



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:02 PM UTC

PDB ID : 7NKX / pdb_00007nkx
EMDB ID : EMD-12449
Title : RNA polymerase II-Spt4/5-nucleosome-Chd1 structure
Authors : Farnung, L.; Ochmann, M.; Engholm, M.; Cramer, P.
Deposited on : 2021-02-19
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

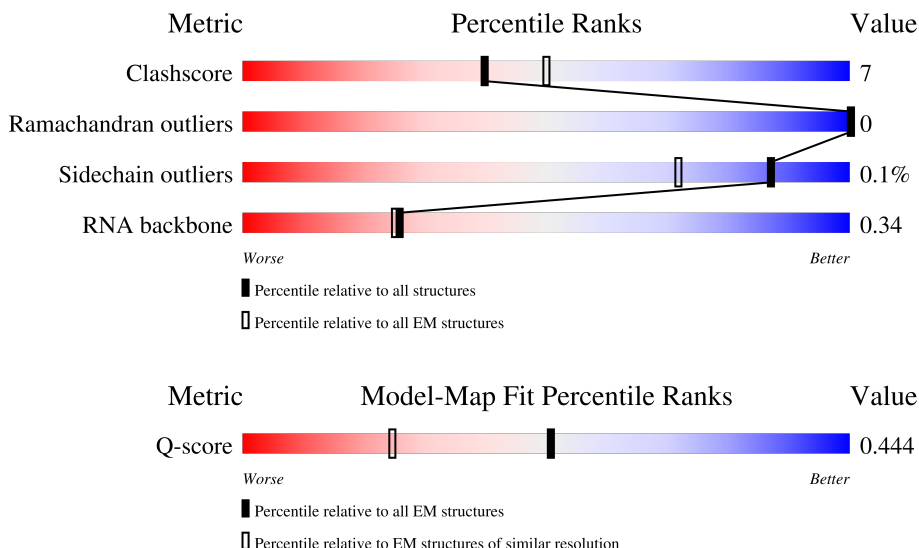
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	E	215	
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	a	136	
11	e	136	
12	b	103	
12	f	103	
13	c	130	
13	g	130	
14	d	123	
14	h	123	
15	T	185	
16	N	176	
17	W	1468	
18	P	69	
19	Y	102	
20	Z	1066	
21	D	221	
22	G	171	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BEF	W	1502	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 49720 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0
			11086	6984	1940	2100	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1116	Total	C	N	O	S	0	0
			8865	5611	1559	1640	55		

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			351	217	70	60	4		

- Molecule 11 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	76	Total	C	N	O	S	0	0
			620	393	115	109	3		
11	e	97	Total	C	N	O	S	0	0
			801	504	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	conflict	UNP P84233
e	102	ALA	GLY	conflict	UNP P84233

- Molecule 12 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 13 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	103	Total	C	N	O		0	0
			795	501	155	139			
13	g	93	Total	C	N	O		0	0
			718	450	142	126			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 14 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
14	h	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	conflict	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	conflict	UNP P02281

- Molecule 15 is a DNA chain called DNA (139-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	139	Total	C	N	O	P	0	0
			2834	1346	526	824	138		

- Molecule 16 is a DNA chain called DNA (128-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	128	Total	C	N	O	P	0	0
			2640	1251	486	775	128		

- Molecule 17 is a protein called Chromo domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	622	Total	C	N	O	S	0	0
			5129	3254	900	953	22		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	16	Total	C	N	O	P	0	0
			330	148	49	117	16		

- Molecule 19 is a protein called Chromatin elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	98	Total	C	N	O	S	0	0
			739	461	126	142	10		

- Molecule 20 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	156	Total	C	N	O	S	0	0
			1252	804	224	221	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-2	SER	-	expression tag	UNP P27692
Z	-1	ASN	-	expression tag	UNP P27692
Z	0	ALA	-	expression tag	UNP P27692
Z	376	LEU	LYS	conflict	UNP P27692
Z	377	GLU	SER	conflict	UNP P27692

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	180	Total	C	N	O	S	0	0
			1444	893	257	291	3		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

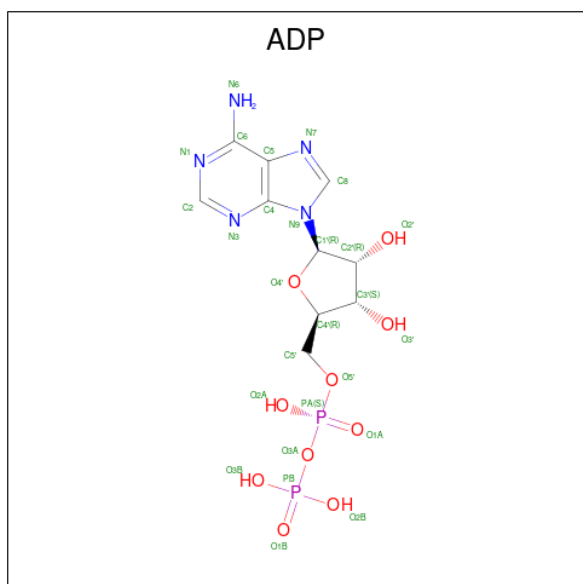
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	C	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	

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

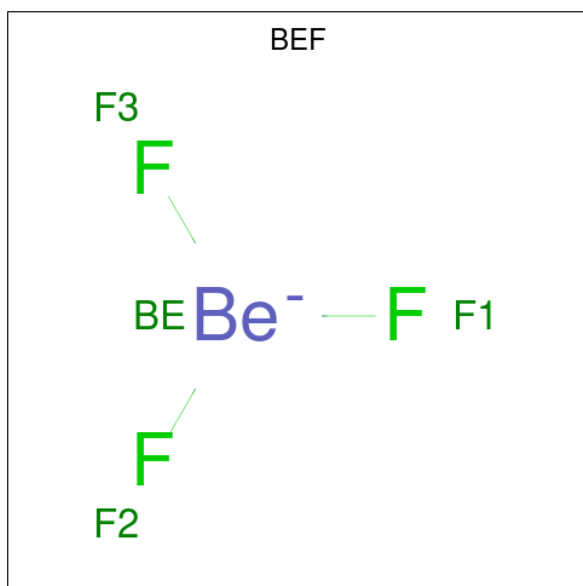
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	

- Molecule 25 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 26 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).

