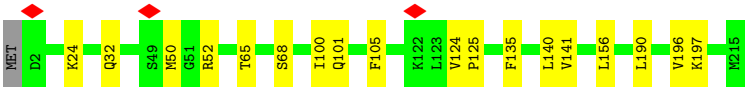
Chain D:



• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1

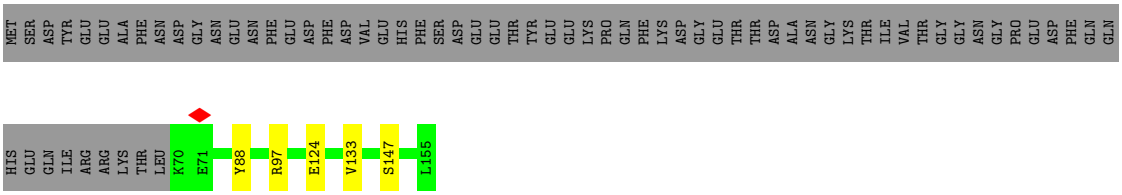
Chain E:





• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

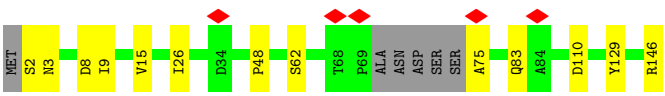


• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G:

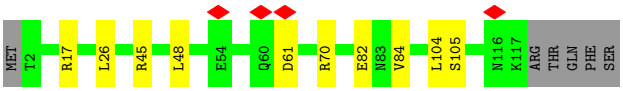
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



• Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I:

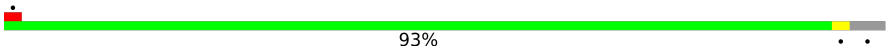


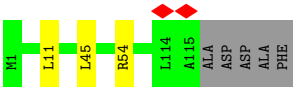
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

• Molecule 19: DNA-directed RNA polymerase II subunit RPB11

Chain K:



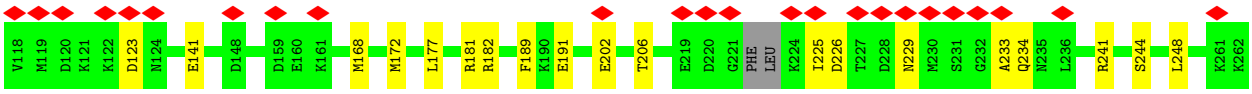


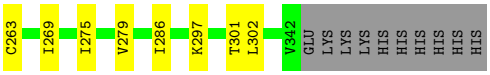
• Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:

• Molecule 21: Transcription initiation factor IIB

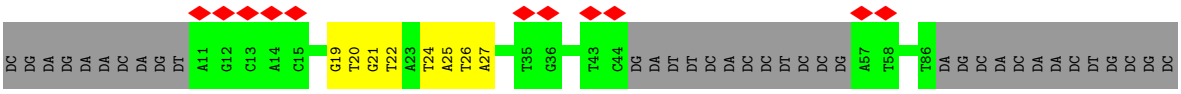
Chain M:

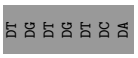




• Molecule 22: Non-template DNA

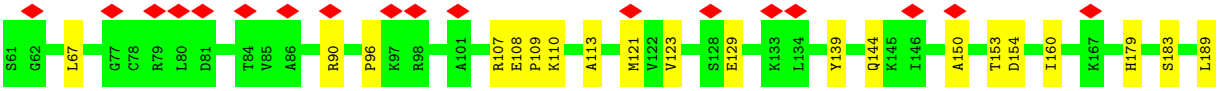
Chain N:

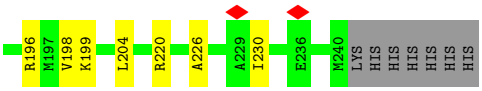




• Molecule 23: TATA-box-binding protein

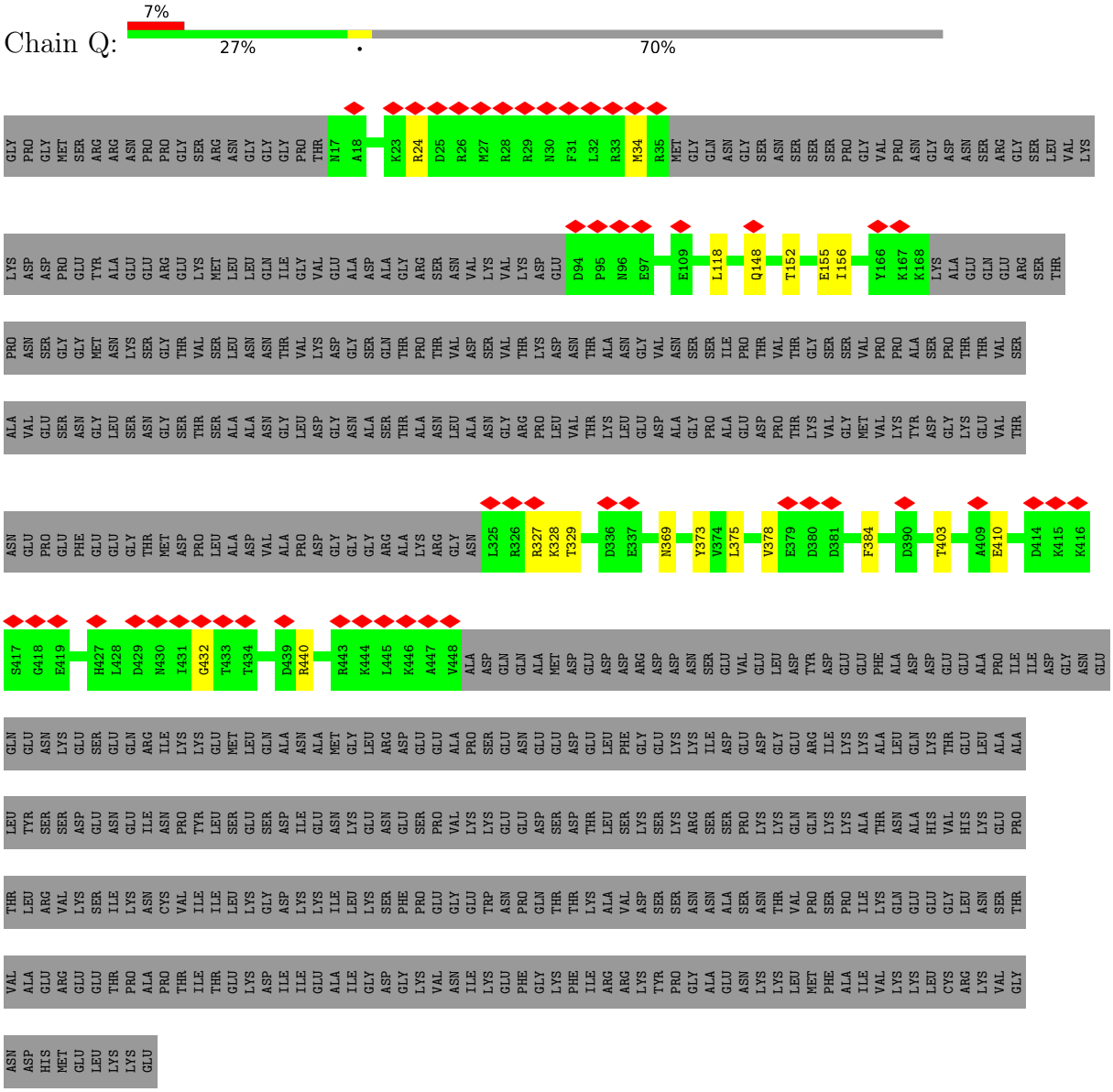
Chain O:





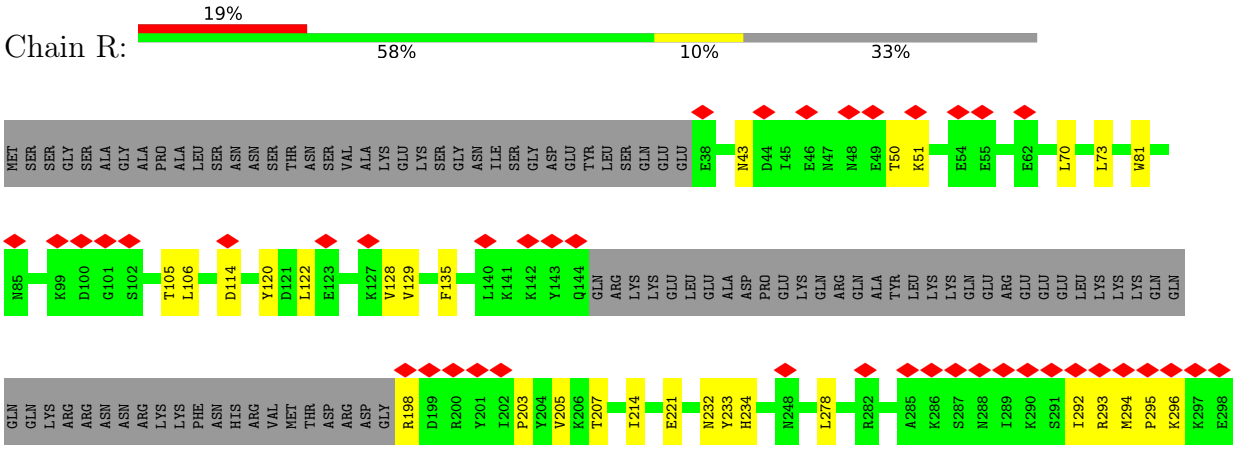
• Molecule 24: Transcription initiation factor IIF subunit alpha

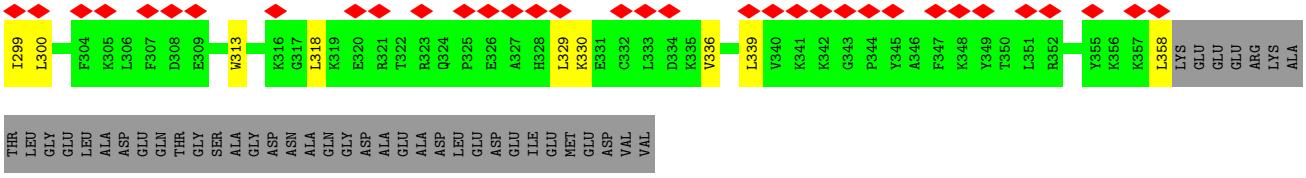
Chain Q:



• Molecule 25: Transcription initiation factor IIF subunit beta

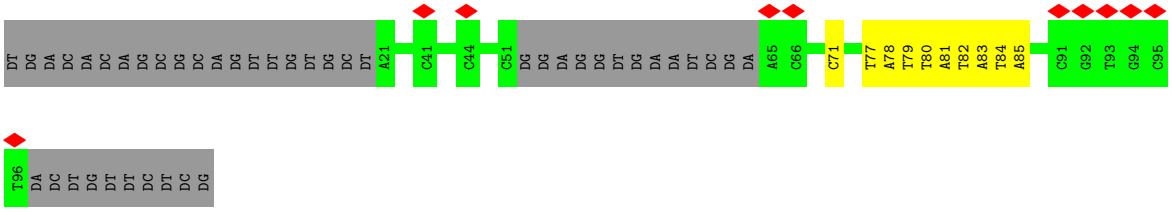
Chain R:





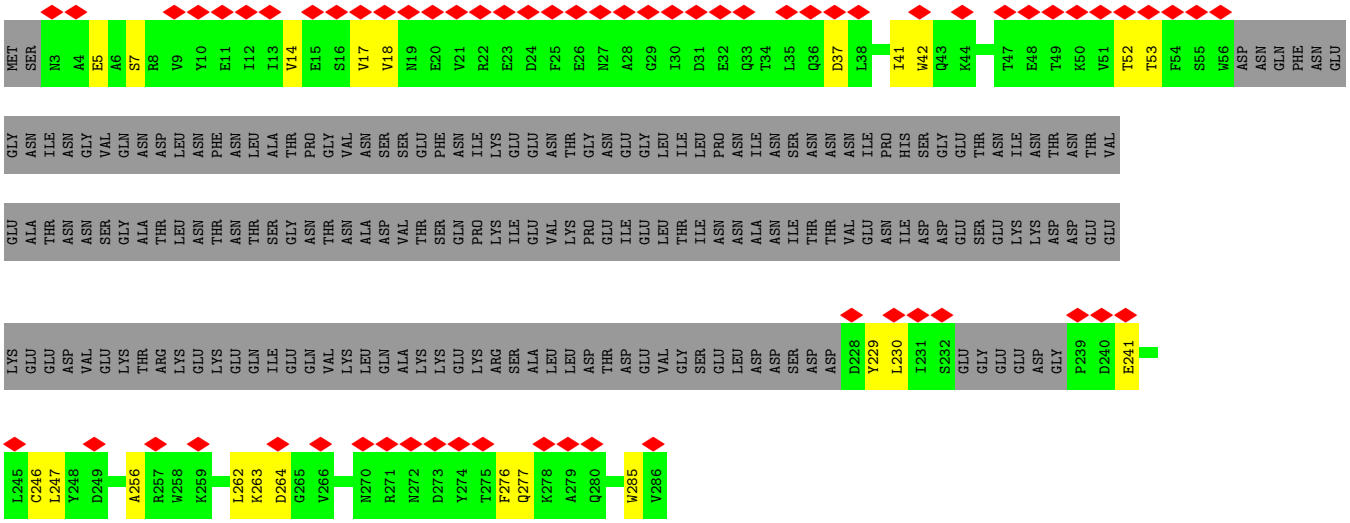
• Molecule 26: Template DNA

Chain T:



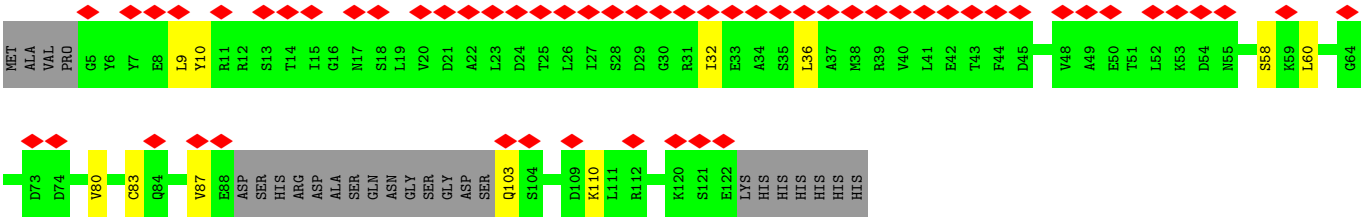
• Molecule 27: Transcription initiation factor IIA large subunit

Chain U:



