



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:38 AM UTC

PDB ID : 8WAU / pdb_00008wau
EMDB ID : EMD-37405
Title : De novo transcribing complex 11 (TC11), the early elongation complex with Pol II positioned 11nt downstream of TSS
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-08
Resolution : 2.78 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

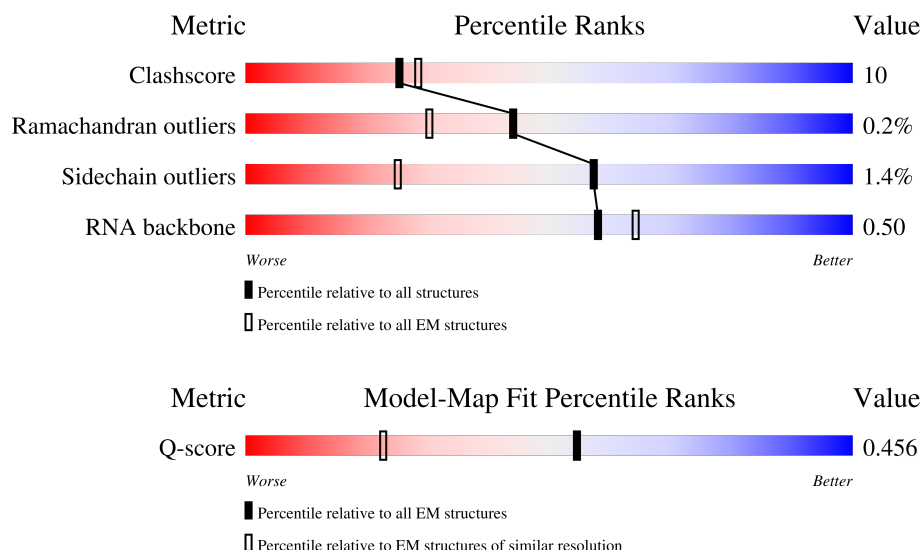
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10754 (2.28 - 3.28)

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

Mol	Chain	Length	Quality of chain
1	N	8	
2	S	517	
3	T	249	

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Mol	Chain	Length	Quality of chain
4	X	99	
5	Y	99	
6	Z	11	
7	o	1970	
8	p	1174	
9	q	275	
10	r	142	
11	s	210	
12	t	127	
13	u	172	
14	v	150	
15	w	125	
16	x	67	
17	y	117	
18	z	58	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 35728 atoms, of which 30 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	8	Total	C	H	N	O	S	
			94	39	30	10	14	1	
								0	0

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	103	Total	C	N	O	S		
			789	492	142	154	1		
								0	0

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	43	Total	C	N	O	P		
			878	418	155	262	43		
								0	0

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	54	Total	C	N	O	P		
			1112	527	211	320	54		
								0	0

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	11	Total	C	N	O	P		
			241	105	40	83	13		
								0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	1146	Total	C	N	O	S	0	0
			9149	5782	1610	1693	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

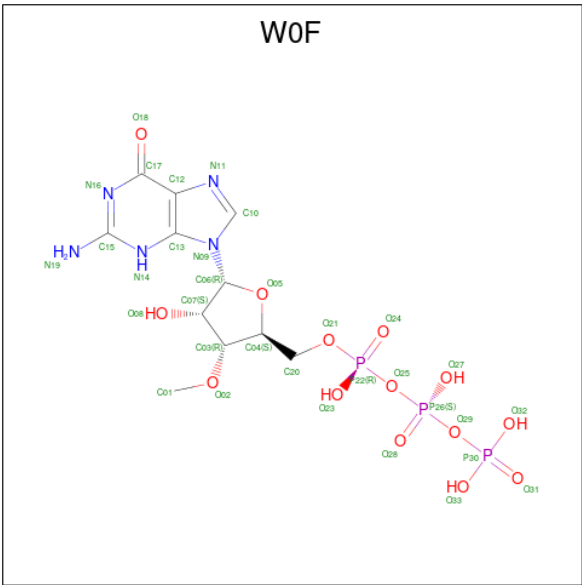
- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	y	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 18 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 19 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	Z	1	Total	C	N	O	P	0
			33	11	5	14	3	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	o	2	Total	Zn	0
			2	2	
20	p	1	Total	Zn	0
			1	1	
20	q	1	Total	Zn	0
			1	1	
20	w	2	Total	Zn	0
			2	2	
20	x	1	Total	Zn	0
			1	1	
20	z	1	Total	Zn	0
			1	1	

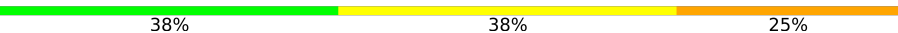
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

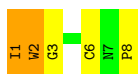
Mol	Chain	Residues	Atoms		AltConf
21	o	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

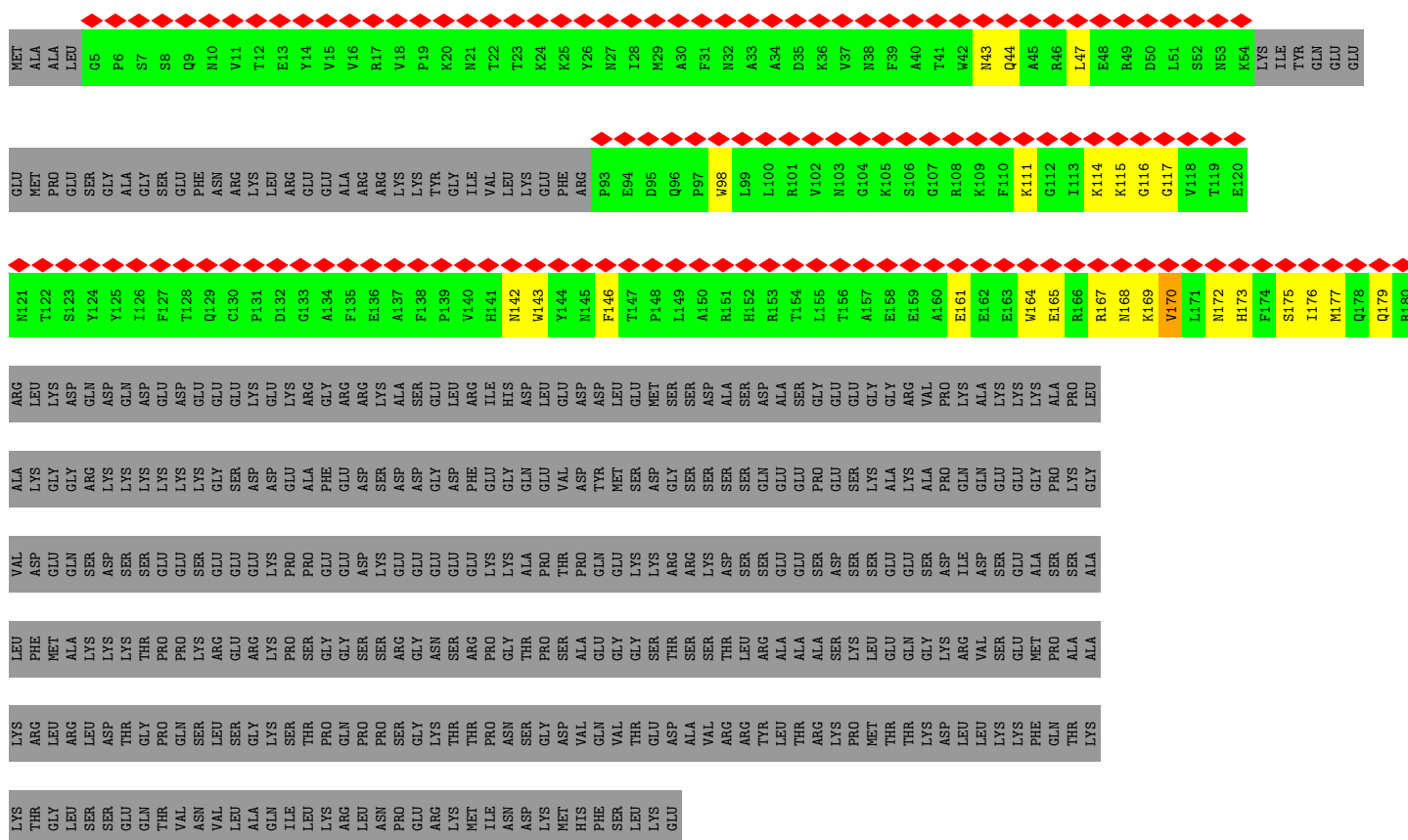
• Molecule 1: Alpha-amanitin

Chain N: 



• Molecule 2: General transcription factor IIF subunit 1

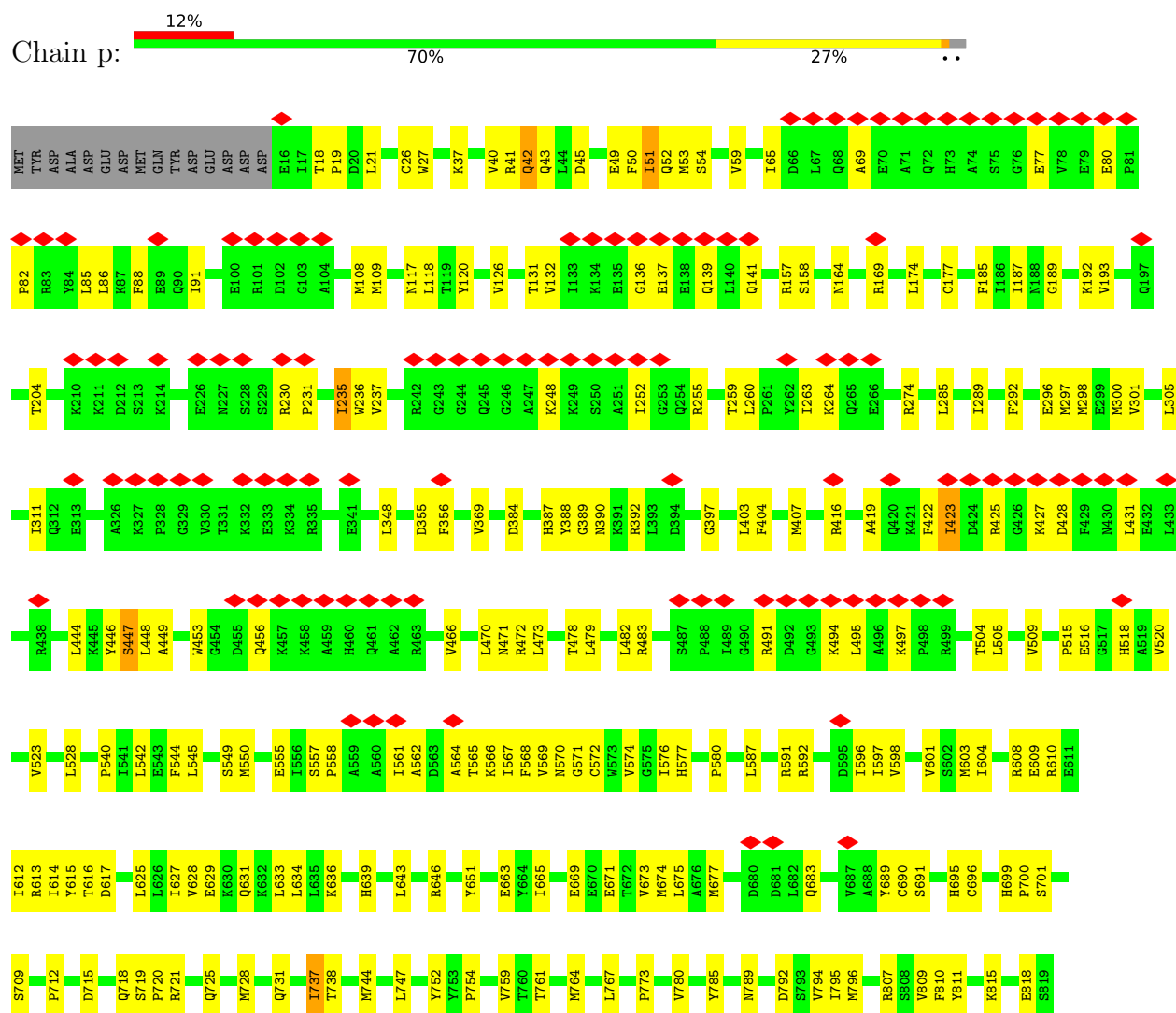
Chain S: 

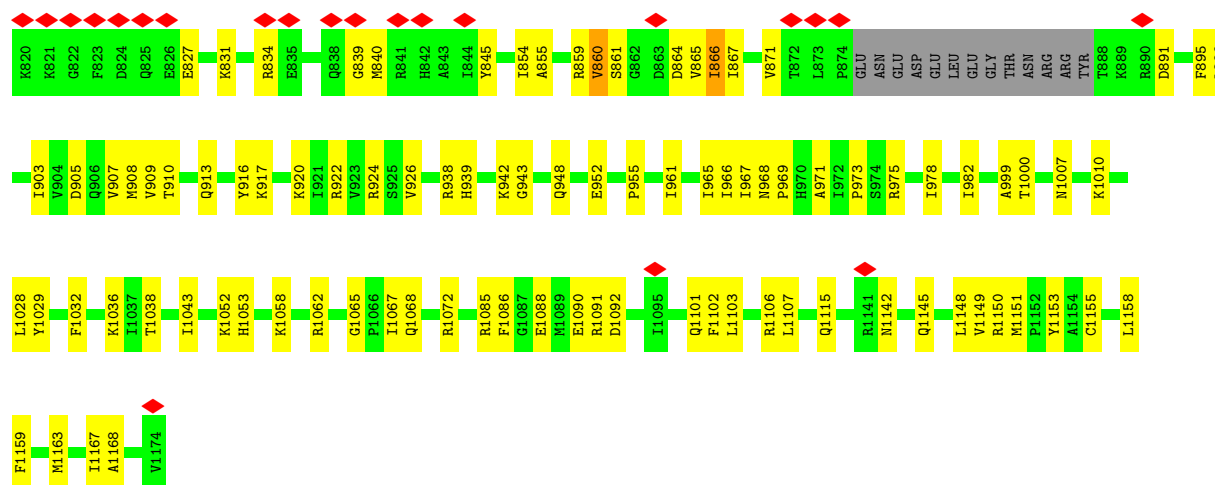


• Molecule 3: General transcription factor IIF subunit 2

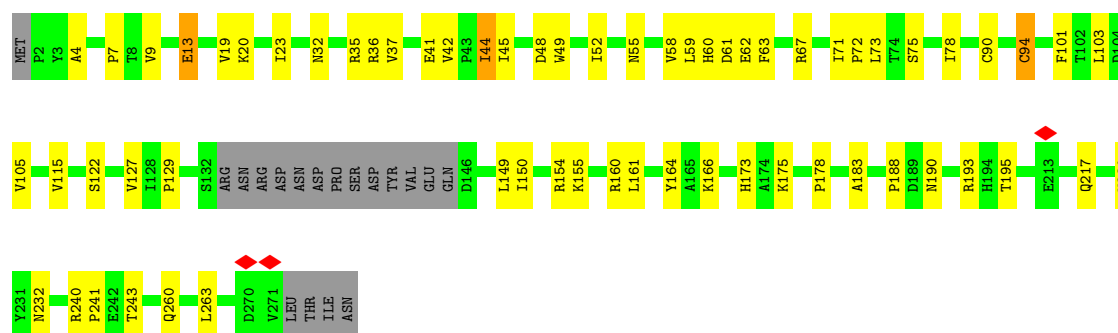
GLY	E1433	L1298	K1219	T1118	V939	G789	L640	M620	G379	S269	ASP	L100	MET
ILE	Q1299	Q1299	T1227	K1255	I948	Q790	L645	V521	V380	A270	GLU	V101	HIS
SER	E1434	G1300				Q791		P522	P381	R271	LEU	K102	GLY
ALA	T1435	V1307	Q1230	I1128	E953	F802	F668	M524	Y413	D282	THR	V106	GLY
MET	M1440		K1234	N1129	E953	T611	V669	V525	R421	I286	LYS	L107	PRO
THR	A1443	Q1313	K1234	I1130	M959	P817	S670	V526	R421		GLU	V110	PRO
TRP	A1444	T1314	I1235	N1130	R960	P817	N671	V527	I427		LYS	F112	SER
ASN	H1445	D1315	N1236	K1135	R963	P817	1672				GLY	F113	ASP
GLN	H1456	N1316		L1139		G821	V675	S530	H432	R292	GLY		S11
GLY	N1457	K1317	F1239	Q1146	P971	F822	1676	R531	P433	G182		L15	
ALA	N1458	K1318	G1240	S1147	T972	V823		R532	G183	G183		I18	
THR	I1458	K1319	D1241	S1147	V978	E824	L680	F533	K434	G184		I18	
PRO	I1320	I1320	D1242	A1148	V978	E824	L680	V534	D437	R186		L26	
ALA	Q1462	I1321	L1243	R1149	L963	L828	H685	M535		Y187		L26	
TYR									H449	A299		L26	
GLY	G1467	E1324	N1248	E1152	L963	L831	1689	A544	I457	R190		L31	
ALA	T1468	R1153	D1249	R1153	W988	F838	T693	V545		S194		L31	
TRP			D1249	I1157	N989	L847	D695	F548	R460	Y199		M34	
SER	F1471	E1327	D1250	L1158	K992	L847	D695	T549	Q461	A200		G40	
PRO	D1472	A1330	N1251	C1159	I956	V852	I706	D552	M469	E201		I41	
SER	N1473	L1331	A1252	R1160	H1005	K853	A709	F554	G471	K203		T46	
VAL	L1474	Q1332	E1253	L1161	P1006	R863	V713	L555	H472	H204		T47	
GLY	E1333	E1333	E1253	E1162	I1007	R863	V713	V560	R473	V205		E48	
SER	A1477	V1346	K1254	H1163	I1077	R863	I717	M665	P478	N206		G49	
GLY	E1478	L1347	L1255	H1163	H1044	L864	I717	M665	V479	K134		G50	
MET	K1479	L1347	L1255	H1163	H1044	L864	I717	M665	V479	R51		R52	
THR	C1480	L1347	L1255	H1163	H1044	L864	I717	M665	V479	K53		K53	
PRO	K1481	T1358	L1256	I1175	H1044	L864	I717	M665	V479	L57		L57	
GLY	Y1482	R1258	R1258	M1180	L1016	L864	I717	M665	V479	M58		Q62	
ALA	G1483	I1259	I1259	P1181	L1020	R866	H721	T569	S480	K212		I65	
ALA	G1483	R1260	R1260	P1181	L1020	R866	H721	T569	S480	I65		E66	
GLY	M1484	I1261	I1261	S1182	V1021	S867	E726	Q576	F482	E66		R67	
PHE	E1485	M1262	M1262	S1182	I1022	Q885	P727	P577	L483	D146		G76	
SER	I1486	N1263	N1263	T1184	H1044	Q885	P727	P577	L483	K149		K151	
PRO	P1487	S1264	S1264	D1189	H1044	D894	L733	L580	V488	E153		E153	
SER		D1265	D1265	Q1190	R1052	V901	T736	P582	T489	E219		E155	
ALA		E1266	E1266	E1191	L1060	L909	F737	L585	P491	R220		GLY	
ALA		N1267	N1267	W1192	L1060	L909	F737	L585	P491	E219		GLY	
ASP	L1398	K1268	K1268	E1198	H1082	K910	L745	K589	D495	V221		GLU	
SER	A1399	M1269	M1269	M1199	V1087	P911	A748	Q590	F496	E219		GLU	
LEU	L1400	Q1270	Q1270	P1200	V1087	S912	R749	T591	D497	K226		GLU	
GLY	L1401	M1270	M1270	P1200	V1087	N913				R227		MET	
PHE	G1402	Q1270	Q1270	P1200	V1087	N913				K357		ASP	
ALA	D1403	E1271	E1271	E1198	H1082	F916	A756	N601	M501	V255		ASP	
GLY	T1404	E1272	E1272	E1198	H1082	F916	A756	N601	M501	P256		ASP	
PRO	C1407	E1273	E1273	F1202	F1202	F920	L760	D625	N502	V260		ASN	
THR	R1408	E1274	E1274	F1202	F1202	F920	L760	D625	N502	V260		ASN	
SER		V1275	V1275	A1205	A1205	R921	I781	K627	L509	V260		LYS	
ALA	L1411	V1276	V1276	R1206	R1206	R921	I781	K627	L509	V260		PHE	
PRO	L1414	D1277	D1277	R1206	R1206	R921	I781	K627	L509	V260		PHE	
TRP	T1415	K1278	K1278	R1206	R1206	R921	I781	K627	L509	V260		GLY	
SER	R1416	M1279	M1279	R1206	R1206	R921	I781	K627	L509	V260		GLY	
THR	H1417	D1280	D1280	R1206	R1206	R921	I781	K627	L509	V260		GLY	
PRO	R1421	D1281	D1281	R1206	R1206	R921	I781	K627	L509	V260		GLY	
GLY		D1282	D1282	R1206	R1206	R921	I781	K627	L509	V260		GLY	
SER		I1288	I1288	R1206	R1206	R921	I781	K627	L509	V260		GLY	
		E1289	E1289	R1206	R1206	R921	I781	K627	L509	V260		GLY	
		L1293	L1293	R1206	R1206	R921	I781	K627	L509	V260		GLY	
		T1294	T1294	R1206	R1206	R921	I781	K627	L509	V260		GLY	
		D1295	D1295	R1206	R1206	R921	I781	K627	L509	V260		GLY	
		M1296	M1296	R1206	R1206	R921	I781	K627	L509	V260		GLY	
		T1297	T1297	R1206	R1206	R921	I781	K627	L509	V260		GLY	