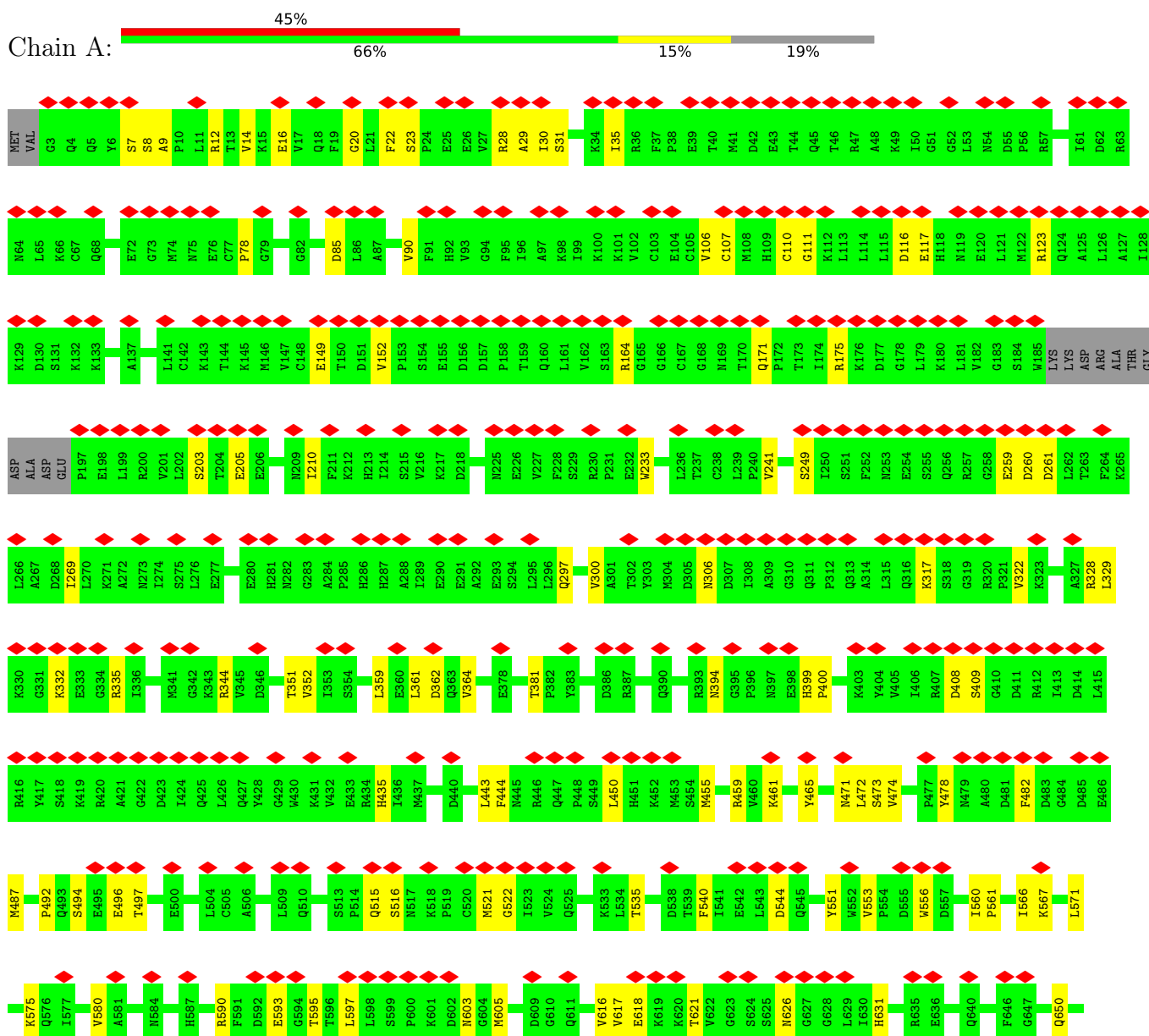


Mol	Chain	Residues	Atoms			AltConf
26	W	1	Total	Be	F	0
			4	1	3	

3 Residue-property plots

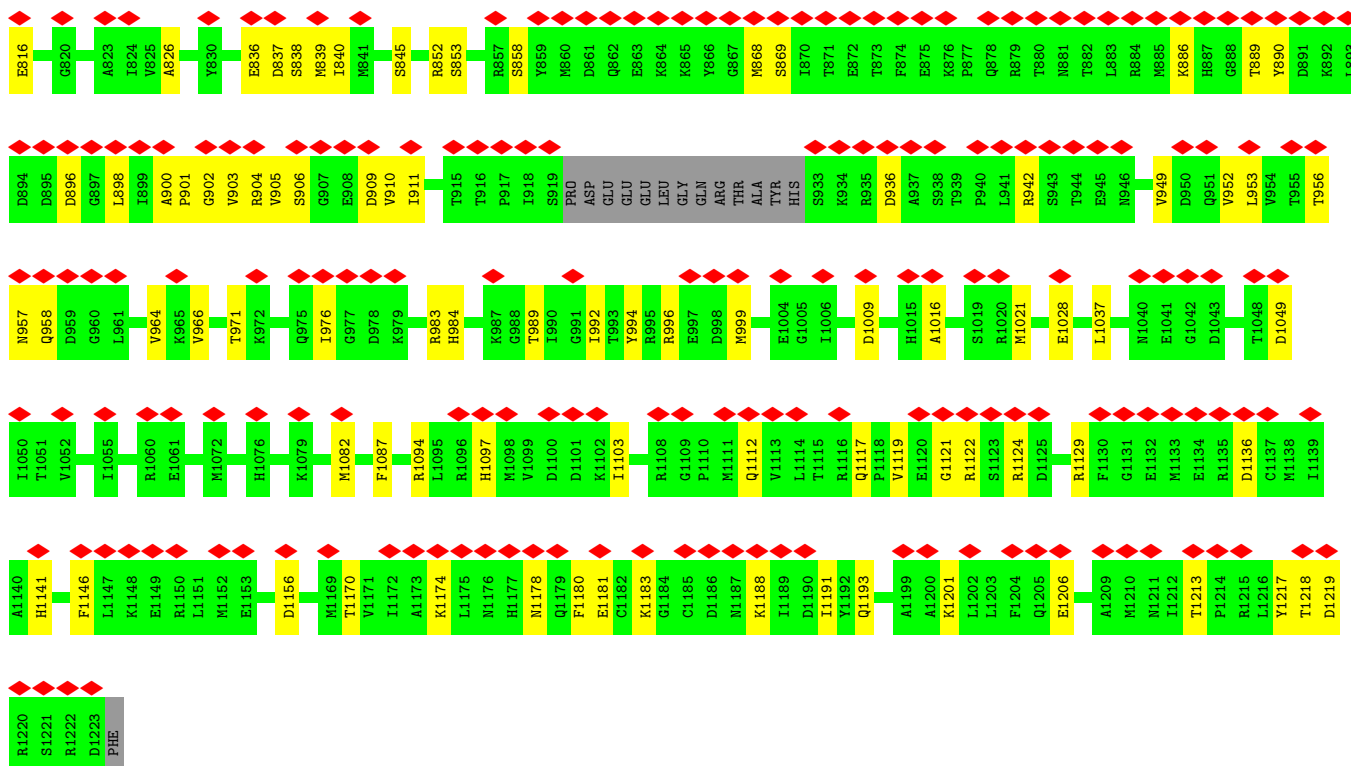
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

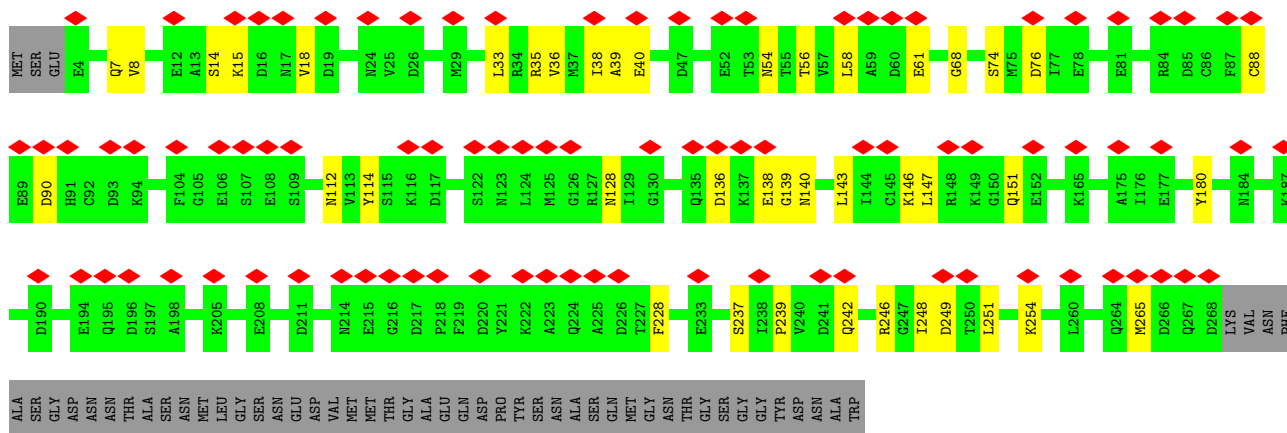




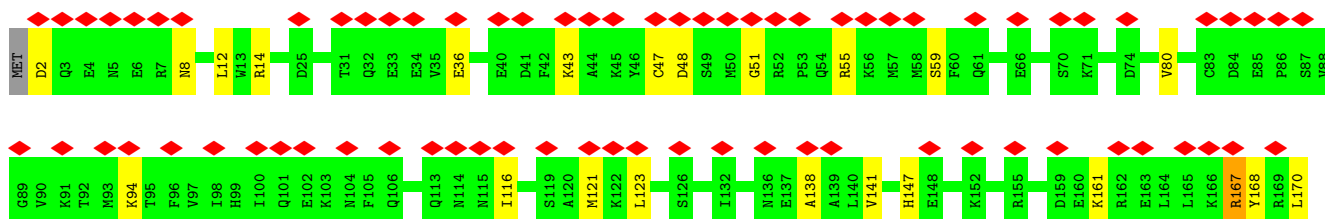
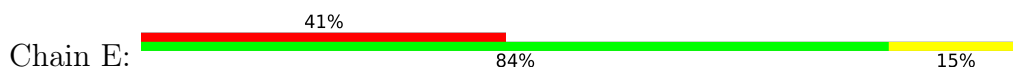


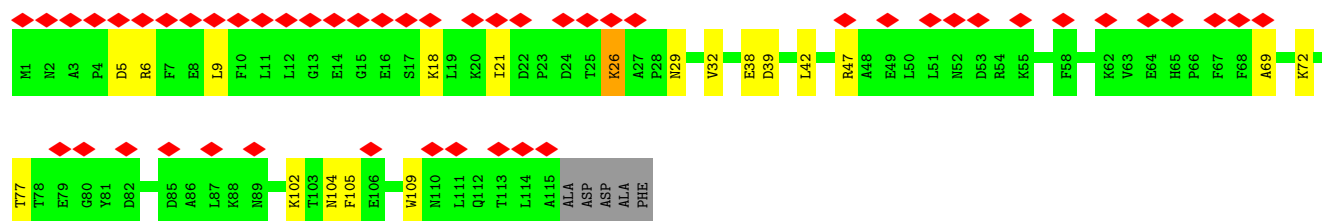


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

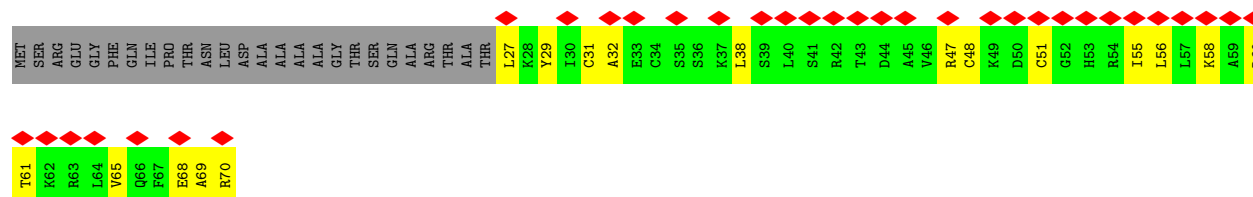


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

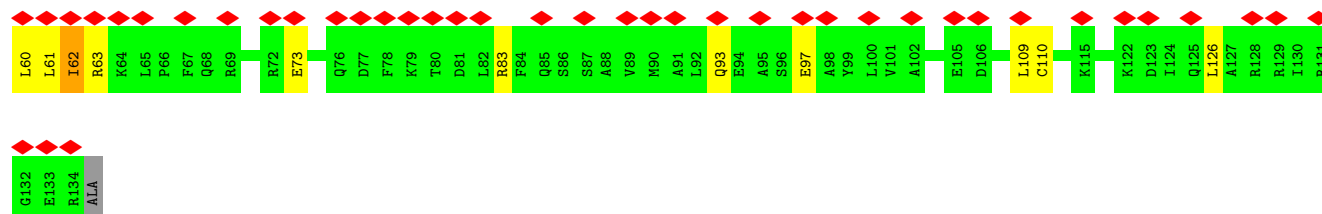
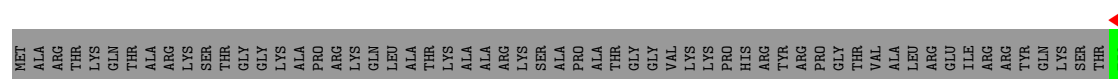




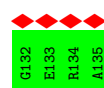
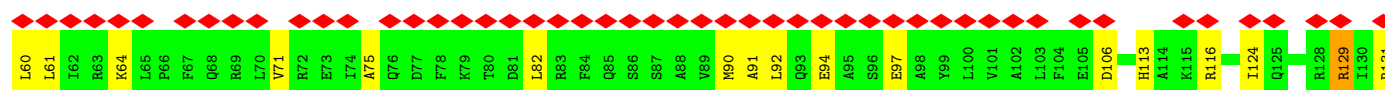
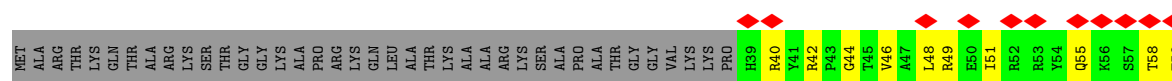
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