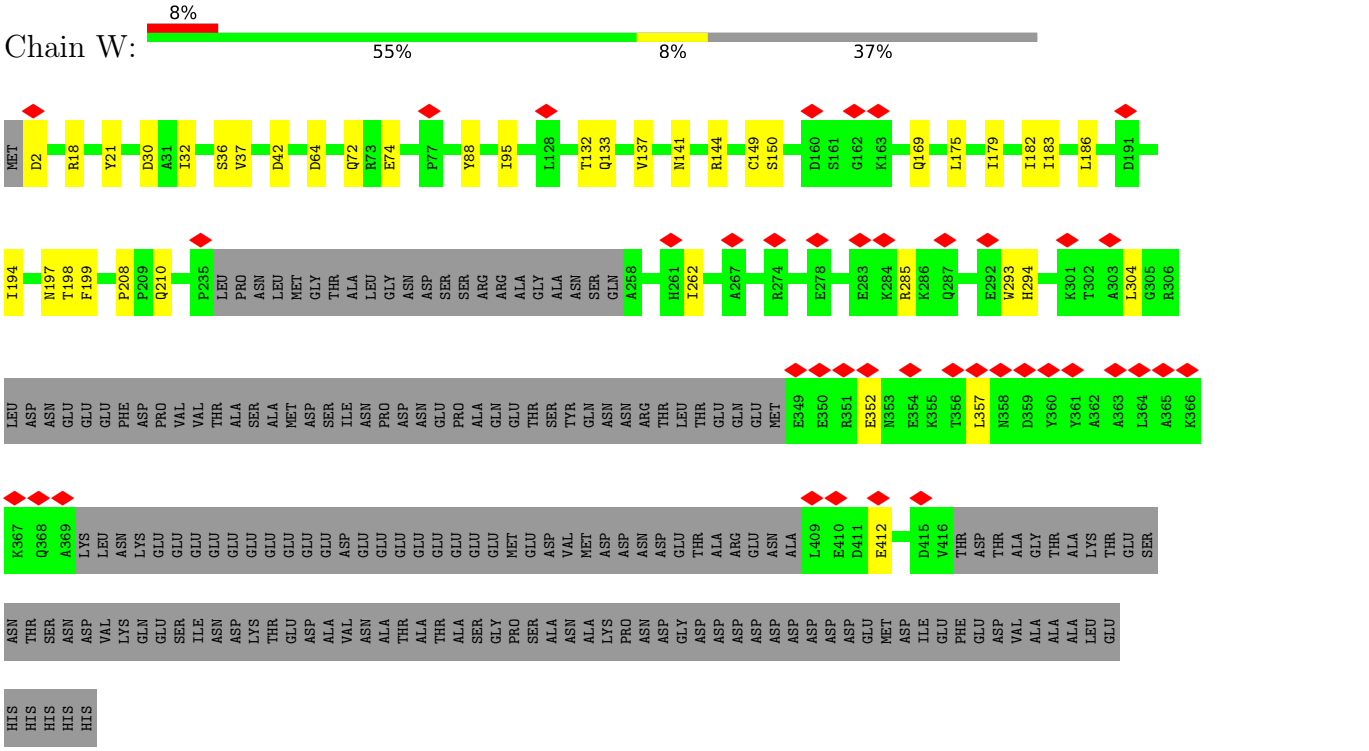
• Molecule 28: Transcription initiation factor IIA subunit 2

Chain V:



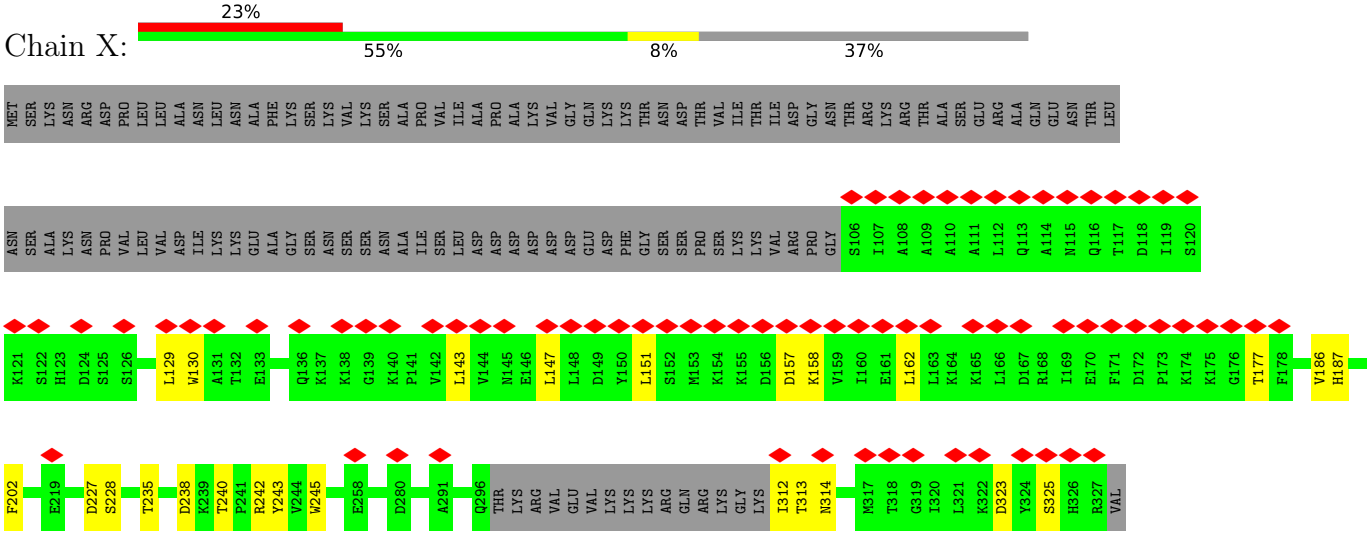
• Molecule 29: Transcription initiation factor IIE subunit alpha

Chain W:



- Molecule 30: Transcription initiation factor IIE subunit beta

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23887	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	62.913	Depositor
Minimum map value	-40.259	Depositor
Average map value	0.041	Depositor
Map value standard deviation	1.024	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	398.99997, 398.99997, 398.99997	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ADP, BEF, SF4

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	0	0.11	0/6209	0.23	0/8384
2	1	0.09	0/4277	0.21	0/5755
3	2	0.08	0/3664	0.21	0/4952
4	3	0.10	0/1109	0.26	0/1492
5	4	0.09	0/2312	0.22	0/3127
6	5	0.09	0/520	0.26	0/701
7	6	0.09	0/3007	0.23	0/4066
8	7	0.10	0/5059	0.27	1/6841 (0.0%)
9	A	0.11	0/11455	0.25	0/15490
10	B	0.11	0/9589	0.26	0/12934
11	C	0.09	0/2130	0.22	0/2887
12	D	0.09	0/1351	0.24	0/1811
13	E	0.10	0/1788	0.23	0/2406
14	F	0.10	0/709	0.23	0/956
15	G	0.10	0/1367	0.21	0/1844
16	H	0.09	0/1139	0.24	0/1544
17	I	0.11	0/962	0.28	0/1295
18	J	0.12	0/578	0.23	0/775
19	K	0.11	0/942	0.21	0/1272
20	L	0.10	0/361	0.25	0/478
21	M	0.09	0/2387	0.23	0/3211
22	N	0.18	0/1474	0.44	0/2272
23	O	0.11	0/1449	0.26	0/1952
24	Q	0.11	0/1885	0.26	0/2526
25	R	0.10	0/2270	0.31	0/3052
26	T	0.20	0/1435	0.46	0/2208
27	U	0.09	0/898	0.27	0/1212
28	V	0.09	0/822	0.24	0/1109
29	W	0.12	0/2575	0.25	0/3473
30	X	0.09	0/1692	0.26	0/2280
All	All	0.11	0/75415	0.26	1/102305 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7	676	HIS	N-CA-C	6.64	119.95	109.39

There are no chirality outliers.

There are no planarity outliers.

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	0	6091	0	6155	50	0
2	1	4214	0	4288	29	0
3	2	3597	0	3687	38	0
4	3	1089	0	1069	8	0
5	4	2274	0	2332	19	0
6	5	514	0	541	5	0
7	6	2946	0	2958	28	0
8	7	4954	0	4946	70	0
9	A	11254	0	11319	86	0
10	B	9404	0	9398	88	0
11	C	2092	0	2050	13	0
12	D	1343	0	1366	6	0
13	E	1752	0	1776	10	0
14	F	697	0	720	4	0
15	G	1339	0	1357	13	0
16	H	1120	0	1086	9	0
17	I	944	0	899	7	0
18	J	569	0	585	5	0
19	K	924	0	934	3	0
20	L	359	0	381	0	0
21	M	2360	0	2467	26	0
22	N	1314	0	728	7	0
23	O	1422	0	1500	26	0
24	Q	1849	0	1866	15	0
25	R	2230	0	2254	37	0
26	T	1283	0	717	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	U	885	0	866	14	0
28	V	815	0	822	7	0
29	W	2532	0	2529	29	0
30	X	1661	0	1694	19	0
31	0	8	0	0	0	0
32	3	2	0	0	0	0
32	4	1	0	0	0	0
32	6	4	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	W	1	0	0	0	0
33	7	4	0	0	0	0
34	7	1	0	0	0	0
34	A	1	0	0	0	0
35	7	27	0	12	1	0
All	All	73885	0	73302	593	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 4.