- Molecule 8: DNA-directed RNA polymerase subunit beta

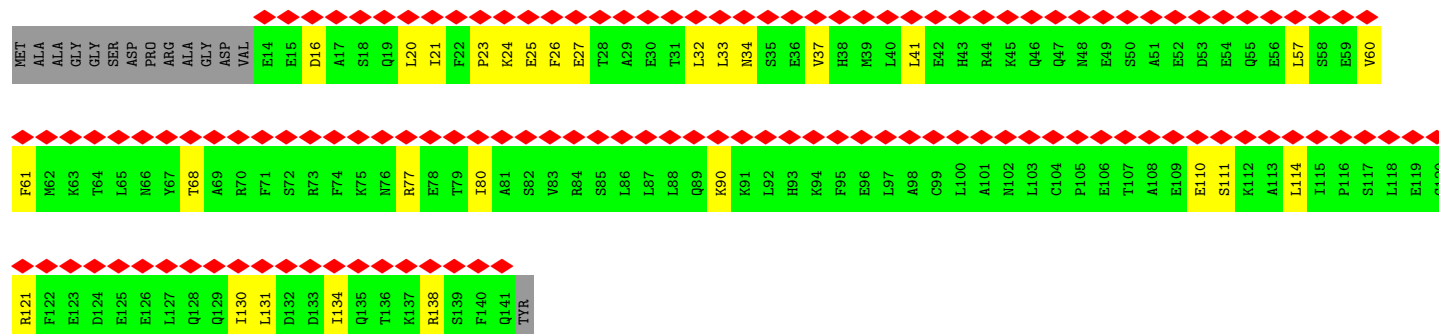
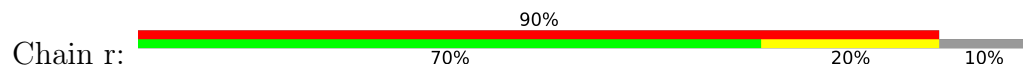




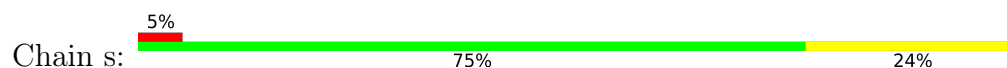
• Molecule 9: DNA-directed RNA polymerase II subunit RPB3

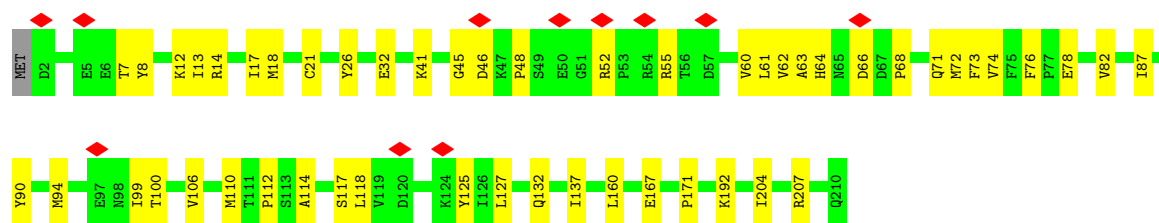


• Molecule 10: DNA-directed RNA polymerase II subunit RPB4

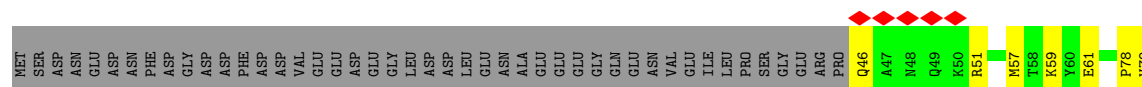


• Molecule 11: DNA-directed RNA polymerase II subunit E

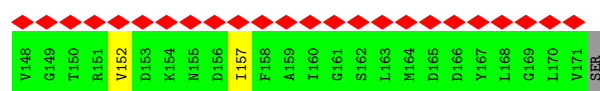
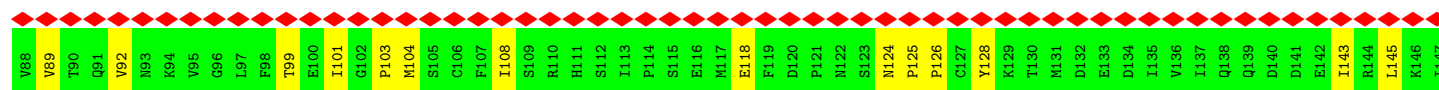
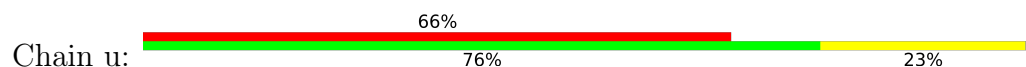




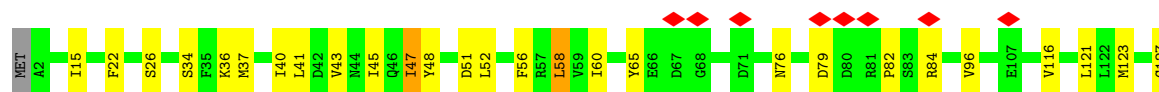
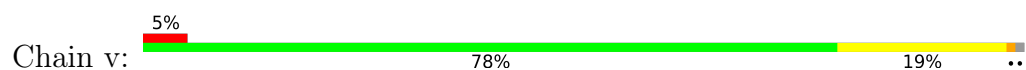
- Molecule 12: DNA-directed RNA polymerase II subunit F



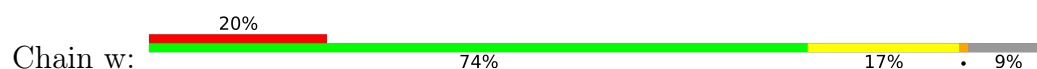
- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

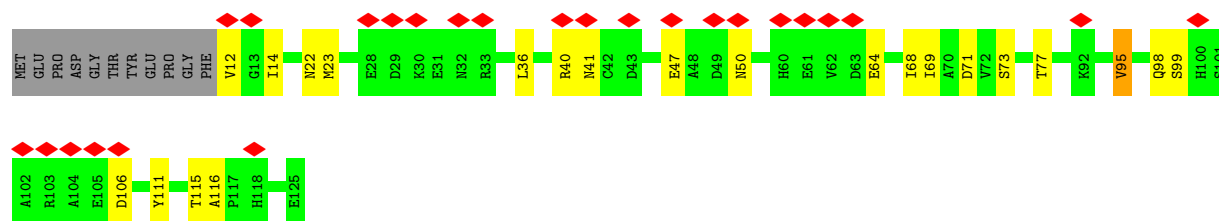


- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

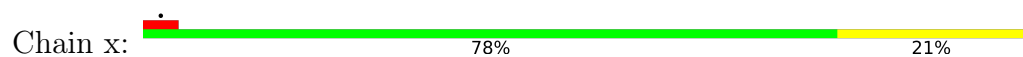


- Molecule 15: DNA-directed RNA polymerase II subunit RPB9

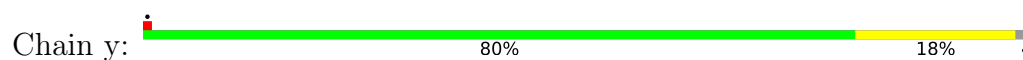




- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 17: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 18: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.464	Depositor
Minimum map value	-5.345	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.93	Depositor
Map size ($\text{\AA}$)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.334, 1.334, 1.334	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: G2L, ATP, ILX, CSX, W0F, MG, TRX, ZN, HYP