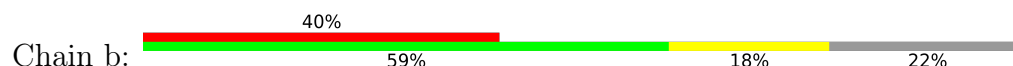
- Molecule 11: Histone H3.2

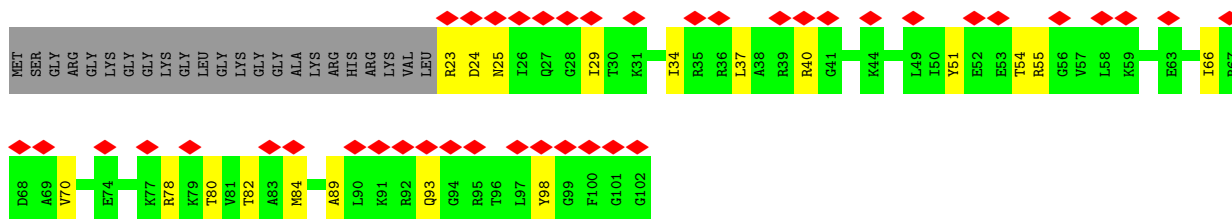


- Molecule 11: Histone H3.2

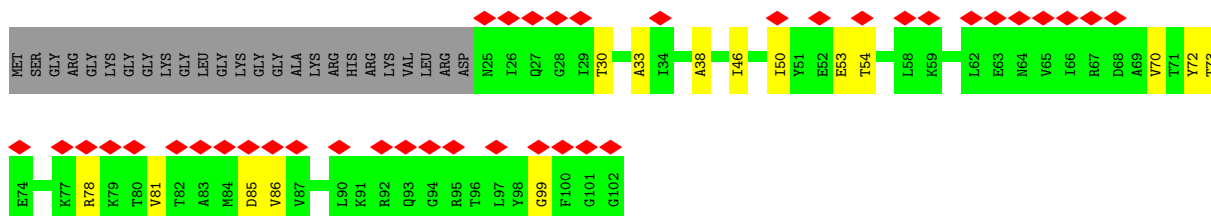


- Molecule 12: Histone H4

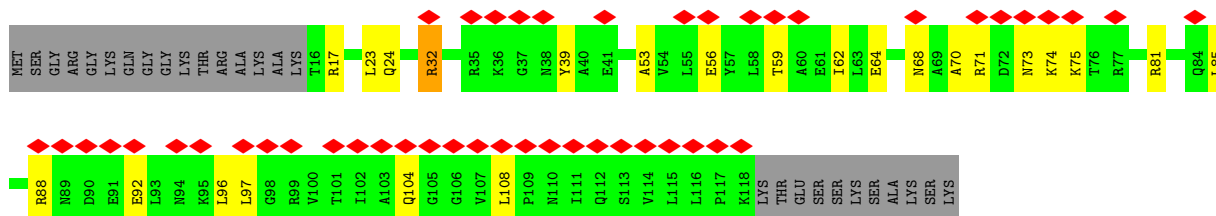




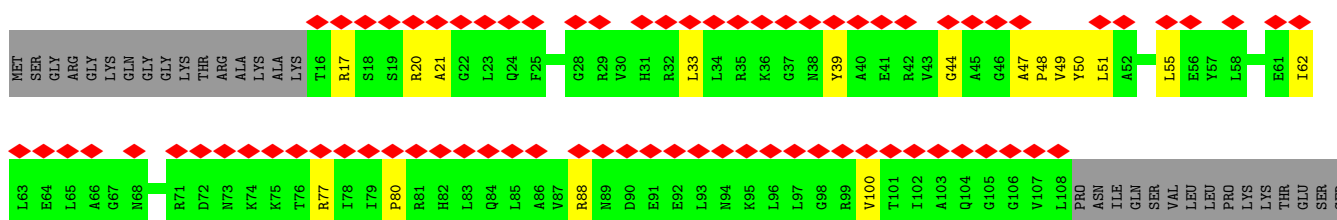
- Molecule 12: Histone H4



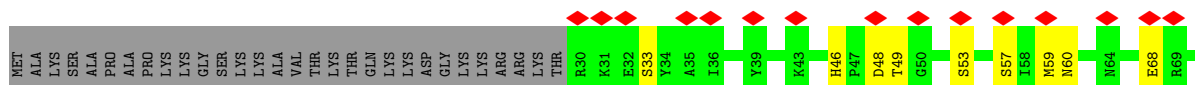
- Molecule 13: Histone H2A type 1

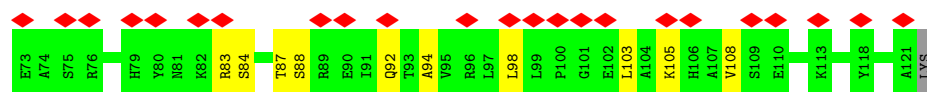


- Molecule 13: Histone H2A type 1

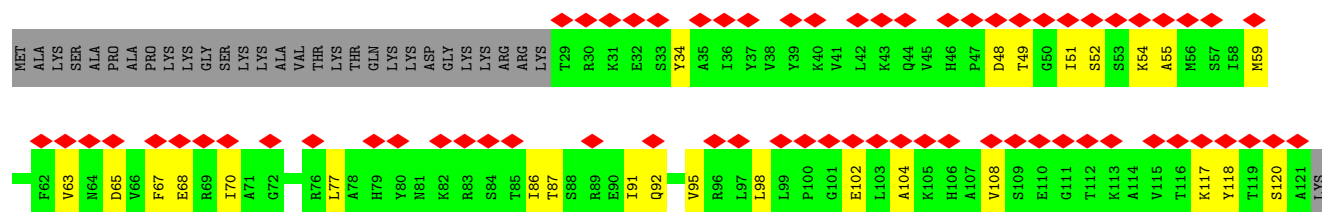


- Molecule 14: Histone H2B 1.1

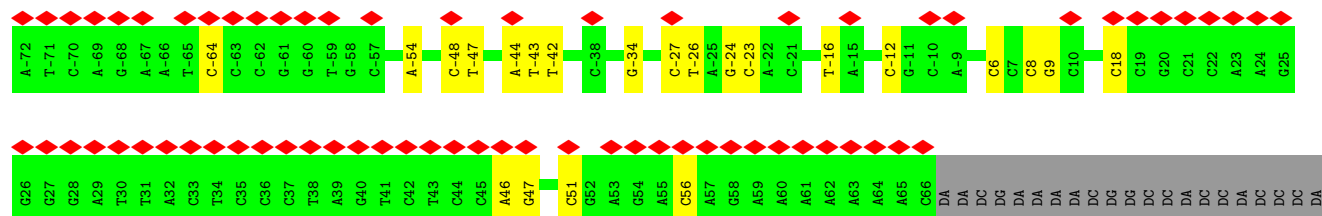




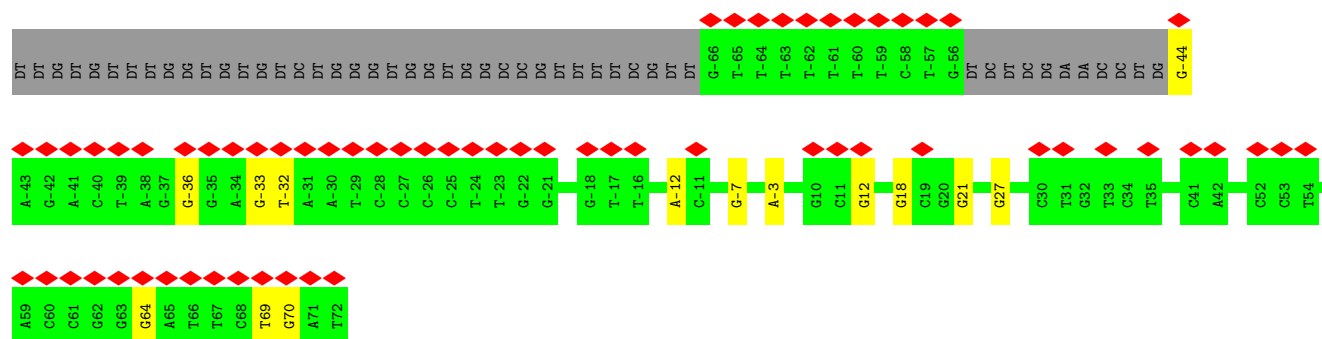
• Molecule 14: Histone H2B 1.1



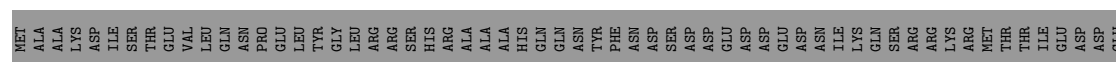
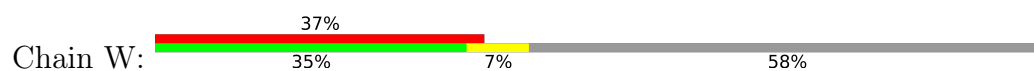
• Molecule 15: DNA (139-MER)



• Molecule 16: DNA (128-MER)



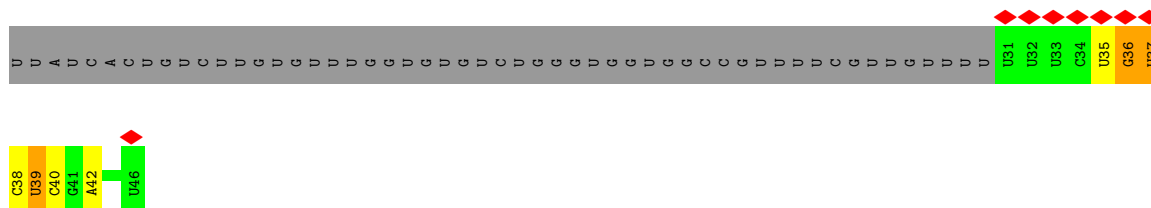
• Molecule 17: Chromo domain-containing protein 1