All (593) 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)
10:B:326:ASP:OD1	10:B:329:THR:OG1	1.92	0.86
9:A:412:ARG:NH2	21:M:42:ASP:OD2	2.08	0.86
8:7:745:ILE:HG21	8:7:748:LEU:HD21	1.59	0.83
9:A:549:MET:HE2	9:A:577:ILE:HG21	1.60	0.83
16:H:2:SER:N	16:H:62:SER:OG	2.12	0.82
9:A:469:ARG:NH2	10:B:991:GLY:O	2.13	0.81
10:B:195:CYS:HG	10:B:783:THR:HG1	1.27	0.81
8:7:601:ARG:NH1	8:7:603:ASP:OD2	2.13	0.81
14:F:97:ARG:NH1	14:F:124:GLU:OE1	2.13	0.81
10:B:868:MET:SD	21:M:182:ARG:NH1	2.55	0.80
10:B:287:ARG:NH1	10:B:292:ILE:O	2.14	0.79
8:7:577:ARG:NH2	8:7:714:GLN:OE1	2.16	0.79
10:B:276:ILE:HG21	10:B:280:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:130:ARG:NH1	8:7:198:ASP:O	2.18	0.76
16:H:48:PRO:O	16:H:146:ARG:NH2	2.19	0.76
8:7:140:ARG:NH1	8:7:172:GLU:OE2	2.20	0.75
4:3:95:THR:OG1	4:3:97:ASP:OD1	2.04	0.74
10:B:336:ARG:NH2	24:Q:410:GLU:OE1	2.16	0.74
21:M:181:ARG:O	21:M:229:ASN:ND2	2.20	0.74
23:O:153:THR:HG22	23:O:154:ASP:H	1.52	0.74
10:B:151:LEU:HD23	10:B:153:ALA:H	1.52	0.74
16:H:83:GLN:OE1	19:K:54:ARG:NH2	2.21	0.74
9:A:120:GLU:OE1	9:A:123:ARG:NH2	2.20	0.73
9:A:840:ARG:NH1	9:A:1106:ASN:OD1	2.22	0.73
23:O:96:PRO:HB2	25:R:292:ILE:HG21	1.71	0.73
10:B:496:ARG:NH2	10:B:540:SER:O	2.21	0.73
10:B:890:TYR:OH	10:B:936:ASP:OD2	2.05	0.73
9:A:451:HIS:O	9:A:454:SER:OG	2.08	0.72
10:B:892:LYS:NZ	10:B:909:ASP:OD2	2.22	0.72
27:U:5:GLU:OE1	28:V:58:SER:OG	2.07	0.72
8:7:421:ARG:NH1	8:7:435:CYS:SG	2.63	0.71
9:A:860:LEU:HD11	9:A:1393:ASN:O	1.91	0.71
21:M:189:PHE:CE2	23:O:189:LEU:HD11	2.25	0.70
9:A:254:GLU:OE1	10:B:935:ARG:NH2	2.25	0.70
10:B:750:GLY:O	10:B:754:SER:OG	2.08	0.70
25:R:233:TYR:O	25:R:234:HIS:ND1	2.25	0.70
25:R:330:LYS:NZ	26:T:71:DC:OP2	2.19	0.70
1:0:48:LYS:NZ	1:0:235:ASP:OD1	2.19	0.70
23:O:121:MET:HE1	23:O:139:TYR:CB	2.22	0.70
9:A:1107:VAL:CG1	9:A:1333:ILE:HD11	2.22	0.69
25:R:114:ASP:OD1	25:R:232:ASN:ND2	2.25	0.69
10:B:925:LEU:HD23	21:M:22:LEU:HD13	1.73	0.69
4:3:42:CYS:O	4:3:46:ILE:HG22	1.93	0.69
12:D:150:ASN:O	15:G:142:ARG:NH2	2.26	0.68
9:A:76:GLU:OE2	10:B:1159:ARG:NH1	2.26	0.68
8:7:519:ARG:NE	8:7:521:ASP:OD1	2.28	0.67
1:0:223:SER:OG	1:0:452:ARG:NH1	2.27	0.67
8:7:166:ARG:NH1	8:7:539:ASN:OD1	2.28	0.67
8:7:190:THR:HG21	8:7:214:LYS:HD3	1.77	0.67
3:2:423:ASP:OD1	29:W:285:ARG:NH1	2.27	0.67
15:G:6:ASP:OD1	15:G:75:ARG:NH1	2.28	0.67
5:4:193:TYR:OH	7:6:373:SER:OG	2.12	0.66
25:R:318:LEU:HD22	25:R:329:LEU:HD21	1.76	0.66
1:0:310:PRO:HB3	1:0:404:THR:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:385:VAL:CG1	1:0:390:VAL:HG21	2.24	0.66
8:7:124:ARG:NH2	8:7:201:SER:O	2.28	0.66
21:M:191:GLU:OE2	21:M:241:ARG:NH1	2.29	0.66
16:H:2:SER:N	16:H:62:SER:HG	1.91	0.66
23:O:113:ALA:HB1	23:O:121:MET:HE3	1.78	0.65
4:3:15:ILE:O	29:W:169:GLN:NE2	2.30	0.65
24:Q:432:GLY:O	25:R:198:ARG:NE	2.29	0.65
3:2:211:ILE:HD13	3:2:221:VAL:HG21	1.79	0.65
9:A:257:ARG:O	21:M:83:SER:OG	2.13	0.64
10:B:169:ARG:NH2	21:M:141:GLU:OE1	2.31	0.64
3:2:141:ASN:O	3:2:145:THR:HG23	1.97	0.63
9:A:107:CYS:SG	9:A:171:GLN:NE2	2.70	0.63
30:X:143:LEU:HD23	30:X:177:THR:OG1	1.99	0.63
2:1:26:GLU:OE1	2:1:26:GLU:N	2.32	0.63
9:A:445:ASN:OD1	9:A:446:ARG:N	2.32	0.63
25:R:106:LEU:HD23	25:R:122:LEU:HD21	1.80	0.63
2:1:174:LEU:HD12	2:1:217:LEU:HB3	1.81	0.63
9:A:1198:ASP:OD2	9:A:1201:ALA:N	2.31	0.63
2:1:440:ASN:OD1	5:4:277:TYR:OH	2.17	0.63
10:B:925:LEU:CD2	21:M:22:LEU:HD13	2.27	0.63
26:T:77:DT:H2"	26:T:78:DA:H8	1.62	0.63
10:B:216:GLU:OE1	10:B:537:LYS:NZ	2.31	0.63
3:2:200:LEU:HD11	3:2:258:LEU:HD11	1.81	0.62
3:2:272:THR:HG22	3:2:273:LYS:H	1.64	0.62
8:7:356:LEU:HD11	8:7:398:THR:HG22	1.80	0.62
8:7:130:ARG:O	8:7:202:LYS:NZ	2.28	0.62
11:C:120:ILE:HG21	11:C:124:LEU:HD21	1.80	0.62
1:0:335:LEU:HD21	1:0:399:LEU:HD22	1.81	0.62
27:U:264:ASP:OD1	27:U:277:GLN:NE2	2.31	0.62
29:W:179:ILE:HG13	29:W:182:ILE:HD12	1.82	0.62
30:X:235:THR:OG1	30:X:238:ASP:O	2.18	0.62
29:W:18:ARG:NH2	29:W:30:ASP:OD2	2.33	0.62
1:0:322:PRO:O	4:3:107:ASN:ND2	2.33	0.62
25:R:318:LEU:HD21	25:R:329:LEU:HD11	1.82	0.62
7:6:113:LYS:HA	7:6:388:THR:HG21	1.81	0.62
1:0:611:ASP:OD2	1:0:671:ARG:NH2	2.33	0.61
9:A:304:MET:HE2	10:B:1210:MET:HA	1.82	0.61
1:0:625:ILE:HG22	1:0:658:ALA:HB1	1.82	0.61
3:2:139:SER:HB2	3:2:272:THR:HG21	1.82	0.61
1:0:385:VAL:HG13	1:0:390:VAL:HG21	1.81	0.61
2:1:564:PHE:HA	2:1:582:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:407:VAL:HG23	8:7:452:LEU:HD12	1.83	0.60
10:B:139:ALA:HB2	10:B:149:TYR:HA	1.81	0.60
11:C:55:THR:HG22	11:C:55:THR:O	2.00	0.60
2:1:437:LEU:HD11	5:4:292:CYS:HB2	1.84	0.60
8:7:384:ILE:HD12	8:7:511:LEU:HD11	1.83	0.60
21:M:301:THR:HG23	21:M:302:LEU:HG	1.83	0.60
11:C:54:ASN:ND2	11:C:60:ASP:OD1	2.33	0.60
1:0:628:GLN:NE2	1:0:657:ASP:OD2	2.35	0.60
2:1:482:ASN:OD1	2:1:483:LYS:N	2.34	0.60
3:2:450:ARG:NH2	8:7:712:ASP:OD2	2.35	0.60
8:7:387:PRO:CG	8:7:543:LEU:HD12	2.31	0.60
9:A:362:ASP:OD2	9:A:459:ARG:NE	2.33	0.60
3:2:420:LEU:HD13	3:2:424:PRO:HA	1.83	0.59
8:7:201:SER:OG	8:7:203:VAL:O	2.21	0.59
9:A:264:PHE:CE1	21:M:92:LEU:HD22	2.37	0.59
24:Q:152:THR:O	24:Q:156:ILE:HD12	2.01	0.59
1:0:22:TYR:CD1	1:0:744:LEU:HD11	2.38	0.59
8:7:407:VAL:CG2	8:7:452:LEU:HD12	2.32	0.59
25:R:313:TRP:HD1	25:R:318:LEU:HD12	1.66	0.59
25:R:43:ASN:ND2	25:R:203:PRO:O	2.35	0.59
10:B:343:ILE:HD12	10:B:348:ARG:HG2	1.85	0.59
9:A:997:LEU:O	9:A:1011:GLN:NE2	2.36	0.59
24:Q:155:GLU:OE2	24:Q:440:ARG:NH1	2.36	0.59
29:W:352:GLU:N	29:W:352:GLU:OE1	2.36	0.58
1:0:5:ILE:HG22	1:0:6:ASP:H	1.68	0.58
10:B:928:ARG:NH1	10:B:929:THR:O	2.36	0.58
29:W:133:GLN:O	29:W:137:VAL:HG23	2.03	0.58
10:B:617:ARG:NH2	17:I:61:ASP:OD2	2.36	0.58
25:R:73:LEU:HD21	25:R:81:TRP:CE3	2.38	0.58
1:0:83:LEU:HD13	1:0:177:SER:HA	1.84	0.58
2:1:198:THR:HG23	2:1:199:VAL:HG23	1.86	0.58
2:1:249:VAL:HG12	29:W:262:ILE:HG22	1.86	0.58
9:A:1166:ASP:OD2	9:A:1239:ARG:NH1	2.36	0.58
9:A:804:TYR:HE2	10:B:1021:MET:HE2	1.69	0.57
10:B:1213:THR:O	10:B:1213:THR:HG23	2.04	0.57
9:A:1062:GLU:OE1	14:F:88:TYR:OH	2.21	0.57
30:X:323:ASP:OD1	30:X:325:SER:OG	2.17	0.57
13:E:100:ILE:HG23	13:E:105:PHE:HB2	1.87	0.57
28:V:32:ILE:HG23	28:V:36:LEU:HD23	1.87	0.57
21:M:177:LEU:HD21	21:M:181:ARG:HE	1.70	0.57
11:C:56:THR:HG22	11:C:147:LEU:CD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:336:VAL:HG12	30:X:129:LEU:CD2	2.35	0.57
27:U:7:SER:OG	27:U:53:THR:O	2.15	0.57
8:7:832:LEU:HD11	9:A:1266:THR:HG21	1.86	0.57
15:G:115:MET:HE1	15:G:130:TYR:CD2	2.39	0.56
25:R:336:VAL:HG12	30:X:129:LEU:HD21	1.87	0.56
9:A:1148:ILE:O	17:I:48:LEU:N	2.38	0.56
9:A:1446:ASP:HB2	14:F:133:VAL:HG13	1.86	0.56
25:R:358:LEU:HB3	30:X:162:LEU:HD13	1.85	0.56
10:B:283:VAL:HG21	10:B:318:VAL:HA	1.88	0.56
10:B:870:ILE:HG23	10:B:917:PRO:HG2	1.86	0.56
9:A:1107:VAL:HG13	9:A:1333:ILE:HD11	1.87	0.56
10:B:18:PHE:CD1	24:Q:34:MET:HE1	2.40	0.56
21:M:91:ASN:ND2	21:M:123:ASP:OD2	2.39	0.56
11:C:77:ILE:HD11	11:C:161:LYS:HB3	1.88	0.56
10:B:1033:LYS:NZ	10:B:1070:GLU:OE2	2.23	0.56
23:O:67:LEU:HD22	23:O:160:ILE:CG2	2.35	0.56
2:1:462:LEU:HD12	2:1:462:LEU:O	2.06	0.55
3:2:139:SER:CB	3:2:272:THR:HG21	2.36	0.55
8:7:445:MET:HE3	8:7:473:VAL:HG13	1.87	0.55
29:W:72:GLN:NE2	29:W:74:GLU:OE2	2.39	0.55
23:O:67:LEU:HD22	23:O:160:ILE:HG22	1.87	0.55
8:7:387:PRO:HG3	8:7:543:LEU:HD12	1.88	0.55
10:B:416:LEU:HD23	10:B:457:LEU:HD23	1.87	0.55
1:0:666:LEU:HD22	1:0:679:MET:HB3	1.87	0.55
10:B:416:LEU:HD21	10:B:460:ALA:CB	2.37	0.55
26:T:82:DT:H2"	26:T:83:DA:C8	2.42	0.55
23:O:121:MET:HE2	23:O:123:VAL:HG22	1.87	0.55
2:1:602:ASN:OD1	2:1:603:GLY:N	2.40	0.55
1:0:24:TYR:CZ	1:0:28:ILE:HD11	2.41	0.55
25:R:106:LEU:HD12	25:R:106:LEU:O	2.06	0.55
1:0:607:SER:O	1:0:664:GLN:NE2	2.40	0.55
29:W:37:VAL:HG12	29:W:88:TYR:HB3	1.88	0.55
10:B:657:HIS:O	10:B:661:LEU:HD23	2.07	0.55
8:7:454:VAL:HG13	8:7:454:VAL:O	2.05	0.55
26:T:82:DT:C2'	26:T:83:DA:C8	2.90	0.54
29:W:412:GLU:OE1	29:W:412:GLU:N	2.38	0.54
30:X:147:LEU:O	30:X:151:LEU:HD23	2.07	0.54
10:B:108:VAL:HG23	21:M:244:SER:HB2	1.89	0.54
10:B:408:LEU:HD21	10:B:545:ILE:HD12	1.88	0.54
2:1:510:ASN:ND2	5:4:264:LYS:O	2.40	0.54
7:6:302:ASN:O	7:6:305:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:338:CYS:SG	7:6:339:HIS:CE1	3.00	0.54
9:A:1318:THR:HG23	13:E:141:VAL:HG11	1.88	0.54
25:R:292:ILE:HG23	25:R:292:ILE:O	2.08	0.54
7:6:400:SER:OG	7:6:402:ASP:OD1	2.25	0.54
9:A:98:LYS:HG2	9:A:234:MET:HE1	1.90	0.54
8:7:181:TYR:OH	8:7:337:VAL:O	2.26	0.54
2:1:35:ASP:OD1	2:1:36:LYS:N	2.41	0.54
3:2:412:ALA:HB1	3:2:430:LEU:HD11	1.90	0.54
13:E:156:LEU:HD11	13:E:197:LYS:HB2	1.90	0.54
15:G:129:SER:OG	15:G:138:THR:HG23	2.08	0.54
24:Q:118:LEU:HD21	24:Q:375:LEU:HD21	1.89	0.54
10:B:737:THR:HG22	10:B:737:THR:O	2.08	0.53
27:U:246:CYS:SG	27:U:262:LEU:HD23	2.49	0.53
29:W:42:ASP:OD1	29:W:210:GLN:NE2	2.41	0.53
25:R:318:LEU:CD2	25:R:329:LEU:HD21	2.39	0.53
1:0:463:ILE:HG23	1:0:463:ILE:O	2.09	0.53
9:A:66:LYS:HG2	21:M:20:ILE:HD11	1.90	0.53
9:A:1220:PHE:CD2	9:A:1224:LEU:HD21	2.43	0.53
3:2:87:LEU:HD21	3:2:98:ILE:HD12	1.91	0.53
10:B:800:GLN:NE2	18:J:52:THR:OG1	2.41	0.53
10:B:848:ARG:NH1	18:J:8:PHE:O	2.41	0.53
23:O:121:MET:HE2	23:O:123:VAL:CG2	2.39	0.53
1:0:620:VAL:CG2	1:0:669:VAL:HG11	2.38	0.53
23:O:129:GLU:OE1	23:O:220:ARG:NH2	2.41	0.53
25:R:358:LEU:HD22	30:X:162:LEU:HB3	1.91	0.53
24:Q:328:LYS:O	24:Q:329:THR:HG23	2.09	0.53
8:7:526:ASP:O	8:7:530:LEU:HD23	2.09	0.53
10:B:358:LYS:O	10:B:366:GLN:NE2	2.42	0.53
17:I:84:VAL:HG13	17:I:104:LEU:HD11	1.91	0.53
22:N:20:DT:C2	22:N:21:DG:C8	2.97	0.53
10:B:893:LEU:HD23	10:B:899:ILE:HG13	1.91	0.53
4:3:73:PHE:N	4:3:79:GLU:OE2	2.35	0.52
7:6:308:LEU:HD12	7:6:309:PRO:HD2	1.91	0.52
30:X:238:ASP:OD1	30:X:240:THR:OG1	2.28	0.52
1:0:108:LEU:HD22	1:0:200:ILE:HD11	1.91	0.52
8:7:445:MET:HE3	8:7:473:VAL:CG1	2.39	0.52
9:A:444:PHE:HE2	9:A:470:LEU:HD13	1.74	0.52
22:N:26:DT:H2'	22:N:27:DA:C8	2.43	0.52
1:0:526:LEU:HD11	1:0:597:ILE:HD11	1.91	0.52
15:G:11:ILE:HD12	15:G:72:VAL:HG21	1.92	0.52
25:R:205:VAL:HG13	25:R:207:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:28:SER:OG	3:2:31:THR:HG22	2.10	0.52
7:6:405:SER:OG	7:6:440:CYS:SG	2.68	0.52
9:A:326:ARG:HG3	9:A:1406:VAL:HG21	1.90	0.52
9:A:985:ASP:OD2	9:A:1039:LYS:NZ	2.24	0.52
10:B:664:THR:HG21	10:B:679:TYR:H	1.75	0.52
22:N:24:DT:H2'	22:N:25:DA:C8	2.45	0.52
23:O:90:ARG:NH2	27:U:230:LEU:O	2.41	0.52
25:R:318:LEU:CD2	25:R:329:LEU:HD11	2.39	0.52
6:5:23:ILE:HD11	6:5:57:LEU:CD1	2.40	0.51
9:A:1260:LEU:HD23	9:A:1263:ILE:HD11	1.91	0.51
14:F:133:VAL:HG12	14:F:147:SER:HA	1.92	0.51
3:2:90:ASN:O	3:2:97:MET:N	2.43	0.51
1:0:690:ARG:HD3	1:0:706:LEU:HD21	1.91	0.51
9:A:156:ASP:OD1	9:A:157:ASP:N	2.41	0.51
30:X:202:PHE:O	30:X:245:TRP:NE1	2.40	0.51
1:0:134:ARG:O	1:0:138:ASN:N	2.40	0.51
1:0:241:ASP:OD1	1:0:242:ASN:N	2.43	0.51
27:U:241:GLU:OE2	28:V:110:LYS:NZ	2.43	0.51
10:B:628:THR:HG22	10:B:628:THR:O	2.10	0.51
2:1:583:TYR:OH	2:1:587:LYS:NZ	2.34	0.51
8:7:186:VAL:HG13	8:7:186:VAL:O	2.10	0.51
9:A:471:ASN:O	9:A:474:VAL:HG12	2.10	0.51
22:N:19:DG:H2'	22:N:20:DT:H71	1.91	0.51
25:R:339:LEU:H	25:R:339:LEU:HD23	1.76	0.51
7:6:429:CYS:O	7:6:433:LYS:N	2.41	0.51
23:O:179:HIS:O	23:O:183:SER:OG	2.29	0.51
5:4:85:TYR:OH	7:6:405:SER:O	2.17	0.51
25:R:128:VAL:HG23	25:R:128:VAL:O	2.11	0.51
8:7:493:VAL:N	8:7:494:PRO:CD	2.74	0.50
12:D:167:LEU:HD21	12:D:214:LEU:HD11	1.93	0.50
10:B:244:LEU:HD23	10:B:244:LEU:H	1.76	0.50
26:T:77:DT:C2'	26:T:78:DA:H8	2.24	0.50
27:U:276:PHE:CD1	28:V:60:LEU:HD12	2.46	0.50
9:A:804:TYR:CE2	10:B:1021:MET:HE2	2.46	0.50
10:B:195:CYS:SG	10:B:783:THR:OG1	2.56	0.50
11:C:84:ARG:HD2	19:K:11:LEU:HD11	1.92	0.50
21:M:168:MET:HE3	21:M:172:MET:HE2	1.92	0.50
7:6:287:PHE:CE1	7:6:308:LEU:HD11	2.46	0.50
8:7:220:TYR:CE1	8:7:338:LEU:HD13	2.47	0.50
9:A:1148:ILE:HD11	9:A:1198:ASP:HB2	1.92	0.50
9:A:1287:TYR:OH	9:A:1307:GLU:OE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:416:LEU:HD21	10:B:460:ALA:HB3	1.92	0.50
21:M:14:ARG:O	21:M:14:ARG:NE	2.43	0.50
24:Q:148:GLN:NE2	24:Q:403:THR:O	2.44	0.50
8:7:683:GLU:OE1	8:7:722:ARG:NH1	2.44	0.50
9:A:500:GLU:OE1	10:B:1145:SER:OG	2.22	0.50
16:H:15:VAL:HG12	16:H:26:ILE:HG22	1.94	0.50
23:O:96:PRO:HB2	25:R:292:ILE:HD13	1.93	0.50
1:0:552:SER:OG	2:1:371:THR:OG1	2.27	0.50
8:7:833:ILE:HG21	9:A:1223:ASP:OD2	2.11	0.50
1:0:289:LEU:HD21	1:0:383:LEU:HD13	1.94	0.49
3:2:272:THR:HG22	3:2:273:LYS:N	2.27	0.49
7:6:102:ILE:HG21	7:6:423:THR:HG21	1.94	0.49
8:7:635:GLU:HB2	30:X:312:ILE:HG22	1.93	0.49
16:H:2:SER:OG	16:H:3:ASN:N	2.44	0.49
25:R:135:PHE:HB3	25:R:214:ILE:HD13	1.94	0.49
7:6:431:ASP:O	7:6:457:LYS:NZ	2.46	0.49
10:B:810:GLU:OE1	24:Q:24:ARG:NH2	2.45	0.49
16:H:110:ASP:O	16:H:129:TYR:N	2.44	0.49
1:0:238:HIS:O	1:0:660:ARG:NH2	2.43	0.49
9:A:474:VAL:HG22	9:A:474:VAL:O	2.12	0.49
25:R:105:THR:OG1	25:R:120:TYR:O	2.25	0.49
6:5:23:ILE:HD11	6:5:57:LEU:HD11	1.94	0.49
9:A:1193:LEU:HD11	9:A:1264:GLU:HB2	1.95	0.49
3:2:186:ASN:OD1	3:2:395:GLN:NE2	2.42	0.49
3:2:211:ILE:CD1	3:2:221:VAL:HG21	2.43	0.49
9:A:895:LYS:O	9:A:1029:ARG:NH1	2.44	0.49
9:A:1279:ILE:HG23	9:A:1308:THR:CG2	2.42	0.49
8:7:742:MET:SD	29:W:304:LEU:HD12	2.53	0.49
13:E:101:GLN:O	13:E:101:GLN:NE2	2.43	0.49
7:6:124:ARG:NH2	7:6:231:GLU:OE1	2.43	0.49
8:7:373:MET:SD	8:7:511:LEU:HD13	2.53	0.49
9:A:66:LYS:CG	21:M:20:ILE:HD11	2.43	0.49
22:N:25:DA:OP1	23:O:196:ARG:NH2	2.45	0.49
5:4:29:ILE:HG23	5:4:152:ALA:HB1	1.95	0.48
1:0:497:ILE:HG21	1:0:525:MET:HE2	1.96	0.48
5:4:64:HIS:O	5:4:71:ASN:ND2	2.42	0.48
9:A:1231:ASP:OD1	9:A:1232:ASN:N	2.46	0.48
10:B:567:GLU:N	10:B:567:GLU:OE1	2.46	0.48
10:B:602:THR:HG22	10:B:606:LYS:HE3	1.95	0.48
10:B:611:PRO:HG2	10:B:685:LEU:HD21	1.94	0.48
7:6:98:LEU:HD22	7:6:413:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:822:ASN:O	18:J:48:ARG:NH1	2.46	0.48
5:4:293:LEU:HD22	7:6:376:LEU:HD22	1.95	0.48
9:A:932:GLU:OE1	9:A:1028:THR:OG1	2.29	0.48
10:B:950:ASP:N	10:B:967:ARG:O	2.42	0.48
3:2:471:LEU:HD13	3:2:504:PHE:HD2	1.79	0.48
9:A:1384:VAL:HG12	9:A:1384:VAL:O	2.13	0.48
26:T:77:DT:H2"	26:T:78:DA:C8	2.46	0.48
21:M:275:ILE:O	21:M:279:VAL:HG23	2.13	0.48
26:T:82:DT:H2'	26:T:83:DA:C8	2.49	0.48
1:0:601:VAL:HG12	1:0:603:ARG:H	1.79	0.48
8:7:354:ILE:HG21	8:7:430:LEU:HD13	1.96	0.48
9:A:1422:ARG:NH2	10:B:1224:PHE:OXT	2.45	0.48
1:0:340:GLU:HG3	4:3:78:VAL:HG21	1.96	0.48
3:2:348:TYR:HB3	3:2:373:MET:HE1	1.95	0.48
5:4:23:PRO:O	5:4:172:LEU:HD12	2.13	0.48
9:A:1151:GLU:OE2	17:I:45:ARG:NH1	2.47	0.48
1:0:70:ILE:N	1:0:231:ILE:O	2.40	0.47
7:6:182:VAL:HG11	7:6:199:ILE:HD11	1.95	0.47
10:B:234:ILE:HD13	10:B:257:LYS:CE	2.44	0.47
13:E:50:MET:HE2	13:E:52:ARG:HD2	1.96	0.47
2:1:442:HIS:ND1	5:4:278:LEU:O	2.46	0.47
3:2:409:ARG:HH21	3:2:432:VAL:HG11	1.79	0.47
5:4:288:ILE:HD12	5:4:293:LEU:HD23	1.96	0.47
27:U:14:VAL:O	27:U:18:VAL:HG22	2.14	0.47
3:2:99:ASN:OD1	3:2:100:LEU:N	2.47	0.47
7:6:221:LEU:HD22	7:6:230:ARG:HG2	1.96	0.47
9:A:881:GLN:NE2	9:A:958:VAL:O	2.46	0.47
10:B:664:THR:HG21	10:B:679:TYR:N	2.29	0.47