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	N	0.41	0/22	0.98	0/26
2	S	0.09	0/1167	0.23	0/1576
3	T	0.09	0/799	0.25	0/1077
4	X	0.30	0/981	0.60	0/1509
5	Y	0.34	0/1249	0.56	0/1926
6	Z	0.32	0/206	0.44	0/317
7	o	0.30	0/11723	0.39	0/15830
8	p	0.33	0/9332	0.42	1/12598 (0.0%)
9	q	0.34	0/2102	0.40	0/2857
10	r	0.13	0/1064	0.22	0/1428
11	s	0.26	0/1751	0.36	1/2366 (0.0%)
12	t	0.31	0/667	0.31	0/901
13	u	0.17	0/1382	0.32	0/1874
14	v	0.32	0/1207	0.36	0/1628
15	w	0.24	0/948	0.35	0/1284
16	x	0.31	0/542	0.34	0/730
17	y	0.32	0/939	0.34	0/1271
18	z	0.26	0/377	0.38	0/500
All	All	0.30	0/36458	0.40	2/49698 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	46	ASP	CB-CA-C	-5.41	109.88	117.23
8	p	355	ASP	CB-CA-C	-5.27	110.06	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	64	30	51	6	0
2	S	1138	0	1103	18	0
3	T	789	0	795	9	0
4	X	878	0	487	27	0
5	Y	1112	0	606	23	0
6	Z	241	0	118	6	0
7	o	11510	0	11616	253	0
8	p	9149	0	9178	251	0
9	q	2059	0	2007	59	0
10	r	1050	0	1033	18	0
11	s	1720	0	1737	39	0
12	t	657	0	684	17	0
13	u	1351	0	1358	26	0
14	v	1186	0	1147	23	0
15	w	927	0	859	17	0
16	x	533	0	553	11	0
17	y	920	0	942	16	0
18	z	372	0	378	8	0
19	Z	33	0	0	6	0
20	o	2	0	0	0	0
20	p	1	0	0	0	0
20	q	1	0	0	0	0
20	w	2	0	0	0	0
20	x	1	0	0	0	0
20	z	1	0	0	0	0
21	o	1	0	0	0	0
All	All	35698	30	34652	731	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 (731) 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)
3:T:91:GLN:HB2	8:p:555:GLU:HG3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:2500:W0F:O32	8:p:975:ARG:NH2	2.11	0.83
8:p:866:ILE:HG22	8:p:867:ILE:HG13	1.62	0.81
8:p:926:VAL:HG21	9:q:62:GLU:HG3	1.63	0.81
4:X:31:DG:H2''	4:X:32:DT:H72	1.61	0.80
7:o:948:ILE:HG12	7:o:1007:ILE:HD11	1.64	0.80
9:q:20:LYS:HG3	9:q:232:ASN:HD22	1.48	0.79
7:o:1458:ILE:HD12	8:p:1091:ARG:HH21	1.48	0.78
8:p:597:ILE:HG23	8:p:601:VAL:HB	1.65	0.78
4:X:14:DC:H2''	4:X:15:DT:H71	1.65	0.77
8:p:108:MET:HE2	8:p:118:LEU:HD12	1.67	0.77
19:Z:2500:W0F:O33	7:o:497:ASP:OD2	2.03	0.76
7:o:922:PHE:H	7:o:1052:ARG:HD2	1.51	0.76
9:q:190:ASN:ND2	9:q:195:THR:O	2.20	0.75
8:p:1142:ASN:HD21	8:p:1145:GLN:HB2	1.51	0.75
4:X:13:DA:H2''	4:X:14:DC:H2'	1.67	0.75
6:Z:11:G2L:OP2	6:Z:11:G2L:H8	1.86	0.73
8:p:910:THR:HG22	18:z:43:ILE:HA	1.70	0.73
5:Y:-11:DC:O2	19:Z:2500:W0F:N19	2.22	0.72
9:q:67:ARG:NH2	16:x:3:ILE:O	2.22	0.72
8:p:567:ILE:HA	8:p:612:ILE:HG22	1.72	0.72
10:r:16:ASP:H	10:r:21:ILE:HB	1.55	0.71
7:o:204:HIS:HA	7:o:211:GLU:HB3	1.72	0.71
7:o:358:ARG:NH2	8:p:1068:GLN:OE1	2.23	0.71
6:Z:1:ATP:H2'	6:Z:1:ATP:N3	2.06	0.71
9:q:193:ARG:HH12	9:q:217:GLN:HB3	1.53	0.70
10:r:25:GLU:HG3	13:u:41:LYS:HE2	1.72	0.70
9:q:48:ASP:HB3	9:q:166:LYS:HE2	1.74	0.70
8:p:274:ARG:NH1	8:p:311:ILE:O	2.23	0.70
7:o:636:ILE:HG22	7:o:637:MET:HG2	1.74	0.69
9:q:42:VAL:HB	9:q:178:PRO:HG3	1.73	0.69
8:p:118:LEU:HD22	8:p:913:GLN:HG3	1.74	0.69
7:o:1148:ALA:HB1	7:o:1333:GLU:HB2	1.74	0.69
11:s:171:PRO:HB2	11:s:207:ARG:HD3	1.74	0.69
17:y:7:PHE:HB2	17:y:11:LEU:HD12	1.75	0.69
1:N:1:ILX:HG23	7:o:791:GLN:NE2	2.07	0.69
5:Y:-1:DA:H8	5:Y:-1:DA:H5''	1.57	0.69
2:S:115:LYS:NZ	2:S:117:GLY:O	2.27	0.68
8:p:544:PHE:HB2	8:p:596:ILE:HD13	1.74	0.68
14:v:26:SER:HB3	14:v:45:ILE:HD11	1.75	0.68
9:q:60:HIS:HD2	9:q:62:GLU:HG2	1.58	0.68
17:y:45:ILE:HG22	17:y:94:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:784:VAL:HG22	8:p:978:ILE:HD11	1.75	0.68
7:o:560:VAL:HG22	7:o:591:ILE:HD11	1.77	0.67
8:p:80:GLU:O	8:p:82:PRO:HD3	1.94	0.67
8:p:193:VAL:HG21	8:p:470:LEU:HD13	1.76	0.67
10:r:33:LEU:HD12	10:r:80:ILE:HG23	1.77	0.67
7:o:576:GLN:O	7:o:590:GLN:NE2	2.29	0.66
8:p:744:MET:HE3	8:p:922:ARG:HB2	1.78	0.66
8:p:505:LEU:HD22	8:p:509:VAL:HB	1.77	0.66
8:p:665:ILE:HG23	8:p:669:GLU:HB3	1.78	0.66
1:N:1:ILX:HG23	7:o:791:GLN:HE22	1.61	0.66
5:Y:-24:DT:H1'	5:Y:-23:DC:H5'	1.77	0.66
9:q:90:CYS:SG	9:q:94:CYS:HB3	2.35	0.66
7:o:478:PRO:O	7:o:483:ARG:NH2	2.28	0.66
8:p:827:GLU:HG2	8:p:871:VAL:HG22	1.77	0.65
11:s:8:TYR:CZ	11:s:12:LYS:HD2	2.32	0.65
7:o:358:ARG:HA	8:p:1085:ARG:HA	1.79	0.65
7:o:1262:MET:HB3	7:o:1265:ASP:HB3	1.77	0.65
7:o:98:GLY:HA3	7:o:1440:MET:HE2	1.78	0.65
7:o:26:LEU:HG	8:p:1168:ALA:HB2	1.79	0.65
8:p:924:ARG:HH11	9:q:60:HIS:HB2	1.63	0.64
4:X:19:DA:H1'	4:X:20:DG:C8	2.32	0.64
8:p:1115:GLN:HB3	8:p:1148:LEU:HD11	1.79	0.64
7:o:527:THR:HB	7:o:534:VAL:HG22	1.80	0.64
7:o:121:SER:HA	7:o:126:ILE:HG21	1.80	0.64
7:o:733:LEU:HB3	15:w:106:ASP:HB2	1.80	0.64
8:p:591:ARG:HH22	8:p:592:ARG:HE	1.46	0.64
7:o:375:ILE:HD11	7:o:669:TYR:HB2	1.80	0.63
8:p:566:LYS:HA	8:p:576:ILE:HG22	1.79	0.63
18:z:17:TYR:HB3	18:z:44:MET:HB3	1.81	0.63
5:Y:-5:DG:H5'	8:p:747:LEU:HD12	1.80	0.63
11:s:82:VAL:HB	11:s:110:MET:HG2	1.81	0.63
8:p:572:CYS:O	8:p:574:VAL:HG23	1.98	0.63
7:o:1213:ARG:NH1	7:o:1215:GLU:OE2	2.31	0.63
7:o:1130:ILE:HD13	7:o:1411:LEU:HB3	1.80	0.63
14:v:58:LEU:HD11	14:v:143:LEU:HD11	1.81	0.63
7:o:141:LEU:HD13	7:o:1445:HIS:HE1	1.63	0.62
8:p:407:MET:HE1	8:p:444:LEU:HG	1.80	0.62
8:p:917:LYS:HG3	18:z:34:ILE:HD11	1.80	0.62
18:z:16:ILE:HG12	18:z:27:GLU:HG2	1.81	0.62
5:Y:-11:DC:H2'	5:Y:-10:DC:C6	2.34	0.62
7:o:1485:GLU:HB3	12:t:78:PRO:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:718:GLN:HG2	8:p:720:PRO:HD2	1.80	0.62
2:S:170:VAL:HG23	7:o:1279:MET:HG3	1.82	0.62
11:s:82:VAL:HG23	11:s:106:VAL:HG13	1.82	0.62
7:o:508:SER:HB3	7:o:511:THR:HG22	1.80	0.62
8:p:545:LEU:HB3	8:p:550:MET:HG3	1.81	0.62
8:p:761:THR:H	8:p:764:MET:HE3	1.63	0.61
3:T:94:THR:HG22	3:T:109:ILE:HG22	1.81	0.61
8:p:387:HIS:HD2	8:p:504:THR:HG21	1.65	0.61
8:p:403:LEU:HD23	8:p:444:LEU:HD23	1.82	0.61
7:o:322:LEU:HB3	7:o:325:LEU:HD12	1.81	0.61
7:o:367:ILE:HG21	7:o:501:MET:HG3	1.82	0.61
7:o:1128:ILE:HG23	7:o:1414:ILE:HB	1.83	0.60
5:Y:-18:DC:H2"	5:Y:-17:DG:C8	2.37	0.60
7:o:201:GLU:HG2	7:o:203:LYS:H	1.66	0.60
7:o:1211:LEU:HD11	7:o:1258:ARG:HB3	1.83	0.60
10:r:60:VAL:HG13	13:u:103:PRO:HB3	1.84	0.60
2:S:167:ARG:O	8:p:248:LYS:NZ	2.34	0.60
9:q:4:ALA:HB2	17:y:93:ASP:HB3	1.82	0.60
8:p:37:LYS:HB3	8:p:41:ARG:HG3	1.84	0.60
8:p:636:LYS:H	8:p:639:HIS:HD2	1.50	0.60
14:v:96:VAL:HG22	14:v:116:VAL:HG22	1.84	0.60
8:p:387:HIS:CD2	8:p:504:THR:HG21	2.37	0.60
7:o:1268:LYS:HD3	7:o:1275:VAL:HG13	1.84	0.59
8:p:834:ARG:HD2	8:p:840:MET:HE2	1.84	0.59
15:w:69:ILE:HG22	15:w:71:ASP:H	1.67	0.59
7:o:1005:HIS:HD2	7:o:1007:ILE:HB	1.67	0.59
13:u:89:VAL:HA	13:u:99:THR:HG22	1.82	0.59
7:o:792:ASN:HD21	7:o:1108:HIS:CE1	2.21	0.59
11:s:45:GLY:HA3	11:s:52:ARG:HB2	1.84	0.59
8:p:157:ARG:NH2	8:p:177:CYS:O	2.36	0.59
8:p:540:PRO:HB2	8:p:596:ILE:HG23	1.85	0.59
5:Y:-2:DG:H2"	5:Y:-1:DA:H5"	1.84	0.58
13:u:99:THR:HG21	13:u:143:ILE:HD11	1.86	0.58
17:y:49:GLN:HB2	17:y:94:LEU:HD21	1.84	0.58
7:o:1403:ASP:O	7:o:1407:CYS:HB2	2.03	0.58
8:p:384:ASP:O	8:p:390:ASN:ND2	2.37	0.58
8:p:550:MET:SD	8:p:577:HIS:HB2	2.44	0.57
7:o:760:LEU:HD11	7:o:781:ILE:HG21	1.86	0.57
7:o:938:LEU:HD22	7:o:1005:HIS:HD1	1.69	0.57
7:o:721:HIS:HE1	15:w:98:GLN:HE21	1.50	0.57
4:X:36:DT:H2"	4:X:37:DA:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:s:17:ILE:HD13	11:s:74:VAL:HG11	1.86	0.57
8:p:859:ARG:HG2	8:p:903:ILE:HG12	1.86	0.57
2:S:168:ASN:HA	8:p:248:LYS:HD3	1.85	0.57
7:o:413:TYR:O	7:o:449:HIS:HD2	1.88	0.57
8:p:1062:ARG:NE	8:p:1065:GLY:H	2.03	0.57
8:p:627:ILE:HD11	8:p:663:GLU:HB2	1.87	0.56
7:o:471:GLY:O	7:o:521:VAL:HG23	2.04	0.56
7:o:996:ILE:HD13	7:o:1060:LEU:HA	1.87	0.56
8:p:860:VAL:HG12	8:p:864:ASP:HB2	1.87	0.56
10:r:32:LEU:HD11	13:u:4:HIS:HB2	1.87	0.56
7:o:1206:ARG:HB2	7:o:1267:ASN:HB2	1.87	0.56
8:p:747:LEU:HD23	8:p:810:PHE:CE1	2.40	0.56
8:p:516:GLU:HA	8:p:520:VAL:HG22	1.87	0.56
8:p:625:LEU:HD13	8:p:675:LEU:HD21	1.88	0.56
16:x:3:ILE:HD12	16:x:4:PRO:HD2	1.86	0.55
7:o:671:ASN:O	7:o:675:VAL:HG13	2.06	0.55
8:p:50:PHE:HB2	8:p:397:GLY:HA2	1.88	0.55
8:p:905:ASP:HB2	8:p:924:ARG:HG3	1.88	0.55
8:p:1062:ARG:HE	8:p:1065:GLY:H	1.55	0.55
4:X:25:DG:H2"	4:X:26:DC:C6	2.42	0.55
7:o:1147:SER:HA	7:o:1153:ARG:HB2	1.89	0.55
9:q:9:VAL:HG11	17:y:105:PHE:HD1	1.72	0.55
7:o:894:ASP:O	7:o:1022:ILE:HD13	2.07	0.55
8:p:392:ARG:NE	8:p:617:ASP:OD2	2.34	0.55
8:p:952:GLU:HB2	9:q:36:ARG:HG3	1.89	0.55
8:p:65:ILE:HB	8:p:86:LEU:HB2	1.89	0.55
11:s:87:ILE:HD12	11:s:114:ALA:HB1	1.89	0.55
7:o:62:GLN:HG3	7:o:84:HIS:O	2.07	0.55
8:p:561:ILE:HB	8:p:610:ARG:HH11	1.71	0.55
9:q:105:VAL:HG11	9:q:115:VAL:HG22	1.89	0.55
9:q:260:GLN:HB2	17:y:91:ILE:HG21	1.89	0.54
4:X:-3:DT:H2"	4:X:-2:DT:H72	1.89	0.54
7:o:549:THR:HG21	7:o:640:LEU:HD12	1.88	0.54
8:p:561:ILE:O	8:p:610:ARG:NH1	2.40	0.54
8:p:709:SER:HB2	8:p:767:LEU:HD11	1.89	0.54
8:p:403:LEU:HD21	8:p:447:SER:OG	2.06	0.54
5:Y:10:DC:H2"	5:Y:11:DT:C6	2.43	0.54
8:p:565:THR:H	8:p:610:ARG:HB3	1.73	0.54
11:s:192:LYS:HE3	11:s:204:ILE:HD13	1.89	0.54
12:t:81:VAL:HG22	12:t:101:LYS:HD3	1.90	0.54
7:o:1381:GLU:O	7:o:1385:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:747:LEU:HD23	8:p:810:PHE:HE1	1.71	0.54
7:o:555:LEU:HD12	7:o:591:ILE:HD12	1.89	0.54
7:o:370:ASP:HB2	7:o:483:ARG:HB3	1.90	0.54
12:t:105:ILE:HG22	12:t:119:GLY:HA2	1.90	0.54
7:o:867:SER:HB3	7:o:1414:ILE:HG23	1.90	0.54
4:X:-1:DC:H2''	4:X:0:DA:C8	2.43	0.53
8:p:565:THR:HA	8:p:610:ARG:O	2.08	0.53
7:o:461:GLN:NE2	8:p:1090:GLU:OE2	2.41	0.53
7:o:1386:ILE:HD12	7:o:1398:LEU:HD21	1.91	0.53
8:p:91:ILE:HD12	8:p:126:VAL:HG22	1.89	0.53
9:q:37:VAL:HG13	9:q:41:GLU:HB2	1.91	0.53
8:p:567:ILE:O	8:p:567:ILE:HG13	2.09	0.53
11:s:18:MET:HE2	11:s:32:GLU:HB3	1.90	0.53
7:o:685:HIS:NE2	7:o:769:MET:HE3	2.24	0.53
11:s:21:CYS:SG	11:s:26:TYR:HB2	2.48	0.53
8:p:569:VAL:O	8:p:571:GLY:N	2.42	0.53
14:v:58:LEU:HD12	14:v:145:MET:HG2	1.90	0.53
7:o:847:LEU:HD11	8:p:720:PRO:HB3	1.91	0.53
8:p:564:ALA:HB3	8:p:580:PRO:HD3	1.91	0.53
7:o:909:LEU:C	7:o:911:PRO:HD2	2.34	0.53
9:q:19:VAL:HG23	9:q:241:PRO:HB2	1.91	0.53
19:Z:2500:W0F:C01	19:Z:2500:W0F:C20	2.85	0.53
7:o:626:THR:OG1	7:o:627:LYS:N	2.40	0.53
7:o:693:ILE:HD13	7:o:828:LEU:HD21	1.90	0.53
7:o:544:ALA:HB2	7:o:680:LEU:HD13	1.91	0.53
8:p:495:LEU:HG	8:p:497:LYS:H	1.74	0.53
7:o:1105:ASN:HB3	7:o:1107:PHE:CD2	2.44	0.52
8:p:789:ASN:O	8:p:968:ASN:HB2	2.10	0.52
13:u:18:PHE:HA	13:u:22:LEU:HD13	1.91	0.52
15:w:115:THR:HG22	15:w:116:ALA:H	1.74	0.52
7:o:1471:PHE:CZ	12:t:61:GLU:HA	2.45	0.52
8:p:591:ARG:NH2	8:p:592:ARG:HG3	2.24	0.52
9:q:78:ILE:HD11	9:q:127:VAL:HG23	1.92	0.52
7:o:1082:HIS:CD2	12:t:59:LYS:HE3	2.45	0.52
7:o:1208:SER:O	7:o:1260:ARG:NH1	2.43	0.52
6:Z:1:ATP:O2'	6:Z:2:U:H5'	2.10	0.52
6:Z:2:U:H2'	6:Z:3:C:C6	2.45	0.52
7:o:769:MET:HE1	8:p:969:PRO:HB2	1.92	0.52
4:X:13:DA:H2''	4:X:14:DC:C2'	2.36	0.52
7:o:525:ILE:HG12	7:o:535:MET:HE3	1.92	0.52
7:o:685:HIS:HE2	7:o:769:MET:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:50:PHE:O	8:p:51:ILE:C	2.51	0.52
13:u:92:VAL:HB	13:u:126:PRO:HB2	1.91	0.52
7:o:924:TYR:OH	7:o:953:GLU:OE2	2.21	0.52
7:o:931:ARG:HG2	7:o:939:VAL:HG11	1.90	0.52
8:p:754:PRO:HB2	8:p:773:PRO:HG2	1.90	0.52
11:s:26:TYR:HB3	11:s:62:VAL:HG12	1.92	0.52
7:o:1347:LEU:HB3	11:s:137:ILE:HD12	1.91	0.52
8:p:472:ARG:NH1	8:p:737:ILE:HD11	2.25	0.52
8:p:570:ASN:OD1	8:p:616:THR:N	2.35	0.52
8:p:924:ARG:NH1	9:q:60:HIS:HB2	2.24	0.52
9:q:44:ILE:HG12	9:q:45:ILE:H	1.74	0.52
9:q:72:PRO:HG3	16:x:13:ILE:HD11	1.91	0.51
13:u:108:ILE:HD11	13:u:145:LEU:HD22	1.92	0.51
15:w:64:GLU:O	15:w:68:ILE:HG12	2.09	0.51
7:o:916:PHE:HE2	7:o:960:ARG:HG2	1.74	0.51
7:o:1262:MET:HB3	7:o:1265:ASP:CB	2.41	0.51
8:p:545:LEU:O	8:p:550:MET:HG2	2.09	0.51
2:S:114:LYS:HB3	8:p:356:PHE:CZ	2.45	0.51
7:o:1163:HIS:CE1	7:o:1297:THR:HG23	2.45	0.51
9:q:52:ILE:HD12	9:q:61:ASP:HB3	1.91	0.51
7:o:577:PRO:HG2	7:o:580:LEU:HD23	1.92	0.51
7:o:1189:ASP:HA	7:o:1192:TRP:CE2	2.45	0.51
7:o:1472:ASP:HB2	12:t:109:TYR:HE2	1.74	0.51
8:p:298:MET:HE3	15:w:14:ILE:HB	1.92	0.51
8:p:759:VAL:HG12	8:p:999:ALA:HB2	1.90	0.51
3:T:97:THR:OG1	3:T:107:GLU:OE2	2.25	0.51
9:q:60:HIS:CD2	9:q:62:GLU:HG2	2.44	0.51
11:s:60:VAL:HG12	11:s:62:VAL:HG23	1.93	0.51
4:X:14:DC:H2''	4:X:15:DT:C7	2.40	0.51
5:Y:10:DC:H2''	5:Y:11:DT:C5	2.45	0.51
7:o:93:PRO:HD2	7:o:219:GLU:HG2	1.92	0.51
14:v:79:ASP:O	14:v:82:PRO:HD2	2.11	0.51
18:z:36:CYS:HB2	18:z:44:MET:HE1	1.93	0.51
12:t:51:ARG:NH1	12:t:122:GLU:OE1	2.44	0.51
2:S:169:LYS:HD2	2:S:173:HIS:CD2	2.46	0.51
5:Y:-22:DG:H5''	11:s:112:PRO:HB3	1.93	0.51
7:o:46:THR:HG22	7:o:47:THR:HG23	1.92	0.51
7:o:1161:LEU:HD22	7:o:1346:VAL:HG22	1.93	0.50
7:o:1230:GLN:HG2	7:o:1234:LYS:HE3	1.92	0.50
8:p:49:GLU:O	8:p:50:PHE:C	2.53	0.50
10:r:20:LEU:HD12	10:r:121:ARG:HH22	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:r:34:ASN:O	10:r:68:THR:OG1	2.29	0.50
7:o:545:VAL:HG11	7:o:645:LEU:HD12	1.93	0.50
7:o:545:VAL:HG22	7:o:676:ILE:HG12	1.91	0.50
8:p:388:TYR:CZ	8:p:505:LEU:HD21	2.47	0.50
7:o:601:ASN:HA	7:o:630:VAL:O	2.11	0.50
7:o:784:VAL:HG13	8:p:978:ILE:HD11	1.93	0.50
8:p:811:TYR:CE2	8:p:924:ARG:HG2	2.47	0.50
13:u:30:LEU:O	13:u:34:VAL:HG22	2.11	0.50
9:q:32:ASN:OD1	9:q:35:ARG:NH1	2.44	0.50
9:q:49:TRP:HB3	9:q:164:TYR:HB2	1.94	0.50
13:u:30:LEU:HD22	13:u:70:VAL:HG11	1.94	0.50
1:N:3:GLY:HA3	7:o:749:ARG:NH1	2.26	0.50
7:o:912:SER:HB2	7:o:1327:GLU:HG2	1.93	0.50
7:o:1443:ALA:HB2	8:p:1167:ILE:HG23	1.92	0.50
5:Y:-1:DA:H5''	5:Y:-1:DA:C8	2.42	0.50
8:p:187:ILE:HD13	8:p:448:LEU:HB3	1.93	0.50
8:p:631:GLN:NE2	8:p:691:SER:O	2.40	0.50
6:Z:6:C:H2'	6:Z:7:U:C6	2.46	0.50
8:p:818:GLU:HG2	8:p:917:LYS:HB3	1.94	0.50
7:o:87:HIS:HD2	7:o:89:GLU:HG3	1.76	0.50
7:o:1458:ILE:HD11	8:p:1103:LEU:HD21	1.94	0.50
8:p:665:ILE:HD13	8:p:673:VAL:HG21	1.93	0.50
13:u:13:LEU:HB3	13:u:66:VAL:HG12	1.94	0.50
7:o:864:LEU:HD23	7:o:1414:ILE:HG21	1.93	0.49
5:Y:-2:DG:H2''	5:Y:-1:DA:C5'	2.43	0.49
7:o:427:ILE:HD13	7:o:437:ASP:HB3	1.94	0.49
7:o:460:ARG:HD3	7:o:492:TYR:O	2.12	0.49
8:p:587:LEU:HB3	8:p:603:MET:SD	2.51	0.49
8:p:591:ARG:HH12	8:p:592:ARG:HE	1.61	0.49
9:q:103:LEU:HB3	9:q:161:LEU:HG	1.93	0.49
12:t:80:MET:HE3	12:t:103:PRO:HG3	1.95	0.49
13:u:53:ASN:HD22	13:u:71:LYS:HE3	1.76	0.49
2:S:164:TRP:CZ2	2:S:167:ARG:HD3	2.47	0.49
5:Y:-6:DA:H2'	5:Y:-5:DG:C8	2.46	0.49
7:o:531:ASN:HD21	7:o:1392:TYR:HE2	1.61	0.49
9:q:58:VAL:HG11	16:x:59:LEU:HB3	1.93	0.49
8:p:109:MET:HE2	8:p:174:LEU:HD22	1.94	0.49
8:p:796:MET:HE3	8:p:948:GLN:HE21	1.76	0.49
8:p:1028:LEU:HD11	8:p:1043:ILE:HD11	1.95	0.49
4:X:-3:DT:C2'	4:X:-2:DT:H72	2.42	0.49
8:p:631:GLN:HE22	8:p:691:SER:C	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:1115:GLN:HG2	8:p:1150:ARG:HG2	1.94	0.49
11:s:7:THR:OG1	11:s:48:PRO:HD3	2.12	0.49
2:S:142:ASN:OD1	2:S:143:TRP:N	2.46	0.49
7:o:581:LYS:HG2	7:o:582:PRO:HA	1.95	0.49
7:o:1180:ASN:O	7:o:1183:SER:OG	2.27	0.49
8:p:404:PHE:HA	8:p:407:MET:HE2	1.95	0.49
8:p:550:MET:HE1	8:p:577:HIS:ND1	2.28	0.49
14:v:40:ILE:O	14:v:123:MET:HA	2.13	0.49
7:o:972:THR:HA	7:o:1320:ILE:HG13	1.95	0.49
8:p:472:ARG:CZ	8:p:737:ILE:HD11	2.42	0.49
2:S:116:GLY:HA2	8:p:356:PHE:HD2	1.78	0.48
4:X:-12:DG:H1'	4:X:-11:DA:C8	2.48	0.48
4:X:18:DG:H2'	4:X:18:DG:OP2	2.13	0.48
7:o:565:MET:HE1	17:y:74:ARG:HB2	1.95	0.48
7:o:802:PHE:HD2	8:p:671:GLU:HG2	1.78	0.48
7:o:375:ILE:HD11	7:o:669:TYR:CB	2.44	0.48
7:o:601:ASN:ND2	7:o:989:ASN:OD1	2.46	0.48
8:p:77:GLU:HA	8:p:80:GLU:HB2	1.94	0.48
4:X:31:DG:H2''	4:X:32:DT:C7	2.38	0.48
7:o:350:VAL:O	7:o:355:MET:HG2	2.13	0.48
7:o:971:PRO:O	7:o:972:THR:OG1	2.27	0.48
8:p:86:LEU:HD22	8:p:431:LEU:HD21	1.95	0.48
3:T:31:TRP:HD1	3:T:62:LEU:HD21	1.78	0.48
7:o:344:LYS:O	7:o:1435:THR:HG21	2.14	0.48
7:o:1347:LEU:HB3	11:s:137:ILE:CD1	2.42	0.48
8:p:69:ALA:H	8:p:82:PRO:HD2	1.77	0.48
8:p:1159:PHE:O	8:p:1163:MET:HG3	2.14	0.48
9:q:52:ILE:HG21	9:q:55:ASN:HB2	1.95	0.48
11:s:21:CYS:SG	11:s:62:VAL:HG11	2.52	0.48
14:v:37:MET:HE3	14:v:127:GLY:HA3	1.96	0.48
8:p:285:LEU:HD11	8:p:305:LEU:HD11	1.94	0.48
8:p:297:MET:O	8:p:301:VAL:HG23	2.13	0.48
8:p:557:SER:N	8:p:558:PRO:HD2	2.28	0.48
2:S:161:GLU:O	2:S:165:GLU:HG2	2.14	0.48
7:o:1321:ILE:HD12	7:o:1331:LEU:HD12	1.96	0.48
9:q:67:ARG:NH1	9:q:149:LEU:O	2.47	0.48
9:q:154:ARG:HD3	16:x:64:PRO:HD3	1.96	0.48
11:s:13:ILE:HD11	11:s:132:GLN:HG3	1.96	0.48
7:o:1427:LEU:HB2	7:o:1456:GLU:HG2	1.96	0.48
8:p:26:CYS:HG	8:p:27:TRP:CD1	2.31	0.48
8:p:574:VAL:HG12	8:p:574:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:u:14:HIS:CD2	13:u:16:ARG:H	2.32	0.48
14:v:65:TYR:CD1	14:v:84:ARG:HG2	2.49	0.48
5:Y:7:DG:H2"	5:Y:8:DA:C8	2.48	0.48
7:o:709:ALA:HB2	7:o:748:ALA:HB2	1.96	0.48
8:p:260:LEU:HB2	8:p:263:ILE:HD12	1.96	0.48
9:q:183:ALA:HB3	9:q:232:ASN:HB3	1.95	0.48
15:w:73:SER:HA	15:w:95:VAL:HG11	1.96	0.48
7:o:1181:PRO:HG3	7:o:1207:ILE:HG21	1.96	0.48
7:o:1467:GLY:O	7:o:1468:THR:OG1	2.26	0.48
8:p:88:PHE:HD2	8:p:126:VAL:HG11	1.79	0.48
18:z:46:LYS:O	18:z:47:LYS:HB3	2.14	0.48
7:o:1374:VAL:HG11	7:o:1411:LEU:HD21	1.95	0.47
10:r:57:LEU:HD13	10:r:61:PHE:CE1	2.48	0.47
11:s:14:ARG:O	11:s:18:MET:HG2	2.13	0.47
15:w:14:ILE:HG21	15:w:23:MET:HE2	1.96	0.47
8:p:192:LYS:NZ	8:p:449:ALA:O	2.43	0.47
8:p:794:VAL:HG22	8:p:967:ILE:HG22	1.96	0.47
8:p:1088:GLU:O	8:p:1091:ARG:HG2	2.13	0.47
19:Z:2500:W0F:O31	8:p:942:LYS:HE2	2.13	0.47
7:o:689:ILE:HD11	8:p:982:ILE:HA	1.96	0.47
9:q:263:LEU:HD22	17:y:87:PHE:HD2	1.79	0.47
7:o:421:ARG:CZ	7:o:427:ILE:HD11	2.44	0.47
7:o:1458:ILE:HD12	8:p:1091:ARG:NH2	2.25	0.47
7:o:756:ALA:HB2	7:o:786:ALA:HB2	1.96	0.47
7:o:909:LEU:O	7:o:910:LYS:HB2	2.14	0.47
7:o:1261:ILE:HG22	7:o:1262:MET:H	1.80	0.47
8:p:677:MET:CE	8:p:700:PRO:HB3	2.44	0.47
11:s:72:MET:HE3	11:s:72:MET:HB2	1.79	0.47
1:N:2:TRX:CE3	7:o:749:ARG:HD2	2.45	0.47
7:o:527:THR:HG22	7:o:532:ARG:O	2.15	0.47
7:o:554:PHE:HZ	14:v:121:LEU:HD11	1.79	0.47
8:p:85:LEU:HB2	8:p:131:THR:OG1	2.15	0.47
8:p:236:TRP:HB2	8:p:259:THR:HB	1.97	0.47
8:p:558:PRO:O	8:p:562:ALA:N	2.48	0.47
8:p:731:GLN:HG2	8:p:1052:LYS:NZ	2.30	0.47
8:p:865:VAL:HG22	8:p:895:PHE:CE1	2.49	0.47
9:q:154:ARG:HB2	16:x:60:LEU:HD22	1.96	0.47