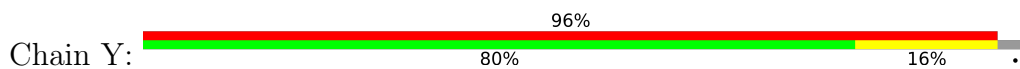


MET	SER	ASN	GLY	PRO	PHE	ASN	ASP	VAL
	LEU	SER	SER	VAL	SER	GLN	GLY	ASN
	ASP	PRO	LYS	ALA	SER	PRO	THR	GLY
	ARG	THR	LEU	LYS	GLY	ASP	LEU	THR
	GLU	PRO	PRO	SER	ASN	ASN	VAL	THR
	TRP	LEU	THR	ALA	THR	PRO	LYS	ALA
	ALA	LYS	GLY	SER	PRO	LEU	SER	ALA
	GLN	SER	PRO	SER	LYS	THR	PHE	ASN
	ILE	LYS	SER	SER	PRO	LEU	GLU	ASN
	LYS	VAL	LYS	ASP	VAL	LEU	LYS	SER
LYS	THR	ARG	ARG	THR	GLN	SER	TYR	ASP
	THR	ARG	ARG	THR	ASN	LEU	GLY	ASP
	GLU	ASN	GLM	PRO	THR	LYS	GLU	ASP
	LEU	ASN	ARG	THR	SER	LYS	THR	ASP
	THR	THR	LYS	PRO	SER	ARG	TYR	SER
	THR	THR	PRO	SER	ASN	GLU	ASP	THR
	ILE	ARG	ALA	LYS	THR	LYS	GLU	SER
	GLY	GLN	ASN	LYS	THR	LYS	GLU	SER
	ASN	SER	HIS	GLY	LYS	ALA	MET	ARG
	LYS	SER	SER	LYS	GLU	VAL	GLU	ARG
HIS	ILE	ASN	LYS	GLY	ASN	LEU	ALA	ARG
	GLU	PRO	SER	ILE	ASP	PHE	ALA	ARG
	SER	SER	MET	THR	GLU	ASN	LYS	ARG
	GLN	SER	THR	GLY	LYS	PHE	ASP	ALA
	LYS	GLY	PRO	SER	LEU	LYS	CYS	ARG
	GLY	SER	GLU	SER	LEU	GLY	VAL	ALA
	SER	ALA	ILE	LYS	ILE	VAL	HIS	ASN
	SER	HIS	THR	LYS	GLY	LYS	GLU	ASP
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	PRO	ASP	ALA	ILE	GLY	GLU	ARG	GLY
	GLU	SER	ASN	HIS	TYR	SER	LYS	SER
	LYS	MET	GLY	LEU	GLY	LEU	GLU	SER
	TYR	ASP	PRO	GLY	SER	LEU	ILE	GLU
	HIS	CYS	LYS	VAL	GLN	VAL	LYS	ALA
	LEU	ASP	ARG	ASP	ILE	GLU	LEU	LEU
	TRP	ARG	MET	TYR	ARG	ASP	GLU	TYR
	SER	HIS	LYS	LEU	ASP	LEU	LYS	LYS
THR	TYR	THR	ALA	LEU	ASP	LYS	HIS	ALA
	SER	MET	PRO	SER	PRO	TYR	ALA	ILE
	ALA	SER	PHE	PHE	PHE	LEU	THR	LEU
	ASN	ASN	LEU	LEU	LYS	LYS	ALA	LYS
	PHE	ILE	GLY	ARG	GLY	ASN	TYR	PHE
	TRP	ARG	PRO	GLY	ILE	LEU	ARG	GLY
	PRO	THR	ALA	GLY	THR	ILE	ALA	GLY
	ALA	SER	ALA	LEU	THR	ILE	ALA	ASN
	ASP	LEU	LEU	LEU	LYS	ASN	LEU	LYS
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LYS	LYS	ARG	ASN	LYS	PHE	TYR	SER	ILE
	SER	LEU	ASN	SER	LEU	LYS	GLY	LEU
	THR	ARG	THR	PRO	GLU	ASP	GLU	ASP
	LYS	GLY	ALA	ALA	GLU	PRO	ILE	GLU
	LEU	GLY	THR	THR	THR	PRO	LYS	LEU
	GLY	GLY	ASP	ASP	HIS	LEU	ALA	ILE
	ASN	GLY	THR	THR	GLY	ASN	LYS	THR
	THR	GLN	SER	THR	THR	LYS	GLU	THR
	GLY	SER	ILE	ILE	THR	ASN	GLY	THR
	ASN	GLN	ASN	LYS	THR	ASN	GLY	MET

- Molecule 18: RNA



- Molecule 19: Chromatin elongation factor SPT4



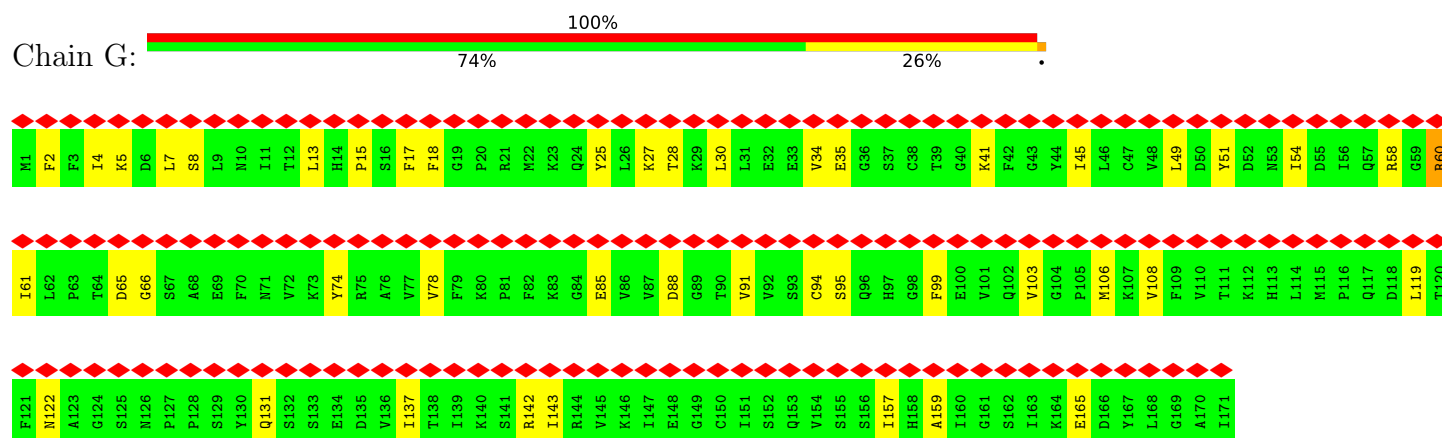
- Molecule 20: Transcription elongation factor SPT5



SER	ASN	ALA	ALA	MET	SER	ASP	ASN	SER	SER	ASP	THR	ASN	ASN	VAL	SER	MET	GLN	ASP	ASP	GLN	GLN	PHE	ALA	ALA	ASP	PRO	VAL	VAL	VAL	PRO	PRO	GLN	SER	THR	ASP	THR	LYS	LYS	ASP	GLU	ASN	THR	SER	SER	SER	ASP	ASP	GLY	ASN	VAL	VAL	THR	THR	THR	THR	SER	GLU	GLU	THR	GLU	ALA	ARG	ALA	GLU	SER
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[illegible]

- Molecule 21: DNA-directed RNA polymerase II subunit RPB4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/11284	0.63	1/15258 (0.0%)
2	B	0.33	0/9037	0.62	2/12184 (0.0%)
3	C	0.33	0/2124	0.62	0/2879
4	E	0.32	0/1788	0.60	1/2406 (0.0%)
5	F	0.42	0/717	0.68	0/967
6	H	0.34	0/1086	0.62	0/1470
7	I	0.35	0/989	0.64	0/1331
8	J	0.36	0/541	0.60	0/727
9	K	0.40	0/938	0.73	1/1267 (0.1%)
10	L	0.35	0/353	0.72	1/468 (0.2%)
11	a	0.36	0/627	0.68	0/841
11	e	0.39	0/812	0.74	1/1088 (0.1%)
12	b	0.32	0/645	0.69	0/862
12	f	0.34	0/626	0.66	0/837
13	c	0.36	0/805	0.74	1/1088 (0.1%)
13	g	0.34	0/726	0.62	0/979
14	d	0.36	0/730	0.73	0/983
14	h	0.35	0/737	0.67	0/993
15	T	0.37	0/3179	0.62	1/4900 (0.0%)
16	N	0.37	0/2961	0.59	0/4571
17	W	0.30	0/5230	0.61	0/7057
18	P	0.25	0/365	0.42	0/564
19	Y	0.26	0/755	0.54	0/1021
20	Z	0.32	0/1271	0.61	0/1702
21	D	0.31	0/1454	0.66	0/1949
22	G	0.42	0/1368	1.03	3/1844 (0.2%)
All	All	0.34	0/51148	0.65	12/70236 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
11	a	0	1
13	c	0	1
14	h	0	1
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	167	ARG	CG-CD-NE	-6.97	96.67	112.00
22	G	60	ARG	CA-CB-CG	6.22	126.54	114.10
2	B	1121	GLY	N-CA-C	5.77	119.46	112.48
1	A	857	ARG	CG-CD-NE	5.68	124.49	112.00
11	e	129	ARG	CB-CG-CD	5.55	124.06	111.30
22	G	85	GLU	N-CA-CB	5.40	118.22	110.06
10	L	60	ARG	CB-CG-CD	5.34	123.59	111.30
13	c	32	ARG	CA-CB-CG	5.25	124.61	114.10
2	B	336	ARG	CB-CG-CD	5.24	123.35	111.30
9	K	26	LYS	CA-CB-CG	5.19	124.48	114.10
22	G	165	GLU	CA-CB-CG	5.06	124.23	114.10
15	T	-24	DG	P-O3'-C3'	5.04	127.75	120.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	90	ASP	Peptide
11	a	62	ILE	Peptide
13	c	74	LYS	Peptide
14	h	102	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11086	0	11155	200	0
2	B	8865	0	8922	159	0
3	C	2086	0	2045	34	0
4	E	1752	0	1776	25	0
5	F	705	0	731	20	0
6	H	1068	0	1040	19	0
7	I	971	0	928	21	0
8	J	532	0	542	11	0
9	K	920	0	929	20	0
10	L	351	0	374	17	0
11	a	620	0	651	13	0
11	e	801	0	838	24	0
12	b	638	0	676	18	0
12	f	619	0	659	15	0
13	c	795	0	846	20	0
13	g	718	0	758	16	0
14	d	719	0	740	16	0
14	h	726	0	747	24	0
15	T	2834	0	1558	25	0
16	N	2640	0	1442	13	0
17	W	5129	0	5097	67	0
18	P	330	0	169	4	0
19	Y	739	0	716	11	0
20	Z	1252	0	1331	21	0
21	D	1444	0	1467	18	0
22	G	1340	0	1357	37	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
24	A	1	0	0	0	0
25	W	27	0	12	3	0
26	W	4	0	0	3	0
All	All	49720	0	47506	687	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 7.