8:7:743:GLU:N	8:7:743:GLU:OE1	2.46	0.47
23:O:121:MET:HE1	23:O:139:TYR:HB3	1.96	0.47
9:A:557:ASP:OD1	9:A:557:ASP:N	2.47	0.47
10:B:1131:GLY:N	10:B:1134:GLU:OE1	2.43	0.47
24:Q:378:VAL:HG22	24:Q:384:PHE:CE1	2.49	0.47
9:A:873:MET:HE1	9:A:1053:PHE:CZ	2.50	0.47
3:2:397:ILE:HD12	3:2:438:VAL:HG22	1.96	0.47
8:7:393:THR:OG1	35:7:903:ADP:O2A	2.25	0.47
8:7:557:VAL:HB	8:7:708:LEU:HD23	1.96	0.47
9:A:1186:ASP:OD1	9:A:1187:GLN:N	2.48	0.47
16:H:8:ASP:OD1	16:H:9:ILE:N	2.45	0.47
22:N:21:DG:C8	22:N:22:DT:H71	2.50	0.47
25:R:129:VAL:HG21	25:R:221:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:9:LEU:HD12	28:V:10:TYR:N	2.30	0.47
1:0:85:GLU:HG2	2:1:419:LEU:HD21	1.97	0.47
1:0:348:VAL:HG11	1:0:352:ILE:HD12	1.97	0.47
8:7:594:LEU:HD22	8:7:706:TYR:CE2	2.50	0.47
11:C:40:GLU:OE1	11:C:254:LYS:NZ	2.46	0.47
8:7:394:LEU:O	8:7:398:THR:HG23	2.15	0.47
8:7:476:PHE:CD2	8:7:477:LEU:HD12	2.50	0.47
10:B:442:PHE:CD1	25:R:278:LEU:HD23	2.50	0.47
2:1:16:ILE:CG1	2:1:27:LEU:HD11	2.45	0.46
8:7:134:ILE:HD11	8:7:197:LEU:HD11	1.97	0.46
9:A:1141:THR:HG23	9:A:1273:LEU:HB2	1.96	0.46
25:R:293:ARG:O	25:R:294:MET:C	2.58	0.46
30:X:227:ASP:O	30:X:228:SER:OG	2.26	0.46
2:1:185:LEU:HD23	29:W:357:LEU:HD11	1.96	0.46
8:7:230:ASN:ND2	8:7:478:THR:O	2.48	0.46
15:G:13:LEU:HD11	15:G:26:LEU:HG	1.97	0.46
3:2:279:THR:HG22	3:2:279:THR:O	2.16	0.46
3:2:375:LEU:HD23	3:2:375:LEU:H	1.80	0.46
8:7:596:GLN:OE1	8:7:745:ILE:HD11	2.16	0.46
23:O:108:GLU:CG	23:O:109:PRO:HD3	2.46	0.46
25:R:300:LEU:HD21	30:X:129:LEU:HD23	1.95	0.46
29:W:293:TRP:CD1	29:W:294:HIS:ND1	2.83	0.46
3:2:213:THR:O	3:2:216:MET:N	2.48	0.46
5:4:258:LEU:H	5:4:258:LEU:HD23	1.80	0.46
10:B:911:ILE:CG2	10:B:966:VAL:HG11	2.46	0.46
29:W:37:VAL:HG11	29:W:199:PHE:CD1	2.50	0.46
5:4:220:GLU:N	5:4:220:GLU:OE1	2.49	0.46
13:E:135:PHE:HB3	13:E:140:LEU:HD11	1.97	0.46
25:R:50:THR:HG23	25:R:51:LYS:HG2	1.97	0.46
1:0:711:ASP:OD1	1:0:712:MET:N	2.48	0.46
21:M:297:LYS:O	21:M:301:THR:HG22	2.15	0.46
30:X:242:ARG:O	30:X:243:TYR:C	2.59	0.46
8:7:670:LEU:HD23	8:7:671:ILE:N	2.30	0.46
9:A:346:ASP:OD1	10:B:1106:ARG:NE	2.49	0.46
24:Q:373:TYR:CD2	25:R:70:LEU:HD11	2.51	0.46
1:0:334:PHE:CE2	1:0:369:ILE:HG23	2.50	0.46
8:7:490:VAL:HG22	8:7:490:VAL:O	2.16	0.46
9:A:466:SER:O	10:B:1103:ILE:HD12	2.16	0.46
9:A:956:LEU:HD13	9:A:1021:LEU:HD22	1.97	0.46
1:0:52:LEU:HD11	1:0:459:THR:HG21	1.97	0.45
3:2:87:LEU:HD21	3:2:98:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:445:MET:HE1	8:7:453:VAL:CG1	2.46	0.45
10:B:90:ILE:HD12	10:B:432:MET:SD	2.56	0.45
10:B:661:LEU:HD21	10:B:684:LEU:HD21	1.97	0.45
29:W:2:ASP:OD1	29:W:2:ASP:N	2.49	0.45
8:7:489:GLU:N	8:7:513:LEU:O	2.49	0.45
10:B:954:VAL:HG12	10:B:964:VAL:HG12	1.97	0.45
23:O:121:MET:HE1	23:O:139:TYR:HB2	1.98	0.45
2:1:185:LEU:HD21	2:1:195:PHE:CD2	2.51	0.45
5:4:316:VAL:HG11	7:6:318:THR:OG1	2.17	0.45
11:C:39:ALA:HA	11:C:164:ALA:HB3	1.99	0.45
12:D:32:GLU:O	15:G:5:LYS:NZ	2.49	0.45
1:0:5:ILE:O	1:0:6:ASP:C	2.60	0.45
17:I:70:ARG:HD3	17:I:84:VAL:HG12	1.98	0.45
23:O:129:GLU:OE2	23:O:220:ARG:NE	2.49	0.45
3:2:155:LEU:HD23	3:2:157:LYS:N	2.32	0.45
5:4:218:SER:O	5:4:237:HIS:NE2	2.49	0.45
8:7:217:THR:HG22	8:7:217:THR:O	2.17	0.45
30:X:313:THR:O	30:X:314:ASN:OD1	2.34	0.45
10:B:540:SER:OG	10:B:748:ILE:O	2.33	0.45
3:2:253:MET:SD	3:2:258:LEU:HD22	2.57	0.45
8:7:408:ILE:HG22	8:7:453:VAL:HB	1.99	0.45
24:Q:156:ILE:HD12	24:Q:156:ILE:H	1.82	0.45
3:2:184:ILE:HD12	3:2:184:ILE:H	1.82	0.45
8:7:448:THR:HG22	8:7:449:GLU:N	2.32	0.45
8:7:569:TYR:HA	8:7:580:LEU:HD23	1.99	0.45
29:W:141:ASN:OD1	29:W:144:ARG:N	2.50	0.45
7:6:111:ALA:O	7:6:114:ASN:ND2	2.50	0.45
10:B:983:ARG:NH2	10:B:1028:GLU:OE2	2.44	0.45
13:E:65:THR:HG23	13:E:68:SER:H	1.82	0.45
23:O:204:LEU:HD22	23:O:230:ILE:HD13	1.99	0.45
3:2:455:GLU:O	3:2:495:LYS:N	2.47	0.44
6:5:17:LYS:O	6:5:21:LEU:HD23	2.18	0.44
9:A:845:LEU:HD22	9:A:1374:VAL:HG21	1.99	0.44
9:A:1233:ASP:OD1	9:A:1234:GLU:N	2.50	0.44
10:B:173:MET:O	10:B:176:SER:OG	2.29	0.44
12:D:34:GLN:O	12:D:37:GLN:NE2	2.50	0.44
27:U:52:THR:HG22	27:U:53:THR:N	2.31	0.44
3:2:471:LEU:HD11	3:2:505:ALA:HA	2.00	0.44
7:6:87:VAL:HG11	8:7:149:LEU:HD21	1.99	0.44
9:A:102:VAL:O	9:A:106:VAL:HG22	2.18	0.44
9:A:224:PHE:HE2	9:A:234:MET:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:77:DT:C2'	26:T:78:DA:C8	2.99	0.44
27:U:256:ALA:O	27:U:285:TRP:N	2.45	0.44
27:U:247:LEU:O	27:U:263:LYS:N	2.50	0.44
29:W:95:ILE:HD12	29:W:194:ILE:HD13	1.98	0.44
4:3:28:PHE:C	4:3:29:LEU:HD22	2.41	0.44
26:T:77:DT:C2	26:T:78:DA:C8	3.06	0.44
26:T:78:DA:C8	26:T:79:DT:H71	2.51	0.44
29:W:132:THR:HG22	29:W:133:GLN:N	2.33	0.44
1:0:5:ILE:HG21	1:0:29:LYS:HD3	1.99	0.44
3:2:207:TYR:HD1	3:2:210:MET:HE2	1.82	0.44
5:4:179:LEU:HD23	5:4:213:VAL:HB	1.99	0.44
8:7:476:PHE:HD2	8:7:477:LEU:HD12	1.83	0.44
9:A:898:ARG:O	9:A:1029:ARG:NH2	2.51	0.44
26:T:80:DT:H2"	26:T:81:DA:C8	2.52	0.44
2:1:170:SER:O	2:1:174:LEU:HD23	2.18	0.44
9:A:157:ASP:OD1	9:A:159:THR:OG1	2.32	0.44
12:D:187:THR:HG23	12:D:190:GLU:H	1.82	0.44
17:I:17:ARG:N	17:I:26:LEU:O	2.48	0.44
2:1:194:VAL:O	2:1:198:THR:HG22	2.18	0.44
8:7:745:ILE:HG21	8:7:748:LEU:CD2	2.40	0.44
9:A:1197:LEU:HD22	9:A:1202:MET:HE1	2.00	0.44
2:1:32:THR:HG21	29:W:208:PRO:HB2	2.00	0.44
10:B:1002:THR:HG22	10:B:1072:MET:HG2	1.99	0.44
21:M:263:CYS:SG	21:M:269:ILE:HD12	2.57	0.44
29:W:175:LEU:O	29:W:179:ILE:HG22	2.18	0.44
1:0:385:VAL:HG12	1:0:390:VAL:HG21	1.99	0.44
1:0:603:ARG:NH1	1:0:626:PRO:O	2.51	0.44
3:2:67:ASN:OD1	3:2:68:SER:N	2.51	0.44
9:A:471:ASN:OD1	9:A:472:LEU:N	2.50	0.44
10:B:531:GLN:N	10:B:531:GLN:OE1	2.51	0.44
29:W:182:ILE:O	29:W:186:LEU:HD13	2.18	0.44
3:2:433:LEU:HD11	3:2:438:VAL:CG2	2.47	0.43
10:B:839:MET:HE1	10:B:980:PHE:HB2	1.98	0.43
26:T:84:DT:H2'	26:T:85:DA:C8	2.53	0.43
15:G:138:THR:HG22	15:G:139:ILE:N	2.33	0.43
15:G:155:SER:O	15:G:155:SER:OG	2.32	0.43
9:A:216:VAL:O	9:A:220:THR:HG23	2.18	0.43
13:E:24:LYS:NZ	13:E:32:GLN:OE1	2.51	0.43
1:0:390:VAL:O	1:0:391:THR:C	2.61	0.43
3:2:433:LEU:HD11	3:2:438:VAL:HG23	2.00	0.43
7:6:128:LEU:N	7:6:170:GLY:O	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:311:ASN:OD1	7:6:312:LYS:N	2.51	0.43
8:7:105:VAL:HG23	8:7:105:VAL:O	2.19	0.43
27:U:229:TYR:C	27:U:230:LEU:HD12	2.42	0.43
29:W:36:SER:O	29:W:37:VAL:C	2.60	0.43
29:W:183:ILE:H	29:W:183:ILE:HD12	1.84	0.43
1:0:24:TYR:CE2	1:0:28:ILE:HD11	2.54	0.43
7:6:181:LEU:HD13	7:6:220:LEU:HD11	2.00	0.43
9:A:1074:GLU:HB3	9:A:1075:PRO:HD3	2.00	0.43
11:C:112:ASN:ND2	18:J:19:GLU:OE2	2.50	0.43
25:R:300:LEU:HD22	30:X:130:TRP:NE1	2.34	0.43
9:A:549:MET:CE	9:A:577:ILE:HG21	2.39	0.43
29:W:197:ASN:OD1	29:W:198:THR:N	2.51	0.43
21:M:79:VAL:HG13	21:M:79:VAL:O	2.18	0.43
25:R:106:LEU:HD12	25:R:106:LEU:C	2.44	0.43
3:2:48:MET:O	3:2:51:VAL:HG12	2.18	0.43
18:J:17:LYS:NZ	18:J:39:LEU:O	2.48	0.43
25:R:313:TRP:CD1	25:R:318:LEU:HD12	2.51	0.43
10:B:995:ARG:NH1	10:B:997:GLU:OE2	2.52	0.43
29:W:149:CYS:SG	29:W:150:SER:N	2.92	0.43
29:W:21:TYR:OH	29:W:64:ASP:OD2	2.34	0.43
6:5:55:ASN:O	6:5:59:SER:N	2.50	0.42
8:7:338:LEU:HD23	8:7:338:LEU:H	1.84	0.42
8:7:742:MET:O	8:7:745:ILE:HG22	2.19	0.42
10:B:684:LEU:HD23	10:B:689:LEU:HD12	1.99	0.42
1:0:643:ARG:NH1	1:0:650:GLU:OE2	2.52	0.42
2:1:328:MET:HE3	2:1:387:MET:HE1	2.01	0.42
8:7:698:ASP:OD1	8:7:698:ASP:N	2.51	0.42
11:C:29:MET:HA	19:K:45:LEU:HD13	2.00	0.42
26:T:80:DT:H2"	26:T:81:DA:H8	1.83	0.42
8:7:510:LYS:NZ	8:7:530:LEU:O	2.45	0.42
9:A:5:GLN:O	10:B:1159:ARG:NH2	2.52	0.42
10:B:732:SER:O	10:B:733:HIS:HB3	2.19	0.42
23:O:144:GLN:NE2	23:O:150:ALA:O	2.46	0.42
24:Q:327:ARG:O	24:Q:328:LYS:HG2	2.19	0.42
1:0:628:GLN:OE1	1:0:635:LEU:HD13	2.19	0.42
8:7:672:GLN:OE1	8:7:722:ARG:NH2	2.52	0.42
9:A:1038:THR:HG22	9:A:1039:LYS:N	2.34	0.42
10:B:806:THR:HG22	10:B:808:ALA:H	1.85	0.42
11:C:55:THR:O	11:C:55:THR:CG2	2.67	0.42
13:E:190:LEU:HD11	13:E:196:VAL:HG11	2.02	0.42
7:6:287:PHE:HE1	7:6:308:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:919:ILE:HG12	9:A:983:ILE:HD12	2.00	0.42
10:B:63:ILE:HD11	10:B:95:ILE:HD12	2.01	0.42
8:7:690:ILE:HD11	8:7:705:PHE:HB2	2.01	0.42
21:M:202:GLU:O	21:M:206:THR:OG1	2.33	0.42
24:Q:369:ASN:ND2	24:Q:373:TYR:OH	2.52	0.42
28:V:87:VAL:O	28:V:103:GLN:N	2.53	0.42
2:1:176:THR:O	2:1:176:THR:HG22	2.20	0.42
2:1:633:TYR:HD1	5:4:326:VAL:HG21	1.85	0.42
8:7:498:PHE:O	8:7:501:VAL:HG22	2.19	0.42
10:B:344:LYS:HG3	10:B:345:LYS:H	1.84	0.42
27:U:37:ASP:O	27:U:41:ILE:HG22	2.20	0.42
2:1:181:GLN:HG2	2:1:217:LEU:HD21	2.02	0.42
7:6:102:ILE:HG21	7:6:423:THR:CG2	2.50	0.42
9:A:493:GLN:N	10:B:1149:GLU:OE2	2.45	0.42
10:B:487:THR:HG23	10:B:490:SER:H	1.85	0.42
13:E:124:VAL:HB	13:E:125:PRO:HD3	2.01	0.42
23:O:107:ARG:O	23:O:110:LYS:N	2.53	0.42
29:W:198:THR:HG22	29:W:199:PHE:N	2.35	0.42
10:B:18:PHE:CG	24:Q:34:MET:HE1	2.55	0.41
12:D:26:THR:HG22	12:D:26:THR:O	2.19	0.41
23:O:121:MET:HE1	23:O:139:TYR:CG	2.54	0.41
3:2:357:ILE:HG12	3:2:374:VAL:HG21	2.02	0.41
9:A:658:LEU:HD13	10:B:830:TYR:O	2.20	0.41
7:6:291:LEU:H	7:6:291:LEU:HD23	1.84	0.41
8:7:205:VAL:HG13	8:7:205:VAL:O	2.19	0.41
9:A:1318:THR:O	9:A:1318:THR:HG22	2.20	0.41
21:M:248:LEU:HD11	21:M:286:ILE:HD11	2.03	0.41
9:A:1331:SER:OG	9:A:1334:ASP:OD2	2.33	0.41
23:O:226:ALA:O	23:O:230:ILE:HG22	2.20	0.41
30:X:157:ASP:OD1	30:X:158:LYS:N	2.54	0.41
7:6:280:THR:O	7:6:280:THR:HG22	2.21	0.41
23:O:108:GLU:HG2	23:O:109:PRO:HD3	2.02	0.41
27:U:17:VAL:HG11	27:U:42:TRP:HZ3	1.86	0.41
3:2:368:ALA:HB3	3:2:375:LEU:HD21	2.03	0.41
9:A:1038:THR:HG22	9:A:1039:LYS:H	1.86	0.41
15:G:46:LEU:HD21	15:G:105:PRO:HG3	2.03	0.41
15:G:119:LEU:HD23	15:G:132:SER:HB2	2.03	0.41
22:N:20:DT:C2	22:N:21:DG:N7	2.89	0.41
23:O:96:PRO:CB	25:R:292:ILE:HD13	2.50	0.41
28:V:80:VAL:HG12	28:V:83:CYS:HB3	2.02	0.41
1:0:267:LEU:HD12	1:0:399:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:633:TYR:CD1	5:4:326:VAL:HG21	2.55	0.41
8:7:474:MET:HE1	8:7:504:THR:HG21	2.02	0.41
9:A:341:MET:HE3	10:B:1135:ARG:CZ	2.51	0.41
17:I:82:GLU:OE2	17:I:105:SER:OG	2.36	0.41
29:W:32:ILE:O	29:W:32:ILE:HG22	2.19	0.41
9:A:464:PRO:O	9:A:465:TYR:HB2	2.20	0.41
1:0:277:VAL:HG23	1:0:278:ASP:N	2.36	0.41
1:0:309:THR:HG23	1:0:309:THR:O	2.20	0.41
1:0:487:LEU:HD11	1:0:490:LYS:HA	2.01	0.41
1:0:620:VAL:HG23	1:0:669:VAL:HG11	2.02	0.41
4:3:16:CYS:SG	4:3:18:THR:OG1	2.70	0.41
8:7:655:SER:OG	8:7:656:LYS:N	2.54	0.41
8:7:662:ILE:O	8:7:689:ARG:NH1	2.53	0.41
9:A:335:ARG:HH22	10:B:1114:LEU:HD21	1.86	0.41
15:G:138:THR:HG22	15:G:139:ILE:H	1.86	0.41
21:M:233:ALA:O	21:M:234:GLN:C	2.64	0.41
26:T:81:DA:H2'	26:T:82:DT:C6	2.56	0.41
2:1:195:PHE:CE1	2:1:199:VAL:HG21	2.55	0.41
5:4:32:ILE:HD11	5:4:132:LEU:HD23	2.02	0.41
7:6:266:LEU:HA	7:6:291:LEU:CD2	2.51	0.41
9:A:20:GLY:C	10:B:1213:THR:HG22	2.46	0.41
11:C:56:THR:HG22	11:C:147:LEU:HD21	2.02	0.41
30:X:186:VAL:O	30:X:187:HIS:ND1	2.54	0.41
9:A:30:ILE:HG23	10:B:1170:THR:HG21	2.03	0.40
9:A:1243:VAL:O	9:A:1243:VAL:HG13	2.21	0.40
10:B:436:VAL:HG22	25:R:278:LEU:HD11	2.03	0.40
11:C:44:LEU:HB2	11:C:77:ILE:HD13	2.02	0.40
21:M:225:ILE:HG13	21:M:226:ASP:N	2.36	0.40
25:R:296:LYS:HA	25:R:299:ILE:HG22	2.03	0.40
1:0:487:LEU:H	1:0:487:LEU:HD23	1.87	0.40
1:0:497:ILE:HG21	1:0:525:MET:CE	2.51	0.40
9:A:559:VAL:HG11	16:H:75:ALA:HB1	2.04	0.40
9:A:830:LYS:NZ	9:A:1077:THR:O	2.55	0.40
8:7:236:THR:OG1	8:7:314:HIS:NE2	2.50	0.40
8:7:445:MET:HE1	8:7:453:VAL:HG13	2.02	0.40
8:7:490:VAL:HG21	8:7:531:ILE:CD1	2.52	0.40
9:A:867:ILE:HD12	9:A:1000:LEU:HD11	2.03	0.40
10:B:698:GLU:OE1	10:B:701:ILE:HD11	2.21	0.40
23:O:198:VAL:HG13	23:O:199:LYS:N	2.37	0.40
6:5:13:ASP:HB2	6:5:14:PRO:HD2	2.04	0.40
8:7:383:ILE:HD11	8:7:527:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:90:THR:O	15:G:102:GLN:N	2.51	0.40
30:X:151:LEU:HD23	30:X:151:LEU:H	1.87	0.40
2:1:251:LEU:HD11	2:1:288:PHE:CE2	2.57	0.40
3:2:25:LEU:O	3:2:31:THR:HG21	2.22	0.40
10:B:230:ALA:O	10:B:232:SER:N	2.54	0.40
10:B:512:ARG:NH1	10:B:533:CYS:O	2.54	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	0	750/778 (96%)	736 (98%)	14 (2%)	0	100	100
2	1	508/645 (79%)	500 (98%)	8 (2%)	0	100	100
3	2	435/517 (84%)	430 (99%)	5 (1%)	0	100	100
4	3	129/324 (40%)	127 (98%)	2 (2%)	0	100	100
5	4	287/341 (84%)	286 (100%)	1 (0%)	0	100	100
6	5	63/76 (83%)	62 (98%)	1 (2%)	0	100	100
7	6	368/464 (79%)	363 (99%)	5 (1%)	0	100	100
8	7	609/843 (72%)	596 (98%)	13 (2%)	0	100	100
9	A	1422/1733 (82%)	1394 (98%)	28 (2%)	0	100	100
10	B	1168/1224 (95%)	1130 (97%)	38 (3%)	0	100	100
11	C	264/347 (76%)	260 (98%)	4 (2%)	0	100	100
12	D	163/221 (74%)	161 (99%)	2 (1%)	0	100	100
13	E	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
14	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
15	G	169/177 (96%)	167 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	H	136/146 (93%)	135 (99%)	1 (1%)	0	100	100
17	I	114/122 (93%)	108 (95%)	6 (5%)	0	100	100
18	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
19	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
20	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
21	M	302/352 (86%)	292 (97%)	10 (3%)	0	100	100
23	O	179/247 (72%)	175 (98%)	4 (2%)	0	100	100
24	Q	212/738 (29%)	200 (94%)	12 (6%)	0	100	100
25	R	264/400 (66%)	252 (96%)	11 (4%)	1 (0%)	30	62
27	U	101/286 (35%)	97 (96%)	4 (4%)	0	100	100
28	V	100/129 (78%)	97 (97%)	3 (3%)	0	100	100
29	W	304/492 (62%)	294 (97%)	10 (3%)	0	100	100
30	X	203/328 (62%)	188 (93%)	15 (7%)	0	100	100
All	All	8769/11560 (76%)	8561 (98%)	207 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	295	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	0	684/707 (97%)	684 (100%)	0	100	100
2	1	483/590 (82%)	483 (100%)	0	100	100
3	2	408/470 (87%)	408 (100%)	0	100	100
4	3	125/305 (41%)	125 (100%)	0	100	100
5	4	260/302 (86%)	260 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	59/68 (87%)	59 (100%)	0	100	100
7	6	338/419 (81%)	338 (100%)	0	100	100
8	7	547/737 (74%)	547 (100%)	0	100	100
9	A	1251/1520 (82%)	1251 (100%)	0	100	100
10	B	1024/1061 (96%)	1024 (100%)	0	100	100
11	C	234/299 (78%)	234 (100%)	0	100	100
12	D	149/200 (74%)	149 (100%)	0	100	100
13	E	196/197 (100%)	196 (100%)	0	100	100
14	F	76/137 (56%)	76 (100%)	0	100	100
15	G	152/158 (96%)	152 (100%)	0	100	100
16	H	123/128 (96%)	123 (100%)	0	100	100
17	I	110/116 (95%)	110 (100%)	0	100	100
18	J	64/65 (98%)	64 (100%)	0	100	100
19	K	99/102 (97%)	99 (100%)	0	100	100
20	L	40/57 (70%)	40 (100%)	0	100	100
21	M	265/306 (87%)	265 (100%)	0	100	100
23	O	153/212 (72%)	153 (100%)	0	100	100
24	Q	202/642 (32%)	202 (100%)	0	100	100
25	R	252/363 (69%)	252 (100%)	0	100	100
27	U	99/260 (38%)	99 (100%)	0	100	100
28	V	94/115 (82%)	94 (100%)	0	100	100
29	W	281/436 (64%)	281 (100%)	0	100	100
30	X	186/295 (63%)	186 (100%)	0	100	100
All	All	7954/10267 (78%)	7954 (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 (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	62	HIS
1	0	88	ASN
1	0	242	ASN
1	0	748	GLN