16:x:27:ALA:O	16:x:28:GLU:HB2	2.14	0.47
4:X:39:DG:H2"	4:X:40:DG:C8	2.49	0.47
7:o:1258:ARG:HH22	7:o:1260:ARG:HH21	1.63	0.47
8:p:427:LYS:HG3	8:p:428:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:q:59:LEU:HD13	9:q:63:PHE:CE1	2.50	0.47
11:s:55:ARG:HE	11:s:76:PHE:HB3	1.80	0.47
4:X:23:DG:H4'	4:X:24:DA:H5'	1.97	0.47
5:Y:-7:DA:H2'	5:Y:-6:DA:H8	1.78	0.47
9:q:101:PHE:CE2	9:q:122:SER:HB3	2.50	0.47
3:T:32:ALA:HA	3:T:35:SER:HB2	1.96	0.47
7:o:201:GLU:HB2	7:o:213:LYS:HG2	1.97	0.47
7:o:552:ASP:OD1	14:v:22:PHE:HB3	2.14	0.47
8:p:675:LEU:HD23	8:p:695:HIS:HB2	1.96	0.47
12:t:57:MET:HE1	12:t:97:LEU:HD11	1.96	0.47
3:T:80:GLU:OE1	3:T:81:HIS:N	2.48	0.46
6:Z:3:C:H2'	6:Z:4:A:C8	2.50	0.46
7:o:76:GLY:HA2	7:o:81:CYS:HB2	1.97	0.46
7:o:675:VAL:HG22	7:o:676:ILE:HD12	1.96	0.46
8:p:1072:ARG:HD2	8:p:1153:TYR:CE1	2.49	0.46
11:s:118:LEU:HD22	11:s:127:LEU:HB2	1.98	0.46
13:u:14:HIS:HD2	13:u:16:ARG:H	1.63	0.46
13:u:124:ASN:HB2	13:u:125:PRO:HD3	1.97	0.46
4:X:15:DT:H2''	4:X:16:DT:O5'	2.14	0.46
7:o:585:LEU:HD12	14:v:47:ILE:HD11	1.97	0.46
8:p:387:HIS:CD2	8:p:389:GLY:H	2.33	0.46
8:p:854:ILE:O	8:p:907:VAL:HG21	2.15	0.46
9:q:9:VAL:HG11	17:y:105:PHE:CD1	2.50	0.46
7:o:421:ARG:NE	7:o:427:ILE:HD11	2.31	0.46
7:o:1016:LEU:O	7:o:1020:LEU:HG	2.16	0.46
8:p:565:THR:HG21	8:p:612:ILE:HB	1.98	0.46
8:p:604:ILE:O	8:p:612:ILE:HA	2.15	0.46
8:p:674:MET:HG2	15:w:77:THR:HA	1.96	0.46
11:s:8:TYR:CE2	11:s:12:LYS:HD2	2.50	0.46
7:o:1208:SER:HB3	7:o:1260:ARG:HB3	1.97	0.46
11:s:62:VAL:O	11:s:71:GLN:HA	2.15	0.46
7:o:530:SER:O	7:o:532:ARG:HG3	2.16	0.46
8:p:561:ILE:HB	8:p:610:ARG:NH1	2.30	0.46
8:p:699:HIS:CD2	8:p:701:SER:H	2.34	0.46
8:p:699:HIS:HD2	8:p:701:SER:H	1.64	0.46
8:p:712:PRO:HD3	8:p:938:ARG:HD2	1.97	0.46
9:q:72:PRO:HG3	16:x:13:ILE:CD1	2.46	0.46
4:X:16:DT:H4'	7:o:1417:HIS:CG	2.50	0.46
4:X:12:DT:H2''	4:X:13:DA:C8	2.51	0.46
7:o:62:GLN:HE22	7:o:255:VAL:HG12	1.81	0.46
8:p:752:TYR:CE2	8:p:807:ARG:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:r:90:LYS:HE2	10:r:130:ILE:HD11	1.98	0.46
14:v:37:MET:HE2	14:v:37:MET:HB3	1.81	0.46
8:p:515:PRO:HG3	8:p:523:VAL:HB	1.97	0.46
8:p:564:ALA:HA	8:p:610:ARG:HD2	1.97	0.46
16:x:17:LYS:HB3	16:x:38:LEU:HD13	1.98	0.46
8:p:50:PHE:O	8:p:54:SER:N	2.40	0.46
8:p:561:ILE:HG21	8:p:610:ARG:HB2	1.97	0.46
7:o:87:HIS:CD2	7:o:89:GLU:HG3	2.51	0.45
7:o:96:HIS:HB3	7:o:99:PHE:HB2	1.97	0.45
7:o:618:TYR:HE1	14:v:40:ILE:HD13	1.81	0.45
7:o:852:VAL:HG13	8:p:494:LYS:HB3	1.98	0.45
10:r:77:ARG:HA	10:r:80:ILE:HD12	1.98	0.45
7:o:601:ASN:HB3	7:o:988:TRP:CE3	2.51	0.45
7:o:631:GLU:HG2	7:o:988:TRP:CZ2	2.52	0.45
7:o:1243:LEU:HD11	7:o:1288:ILE:HD13	1.99	0.45
7:o:1479:LYS:HD2	12:t:103:PRO:HA	1.98	0.45
9:q:103:LEU:O	9:q:160:ARG:HA	2.17	0.45
7:o:123:ASN:HD21	7:o:125:LYS:HB2	1.81	0.45
7:o:548:PHE:HE1	7:o:555:LEU:HD11	1.81	0.45
7:o:569:THR:HG23	7:o:671:ASN:HD21	1.80	0.45
10:r:37:VAL:O	10:r:41:LEU:HG	2.16	0.45
12:t:46:GLN:N	12:t:116:GLU:HA	2.32	0.45
12:t:81:VAL:HG23	12:t:96:GLU:HG2	1.96	0.45
7:o:357:LYS:HD2	8:p:1107:LEU:O	2.17	0.45
7:o:381:PRO:HB3	7:o:480:SER:HA	1.98	0.45
13:u:79:PRO:HG3	13:u:104:MET:SD	2.56	0.45
7:o:733:LEU:HA	7:o:736:THR:HG22	1.99	0.45
7:o:769:MET:SD	8:p:973:PRO:HG3	2.57	0.45
8:p:569:VAL:HG13	8:p:570:ASN:N	2.32	0.45
17:y:84:GLN:O	17:y:88:THR:HG23	2.16	0.45
7:o:865:ILE:HG21	8:p:1092:ASP:CG	2.41	0.45
7:o:1318:LYS:HE2	7:o:1330:ALA:HB1	1.98	0.45
7:o:1434:GLU:C	7:o:1435:THR:HG1	2.22	0.45
7:o:1440:MET:SD	8:p:1167:ILE:HD11	2.56	0.45
7:o:1487:PRO:HD2	12:t:79:VAL:H	1.82	0.45
8:p:561:ILE:HG21	8:p:610:ARG:CB	2.47	0.45
7:o:194:SER:HB3	7:o:199:TYR:HE2	1.81	0.45
7:o:913:ASN:OD1	7:o:963:ARG:NH1	2.49	0.45
8:p:422:PHE:HB3	8:p:428:ASP:O	2.16	0.45
9:q:240:ARG:O	9:q:243:THR:HG22	2.16	0.45
7:o:155:GLU:H	7:o:181:HIS:CD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:727:PRO:HA	7:o:736:THR:HG21	1.98	0.45
8:p:569:VAL:HG12	8:p:572:CYS:HB2	1.97	0.45
8:p:926:VAL:CG2	9:q:62:GLU:HG3	2.39	0.45
8:p:968:ASN:OD1	8:p:969:PRO:HD2	2.16	0.45
10:r:23:PRO:HG2	10:r:26:PHE:HB2	1.98	0.45
7:o:1474:LEU:HB2	12:t:105:ILE:HG13	1.98	0.45
7:o:721:HIS:CE1	15:w:98:GLN:HE21	2.31	0.45
8:p:1038:THR:HA	9:q:195:THR:HA	1.99	0.45
9:q:13:GLU:HB2	9:q:20:LYS:HB2	1.98	0.45
7:o:469:MET:HE1	8:p:1086:PHE:CZ	2.52	0.44
2:S:172:ASN:HB2	7:o:1280:ASP:OD1	2.17	0.44
5:Y:-5:DG:H2'	5:Y:-4:DT:H71	1.98	0.44
7:o:226:LYS:HG2	7:o:246:GLU:OE1	2.18	0.44
7:o:948:ILE:HG23	7:o:1007:ILE:HG13	1.99	0.44
8:p:643:LEU:O	8:p:646:ARG:HB2	2.17	0.44
8:p:1007:ASN:HB2	8:p:1010:LYS:HG3	1.99	0.44
11:s:160:LEU:HD11	11:s:167:GLU:HG2	1.98	0.44
15:w:12:VAL:HG23	15:w:50:ASN:HD21	1.82	0.44
15:w:22:ASN:ND2	15:w:41:ASN:HD22	2.15	0.44
7:o:952:LEU:HD21	7:o:1006:PRO:HB2	1.99	0.44
7:o:1477:ALA:O	7:o:1481:LYS:HG2	2.17	0.44
5:Y:-6:DA:H8	5:Y:-6:DA:H5''	1.83	0.44
7:o:26:LEU:HD13	7:o:31:LEU:HD21	1.98	0.44
7:o:113:PHE:CE1	7:o:186:ARG:HD2	2.52	0.44
8:p:158:SER:O	8:p:164:ASN:HB2	2.18	0.44
8:p:252:ILE:HD12	8:p:255:ARG:HD3	1.99	0.44
8:p:1028:LEU:HD23	8:p:1028:LEU:HA	1.77	0.44
7:o:18:ILE:HD11	8:p:1149:VAL:HG11	1.99	0.44
7:o:631:GLU:HG2	7:o:988:TRP:HZ2	1.81	0.44
11:s:94:MET:HE3	11:s:99:ILE:O	2.17	0.44
2:S:175:SER:O	2:S:179:GLN:HG2	2.18	0.44
5:Y:-7:DA:H2'	5:Y:-6:DA:C8	2.52	0.44
7:o:460:ARG:HB2	7:o:501:MET:SD	2.58	0.44
8:p:491:ARG:HB3	8:p:518:HIS:HB3	2.00	0.44
8:p:591:ARG:NH2	8:p:592:ARG:HE	2.13	0.44
9:q:7:PRO:HB2	17:y:101:LEU:HD13	2.00	0.44
15:w:106:ASP:OD1	15:w:106:ASP:N	2.50	0.44
7:o:517:GLU:O	7:o:523:ARG:HD2	2.17	0.44
7:o:1263:ASN:OD1	7:o:1263:ASN:N	2.45	0.44
7:o:1268:LYS:HG3	7:o:1271:GLU:OE2	2.18	0.44
8:p:1142:ASN:ND2	8:p:1145:GLN:HB2	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:s:100:THR:HA	11:s:125:TYR:HD1	1.82	0.44
7:o:860:ILE:HD11	7:o:1125:LYS:HG3	1.98	0.44
8:p:40:VAL:HG11	8:p:482:LEU:HD13	2.00	0.44
9:q:9:VAL:HG22	9:q:23:ILE:HG12	2.00	0.44
7:o:353:ASN:O	7:o:357:LYS:HE2	2.18	0.44
7:o:510:GLU:O	7:o:514:GLU:HG3	2.18	0.44
7:o:516:GLN:O	7:o:520:MET:HB2	2.17	0.44
7:o:1347:LEU:C	11:s:137:ILE:HD11	2.43	0.44
8:p:51:ILE:O	8:p:52:GLN:C	2.59	0.44
11:s:26:TYR:HA	11:s:64:HIS:HA	1.99	0.44
7:o:706:ILE:HD13	7:o:824:GLU:HB2	2.00	0.43
8:p:419:ALA:O	8:p:423:ILE:HG12	2.18	0.43
8:p:528:LEU:HA	8:p:528:LEU:HD23	1.70	0.43
8:p:831:LYS:HE3	8:p:845:TYR:O	2.17	0.43
8:p:971:ALA:O	8:p:975:ARG:HD2	2.17	0.43
11:s:63:ALA:HB1	11:s:68:PRO:HA	2.00	0.43
7:o:282:ASP:O	7:o:286:ILE:HG12	2.19	0.43
8:p:839:GLY:O	8:p:891:ASP:HB2	2.18	0.43
8:p:1072:ARG:HB2	8:p:1153:TYR:CD2	2.53	0.43
11:s:73:PHE:HE1	11:s:99:ILE:HD13	1.83	0.43
13:u:12:LEU:HD11	13:u:67:LEU:HD12	2.00	0.43
5:Y:-32:DA:H2"	5:Y:-31:DC:C5	2.53	0.43
7:o:901:VAL:HB	7:o:978:VAL:HG12	2.01	0.43
8:p:633:LEU:HD21	8:p:696:CYS:HB3	1.99	0.43
14:v:52:LEU:HD23	14:v:52:LEU:HA	1.78	0.43
7:o:210:GLN:HB2	7:o:214:ILE:HD11	1.99	0.43
8:p:542:LEU:HD22	8:p:574:VAL:HG11	1.99	0.43
11:s:90:TYR:O	11:s:94:MET:HG2	2.18	0.43
10:r:24:LYS:HA	10:r:27:GLU:CD	2.43	0.43
10:r:110:GLU:O	10:r:114:LEU:HG	2.17	0.43
10:r:121:ARG:HD3	10:r:121:ARG:HA	1.79	0.43
7:o:343:LEU:HD22	8:p:1158:LEU:HD12	2.00	0.43
7:o:821:GLY:HA2	7:o:838:PHE:CD2	2.54	0.43
7:o:910:LYS:N	7:o:911:PRO:HD2	2.34	0.43
7:o:916:PHE:CE2	7:o:960:ARG:HG2	2.53	0.43
7:o:920:PHE:CD1	7:o:959:MET:HE1	2.54	0.43
7:o:1400:LEU:O	7:o:1404:THR:HG23	2.19	0.43
8:p:237:VAL:HG11	8:p:369:VAL:HG22	2.00	0.43
8:p:264:LYS:HE2	8:p:264:LYS:HB3	1.86	0.43
8:p:961:ILE:HG23	16:x:9:THR:HG21	1.99	0.43
15:w:36:LEU:HD23	15:w:47:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:360:ASP:O	8:p:1106:ARG:NH2	2.52	0.43
8:p:169:ARG:H	8:p:169:ARG:HG3	1.68	0.43
8:p:193:VAL:HG23	8:p:470:LEU:HB2	2.01	0.43
8:p:470:LEU:HD11	8:p:478:THR:HG23	2.00	0.43
12:t:51:ARG:HD3	12:t:118:TRP:CE2	2.54	0.43
8:p:117:ASN:HA	8:p:189:GLY:HA3	2.01	0.43
8:p:296:GLU:O	8:p:300:MET:HG2	2.19	0.43
8:p:1151:MET:HE2	8:p:1155:CYS:HB3	2.00	0.43
17:y:64:PRO:HG3	17:y:70:LYS:HE2	2.01	0.43
4:X:24:DA:C6	4:X:25:DG:C6	3.07	0.43
5:Y:-22:DG:C6	5:Y:-21:DG:C6	3.07	0.43
5:Y:-15:DA:H2"	5:Y:-14:DG:C8	2.54	0.43
7:o:53:LYS:HE3	7:o:53:LYS:HB2	1.73	0.43
7:o:1215:GLU:HG2	7:o:1256:VAL:HG22	2.01	0.43
8:p:19:PRO:C	8:p:21:LEU:H	2.26	0.43
10:r:134:ILE:O	10:r:138:ARG:HG3	2.19	0.43
4:X:-3:DT:H2"	4:X:-2:DT:C7	2.47	0.43
7:o:41:ILE:HG21	7:o:57:LEU:HD23	2.00	0.43
7:o:123:ASN:ND2	7:o:125:LYS:HB2	2.34	0.43
7:o:377:GLN:HA	7:o:473:ARG:O	2.19	0.43
8:p:818:GLU:O	8:p:916:TYR:HB3	2.19	0.43
16:x:22:LEU:O	16:x:26:GLN:HG2	2.19	0.43
1:N:1:ILX:CG2	7:o:791:GLN:HE22	2.28	0.42
2:S:177:MET:HG2	15:w:40:ARG:O	2.19	0.42
5:Y:-37:DT:H2"	5:Y:-36:DA:C8	2.53	0.42
7:o:112:PHE:HD1	7:o:113:PHE:CD2	2.37	0.42
7:o:362:SER:HA	7:o:503:LEU:O	2.19	0.42
7:o:936:GLU:HA	7:o:939:VAL:HG12	2.01	0.42
7:o:1416:ARG:HB3	7:o:1433:GLU:OE1	2.19	0.42
7:o:1421:ARG:HA	7:o:1421:ARG:HD3	1.86	0.42
8:p:65:ILE:HG23	8:p:416:ARG:HD3	2.01	0.42
8:p:565:THR:HA	8:p:610:ARG:C	2.43	0.42
8:p:809:VAL:HG21	9:q:60:HIS:CE1	2.53	0.42
11:s:114:ALA:O	11:s:117:SER:HB2	2.19	0.42
8:p:785:TYR:CZ	8:p:955:PRO:HD3	2.54	0.42
10:r:111:SER:HB2	10:r:131:LEU:HD21	2.01	0.42
13:u:84:VAL:HA	13:u:145:LEU:O	2.20	0.42
13:u:87:ALA:HB2	13:u:101:ILE:HG12	2.00	0.42
7:o:102:LYS:HB3	7:o:102:LYS:HE3	1.79	0.42
7:o:457:ILE:HG12	7:o:515:ILE:HD13	2.01	0.42
7:o:668:PHE:CZ	7:o:672:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:1289:GLU:O	7:o:1293:LEU:HG	2.19	0.42
8:p:674:MET:HE2	8:p:690:CYS:SG	2.59	0.42
9:q:44:ILE:HG12	9:q:45:ILE:N	2.34	0.42
9:q:173:HIS:ND1	9:q:175:LYS:HB3	2.33	0.42
8:p:815:LYS:HG2	8:p:920:LYS:HE2	2.02	0.42
8:p:955:PRO:HB2	8:p:1028:LEU:HD13	2.00	0.42
11:s:106:VAL:HG21	11:s:110:MET:HG3	2.02	0.42
2:S:43:ASN:OD1	2:S:44:GLN:N	2.52	0.42
7:o:212:LYS:H	7:o:212:LYS:HD3	1.83	0.42
7:o:379:GLY:O	7:o:482:PHE:HA	2.19	0.42
7:o:515:ILE:HD11	8:p:1102:PHE:CD1	2.55	0.42
7:o:1153:ARG:O	7:o:1157:ILE:HG12	2.20	0.42
8:p:204:THR:HG22	8:p:615:TYR:OH	2.20	0.42
8:p:608:ARG:O	8:p:609:GLU:HB2	2.19	0.42
11:s:61:LEU:HD13	11:s:73:PHE:CE1	2.55	0.42
13:u:25:THR:O	13:u:29:LYS:HG2	2.20	0.42
13:u:104:MET:HE2	13:u:104:MET:HB3	1.92	0.42
13:u:152:VAL:HG22	13:u:157:ILE:HG12	2.00	0.42
7:o:34:MET:HE2	7:o:34:MET:HB3	1.92	0.42
7:o:983:LEU:HD12	7:o:1044:HIS:CD2	2.55	0.42
7:o:1282:ASP:N	7:o:1282:ASP:OD1	2.52	0.42
8:p:780:VAL:HA	8:p:965:ILE:O	2.18	0.42
8:p:792:ASP:O	8:p:943:GLY:HA3	2.19	0.42
8:p:1032:PHE:HA	9:q:36:ARG:HH21	1.85	0.42
9:q:190:ASN:HD22	9:q:217:GLN:NE2	2.17	0.42
4:X:-1:DC:H2"	4:X:0:DA:N7	2.35	0.42
7:o:15:LEU:HD11	8:p:1150:ARG:HG3	2.02	0.42
8:p:603:MET:HE3	8:p:603:MET:HB2	1.89	0.42
8:p:629:GLU:HG3	8:p:634:LEU:HD21	2.02	0.42
8:p:721:ARG:HD3	8:p:721:ARG:HA	1.84	0.42
7:o:93:PRO:HB2	7:o:218:PRO:HB2	2.00	0.42
8:p:761:THR:HG23	8:p:1000:THR:HA	2.02	0.42
17:y:58:PHE:HB3	17:y:76:GLN:HB3	2.02	0.42
7:o:1184:THR:HG21	7:o:1190:GLN:HA	2.01	0.42
8:p:185:PHE:HB2	8:p:187:ILE:HD11	2.02	0.42
8:p:591:ARG:HH12	8:p:592:ARG:NE	2.17	0.42
9:q:59:LEU:HD13	9:q:63:PHE:CD1	2.55	0.42
9:q:78:ILE:HD11	9:q:127:VAL:CG2	2.49	0.42
7:o:853:LYS:HA	7:o:1104:LEU:HD21	2.00	0.42
4:X:-2:DT:H2"	4:X:-1:DC:C6	2.54	0.41
4:X:33:DG:H2"	4:X:34:DC:C5	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:2500:W0F:O32	8:p:975:ARG:CZ	2.68	0.41
7:o:788:VAL:HG21	7:o:831:LEU:HD21	2.01	0.41
7:o:992:LYS:HA	7:o:992:LYS:HD3	1.84	0.41
8:p:628:VAL:HG21	8:p:683:GLN:NE2	2.35	0.41
9:q:154:ARG:HG2	9:q:155:LYS:N	2.35	0.41
14:v:76:ASN:HB3	14:v:79:ASP:HB2	2.01	0.41
2:S:47:LEU:HD11	2:S:98:TRP:HB3	2.01	0.41
3:T:9:LEU:O	3:T:13:LYS:HG2	2.20	0.41
7:o:102:LYS:HZ1	7:o:141:LEU:HD13	1.85	0.41
8:p:568:PHE:HB2	8:p:613:ARG:HA	2.01	0.41
8:p:712:PRO:O	8:p:939:HIS:HE1	2.02	0.41
13:u:101:ILE:HD11	13:u:145:LEU:HD11	2.01	0.41
14:v:36:LYS:HA	14:v:36:LYS:HD2	1.84	0.41
2:S:111:LYS:O	2:S:146:PHE:HA	2.20	0.41
7:o:107:LEU:HD21	7:o:221:VAL:HG13	2.02	0.41
7:o:745:LEU:HD21	7:o:817:PRO:HB3	2.01	0.41
7:o:1118:THR:HG21	7:o:1135:LYS:HB2	2.02	0.41
7:o:1139:LEU:HD12	7:o:1358:THR:O	2.19	0.41
7:o:1175:ILE:HG12	7:o:1212:LEU:HD12	2.02	0.41
7:o:1206:ARG:HA	7:o:1206:ARG:HD3	1.74	0.41
8:p:289:ILE:HD11	8:p:301:VAL:HG21	2.02	0.41
9:q:101:PHE:HZ	9:q:127:VAL:HG12	1.86	0.41
1:N:2:TRX:O	7:o:790:GLN:N	2.53	0.41
7:o:589:LYS:HZ1	7:o:625:ASP:CG	2.29	0.41
8:p:108:MET:O	8:p:120:TYR:HE1	2.03	0.41
11:s:7:THR:HG21	11:s:41:LYS:HG2	2.01	0.41
13:u:8:GLU:OE1	13:u:71:LYS:HG2	2.20	0.41
14:v:65:TYR:HD1	14:v:84:ARG:HG2	1.85	0.41
17:y:11:LEU:HD23	17:y:11:LEU:HA	1.96	0.41
17:y:47:LYS:HD3	17:y:61:TYR:HD1	1.86	0.41
4:X:36:DT:H2"	4:X:37:DA:N7	2.36	0.41
7:o:1243:LEU:HD21	7:o:1288:ILE:HG21	2.02	0.41
14:v:56:PHE:HE1	14:v:58:LEU:HD13	1.86	0.41
14:v:60:ILE:HG23	14:v:141:VAL:HG13	2.03	0.41
3:T:43:LEU:HD12	3:T:55:SER:O	2.21	0.41
7:o:18:ILE:H	7:o:1462:GLN:NE2	2.18	0.41
7:o:154:CYS:O	7:o:185:GLY:HA2	2.20	0.41
7:o:811:ILE:HG13	8:p:689:TYR:CE2	2.55	0.41
7:o:1212:LEU:HD23	7:o:1259:ILE:HD12	2.02	0.41
8:p:298:MET:HB3	15:w:14:ILE:HD12	2.03	0.41
8:p:715:ASP:OD1	8:p:715:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:u:118:GLU:O	13:u:128:TYR:HA	2.21	0.41
4:X:16:DT:H4'	7:o:1417:HIS:ND1	2.35	0.41
7:o:885:GLN:HE22	7:o:1408:ARG:HH12	1.69	0.41
8:p:446:TYR:CD2	8:p:456:GLN:HG2	2.55	0.41
12:t:94:MET:HE3	12:t:94:MET:HB3	1.96	0.41
7:o:106:VAL:O	7:o:110:VAL:HG23	2.19	0.41
8:p:235:ILE:HG21	8:p:348:LEU:HD12	2.03	0.41
8:p:403:LEU:HD22	8:p:453:TRP:CZ2	2.55	0.41
8:p:473:LEU:HD22	8:p:1052:LYS:HD3	2.02	0.41
8:p:764:MET:HE1	8:p:938:ARG:NH1	2.36	0.41
8:p:795:ILE:HB	8:p:966:ILE:HB	2.03	0.41
8:p:855:ALA:HA	18:z:46:LYS:HG2	2.02	0.41
9:q:49:TRP:CE3	9:q:164:TYR:HD2	2.38	0.41
9:q:63:PHE:CE1	9:q:67:ARG:HD2	2.56	0.41
9:q:73:LEU:HD23	9:q:129:PRO:HA	2.03	0.41
14:v:41:LEU:HG	14:v:43:VAL:HG23	2.01	0.41
15:w:99:SER:HA	15:w:111:TYR:HE2	1.86	0.41
4:X:17:DC:H2''	4:X:18:DG:C8	2.55	0.41
5:Y:-25:DC:H2''	5:Y:-24:DT:C5'	2.51	0.41
7:o:514:GLU:CD	8:p:1101:GLN:HB3	2.46	0.41
7:o:552:ASP:CG	14:v:22:PHE:HB3	2.45	0.41
7:o:823:VAL:HG11	7:o:831:LEU:HD22	2.02	0.41
7:o:1128:ILE:HD11	7:o:1401:LEU:HD21	2.03	0.41
7:o:1160:ARG:O	7:o:1300:GLY:HA2	2.20	0.41
8:p:479:LEU:O	8:p:483:ARG:HG3	2.21	0.41
8:p:725:GLN:HA	8:p:728:MET:HE2	2.03	0.41
8:p:794:VAL:HG13	8:p:965:ILE:HG23	2.03	0.41
8:p:1102:PHE:CE1	8:p:1106:ARG:HD3	2.56	0.41
14:v:48:TYR:OH	14:v:147:LYS:HG3	2.21	0.41
2:S:172:ASN:O	2:S:176:ILE:HG12	2.21	0.41
7:o:717:ILE:HG12	7:o:737:PHE:CZ	2.56	0.41
7:o:811:ILE:HD11	8:p:690:CYS:HB2	2.03	0.41
8:p:132:VAL:O	8:p:139:GLN:HA	2.21	0.41
8:p:230:ARG:O	8:p:231:PRO:C	2.64	0.41
8:p:737:ILE:HG22	8:p:738:THR:N	2.36	0.41
9:q:188:PRO:HD3	9:q:230:TYR:HE2	1.86	0.41
18:z:36:CYS:HB3	18:z:39:CYS:SG	2.61	0.41
8:p:131:THR:HG22	8:p:141:GLN:HB3	2.03	0.40
8:p:425:ARG:HB3	8:p:427:LYS:HE3	2.03	0.40
8:p:646:ARG:HG3	8:p:651:TYR:O	2.21	0.40
8:p:861:SER:O	8:p:896:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:1029:TYR:CE2	8:p:1036:LYS:HG2	2.56	0.40
13:u:31:PHE:O	13:u:35:GLU:HB2	2.21	0.40
2:S:164:TRP:CH2	2:S:167:ARG:HD3	2.56	0.40
7:o:256:PRO:HB2	7:o:260:VAL:HB	2.03	0.40
7:o:267:GLN:C	7:o:269:SER:H	2.29	0.40
7:o:472:HIS:CE1	7:o:521:VAL:HG21	2.57	0.40
7:o:784:VAL:HG13	8:p:978:ILE:CD1	2.51	0.40
7:o:1234:LYS:HZ3	7:o:1298:LEU:C	2.28	0.40
11:s:63:ALA:HA	11:s:71:GLN:HA	2.02	0.40
11:s:64:HIS:HD2	11:s:66:ASP:HB2	1.86	0.40
3:T:30:GLN:O	3:T:62:LEU:HD11	2.22	0.40
7:o:58:MET:HE3	7:o:65:ILE:HD13	2.02	0.40
7:o:92:LYS:HE2	7:o:307:VAL:HG21	2.04	0.40
7:o:346:LYS:HE2	7:o:346:LYS:HB3	1.92	0.40
8:p:136:GLY:O	8:p:137:GLU:HG2	2.22	0.40
10:r:41:LEU:HD22	10:r:61:PHE:CE2	2.56	0.40
11:s:55:ARG:HB2	11:s:78:GLU:HG2	2.02	0.40
12:t:81:VAL:HG21	12:t:96:GLU:HA	2.03	0.40
14:v:15:ILE:HD11	14:v:51:ASP:HA	2.01	0.40
7:o:40:GLY:HA2	7:o:87:HIS:O	2.20	0.40
8:p:42:GLN:HG3	8:p:43:GLN:H	1.86	0.40
8:p:52:GLN:O	8:p:53:MET:C	2.65	0.40
8:p:497:LYS:HA	8:p:497:LYS:HD2	1.75	0.40
8:p:576:ILE:HD13	8:p:576:ILE:HG21	1.69	0.40
8:p:1053:HIS:HB3	8:p:1058:LYS:HE3	2.03	0.40
7:o:376:ASP:N	7:o:376:ASP:OD1	2.52	0.40
7:o:713:VAL:O	7:o:717:ILE:HG13	2.21	0.40
7:o:1158:LEU:HG	7:o:1307:VAL:HB	2.04	0.40
7:o:1486:ILE:HB	7:o:1487:PRO:HD3	2.03	0.40
8:p:41:ARG:O	8:p:45:ASP:HB2	2.22	0.40
8:p:719:SER:OG	8:p:720:PRO:HD3	2.21	0.40
9:q:36:ARG:HD3	17:y:41:THR:OG1	2.21	0.40
9:q:71:ILE:HD11	9:q:150:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
2	S	134/517 (26%)	134 (100%)	0	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1395 (96%)	51 (4%)	2 (0%)	48	75
8	p	1142/1174 (97%)	1076 (94%)	64 (6%)	2 (0%)	43	70
9	q	253/275 (92%)	244 (96%)	9 (4%)	0	100	100
10	r	126/142 (89%)	126 (100%)	0	0	100	100
11	s	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
12	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
13	u	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
14	v	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	18	44
15	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	3	10
17	y	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
18	z	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
All	All	4140/5361 (77%)	3970 (96%)	163 (4%)	7 (0%)	44	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	549	SER
14	v	34	SER
16	x	6	ARG
7	o	184	CYS
8	p	614	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	2/2 (100%)	2 (100%)	0	100	100
2	S	121/448 (27%)	120 (99%)	1 (1%)	73	89
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1257 (98%)	23 (2%)	51	79
8	p	1001/1027 (98%)	984 (98%)	17 (2%)	53	80
9	q	234/252 (93%)	230 (98%)	4 (2%)	53	80
10	r	118/126 (94%)	118 (100%)	0	100	100
11	s	191/192 (100%)	191 (100%)	0	100	100
12	t	71/111 (64%)	71 (100%)	0	100	100
13	u	152/153 (99%)	151 (99%)	1 (1%)	76	90
14	v	129/131 (98%)	127 (98%)	2 (2%)	55	81
15	w	103/112 (92%)	102 (99%)	1 (1%)	68	86
16	x	56/56 (100%)	55 (98%)	1 (2%)	51	79
17	y	104/106 (98%)	103 (99%)	1 (1%)	68	86
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3637 (99%)	51 (1%)	57	82