All (687) 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)
13:c:59:THR:HG23	14:d:59:MET:HE2	1.49	0.94
17:W:430:ILE:HD13	17:W:511:ALA:HB3	1.57	0.85
17:W:701:ASP:OD1	17:W:730:TYR:OH	1.95	0.85
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.11	0.84
1:A:551:TYR:OH	9:K:72:LYS:NZ	2.10	0.83
1:A:1328:TYR:OH	1:A:1351:GLU:OE2	1.96	0.82
2:B:971:THR:OG1	3:C:61:GLU:OE1	1.98	0.82
1:A:450:LEU:HD23	1:A:1077:THR:HG21	1.61	0.81
1:A:494:SER:HG	1:A:497:THR:HG1	1.24	0.81
1:A:806:ARG:NH2	2:B:727:LYS:O	2.13	0.80
17:W:283:GLU:OE1	17:W:313:ARG:NE	2.15	0.80
16:N:21:DG:OP1	17:W:523:SER:OG	2.00	0.79
20:Z:329:ASP:O	20:Z:332:THR:OG1	2.00	0.79
1:A:1062:GLU:OE2	5:F:88:TYR:OH	2.01	0.79
21:D:127:ASP:OD2	21:D:142:LYS:NZ	2.16	0.79
2:B:118:ARG:NH1	2:B:209:GLU:OE1	2.16	0.79
21:D:56:ARG:NH1	21:D:152:SER:OG	2.16	0.78
13:g:77:ARG:NH2	14:h:52:SER:OG	2.17	0.78
8:J:21:TYR:OH	8:J:32:GLU:OE1	2.02	0.78
1:A:1100:ARG:NH2	1:A:1330:ASN:OD1	2.16	0.77
1:A:1323:ASP:OD1	1:A:1325:THR:OG1	2.02	0.77
14:h:70:ILE:HD13	14:h:98:LEU:HD22	1.66	0.77
1:A:871:ASP:OD1	4:E:204:THR:OG1	2.02	0.76
2:B:393:LYS:O	7:I:91:ARG:NH2	2.18	0.76
1:A:1348:LEU:HD22	1:A:1372:VAL:HG12	1.68	0.76
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.19	0.75
3:C:249:ASP:OD2	9:K:102:LYS:NZ	2.19	0.75
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.68	0.75
1:A:871:ASP:OD2	4:E:205:SER:OG	2.03	0.75
20:Z:324:SER:OG	20:Z:338:GLU:OE2	2.00	0.75
7:I:8:ARG:NH1	7:I:9:ASP:OD1	2.20	0.75
1:A:394:ASN:ND2	1:A:400:PRO:O	2.19	0.74
21:D:32:GLU:OE2	22:G:41:LYS:NZ	2.20	0.74
1:A:744:LYS:NZ	1:A:748:MET:SD	2.59	0.74
19:Y:4:GLU:OE1	20:Z:302:ARG:NH2	2.19	0.74
2:B:906:SER:OG	20:Z:830:GLU:OE1	2.03	0.74
17:W:228:GLU:OE2	17:W:232:SER:OG	2.04	0.73
1:A:886:ILE:O	1:A:944:ARG:NH1	2.20	0.73
13:c:39:TYR:OH	14:d:68:GLU:OE1	2.07	0.73
19:Y:15:THR:OG1	19:Y:17:ASN:OD1	2.06	0.73
2:B:845:SER:OG	2:B:1009:ASP:OD1	2.04	0.72
3:C:114:TYR:OH	8:J:19:GLU:OE1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:104:GLN:N	11:e:94:GLU:OE2	2.21	0.72
19:Y:37:SER:OG	19:Y:40:GLU:OE2	2.06	0.72
19:Y:26:ASN:OD1	19:Y:74:TYR:OH	2.05	0.72
2:B:301:ILE:HG21	2:B:314:LEU:HD11	1.71	0.72
17:W:759:SER:OG	17:W:761:ASP:O	2.08	0.72
1:A:535:THR:O	1:A:575:LYS:NZ	2.23	0.71
1:A:669:THR:O	1:A:762:SER:OG	2.03	0.71
2:B:889:THR:OG1	2:B:909:ASP:OD1	2.08	0.71
2:B:493:SER:OG	2:B:526:GLU:OE1	2.06	0.71
2:B:1181:GLU:OE2	2:B:1188:LYS:NZ	2.23	0.71
20:Z:339:ALA:HB3	20:Z:345:ILE:HD11	1.73	0.70
1:A:1342:GLU:OE1	4:E:212:ARG:NE	2.23	0.70
2:B:39:ARG:NH1	2:B:665:GLU:OE2	2.25	0.70
1:A:556:TRP:O	9:K:26:LYS:NZ	2.24	0.70
11:e:42:ARG:NH2	16:N:69:DT:O3'	2.24	0.70
1:A:665:GLY:N	1:A:668:ASP:OD2	2.25	0.70
2:B:540:SER:OG	2:B:747:MET:O	2.10	0.69
1:A:344:ARG:NH1	2:B:1119:VAL:O	2.25	0.69
7:I:19:ASP:O	7:I:23:ASN:N	2.25	0.69
13:g:88:ARG:NH2	13:g:100:VAL:O	2.25	0.69
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.25	0.69
2:B:942:ARG:NH2	15:T:51:DC:OP2	2.25	0.69
10:L:68:GLU:N	10:L:68:GLU:OE2	2.25	0.69
21:D:146:GLN:O	21:D:150:ASN:ND2	2.25	0.69
13:g:39:TYR:OH	14:h:68:GLU:OE1	2.10	0.69
11:e:40:ARG:NH2	15:T:9:DG:O3'	2.26	0.69
13:g:50:TYR:OH	14:h:92:GLN:OE1	2.04	0.69
1:A:1070:GLN:NE2	2:B:1136:ASP:OD2	2.26	0.68
17:W:401:ASP:OD2	17:W:407:LYS:NZ	2.24	0.68
2:B:398:ARG:NH2	16:N:-44:DG:OP2	2.27	0.68
4:E:177:ARG:NH1	4:E:215:MET:SD	2.66	0.68
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.05	0.68
3:C:35:ARG:NH2	9:K:39:ASP:OD1	2.26	0.68
2:B:1219:ASP:OD1	21:D:14:ARG:NH1	2.26	0.68
7:I:29:CYS:SG	7:I:31:THR:OG1	2.52	0.68
2:B:512:ARG:NH1	2:B:533:CYS:O	2.28	0.67
1:A:1394:THR:O	1:A:1399:ARG:NH1	2.28	0.67
12:f:50:ILE:O	12:f:54:THR:OG1	2.09	0.67
1:A:332:LYS:NZ	15:T:47:DG:OP2	2.27	0.67
4:E:59:SER:OG	4:E:80:VAL:O	2.12	0.67
11:a:61:LEU:HD13	12:b:40:ARG:NH2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:7:LEU:HD11	22:G:74:TYR:CZ	2.30	0.66
1:A:709:THR:OG1	7:I:93:LYS:O	2.07	0.66
17:W:474:ASN:ND2	17:W:475:PRO:O	2.28	0.66
1:A:78:PRO:O	2:B:1201:LYS:NZ	2.28	0.66
6:H:8:ASP:OD1	6:H:9:ILE:N	2.29	0.66
14:d:103:LEU:O	14:d:105:LYS:NZ	2.28	0.66
2:B:816:GLU:N	2:B:816:GLU:OE1	2.29	0.66
1:A:593:GLU:OE1	1:A:603:ASN:ND2	2.29	0.66
2:B:853:SER:OG	2:B:1094:ARG:NH1	2.29	0.65
10:L:47:ARG:NH1	10:L:51:CYS:O	2.30	0.65
22:G:30:LEU:O	22:G:34:VAL:HG22	1.97	0.65
11:e:75:ALA:HB1	11:e:82:LEU:HD23	1.77	0.65
1:A:1134:ILE:O	1:A:1138:ILE:HG22	1.96	0.65
12:f:78:ARG:NH2	12:f:85:ASP:OD2	2.29	0.65
2:B:901:PRO:O	10:L:61:THR:N	2.30	0.65
1:A:846:GLU:OE2	1:A:1425:SER:OG	2.09	0.64
1:A:1445:ILE:HD11	22:G:61:ILE:HD11	1.78	0.64
1:A:571:LEU:HD12	6:H:46:LEU:HD11	1.79	0.64
1:A:175:ARG:NH1	16:N:-36:DG:OP2	2.30	0.64
1:A:870:GLU:O	4:E:205:SER:OG	2.14	0.64
17:W:183:ILE:O	17:W:184:ASN:ND2	2.30	0.64
13:c:64:GLU:OE1	14:d:46:HIS:NE2	2.29	0.64
2:B:636:PRO:O	2:B:637:LEU:HD23	1.98	0.63
17:W:431:VAL:CG2	17:W:512:VAL:HG12	2.27	0.63
1:A:739:ASP:OD1	6:H:19:ARG:NH2	2.32	0.63
1:A:152:VAL:HG23	1:A:164:ARG:NH1	2.14	0.63
1:A:472:LEU:HD21	2:B:836:GLU:OE2	1.98	0.63
1:A:873:MET:O	1:A:1366:ARG:NH1	2.32	0.63
21:D:199:ASN:OD1	21:D:200:ASN:N	2.32	0.63
22:G:45:ILE:HA	22:G:78:VAL:HG12	1.80	0.63
1:A:117:GLU:O	1:A:123:ARG:NE	2.32	0.62
1:A:1150:SER:O	7:I:46:HIS:NE2	2.22	0.62
17:W:808:ILE:HD11	25:W:1501:ADP:C8	2.34	0.62
1:A:496:GLU:OE1	5:F:99:LEU:HD12	1.98	0.62
13:g:21:ALA:O	14:h:117:LYS:NZ	2.32	0.62
17:W:713:ARG:NH1	17:W:782:THR:O	2.32	0.62
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.82	0.62
1:A:850:VAL:HG13	1:A:1060:PRO:HA	1.80	0.62
17:W:661:HIS:HB3	17:W:723:MET:HE1	1.82	0.62
1:A:20:GLY:N	2:B:1213:THR:OG1	2.34	0.61
5:F:140:ASP:OD2	5:F:142:SER:OG	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:-64:DC:O2	16:N:64:DG:N2	2.27	0.61
1:A:473:SER:OG	1:A:522:GLY:O	2.17	0.61
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.13	0.61
12:f:38:ALA:HB3	12:f:46:ILE:HD11	1.82	0.61
1:A:515:GLN:NE2	1:A:516:SER:OG	2.33	0.61
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.34	0.61
2:B:1174:LYS:O	2:B:1178:ASN:N	2.33	0.61
11:a:73:GLU:OE2	12:b:25:ASN:ND2	2.33	0.61
1:A:966:ASN:O	1:A:970:THR:HG22	2.01	0.61
1:A:1318:THR:O	4:E:14:ARG:NH2	2.33	0.61
2:B:206:ASN:HD22	2:B:206:ASN:C	2.08	0.61
2:B:301:ILE:HD12	2:B:382:ILE:HG21	1.83	0.61