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Mol	Chain	Res	Type
2	1	49	GLN
5	4	62	ASN
6	5	39	HIS
7	6	227	HIS
7	6	351	ASN
8	7	171	HIS
8	7	230	ASN
8	7	641	GLN
8	7	650	ASN
8	7	738	HIS
9	A	5	GLN
9	A	169	ASN
9	A	213	HIS
9	A	225	ASN
9	A	313	GLN
9	A	339	ASN
9	A	358	ASN
9	A	745	GLN
9	A	935	GLN
9	A	953	ASN
9	A	972	HIS
9	A	1008	GLN
9	A	1033	GLN
10	B	767	ASN
10	B	770	GLN
10	B	835	GLN
10	B	881	ASN
10	B	1097	HIS
10	B	1195	HIS
10	B	1205	GLN
11	C	7	GLN
11	C	73	GLN
11	C	131	HIS
12	D	31	GLN
12	D	132	GLN
12	D	150	ASN
12	D	165	GLN
13	E	63	ASN
13	E	136	ASN
13	E	174	GLN
17	I	22	ASN
21	M	197	HIS

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Mol	Chain	Res	Type
21	M	319	HIS
23	O	68	GLN
24	Q	150	GLN
25	R	67	GLN
25	R	328	HIS
27	U	280	GLN
29	W	72	GLN
29	W	261	HIS
30	X	270	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 22 ligands modelled in this entry, 19 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
35	ADP	7	903	33,34	27,29,29	0.43	0	42,45,45	0.57	0
31	SF4	0	801	1	0,12,12	-	-	-		
33	BEF	7	901	35	0,3,3	-	-	-		