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	170	VAL
7	o	46	THR
7	o	48	GLU
7	o	184	CYS
7	o	227	ARG
7	o	302	VAL
7	o	484	LEU
7	o	488	VAL
7	o	490	THR
7	o	495	ASP

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Mol	Chain	Res	Type
7	o	503	LEU
7	o	534	VAL
7	o	626	THR
7	o	636	ILE
7	o	675	VAL
7	o	676	ILE
7	o	689	ILE
7	o	695	ASP
7	o	863	ARG
7	o	1087	VAL
7	o	1207	ILE
7	o	1279	MET
7	o	1385	VAL
7	o	1458	ILE
8	p	18	THR
8	p	42	GLN
8	p	51	ILE
8	p	59	VAL
8	p	235	ILE
8	p	292	PHE
8	p	423	ILE
8	p	447	SER
8	p	466	VAL
8	p	471	ASN
8	p	598	VAL
8	p	737	ILE
8	p	860	VAL
8	p	866	ILE
8	p	908	MET
8	p	909	VAL
8	p	1067	ILE
9	q	13	GLU
9	q	44	ILE
9	q	75	SER
9	q	94	CYS
13	u	85	VAL
14	v	47	ILE
14	v	58	LEU
15	w	95	VAL
16	x	14	VAL
17	y	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76)