4:E:48:ASP:OD2	4:E:51:GLY:N	2.34	0.60
1:A:31:SER:O	2:B:1183:LYS:NZ	2.19	0.60
4:E:36:GLU:OE1	4:E:36:GLU:N	2.34	0.60
1:A:455:MET:O	2:B:1141:HIS:NE2	2.34	0.60
2:B:727:LYS:NZ	2:B:1049:ASP:O	2.34	0.60
2:B:957:ASN:OD1	2:B:958:GLN:N	2.31	0.60
19:Y:69:SER:OG	19:Y:74:TYR:OH	2.10	0.60
13:c:62:ILE:CG2	14:d:59:MET:HE1	2.31	0.60
6:H:25:ARG:NE	6:H:41:ASP:OD2	2.34	0.60
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.37	0.60
4:E:180:ARG:NH2	4:E:215:MET:OXT	2.35	0.60
14:d:53:SER:N	15:T:-54:DA:OP1	2.34	0.60
2:B:287:ARG:NH1	2:B:292:ILE:O	2.35	0.60
3:C:265:MET:CE	9:K:21:ILE:HD12	2.32	0.59
1:A:149:GLU:O	1:A:164:ARG:NH2	2.35	0.59
2:B:197:PHE:O	2:B:488:TYR:OH	2.18	0.59
3:C:18:VAL:HG21	9:K:109:TRP:CZ3	2.37	0.59
1:A:23:SER:OG	1:A:233:TRP:NE1	2.35	0.59
1:A:362:ASP:OD1	1:A:459:ARG:NH2	2.35	0.59
1:A:626:ASN:O	1:A:631:HIS:ND1	2.36	0.59
14:d:83:ARG:NH2	15:T:-34:DG:O5'	2.33	0.59
3:C:138:GLU:OE1	3:C:140:ASN:N	2.36	0.59
10:L:31:CYS:SG	10:L:32:ALA:N	2.74	0.59
1:A:306:ASN:ND2	1:A:322:VAL:O	2.36	0.59
2:B:115:GLN:O	2:B:119:LEU:HD23	2.03	0.59
1:A:566:ILE:CG2	6:H:96:VAL:HG13	2.33	0.59
1:A:359:LEU:HD21	1:A:461:LYS:HD3	1.83	0.59
17:W:406:GLY:N	25:W:1501:ADP:O1A	2.35	0.59
22:G:91:VAL:HG22	22:G:99:PHE:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:ASP:OD1	10:L:29:TYR:OH	2.15	0.58
2:B:103:ASN:O	2:B:958:GLN:NE2	2.36	0.58
22:G:65:ASP:OD2	22:G:66:GLY:N	2.37	0.58
11:a:109:LEU:HD11	11:e:129:ARG:NH2	2.19	0.58
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.34	0.58
1:A:328:ARG:NH2	2:B:1206:GLU:OE1	2.36	0.58
1:A:16:GLU:OE2	2:B:1217:TYR:N	2.37	0.58
2:B:542:MET:HE2	2:B:747:MET:HG3	1.86	0.57
17:W:175:ASP:OD2	17:W:176:PHE:N	2.37	0.57
2:B:206:ASN:O	2:B:206:ASN:ND2	2.28	0.57
17:W:660:ASN:ND2	17:W:720:MET:HE1	2.19	0.57
1:A:1234:GLU:N	1:A:1234:GLU:OE1	2.37	0.57
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.87	0.57
6:H:5:LEU:HD11	6:H:61:SER:OG	2.04	0.57
2:B:852:ARG:NH2	10:L:70:ARG:O	2.38	0.57
12:b:98:TYR:OH	14:h:65:ASP:OD1	2.11	0.57
17:W:206:ASN:ND2	17:W:210:ASN:OD1	2.34	0.57
12:b:29:ILE:O	12:b:55:ARG:NH1	2.37	0.57
13:g:33:LEU:HD22	14:h:67:PHE:CZ	2.40	0.57
1:A:894:GLU:OE1	1:A:933:TYR:OH	2.09	0.57
1:A:1348:LEU:CD2	1:A:1372:VAL:HG12	2.34	0.57
1:A:106:VAL:O	1:A:171:GLN:NE2	2.38	0.56
1:A:472:LEU:O	1:A:472:LEU:HD23	2.04	0.56
17:W:574:ASN:OD1	17:W:579:GLN:NE2	2.38	0.56
1:A:1004:ASN:OD1	4:E:167:ARG:NH2	2.38	0.56
14:d:33:SER:OG	14:d:60:ASN:ND2	2.38	0.56
2:B:1037:LEU:O	8:J:47:ARG:NH2	2.39	0.56
1:A:116:ASP:OD2	1:A:117:GLU:N	2.38	0.56
2:B:195:CYS:SG	2:B:783:THR:OG1	2.56	0.56
11:a:63:ARG:NH1	16:N:18:DG:OP2	2.28	0.56
11:a:83:ARG:O	12:b:80:THR:HG23	2.04	0.56
11:e:59:GLU:N	11:e:59:GLU:OE2	2.37	0.56
5:F:145:ASP:OD1	22:G:58:ARG:NH2	2.39	0.56
11:e:106:ASP:OD2	11:e:131:ARG:NH1	2.39	0.56
14:h:91:ILE:O	14:h:95:VAL:HG23	2.06	0.56
2:B:332:ASP:O	2:B:336:ARG:NE	2.31	0.56
2:B:953:LEU:HD11	10:L:55:ILE:HG23	1.87	0.55
2:B:953:LEU:HD11	10:L:55:ILE:CG2	2.36	0.55
6:H:13:SER:OG	6:H:27:GLU:O	2.22	0.55
2:B:44:VAL:CG1	2:B:495:LEU:HD23	2.36	0.55
2:B:90:ILE:N	2:B:133:LYS:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:VAL:HG13	2:B:385:LEU:HD12	1.88	0.55
7:I:77:LYS:NZ	7:I:106:CYS:SG	2.80	0.55
1:A:1169:ILE:HG23	1:A:1170:ILE:HG23	1.89	0.55
1:A:767:GLN:NE2	1:A:768:GLN:O	2.39	0.55
2:B:886:LYS:NZ	2:B:936:ASP:OD1	2.39	0.55
17:W:796:GLN:NE2	17:W:840:GLU:OE2	2.39	0.55
1:A:465:TYR:HB3	2:B:976:ILE:HD11	1.89	0.55
1:A:1217:LYS:O	1:A:1220:PHE:C	2.50	0.55
17:W:410:GLN:OE1	17:W:597:ARG:NH1	2.40	0.55
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.89	0.55
2:B:604:ARG:NH2	2:B:691:GLU:OE1	2.40	0.55
17:W:776:LEU:O	26:W:1502:BEF:F2	2.15	0.55
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.87	0.55
2:B:181:LEU:HD22	2:B:189:LEU:HD23	1.90	0.54
2:B:610:ASN:O	2:B:613:VAL:HG12	2.06	0.54
2:B:318:VAL:HG22	7:I:13:MET:HE2	1.89	0.54
2:B:1129:ARG:NH1	15:T:47:DG:H4'	2.22	0.54
3:C:112:ASN:ND2	8:J:19:GLU:OE2	2.40	0.54
1:A:1445:ILE:HD12	22:G:18:PHE:CE2	2.42	0.54
3:C:58:LEU:HD11	8:J:2:ILE:HD11	1.89	0.54
20:Z:287:ILE:HG23	20:Z:363:ILE:HB	1.89	0.54
11:e:61:LEU:N	11:e:97:GLU:OE1	2.36	0.54
16:N:-33:DG:H2'	16:N:-32:DT:H72	1.89	0.54
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.73	0.54
1:A:1442:ASP:HB3	1:A:1444:MET:HE1	1.90	0.54
2:B:781:PHE:HE2	2:B:793:ALA:HB1	1.73	0.54
11:e:71:VAL:HG21	11:e:92:LEU:HD23	1.89	0.54
14:h:104:ALA:O	14:h:108:VAL:HG23	2.08	0.54
2:B:567:GLU:N	2:B:567:GLU:OE1	2.41	0.54
17:W:404:GLY:O	17:W:405:LEU:HD22	2.08	0.54
17:W:483:MET:SD	17:W:483:MET:N	2.80	0.54
22:G:4:ILE:CD1	22:G:49:LEU:HD21	2.38	0.54
1:A:739:ASP:OD2	1:A:748:MET:HE1	2.08	0.53
2:B:551:PRO:O	2:B:555:ILE:HD12	2.08	0.53
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.90	0.53
11:e:42:ARG:NE	16:N:70:DG:O5'	2.42	0.53
17:W:292:ASP:OD2	17:W:293:SER:N	2.42	0.53
17:W:727:LEU:HD11	17:W:789:PHE:HE1	1.73	0.53
19:Y:3:SER:OG	19:Y:4:GLU:N	2.41	0.53
1:A:567:LYS:HB2	6:H:96:VAL:HG12	1.89	0.53
1:A:782:ARG:NH2	7:I:67:THR:HG23	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:ASP:C	1:A:1224:LEU:HD12	2.34	0.53
3:C:74:SER:HG	3:C:237:SER:HG	1.57	0.53
5:F:103:MET:HE2	22:G:15:PRO:CG	2.39	0.53
16:N:12:DG:O3'	17:W:241:ARG:NH2	2.41	0.53
17:W:713:ARG:NH1	17:W:782:THR:OG1	2.42	0.53
1:A:111:GLY:CA	1:A:210:ILE:HD11	2.39	0.53
1:A:1444:MET:HE3	5:F:135:ARG:HG2	1.90	0.53
12:b:78:ARG:NH2	12:b:80:THR:OG1	2.42	0.53
2:B:416:LEU:O	2:B:420:LEU:HD23	2.08	0.53
11:a:126:LEU:HD22	11:e:113:HIS:CG	2.43	0.53
14:h:48:ASP:OD2	14:h:49:THR:N	2.41	0.53
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.44	0.53
1:A:482:PHE:O	2:B:989:THR:HG22	2.09	0.53
1:A:920:LEU:HD23	1:A:921:GLY:N	2.24	0.53
1:A:1168:GLU:OE2	1:A:1168:GLU:N	2.41	0.53
12:f:30:THR:OG1	16:N:-12:DA:OP2	2.26	0.53
17:W:690:LEU:HD21	17:W:697:MET:HE3	1.90	0.53
13:c:17:ARG:NH2	15:T:-43:DT:OP2	2.43	0.52
17:W:381:LEU:O	17:W:385:ASN:ND2	2.42	0.52
17:W:804:ARG:NH1	26:W:1502:BEF:F1	2.29	0.52
1:A:515:GLN:HE21	1:A:1363:VAL:HG22	1.74	0.52
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.24	0.52
1:A:332:LYS:NZ	15:T:46:DA:OP2	2.42	0.52
2:B:236:HIS:O	2:B:385:LEU:HD11	2.09	0.52
2:B:790:ASP:O	2:B:858:SER:OG	2.22	0.52
5:F:85:MET:SD	5:F:153:VAL:HG22	2.49	0.52
17:W:384:ILE:HD11	17:W:413:ALA:HB3	1.91	0.52