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
35	ADP	7	903	33,34	-	3/16/32/32	0/3/3/3
31	SF4	0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	7	903	ADP	PA-O3A-PB-O3B
35	7	903	ADP	PA-O3A-PB-O1B
35	7	903	ADP	PA-O3A-PB-O2B

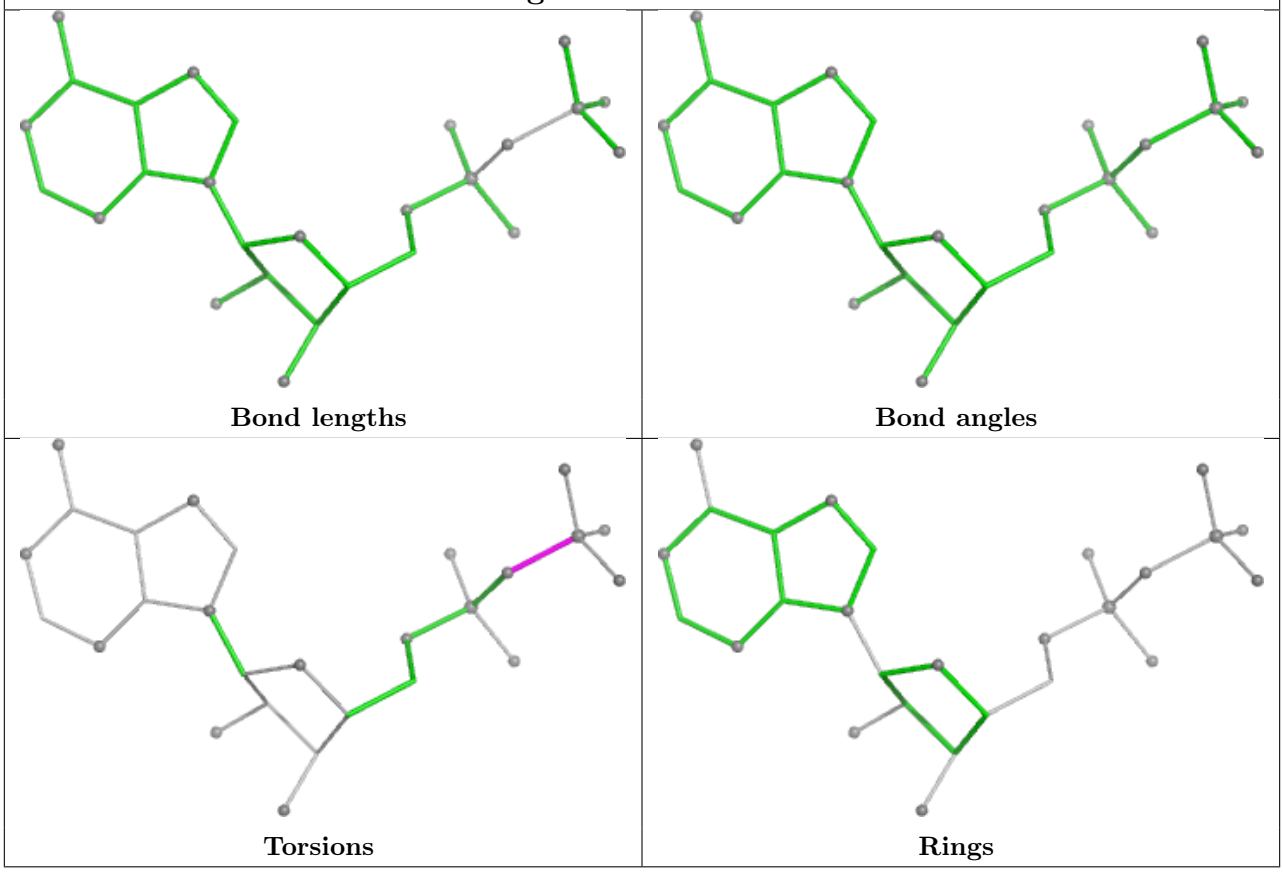
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	7	903	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP 7 903



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.

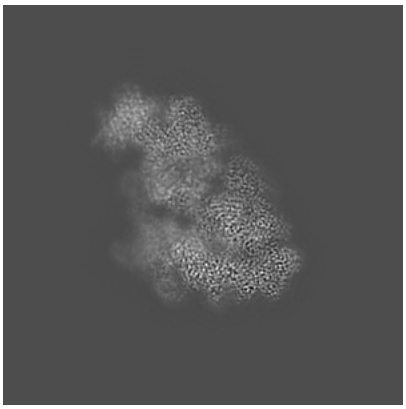
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12745. These allow visual inspection of the internal detail of the map and identification of artifacts.

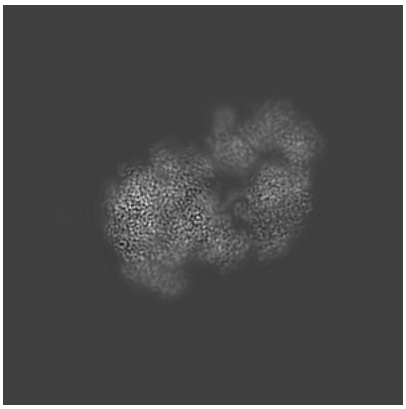
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

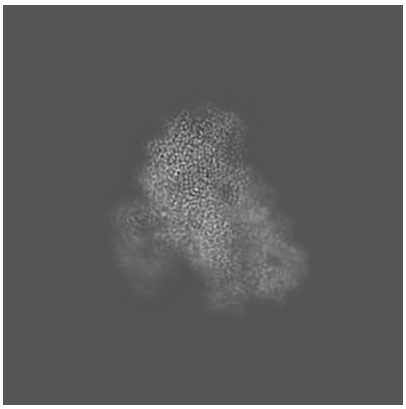
6.1.1 Primary map



X

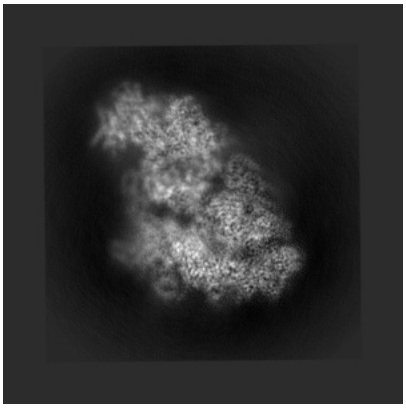


Y

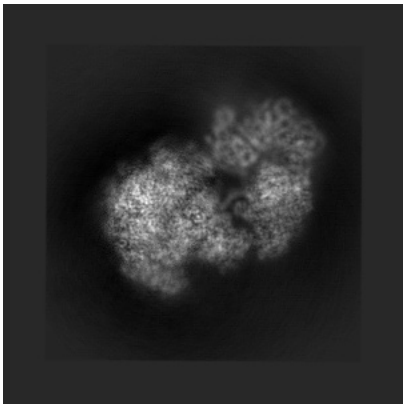


Z

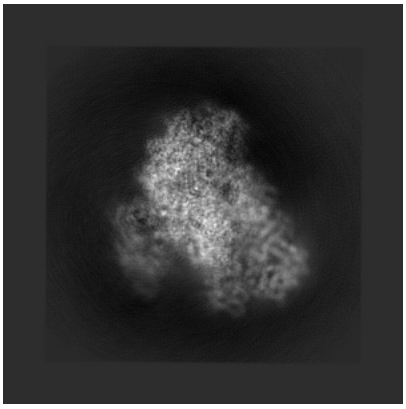
6.1.2 Raw map



X



Y

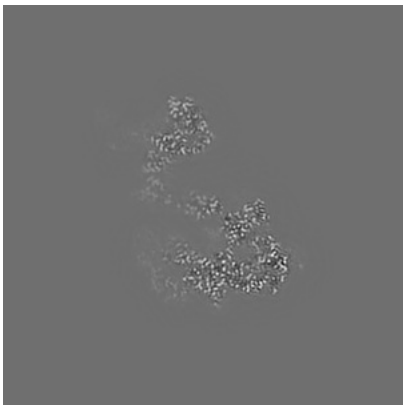


Z

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

6.2 Central slices (i)

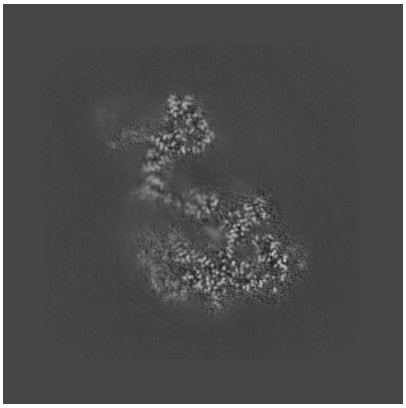
6.2.1 Primary map

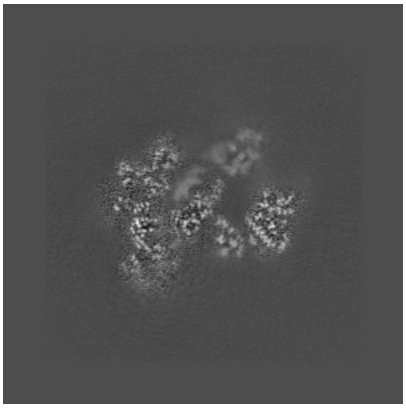

X Index: 190

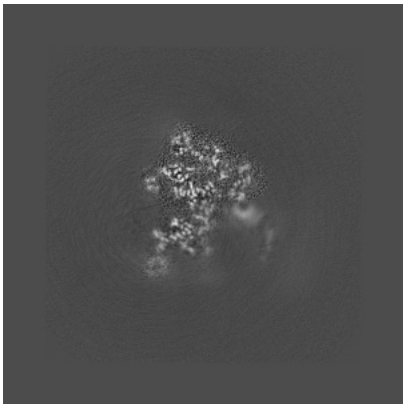
Y Index: 190

Z Index: 190

6.2.2 Raw map


X Index: 190

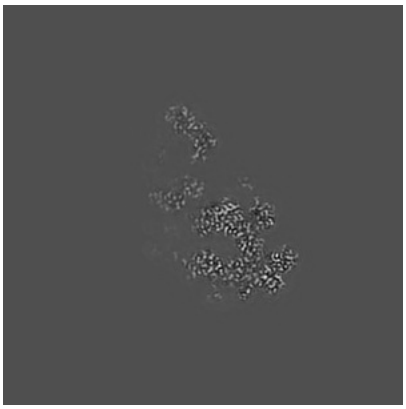

Y Index: 190

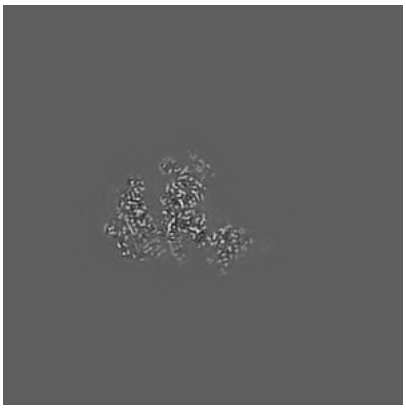

Z Index: 190

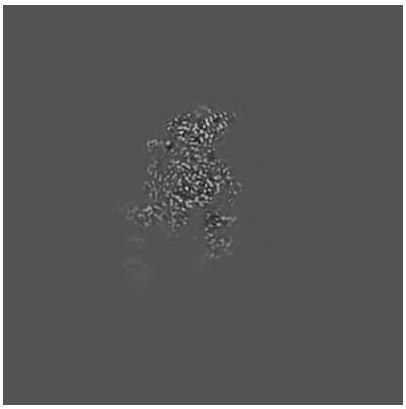
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

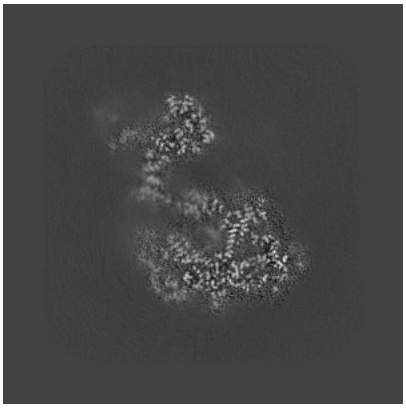
6.3.1 Primary map

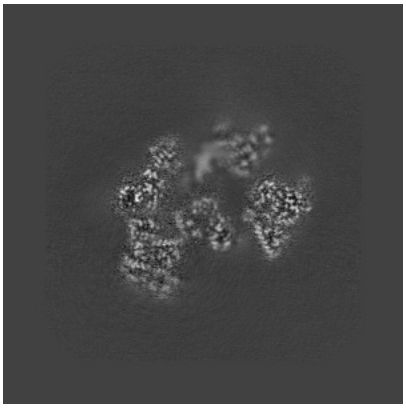

X Index: 174

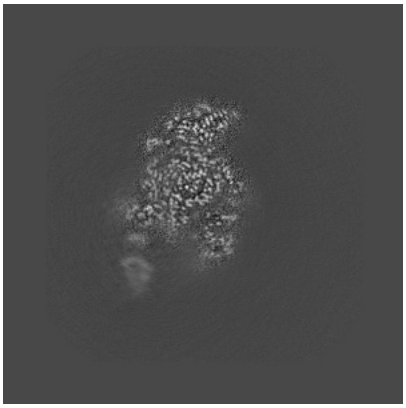

Y Index: 223


Z Index: 132

6.3.2 Raw map


X Index: 191

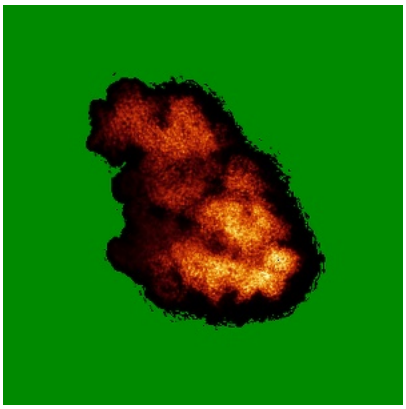

Y Index: 180

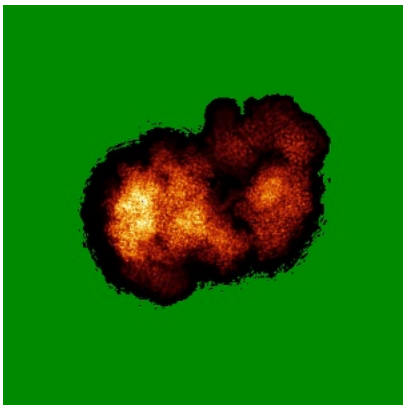

Z Index: 132

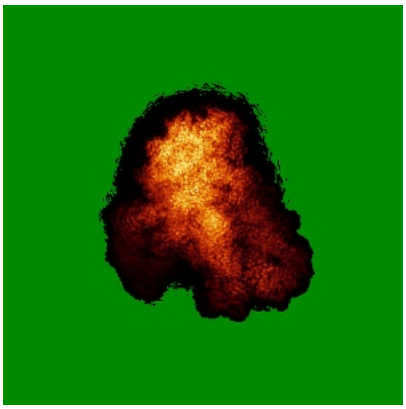
The images above show the largest variance slices of the map in three orthogonal directions.