such sidechains are listed below:

Mol	Chain	Res	Type
2	S	44	GLN
2	S	178	GLN
3	T	59	ASN
3	T	64	ASN
7	o	62	GLN
7	o	181	HIS
7	o	341	GLN
7	o	449	HIS
7	o	531	ASN
7	o	539	GLN
7	o	599	HIS
7	o	671	ASN
7	o	721	HIS
7	o	780	ASN
7	o	791	GLN
7	o	792	ASN
7	o	804	HIS
7	o	904	GLN
7	o	1032	GLN
7	o	1044	HIS
7	o	1082	HIS
7	o	1093	GLN
7	o	1163	HIS
7	o	1190	GLN
7	o	1230	GLN
7	o	1384	HIS
7	o	1410	HIS
7	o	1422	GLN
7	o	1445	HIS
7	o	1462	GLN
8	p	43	GLN
8	p	68	GLN
8	p	117	ASN
8	p	144	HIS
8	p	164	ASN
8	p	245	GLN
8	p	312	GLN
8	p	387	HIS
8	p	430	ASN
8	p	452	ASN
8	p	481	HIS
8	p	500	GLN

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Mol	Chain	Res	Type
8	p	518	HIS
8	p	525	ASN
8	p	639	HIS
8	p	699	HIS
8	p	717	ASN
8	p	725	GLN
8	p	755	GLN
8	p	797	ASN
8	p	838	GLN
8	p	941	GLN
8	p	948	GLN
8	p	986	GLN
8	p	1071	ASN
8	p	1094	GLN
8	p	1142	ASN
9	q	18	ASN
9	q	190	ASN
9	q	232	ASN
9	q	262	GLN
9	q	265	HIS
10	r	66	ASN
10	r	129	GLN
11	s	35	GLN
11	s	64	HIS
12	t	46	GLN
13	u	14	HIS
13	u	53	ASN
14	v	131	ASN
14	v	133	HIS
15	w	41	ASN
15	w	118	HIS
17	y	49	GLN
17	y	69	HIS
17	y	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	10/11 (90%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	4	A
6	Z	11	G2L

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	Z	1	ATP

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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
6	G2L	Z	11	5,21,6	23,26,30	1.38	4 (17%)	31,38,44	3.15	15 (48%)
1	HYP	N	8	1	7,8,9	0.84	0	5,10,12	2.35	2 (40%)
1	TRX	N	2	1	15,16,17	1.12	1 (6%)	17,22,24	0.97	0
1	CSX	N	6	1	3,6,7	1.08	0	1,6,8	2.10	1 (100%)
1	ILX	N	1	1	8,9,10	0.61	0	8,11,13	1.41	1 (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
6	G2L	Z	11	5,21,6	-	2/9/27/31	0/3/3/3
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1
1	TRX	N	2	1	-	2/5/6/8	0/2/2/2
1	CSX	N	6	1	-	2/2/5/7	-
1	ILX	N	1	1	-	7/11/12/14	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	11	G2L	C5-C4	3.11	1.47	1.38
6	Z	11	G2L	C6-N1	-2.42	1.34	1.38
1	N	2	TRX	CD2-CE2	2.40	1.44	1.41
6	Z	11	G2L	O4'-C4'	-2.31	1.39	1.45
6	Z	11	G2L	C5-N7	-2.14	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	11	G2L	O4'-C4'-C5'	-6.90	87.22	109.33
6	Z	11	G2L	O4'-C1'-N9	6.66	123.44	108.36
6	Z	11	G2L	C5-C4-N3	-6.17	118.57	128.39
6	Z	11	G2L	C2-N3-C4	5.10	121.09	112.30
6	Z	11	G2L	O2'-C2'-C1'	-4.88	93.32	110.10
6	Z	11	G2L	N9-C4-N3	4.34	134.63	125.95
6	Z	11	G2L	C4'-O4'-C1'	3.85	117.98	109.47
6	Z	11	G2L	C2'-C1'-N9	-3.67	103.04	113.25
6	Z	11	G2L	C5'-C4'-C3'	3.55	126.19	114.38
6	Z	11	G2L	C6-C5-N7	3.41	136.49	130.29
1	N	8	HYP	CB-CG-CD	3.39	106.94	103.16
1	N	8	HYP	O-C-CA	-3.33	116.20	124.77
1	N	1	ILX	OD1-CD1-CG1	-3.06	104.74	111.16
6	Z	11	G2L	O4'-C1'-C2'	-3.02	100.16	106.62
6	Z	11	G2L	C4-C5-N7	-2.76	106.30	110.67
6	Z	11	G2L	O4'-C4'-C3'	-2.58	99.48	104.92
6	Z	11	G2L	O2'-C2'-C3'	2.52	118.25	111.19
1	N	6	CSX	CA-CB-SG	2.10	118.11	113.17
6	Z	11	G2L	O6-C6-C5	-2.07	121.06	126.53

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	ILX	C-CA-CB-CG2
1	N	1	ILX	OD1-CD1-CG1-CB
1	N	1	ILX	OD1-CD1-CG1-OG1
1	N	6	CSX	N-CA-CB-SG
1	N	6	CSX	C-CA-CB-SG
1	N	2	TRX	CA-CB-CG-CD2
6	Z	11	G2L	O4'-C4'-C5'-O5'
1	N	2	TRX	CA-CB-CG-CD1
1	N	1	ILX	C-CA-CB-CG1

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Mol	Chain	Res	Type	Atoms
6	Z	11	G2L	C4'-C5'-O5'-P
1	N	1	ILX	N-CA-CB-CG2
1	N	1	ILX	CG2-CB-CG1-CD1
1	N	1	ILX	CG2-CB-CG1-OG1

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	11	G2L	1	0
1	N	2	TRX	2	0
1	N	1	ILX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	$\# Z > 2$
19	W0F	Z	2500	-	34,35,35	4.06	14 (41%)	43,55,55	3.45	17 (39%)

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
19	W0F	Z	2500	-	-	3/24/40/40	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	2500	W0F	P26-O29	13.80	1.74	1.59
19	Z	2500	W0F	C03-C04	-9.77	1.27	1.52
19	Z	2500	W0F	P22-O25	8.44	1.68	1.59
19	Z	2500	W0F	O05-C04	6.86	1.60	1.45
19	Z	2500	W0F	O05-C06	-6.01	1.28	1.42
19	Z	2500	W0F	C12-C13	5.67	1.47	1.38
19	Z	2500	W0F	P26-O25	5.30	1.65	1.59
19	Z	2500	W0F	C13-N09	-3.12	1.34	1.37
19	Z	2500	W0F	C07-C03	-2.96	1.46	1.53
19	Z	2500	W0F	C20-C04	2.56	1.59	1.51
19	Z	2500	W0F	C06-N09	2.32	1.54	1.47
19	Z	2500	W0F	P22-O21	2.16	1.67	1.59
19	Z	2500	W0F	C12-N11	-2.12	1.34	1.39
19	Z	2500	W0F	C17-N16	-2.08	1.34	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	2500	W0F	O05-C06-N09	-14.54	75.41	108.36
19	Z	2500	W0F	C07-C06-N09	8.28	136.30	113.25
19	Z	2500	W0F	O05-C04-C03	-5.80	92.69	104.92
19	Z	2500	W0F	O27-P26-O25	-5.27	93.03	107.27
19	Z	2500	W0F	O05-C04-C20	4.93	125.14	109.33
19	Z	2500	W0F	O05-C06-C07	-4.16	97.71	106.62
19	Z	2500	W0F	O21-C20-C04	3.98	122.53	108.99
19	Z	2500	W0F	O32-P30-O29	3.90	117.72	104.64
19	Z	2500	W0F	O33-P30-O31	-3.36	97.74	110.83
19	Z	2500	W0F	C06-N09-C10	-3.25	117.50	126.73
19	Z	2500	W0F	O08-C07-C06	2.82	119.83	110.10
19	Z	2500	W0F	O33-P30-O29	2.65	113.53	104.64
19	Z	2500	W0F	O21-P22-O24	-2.28	99.89	108.94
19	Z	2500	W0F	O29-P26-O28	2.26	117.52	110.70
19	Z	2500	W0F	O27-P26-O29	2.16	113.10	107.27
19	Z	2500	W0F	C13-C12-N11	-2.09	106.55	109.26
19	Z	2500	W0F	C10-N09-C13	2.08	108.42	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Z	2500	W0F	C20-O21-P22-O24

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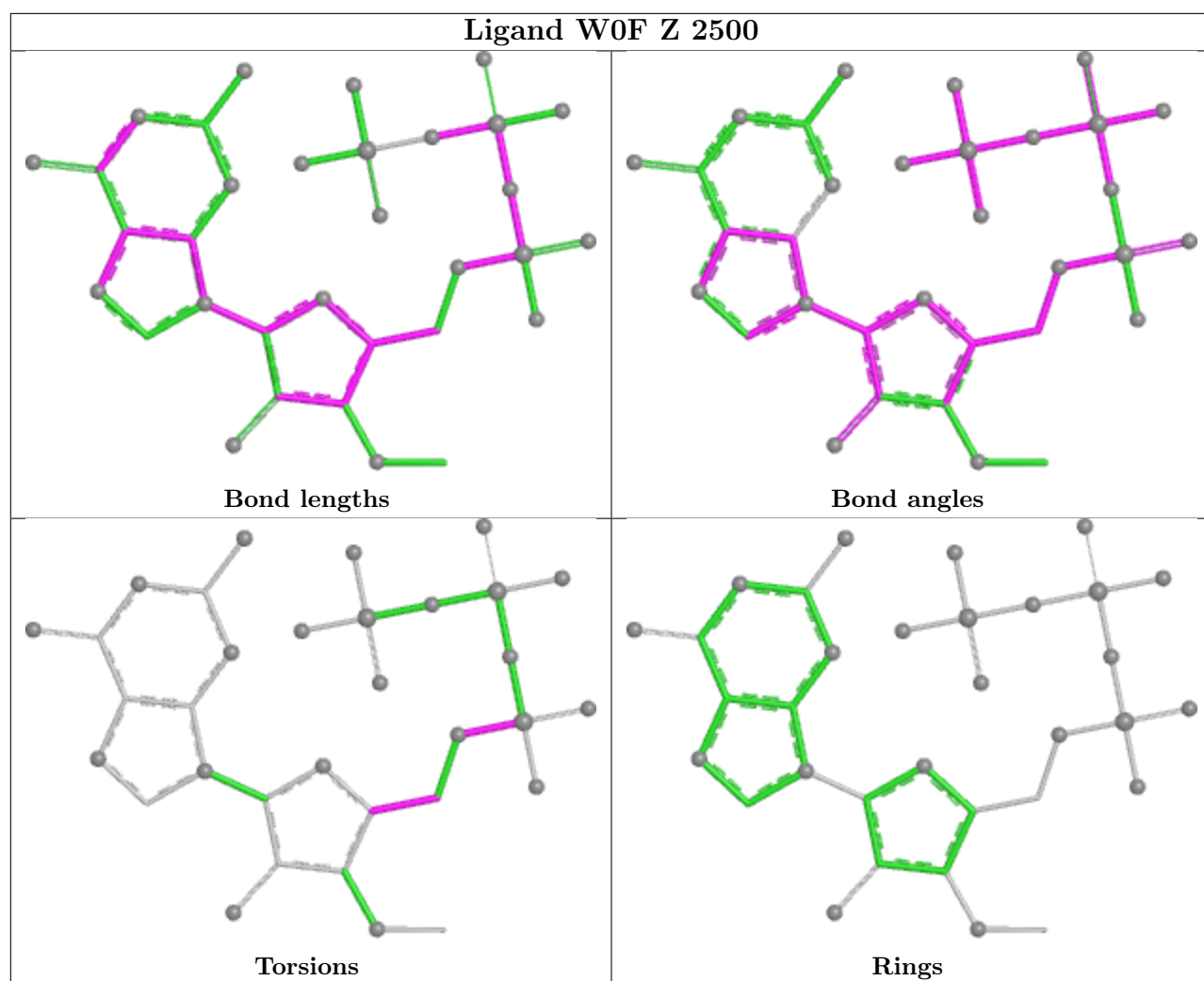
Mol	Chain	Res	Type	Atoms
19	Z	2500	W0F	C20-O21-P22-O25
19	Z	2500	W0F	C03-C04-C20-O21

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	2500	W0F	6	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 than 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.



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.

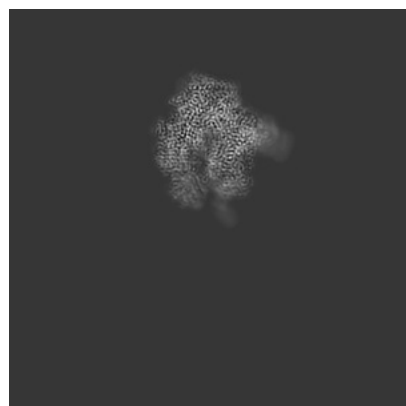
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37405. These allow visual inspection of the internal detail of the map and identification of artifacts.