17:W:548:ASN:OD1	17:W:549:ILE:N	2.43	0.52
1:A:1444:MET:SD	22:G:60:ARG:NH2	2.78	0.52
20:Z:805:VAL:HG12	20:Z:847:TYR:HD1	1.75	0.52
21:D:5:THR:CG2	22:G:7:LEU:HD13	2.40	0.52
1:A:203:SER:OG	1:A:205:GLU:OE1	2.28	0.52
13:g:47:ALA:HB2	14:h:87:THR:HA	1.92	0.52
3:C:39:ALA:HB3	3:C:40:GLU:OE2	2.10	0.51
3:C:88:CYS:O	20:Z:808:ARG:NH2	2.41	0.51
19:Y:30:ILE:HG23	19:Y:89:LEU:HD22	1.92	0.51
22:G:119:LEU:HD11	22:G:137:ILE:HD12	1.91	0.51
1:A:760:GLN:HB2	2:B:1021:MET:HE1	1.92	0.51
2:B:776:GLN:OE1	2:B:1097:HIS:NE2	2.38	0.51
2:B:902:GLY:HA3	10:L:61:THR:HG22	1.93	0.51
11:a:61:LEU:HD13	12:b:40:ARG:CZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:156:ASP:HB2	21:D:159:THR:HG23	1.91	0.51
6:H:77:ARG:NH2	6:H:141:TYR:OH	2.44	0.51
7:I:50:THR:HG22	7:I:92:ARG:HH22	1.75	0.51
2:B:838:SER:OG	2:B:839:MET:N	2.43	0.51
2:B:1124:ARG:HD3	18:P:36:G:H21	1.75	0.51
6:H:104:PHE:HD2	6:H:114:VAL:HG22	1.75	0.51
9:K:29:ASN:OD1	9:K:77:THR:OG1	2.23	0.51
12:f:72:TYR:CD1	14:h:77:LEU:HD21	2.45	0.51
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.93	0.51
19:Y:17:ASN:OD1	19:Y:18:GLU:N	2.44	0.51
11:e:46:VAL:HG11	15:T:9:DG:H3'	1.93	0.51
17:W:434:LEU:O	17:W:435:SER:OG	2.25	0.51
17:W:474:ASN:OD1	17:W:481:LYS:NZ	2.44	0.51
7:I:60:GLN:N	7:I:60:GLN:OE1	2.44	0.51
8:J:1:MET:HB3	8:J:2:ILE:HD12	1.92	0.51
13:g:17:ARG:O	13:g:20:ARG:NH2	2.44	0.51
14:d:48:ASP:OD2	14:d:49:THR:HG23	2.11	0.51
11:e:91:ALA:HB3	12:f:86:VAL:HG11	1.93	0.51
1:A:317:LYS:NZ	15:T:56:DC:OP2	2.44	0.51
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.93	0.51
10:L:38:LEU:HD22	10:L:56:LEU:HD11	1.93	0.51
11:a:62:ILE:O	11:a:93:GLN:NE2	2.43	0.51
14:d:92:GLN:OE1	14:d:108:VAL:HG13	2.10	0.51
5:F:112:GLU:OE1	5:F:112:GLU:N	2.39	0.50
13:g:80:PRO:HD3	14:h:54:LYS:HZ1	1.76	0.50
1:A:804:TYR:O	2:B:761:HIS:ND1	2.39	0.50
12:b:89:ALA:O	12:b:93:GLN:NE2	2.44	0.50
11:e:60:LEU:HD12	11:e:90:MET:HE1	1.94	0.50
13:g:49:VAL:HG21	14:h:118:TYR:CD2	2.47	0.50
1:A:666:ILE:HG22	1:A:670:ILE:HD11	1.94	0.50
1:A:1054:LEU:HD13	5:F:84:TYR:CZ	2.46	0.50
2:B:629:ASP:O	2:B:632:ARG:NH1	2.45	0.50
1:A:866:PHE:N	4:E:208:TYR:OH	2.44	0.50
22:G:13:LEU:HD11	22:G:17:PHE:HB2	1.93	0.50
13:c:96:LEU:HD23	13:c:97:LEU:HG	1.94	0.50
22:G:91:VAL:HG13	22:G:99:PHE:HD1	1.77	0.50
11:a:83:ARG:NH2	15:T:-23:DC:O4'	2.44	0.50
1:A:7:SER:OG	1:A:8:SER:N	2.45	0.50
1:A:22:PHE:CD1	2:B:1213:THR:HG22	2.47	0.50
1:A:1073:GLY:O	1:A:1077:THR:HG23	2.12	0.50
2:B:223:VAL:O	2:B:384:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:357:GLN:OE1	17:W:358:ARG:N	2.45	0.50
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.94	0.49
2:B:996:ARG:NH1	3:C:38:ILE:HD11	2.27	0.49
1:A:1212:VAL:HG23	1:A:1273:LEU:HD23	1.94	0.49
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.94	0.49
1:A:9:ALA:HB3	2:B:1193:GLN:OE1	2.12	0.49
4:E:123:LEU:O	4:E:123:LEU:HD12	2.12	0.49
8:J:45:CYS:SG	8:J:46:CYS:N	2.85	0.49
13:c:17:ARG:NH1	15:T:-43:DT:O5'	2.45	0.49
17:W:591:GLN:HA	17:W:594:ILE:HG22	1.95	0.49
25:W:1501:ADP:O2B	26:W:1502:BEF:F1	2.21	0.49
4:E:8:ASN:O	4:E:12:LEU:HD23	2.12	0.49
2:B:384:ARG:HE	2:B:393:LYS:NZ	2.11	0.49
22:G:108:VAL:HG22	22:G:159:ALA:HB3	1.95	0.49
1:A:560:ILE:HG22	1:A:561:PRO:O	2.13	0.49
1:A:1144:LYS:HE2	1:A:1268:LEU:HD23	1.95	0.49
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.48	0.49
17:W:778:ILE:O	17:W:807:ARG:NH1	2.46	0.49
1:A:818:MET:HA	2:B:514:LEU:HD21	1.94	0.49
1:A:970:THR:HG23	1:A:971:PHE:HD2	1.78	0.49
2:B:173:MET:O	2:B:176:SER:OG	2.31	0.49
2:B:332:ASP:OD1	2:B:349:ILE:HD12	2.12	0.49
1:A:260:ASP:OD1	1:A:261:ASP:N	2.45	0.48
2:B:120:ARG:NH1	2:B:956:THR:O	2.46	0.48
2:B:499:ASN:OD1	2:B:500:THR:N	2.43	0.48
21:D:4:SER:OG	21:D:5:THR:N	2.46	0.48
22:G:4:ILE:HD12	22:G:49:LEU:HD21	1.94	0.48
1:A:399:HIS:O	1:A:435:HIS:ND1	2.42	0.48
3:C:248:ILE:HG21	9:K:102:LYS:HB2	1.95	0.48
14:d:94:ALA:O	14:d:98:LEU:HD23	2.13	0.48
2:B:247:GLY:O	2:B:248:SER:OG	2.23	0.48
22:G:106:MET:HE2	22:G:157:ILE:HB	1.96	0.48
22:G:137:ILE:HG12	22:G:143:ILE:HD11	1.94	0.48
2:B:542:MET:HE1	2:B:743:ILE:HB	1.96	0.48
3:C:18:VAL:HG21	9:K:109:TRP:HZ3	1.79	0.48
6:H:56:THR:HG21	6:H:145:ARG:HH12	1.79	0.48
11:e:48:LEU:HA	11:e:51:ILE:HD12	1.96	0.48
22:G:27:LYS:HZ3	22:G:54:ILE:HD13	1.79	0.48
1:A:90:VAL:HG13	1:A:297:GLN:HG3	1.96	0.48
2:B:1180:PHE:HD1	2:B:1191:ILE:HG21	1.79	0.48
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.45	0.47
11:e:92:LEU:CD1	12:f:86:VAL:HG13	2.44	0.47
15:T:-27:DC:H2'	15:T:-26:DT:H72	1.95	0.47
2:B:898:LEU:HD11	2:B:964:VAL:HG11	1.96	0.47
2:B:1129:ARG:HH11	2:B:1129:ARG:HG3	1.79	0.47
3:C:147:LEU:HD12	3:C:151:GLN:HB2	1.95	0.47
7:I:32:CYS:O	7:I:34:TYR:N	2.45	0.47
1:A:111:GLY:HA2	1:A:210:ILE:HD11	1.96	0.47
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.96	0.47
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.47	0.47
2:B:711:GLU:N	2:B:711:GLU:OE1	2.47	0.47
3:C:136:ASP:OD1	3:C:139:GLY:N	2.43	0.47
14:h:117:LYS:O	14:h:120:SER:OG	2.32	0.47
1:A:494:SER:OG	1:A:497:THR:OG1	2.08	0.47
1:A:709:THR:HG23	1:A:712:GLU:H	1.79	0.47
1:A:1193:LEU:CD2	1:A:1260:LEU:HD11	2.45	0.47
2:B:635:ARG:NH1	2:B:637:LEU:HD21	2.28	0.47
12:b:78:ARG:NH2	16:N:27:DG:O3'	2.47	0.47
4:E:43:LYS:O	4:E:47:CYS:N	2.48	0.47
11:a:110:CYS:SG	11:a:126:LEU:HD23	2.54	0.47
15:T:-27:DC:C2'	15:T:-26:DT:H72	2.44	0.47
1:A:1224:LEU:HD23	1:A:1240:CYS:SG	2.54	0.47
2:B:596:LEU:HD23	2:B:624:LEU:HD13	1.95	0.47
12:b:24:ASP:OD2	12:b:25:ASN:N	2.47	0.47
1:A:837:ILE:CG2	1:A:1105:LEU:HD12	2.45	0.47
2:B:803:LEU:HD22	8:J:52:THR:HG21	1.96	0.47
10:L:47:ARG:NH1	10:L:48:CYS:O	2.47	0.47
13:g:44:GLY:N	14:h:86:ILE:O	2.43	0.47
14:h:51:ILE:HG12	14:h:55:ALA:HB3	1.95	0.47
17:W:362:GLU:N	17:W:362:GLU:OE2	2.47	0.47
3:C:254:LYS:HD2	9:K:42:LEU:HD21	1.96	0.47
11:e:116:ARG:NH2	16:N:-3:DA:OP1	2.48	0.47
13:g:80:PRO:CD	14:h:54:LYS:HZ1	2.27	0.47
2:B:416:LEU:HD11	2:B:460:ALA:HB1	1.97	0.47
1:A:544:ASP:OD2	9:K:47:ARG:NH1	2.48	0.46
2:B:890:TYR:CE1	2:B:910:VAL:HG11	2.51	0.46
1:A:944:ARG:NH2	1:A:1296:GLY:O	2.48	0.46
1:A:473:SER:HB2	1:A:650:GLN:NE2	2.30	0.46
1:A:1399:ARG:NH2	1:A:1417:GLU:OE1	2.48	0.46
10:L:27:LEU:HD23	10:L:27:LEU:O	2.14	0.46
12:b:82:THR:HG22	12:b:84:MET:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:57:SER:OG	12:f:99:GLY:O	2.15	0.46