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

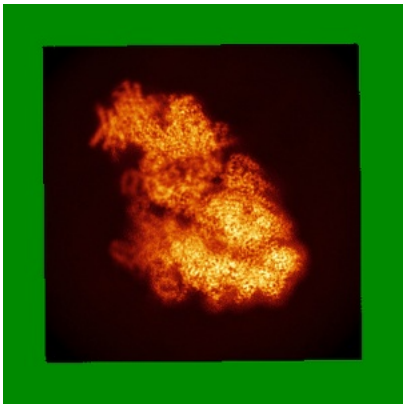
6.4.1 Primary map

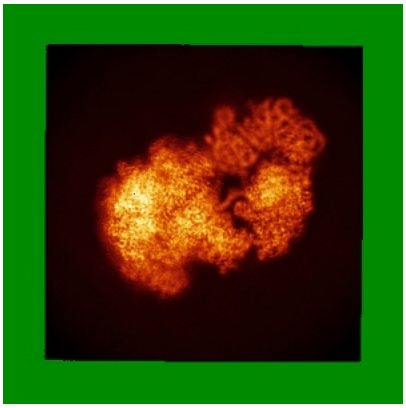

X

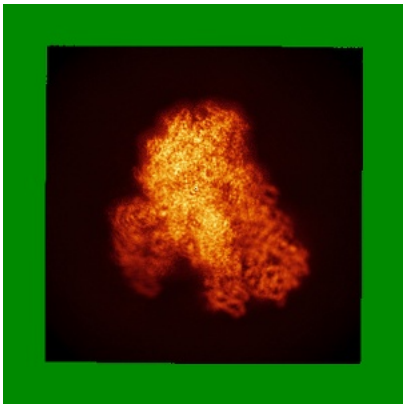

Y


Z

6.4.2 Raw map


X

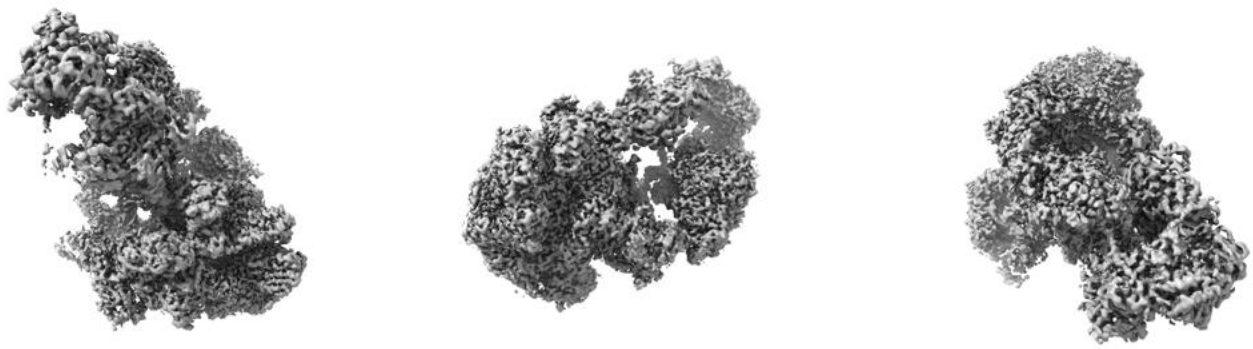

Y


Z

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

6.5 Orthogonal surface views (i)

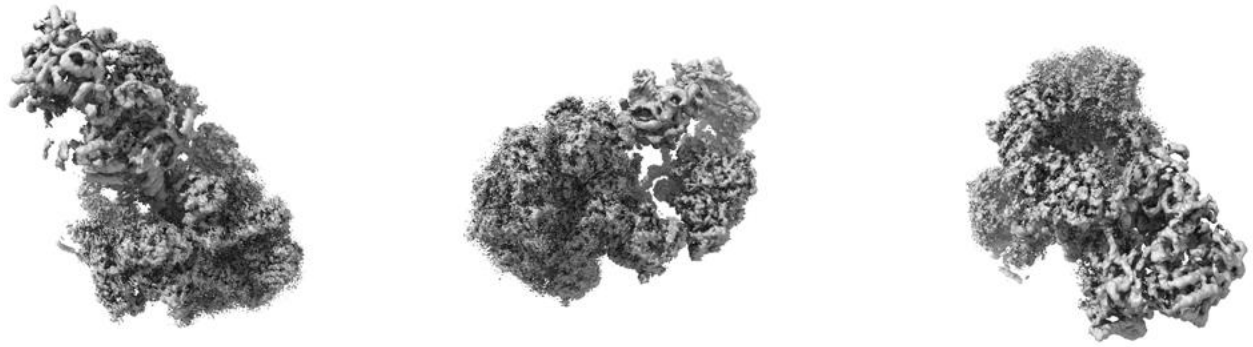
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

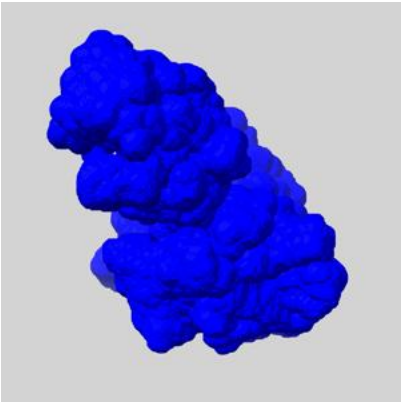
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

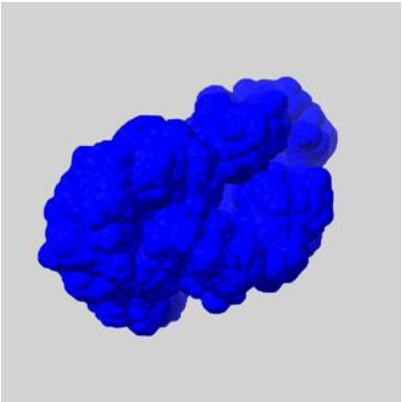
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

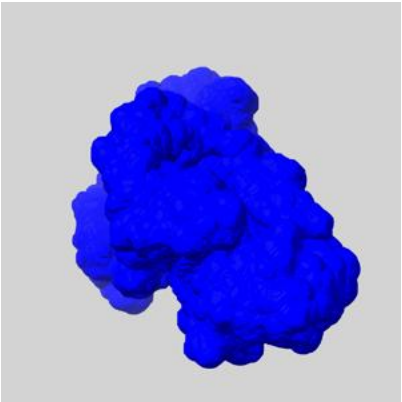
6.6.1 emd_12745_msk_1.map (i)



X



Y

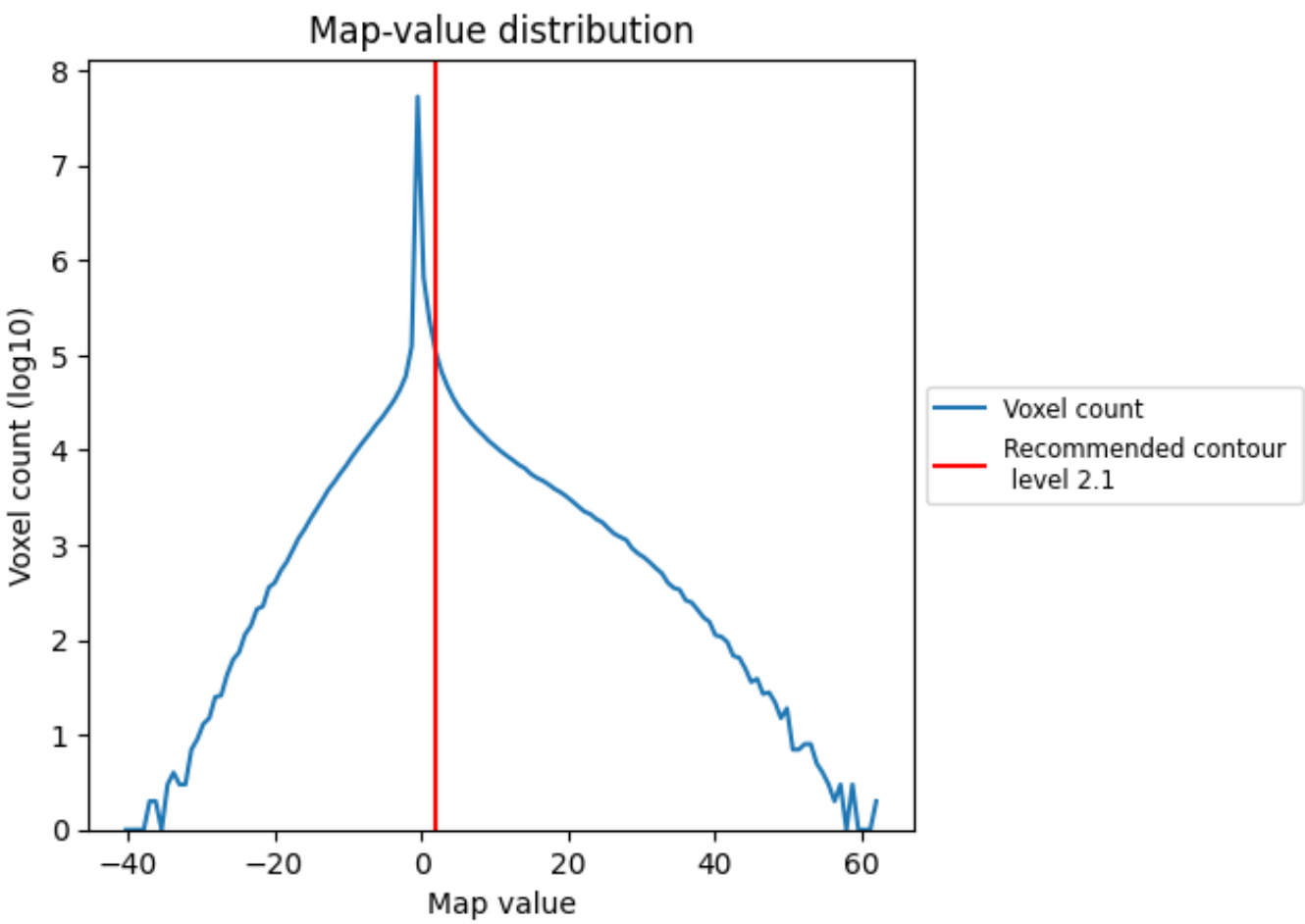


Z

7 Map analysis (i)

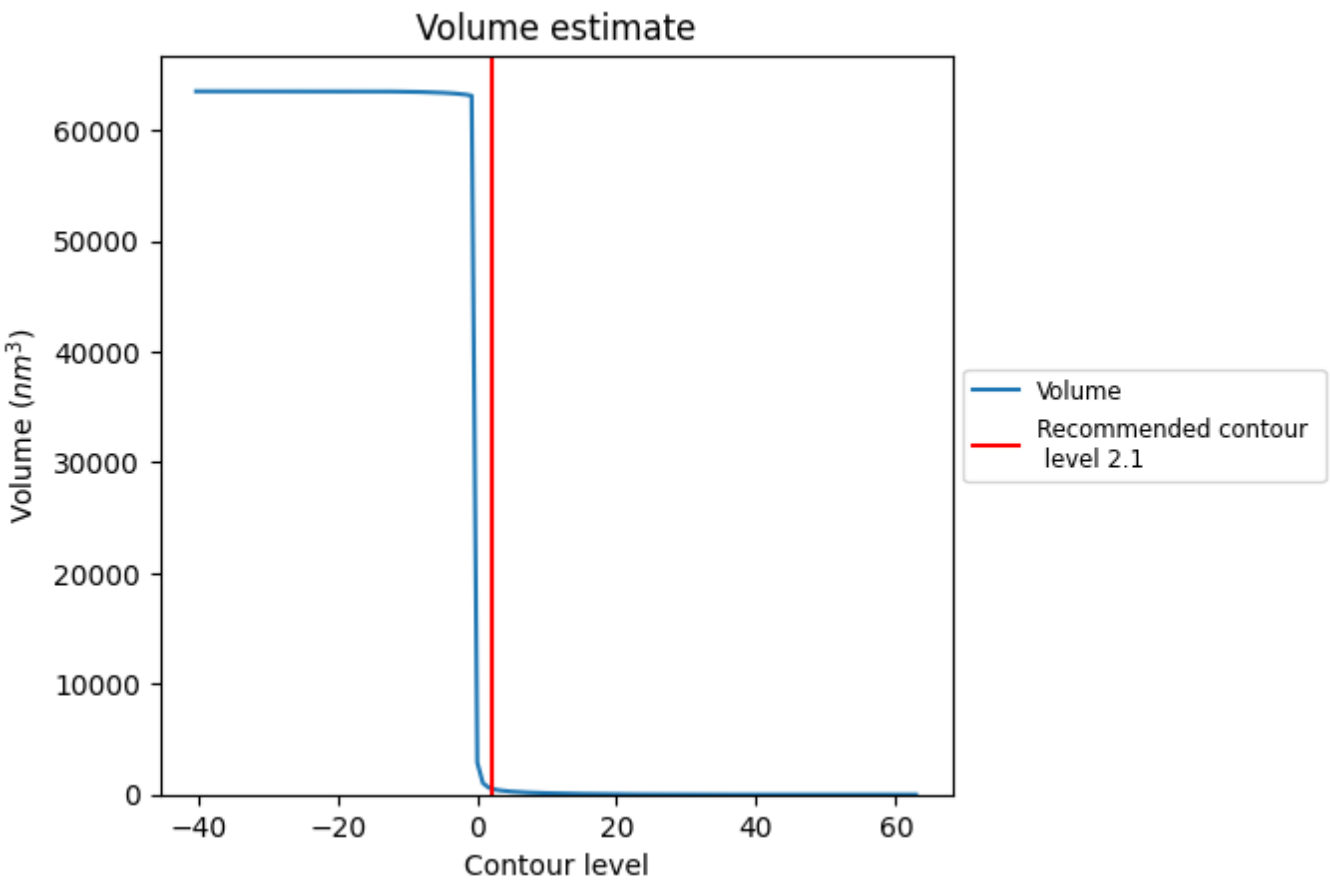
This section contains the results of statistical analysis of the map.

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.