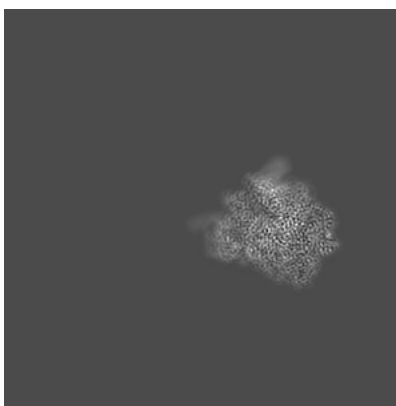
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

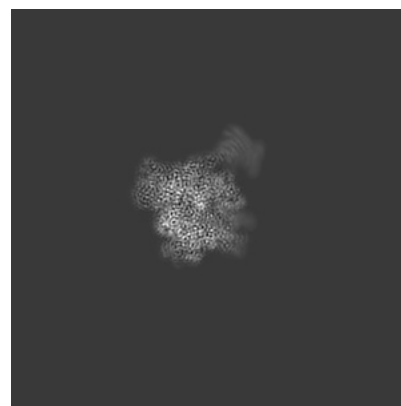
6.1.1 Primary map



X

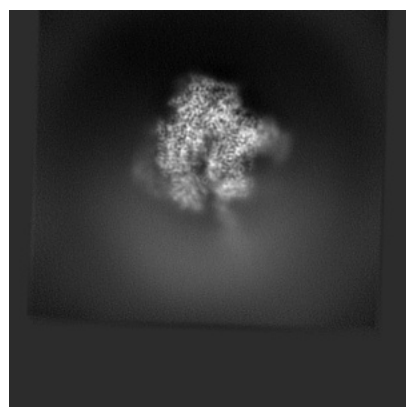


Y

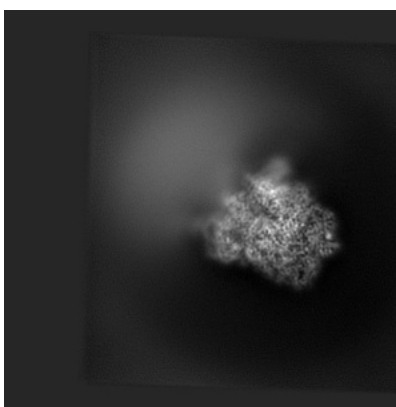


Z

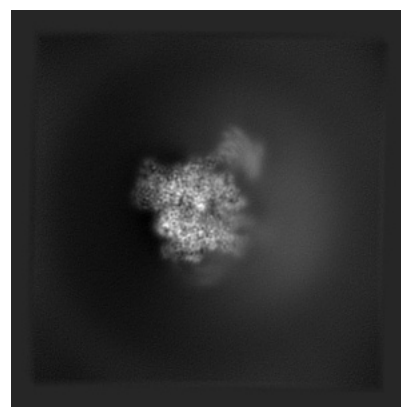
6.1.2 Raw map



X



Y

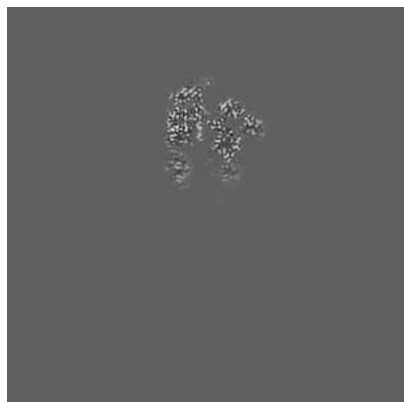


Z

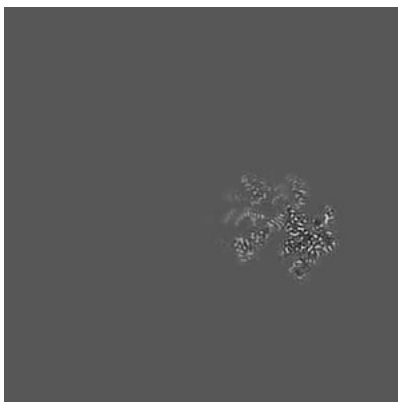
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

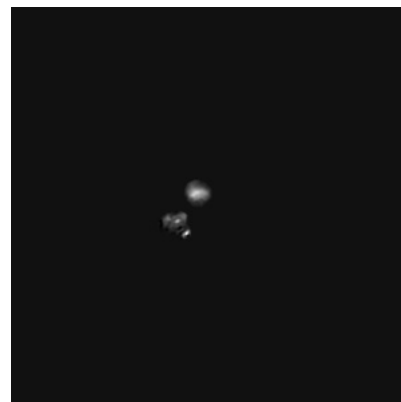
6.2.1 Primary map



X Index: 160

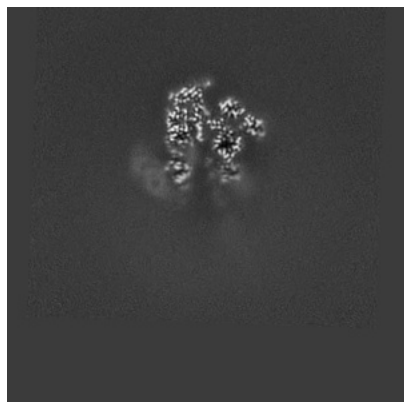


Y Index: 160

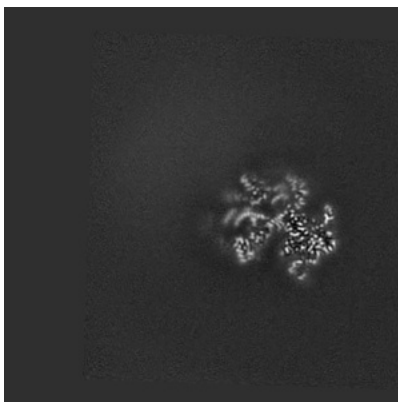


Z Index: 160

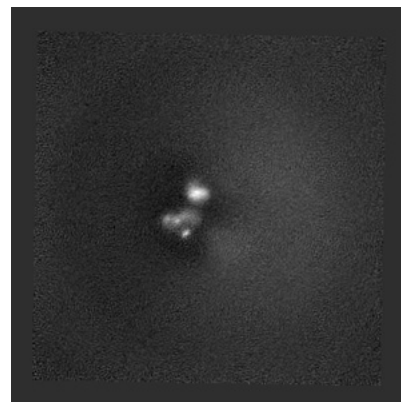
6.2.2 Raw map



X Index: 160



Y Index: 160

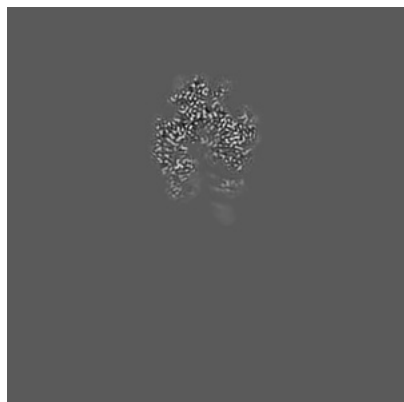


Z Index: 160

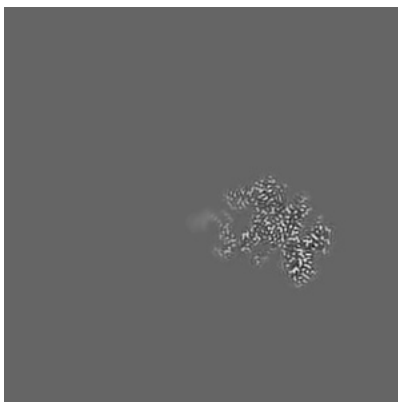
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

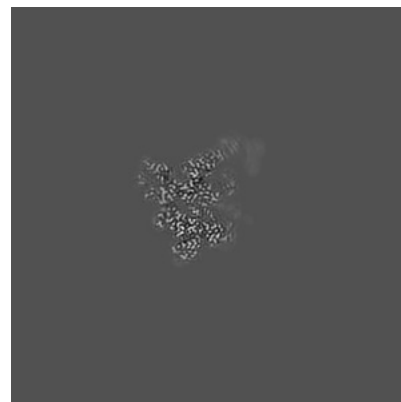
6.3.1 Primary map



X Index: 144

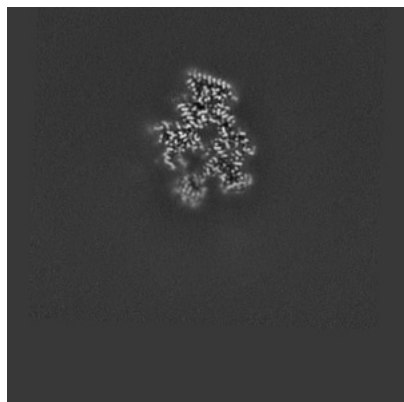


Y Index: 172

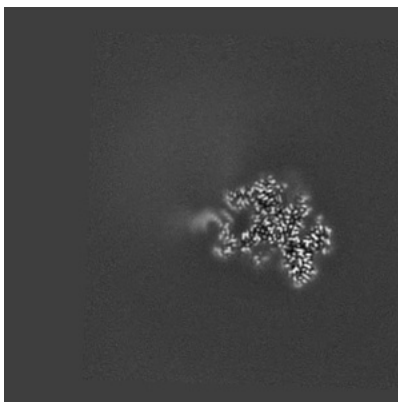


Z Index: 224

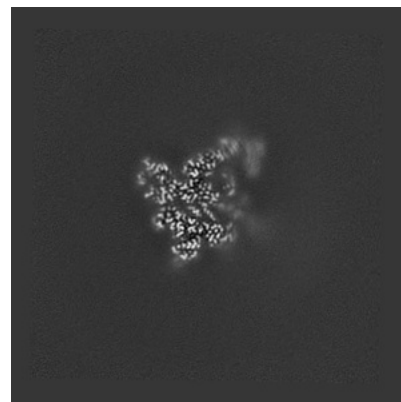
6.3.2 Raw map



X Index: 133



Y Index: 172

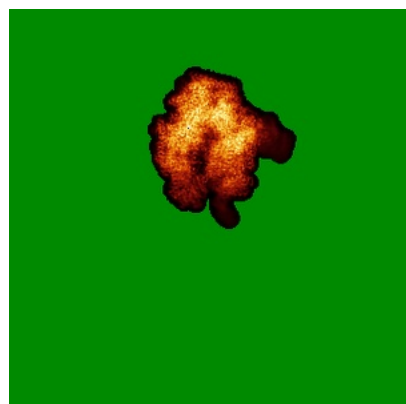


Z Index: 224

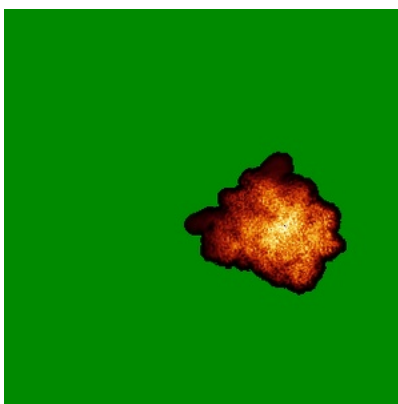
The images above show the largest variance slices of the map in three orthogonal directions.

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

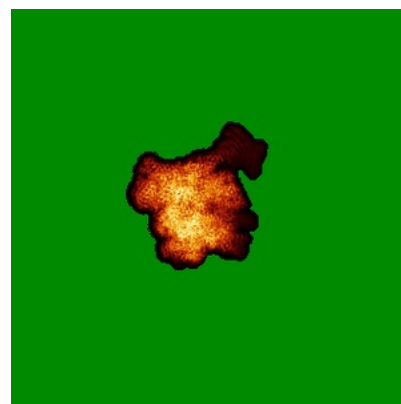
6.4.1 Primary map



X



Y

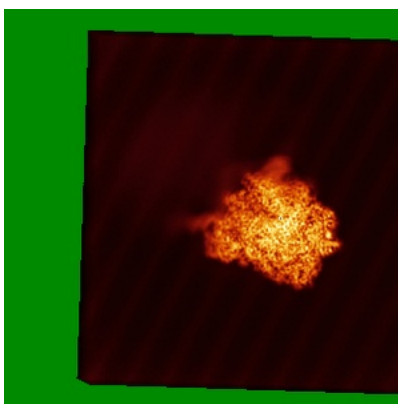


Z

6.4.2 Raw map



X



Y

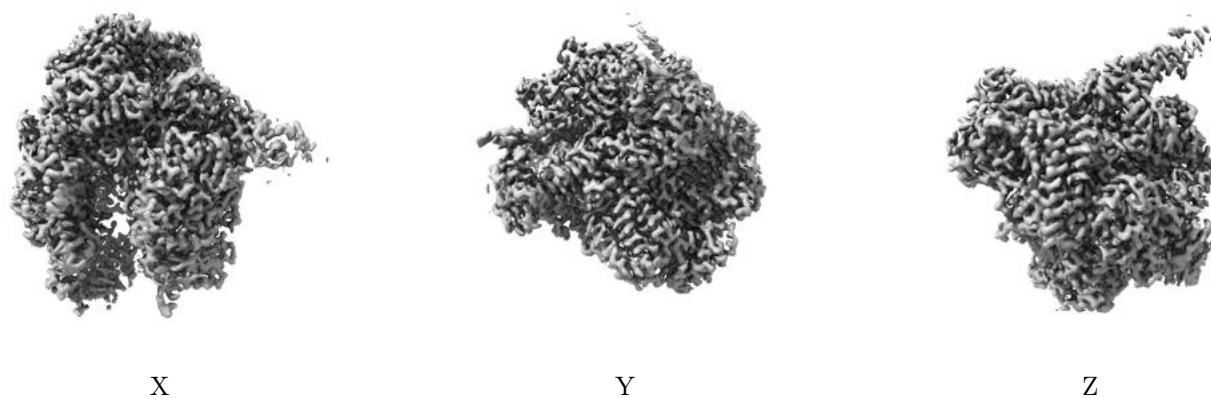


Z

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.

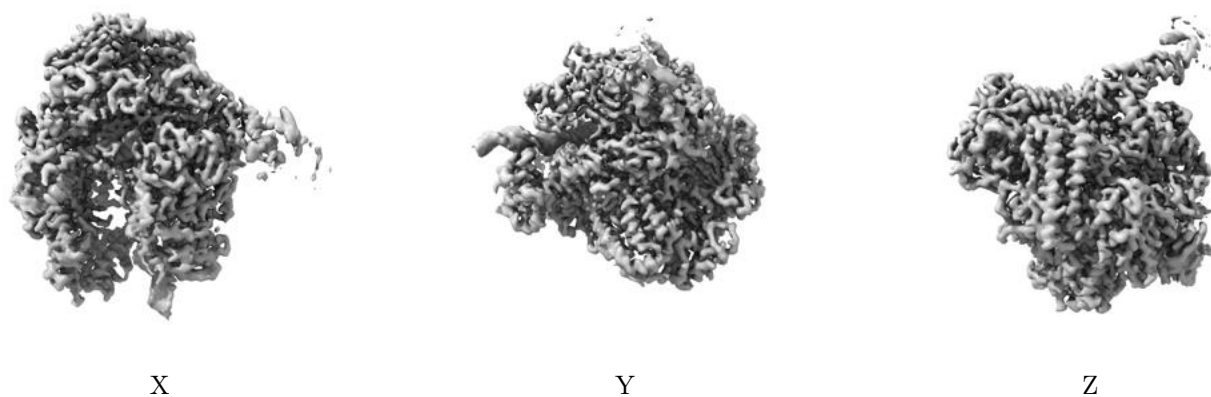
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.93. 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



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.

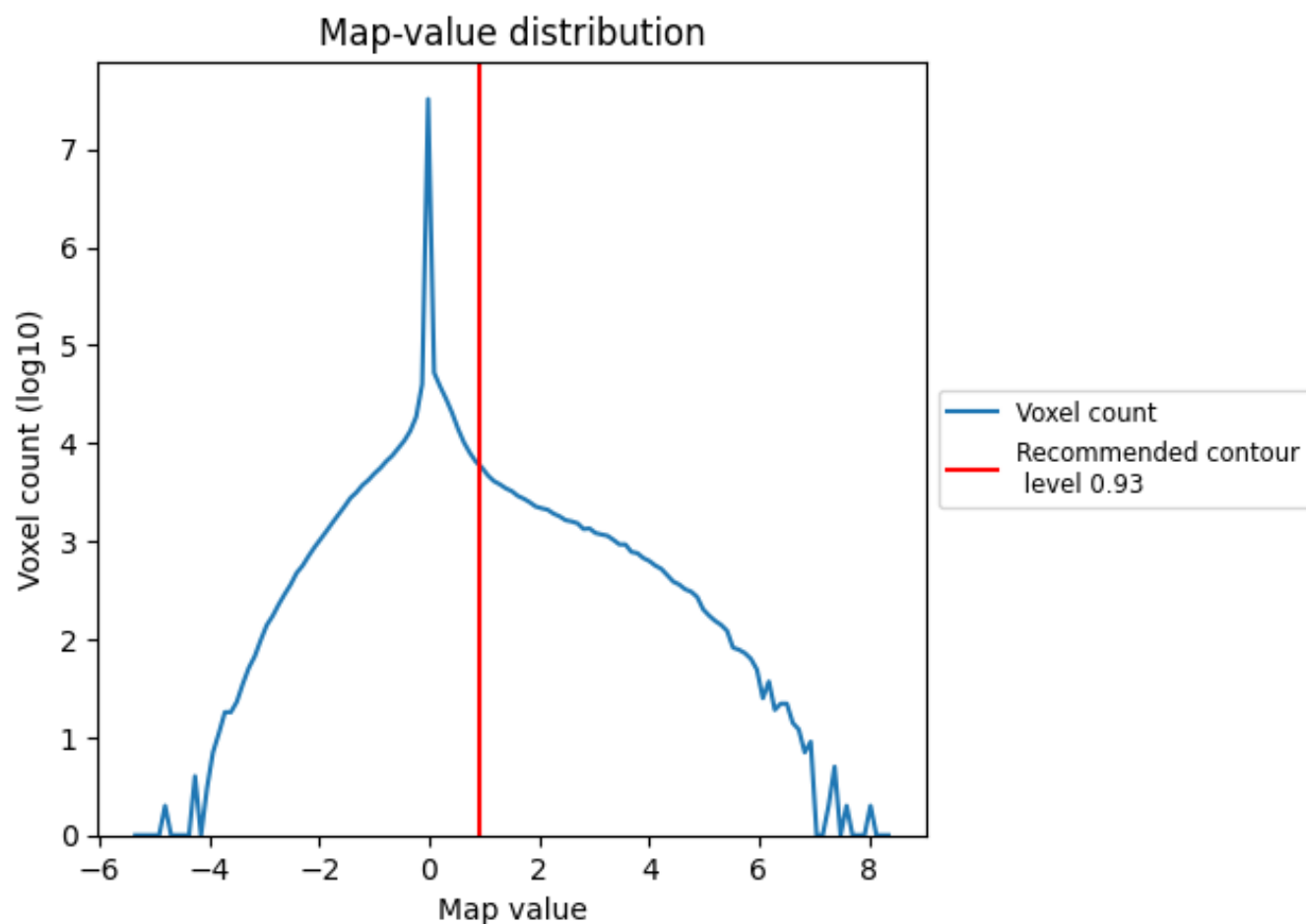
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

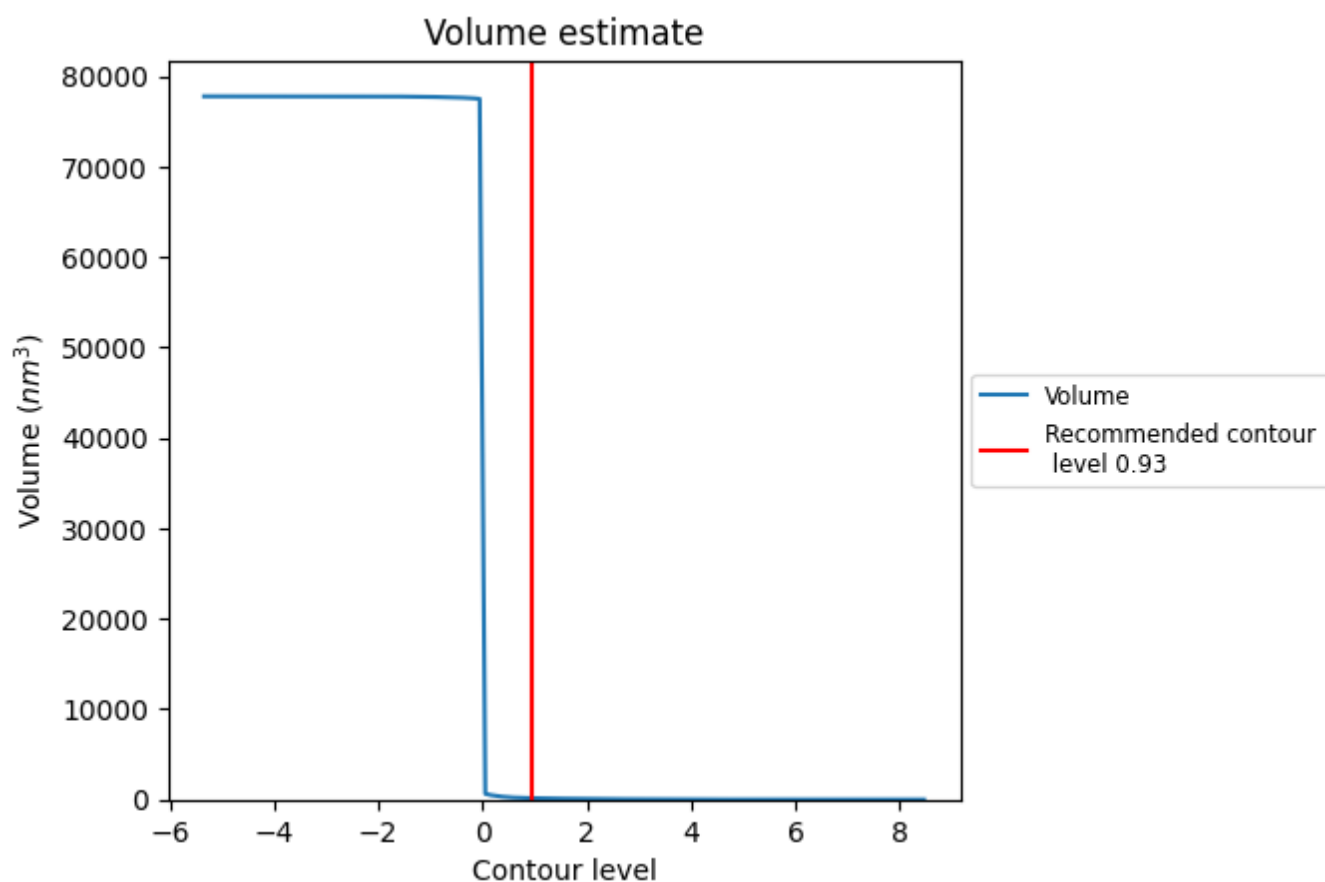
This section contains the results of statistical analysis of the map.

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.

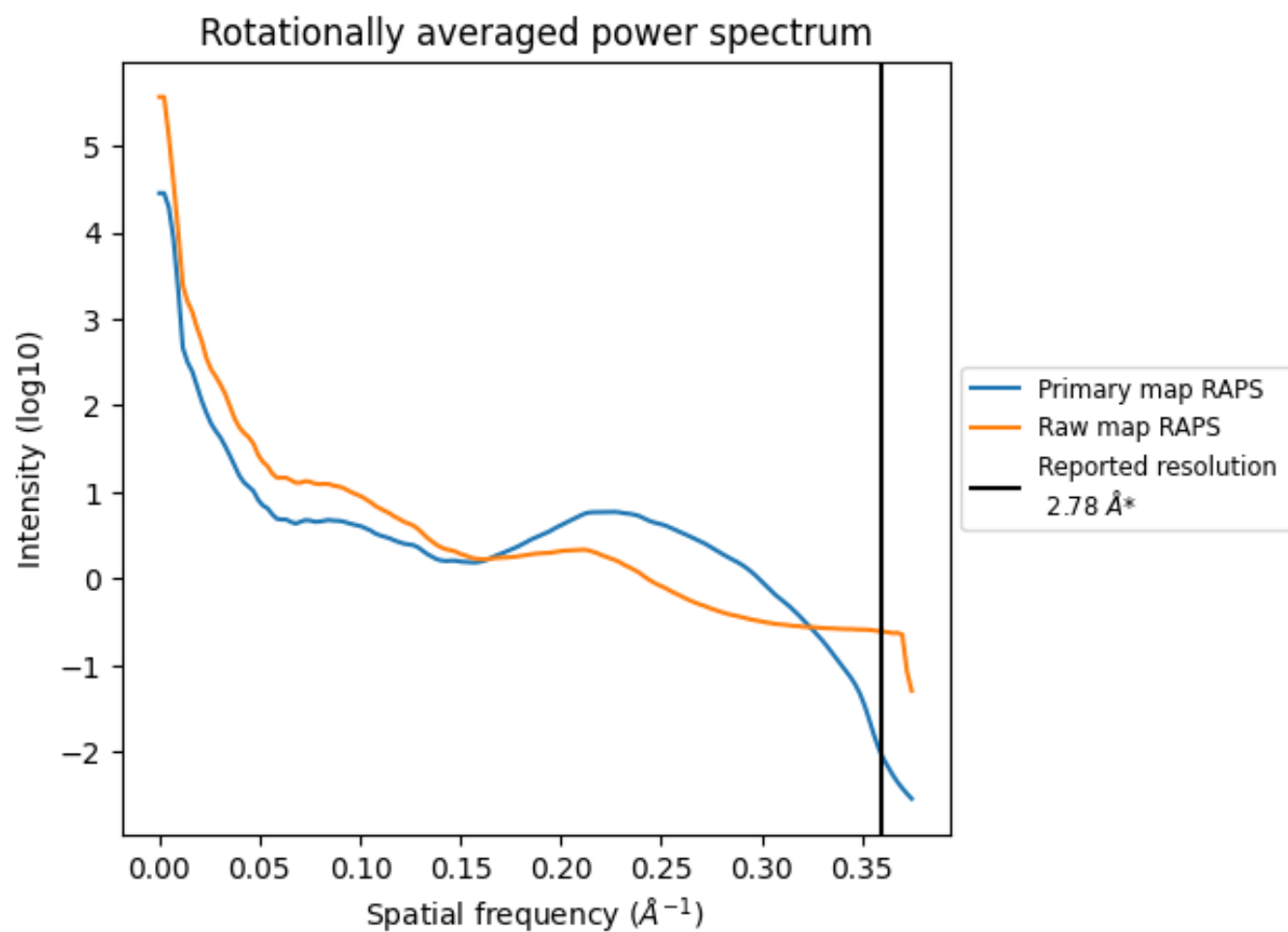
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm^3 ; this corresponds to an approximate mass of 142 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

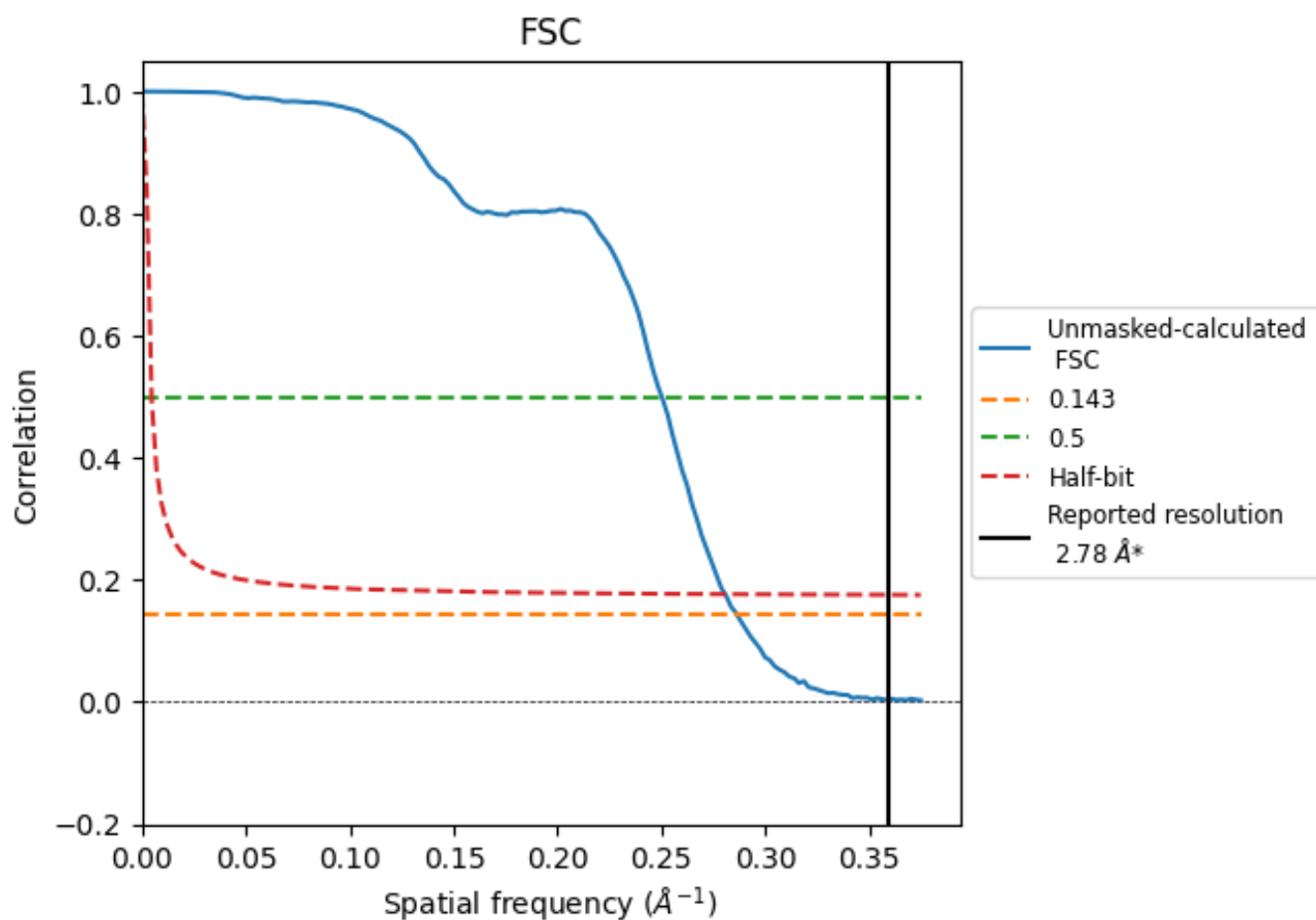


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

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 $0.360 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	4.00	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.78 by more than 10 %

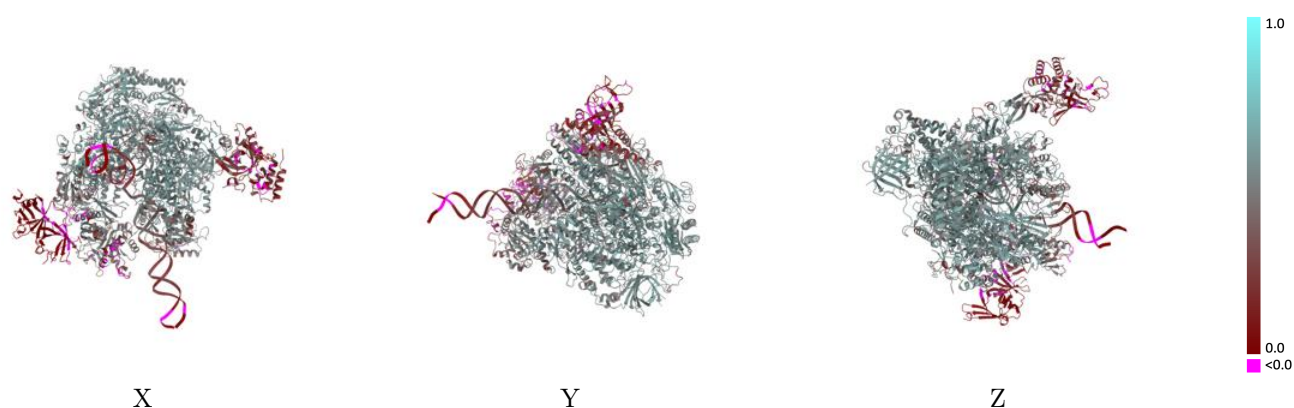
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37405 and PDB model 8WAU. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

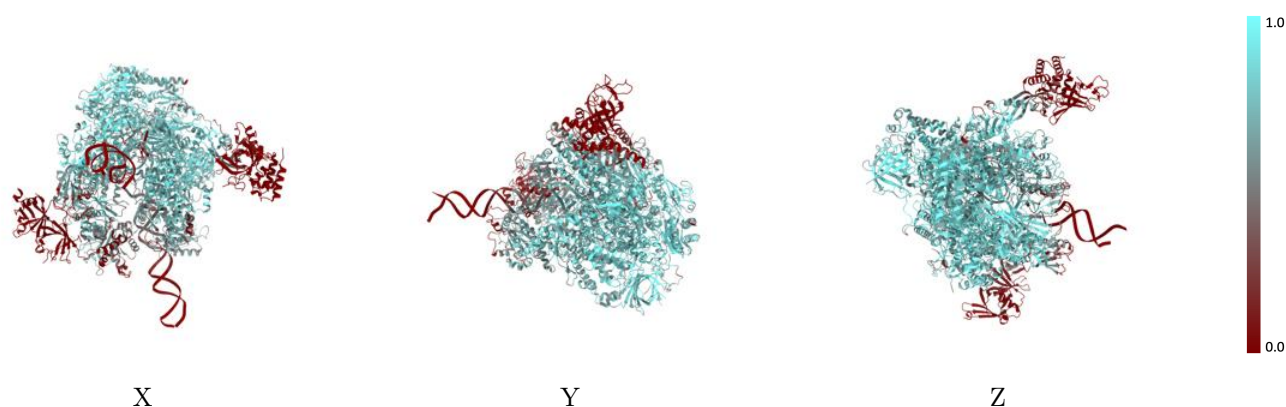
This section was not generated.

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



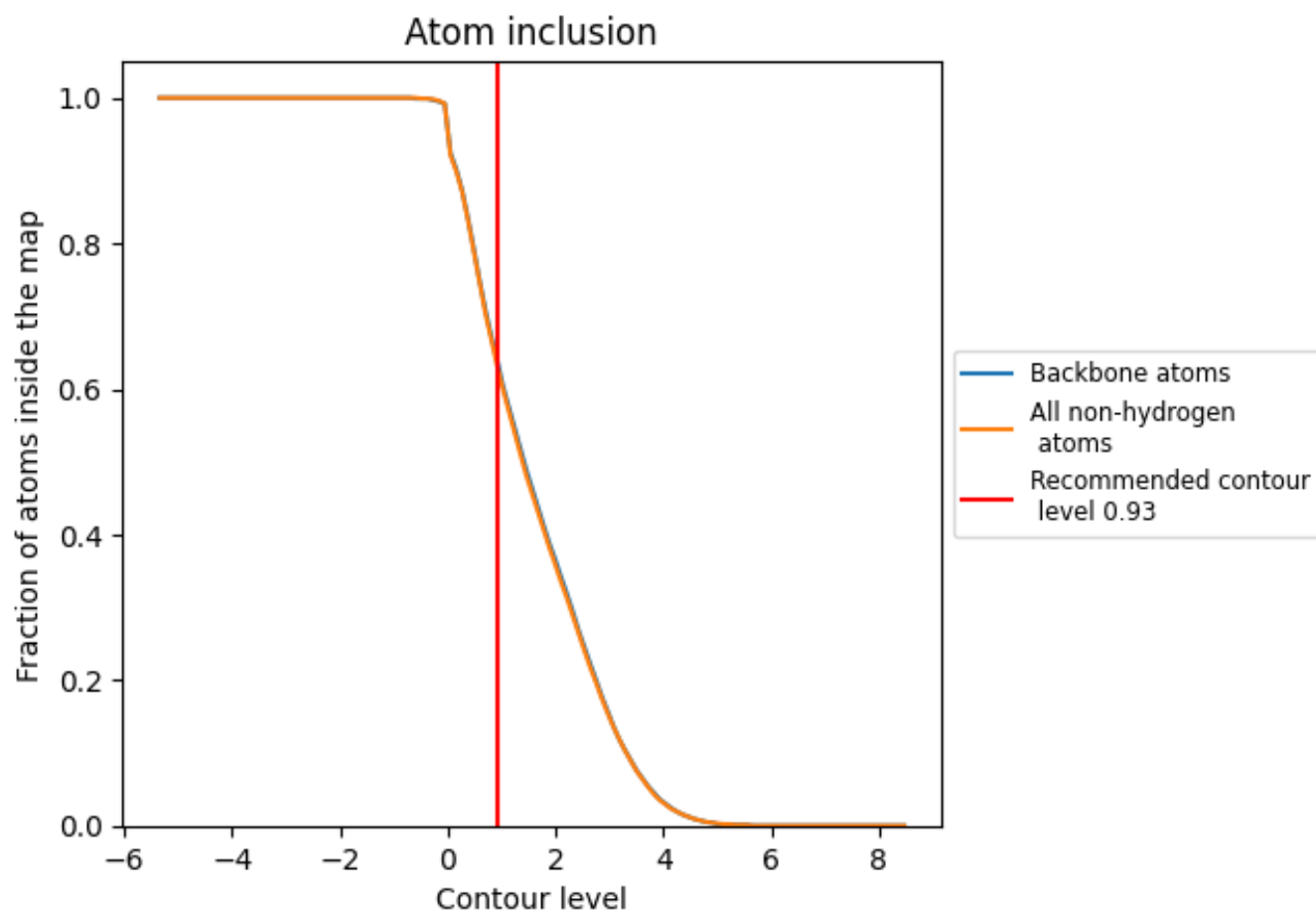
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.93).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.93) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6270	 0.4560
N	 0.9030	 0.5800
S	 0.0000	 0.0210
T	 0.0000	 -0.0050
X	 0.1900	 0.2020
Y	 0.3290	 0.2900
Z	 0.6570	 0.4760
o	 0.7270	 0.5170
p	 0.7300	 0.5100
q	 0.8260	 0.5460
r	 0.0240	 0.1930
s	 0.7310	 0.5000
t	 0.7820	 0.5400
u	 0.2670	 0.2870
v	 0.7810	 0.5200
w	 0.6230	 0.4430
x	 0.8310	 0.5700
y	 0.8190	 0.5580
z	 0.6990	 0.4840