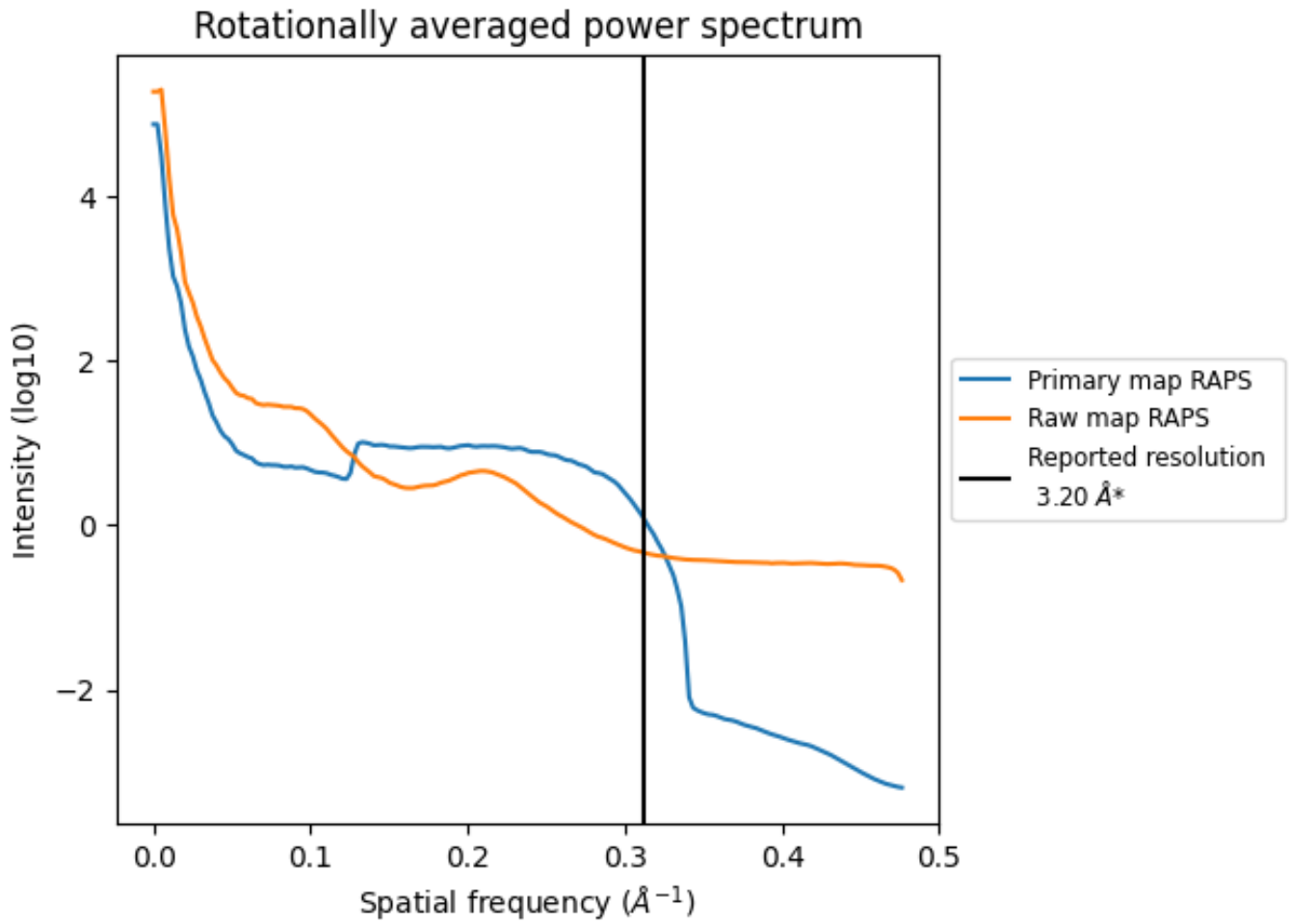
7.2 Volume estimate (i)



The volume at the recommended contour level is 545 nm^3; this corresponds to an approximate mass of 492 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)

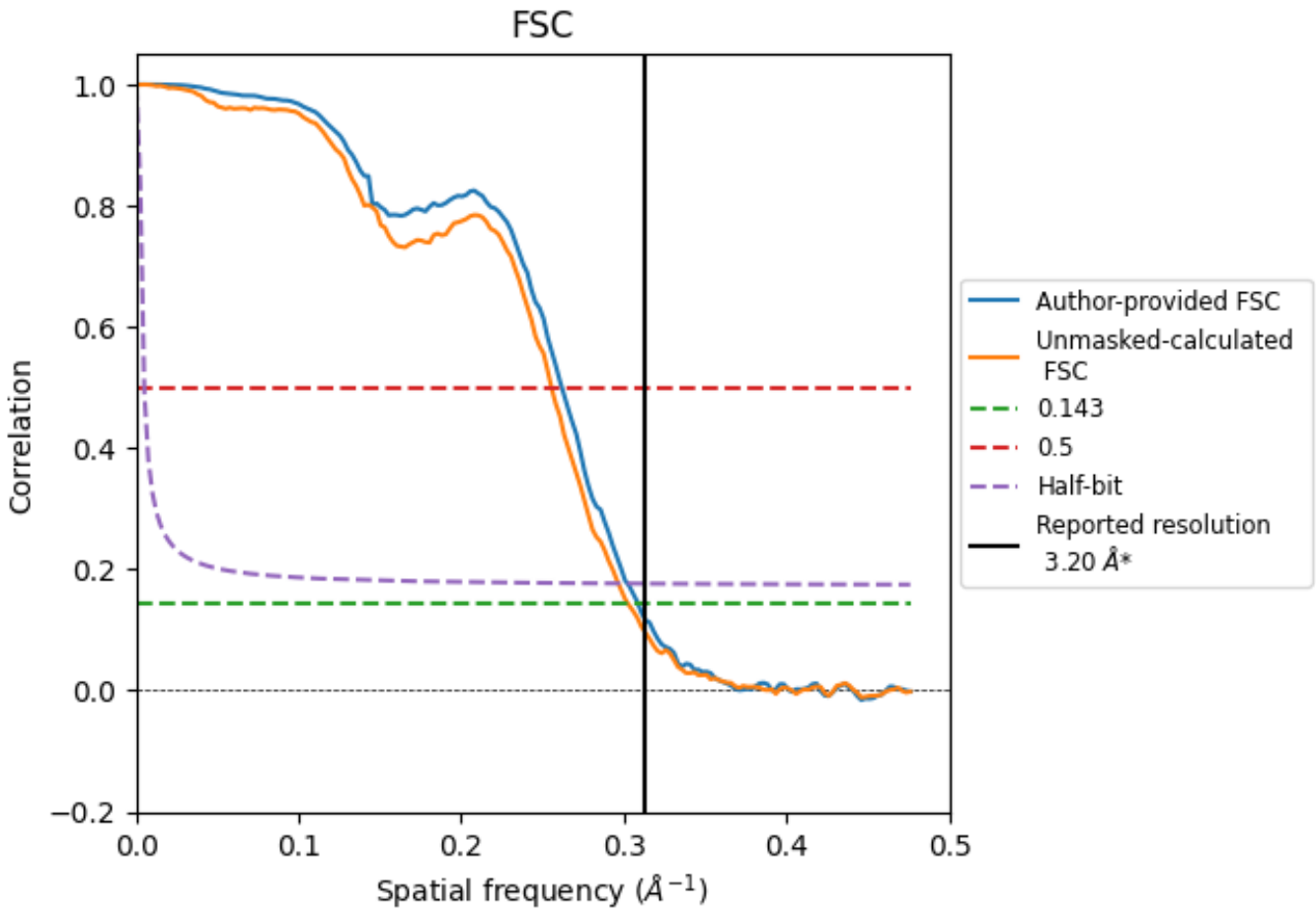


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

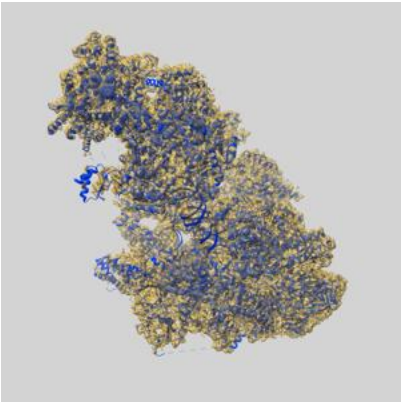
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.82	3.31
Unmasked-calculated*	3.31	3.91	3.37

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

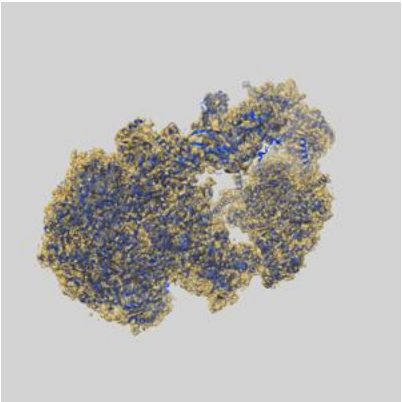
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12745 and PDB model 7O75. Per-residue inclusion information can be found in section 3 on page 16.

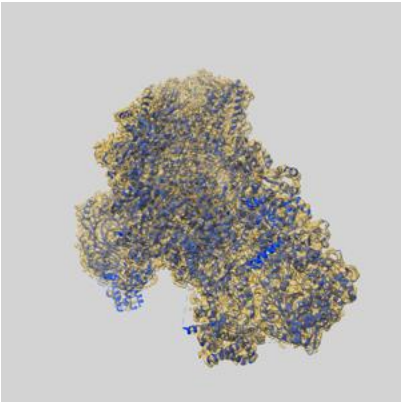
9.1 Map-model overlay (i)



X



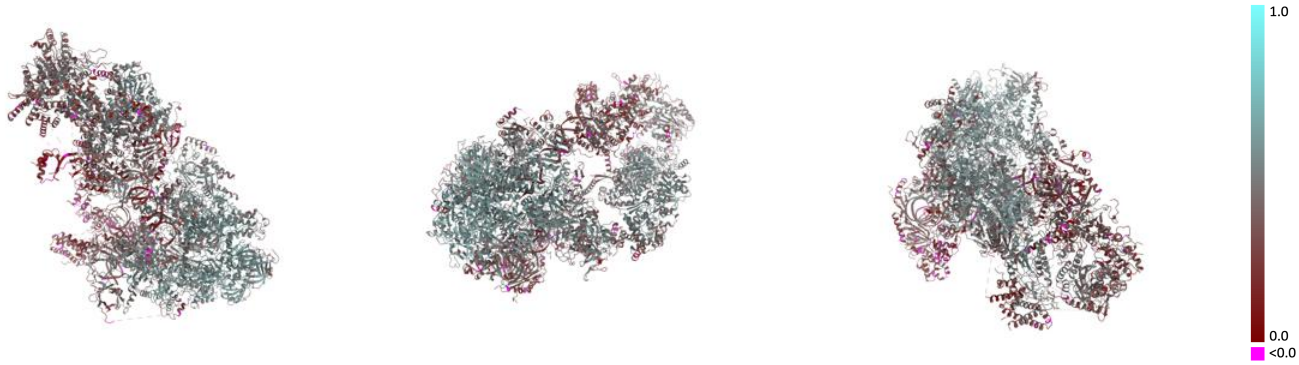
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

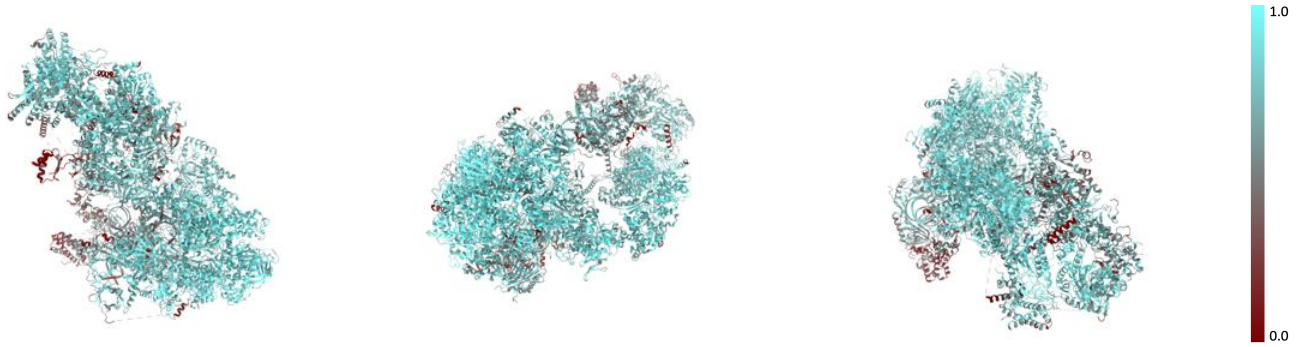
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

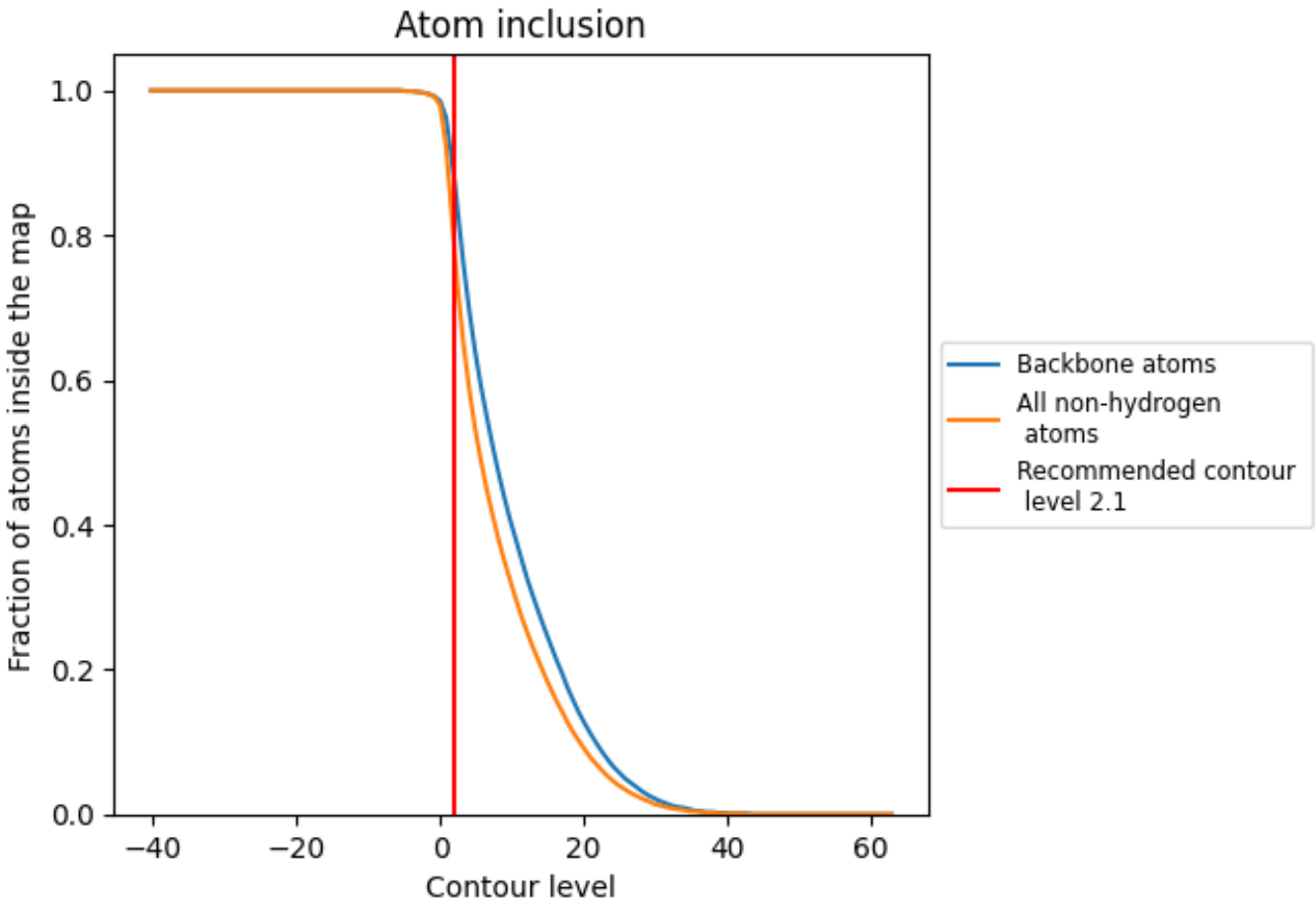
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.1).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 77% 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 (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.4280
0	0.8710	0.5050
1	0.7400	0.3820
2	0.6100	0.3120
3	0.7820	0.4030
4	0.8160	0.4210
5	0.4520	0.2380
6	0.7760	0.4360
7	0.6530	0.3180
A	0.8760	0.5150
B	0.8750	0.5180
C	0.9200	0.5550
D	0.7650	0.4110
E	0.8220	0.4570
F	0.8980	0.5390
G	0.8710	0.5070
H	0.8590	0.5030
I	0.8560	0.4770
J	0.9090	0.5550
K	0.9370	0.5680
L	0.8530	0.4970
M	0.7200	0.4170
N	0.6320	0.2100
O	0.6580	0.2930
Q	0.6290	0.3560
R	0.5650	0.2950
T	0.6520	0.2490
U	0.3140	0.1690
V	0.3520	0.2220
W	0.7210	0.3940
X	0.5480	0.3040