17:W:560:MET:HE1	17:W:593:PHE:CD2	2.51	0.46
1:A:660:ASN:O	2:B:1082:MET:N	2.49	0.46
2:B:704:ALA:HB3	2:B:741:CYS:CB	2.45	0.46
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.46
15:T:-16:DT:OP1	17:W:463:ARG:NH2	2.49	0.46
1:A:605:MET:CE	1:A:617:VAL:HG22	2.46	0.46
2:B:540:SER:OG	2:B:541:LEU:N	2.48	0.46
12:b:66:ILE:O	12:b:70:VAL:HG23	2.15	0.46
17:W:214:LEU:HD11	17:W:225:ASN:HB3	1.97	0.46
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.49	0.46
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.97	0.46
6:H:58:THR:HG21	6:H:93:TYR:OH	2.16	0.46
1:A:881:GLN:OE1	1:A:1021:LEU:HD21	2.16	0.46
1:A:888:GLY:N	1:A:1297:GLU:OE1	2.49	0.46
2:B:345:LYS:O	2:B:349:ILE:HG22	2.16	0.46
13:g:33:LEU:HD22	14:h:67:PHE:CE1	2.51	0.46
13:g:47:ALA:HB3	13:g:48:PRO:HD3	1.96	0.46
1:A:29:ALA:O	2:B:1183:LYS:NZ	2.38	0.46
9:K:32:VAL:CG1	9:K:72:LYS:HE2	2.45	0.46
11:e:64:LYS:NZ	15:T:18:DC:OP1	2.46	0.46
11:e:124:ILE:HG21	12:f:53:GLU:OE1	2.16	0.46
12:f:73:THR:HG21	12:f:81:VAL:HG12	1.98	0.46
1:A:1444:MET:HE3	5:F:135:ARG:CG	2.45	0.46
7:I:103:CYS:O	7:I:107:SER:N	2.46	0.46
17:W:576:ASP:OD1	17:W:577:GLU:N	2.49	0.46
1:A:1325:THR:O	4:E:147:HIS:ND1	2.49	0.46
11:e:44:GLY:N	15:T:9:DG:OP1	2.43	0.46
12:f:46:ILE:N	15:T:8:DC:OP1	2.44	0.46
17:W:454:ILE:HD11	17:W:469:TYR:HE2	1.80	0.46
1:A:28:ARG:NH2	1:A:85:ASP:OD1	2.49	0.45
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.98	0.45
2:B:498:THR:N	2:B:537:LYS:O	2.49	0.45
2:B:904:ARG:NH2	20:Z:832:HIS:O	2.49	0.45
5:F:103:MET:HE2	22:G:15:PRO:HG3	1.97	0.45
6:H:104:PHE:CD2	6:H:114:VAL:HG22	2.51	0.45
13:c:104:GLN:O	11:e:58:THR:OG1	2.34	0.45
14:h:54:LYS:HE3	14:h:55:ALA:HB2	1.98	0.45
20:Z:812:TYR:CD2	20:Z:838:ILE:HD13	2.51	0.45
1:A:1054:LEU:HD13	5:F:84:TYR:CE2	2.51	0.45
2:B:277:LYS:NZ	2:B:338:GLY:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:HG22	6:H:96:VAL:HG13	1.99	0.45
1:A:1063:MET:HE2	1:A:1436:ILE:HA	1.97	0.45
11:e:46:VAL:HG23	11:e:49:ARG:NH1	2.31	0.45
11:a:97:GLU:OE1	12:b:40:ARG:NH1	2.45	0.45
21:D:59:ILE:O	21:D:63:LEU:HD23	2.16	0.45
2:B:394:ASP:HA	7:I:91:ARG:HH12	1.81	0.45
4:E:171:LYS:N	4:E:174:GLN:OE1	2.42	0.45
2:B:517:THR:CG2	2:B:695:ALA:HB1	2.47	0.45
13:c:24:GLN:N	13:c:56:GLU:OE2	2.42	0.45
15:T:-43:DT:H2'	15:T:-42:DT:H71	1.99	0.45
17:W:378:ASP:OD1	17:W:378:ASP:N	2.49	0.45
4:E:12:LEU:HD21	4:E:55:ARG:NH2	2.32	0.45
13:c:81:ARG:NH2	11:e:55:GLN:O	2.49	0.45
20:Z:315:MET:SD	20:Z:316:GLY:N	2.90	0.45
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.98	0.45
6:H:34:ASP:OD2	6:H:34:ASP:N	2.50	0.45
20:Z:832:HIS:O	20:Z:832:HIS:ND1	2.47	0.45
8:J:48:ARG:NH1	8:J:49:MET:SD	2.90	0.45
12:b:23:ARG:NH2	15:T:-12:DC:OP1	2.47	0.45
19:Y:13:VAL:HG11	20:Z:302:ARG:HH22	1.82	0.45
1:A:553:VAL:HG21	1:A:580:VAL:HG23	1.98	0.45
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.47	0.45
3:C:265:MET:HE3	9:K:21:ILE:HD12	1.99	0.45
1:A:9:ALA:HB1	2:B:1191:ILE:O	2.16	0.44
2:B:261:ARG:NH2	2:B:262:GLU:OE1	2.51	0.44
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.44	0.44
2:B:186:GLU:OE2	8:J:62:ARG:NH2	2.50	0.44
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.99	0.44
11:a:62:ILE:HD11	12:b:37:LEU:HD11	1.99	0.44
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.99	0.44
13:c:68:ASN:OD1	13:c:71:ARG:NH1	2.50	0.44
13:c:73:ASN:ND2	13:c:73:ASN:O	2.50	0.44
17:W:398:ILE:HG23	17:W:539:LEU:HB2	1.99	0.44
17:W:412:VAL:HG21	17:W:443:THR:HG22	1.99	0.44
21:D:50:LEU:HD12	21:D:54:GLU:HG2	1.99	0.44
1:A:329:LEU:HD21	2:B:1206:GLU:OE2	2.18	0.44
1:A:1450:LEU:HD23	1:A:1450:LEU:O	2.17	0.44
2:B:481:GLN:NE2	18:P:42:A:O3'	2.49	0.44
5:F:114:GLU:OE1	5:F:119:ARG:NH1	2.50	0.44
12:f:30:THR:HG23	12:f:33:ALA:H	1.83	0.44
17:W:575:GLN:NE2	17:W:576:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:92:GLN:OE1	14:h:108:VAL:HG13	2.18	0.44
1:A:1106:ASN:OD1	1:A:1385:THR:HG22	2.18	0.44
5:F:103:MET:HE2	22:G:15:PRO:HG2	2.00	0.44
7:I:84:VAL:HG13	7:I:104:LEU:HD11	1.98	0.44
12:b:34:ILE:HD12	12:b:54:THR:HG21	2.00	0.44
12:f:38:ALA:CB	12:f:46:ILE:HD11	2.48	0.44
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.98	0.44
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.00	0.44
9:K:32:VAL:HG13	9:K:72:LYS:HE2	1.99	0.44
17:W:611:GLU:OE1	17:W:611:GLU:N	2.50	0.44
1:A:474:VAL:HG23	1:A:521:MET:HE1	1.99	0.44
2:B:704:ALA:HB3	2:B:741:CYS:HB2	1.99	0.44
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.99	0.44
3:C:242:GLN:O	3:C:246:ARG:HG3	2.17	0.44
21:D:148:LEU:HD21	22:G:2:PHE:CZ	2.53	0.44
1:A:408:ASP:OD2	1:A:409:SER:N	2.51	0.44
1:A:616:VAL:HG13	1:A:618:GLU:OE1	2.17	0.44
1:A:913:LEU:HD23	1:A:913:LEU:H	1.83	0.44
1:A:974:ASP:OD1	1:A:977:LYS:N	2.46	0.44
1:A:1257:ASP:O	1:A:1261:LYS:NZ	2.28	0.44
2:B:466:TRP:HB2	2:B:479:VAL:HG21	2.00	0.44
2:B:996:ARG:CZ	3:C:38:ILE:HD11	2.48	0.44
22:G:91:VAL:HG22	22:G:99:PHE:HE1	1.81	0.44
1:A:885:THR:O	1:A:940:ARG:NH1	2.52	0.43
2:B:903:VAL:O	2:B:949:VAL:HG12	2.18	0.43
5:F:97:ARG:HD3	5:F:130:ILE:HG23	2.00	0.43
5:F:133:VAL:O	5:F:134:ILE:HD13	2.17	0.43
17:W:419:ILE:HD13	17:W:451:LEU:HD11	2.00	0.43
17:W:683:ARG:NH1	17:W:687:LEU:HD23	2.33	0.43
1:A:364:VAL:HG21	1:A:444:PHE:CE2	2.53	0.43
9:K:9:LEU:HD12	9:K:69:ALA:HB2	2.00	0.43
17:W:660:ASN:HD22	17:W:720:MET:HE1	1.81	0.43
19:Y:22:ASP:OD1	19:Y:22:ASP:N	2.48	0.43
1:A:863:VAL:O	1:A:863:VAL:HG23	2.18	0.43
1:A:1193:LEU:HD21	1:A:1260:LEU:HD11	1.98	0.43
2:B:416:LEU:HD13	2:B:457:LEU:HD12	1.99	0.43
3:C:8:VAL:HG21	9:K:105:PHE:HD1	1.83	0.43
4:E:138:ALA:O	4:E:141:VAL:HG12	2.17	0.43
10:L:38:LEU:HD21	10:L:48:CYS:HA	2.01	0.43
10:L:68:GLU:OE2	20:Z:833:SER:HB2	2.17	0.43
13:c:32:ARG:NH1	15:T:-44:DA:OP1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:431:VAL:HG21	17:W:512:VAL:HG12	2.00	0.43
21:D:162:ALA:O	21:D:166:LEU:HD13	2.18	0.43
1:A:1143:LEU:O	1:A:1147:THR:HG23	2.18	0.43
3:C:36:VAL:HG21	3:C:251:LEU:HB2	2.00	0.43
7:I:96:SER:OG	7:I:98:VAL:HG23	2.18	0.43
13:c:23:LEU:HD21	13:c:53:ALA:N	2.34	0.43
1:A:361:LEU:HD11	1:A:521:MET:HE2	2.00	0.43
20:Z:287:ILE:HD13	20:Z:338:GLU:HG3	1.99	0.43
1:A:544:ASP:O	9:K:47:ARG:NH2	2.52	0.43
1:A:981:LEU:HD13	1:A:986:ILE:HD11	2.00	0.43
1:A:993:LEU:HD21	1:A:1049:ILE:HG21	1.99	0.43
2:B:56:ASP:OD2	2:B:177:LYS:NZ	2.29	0.43
2:B:514:LEU:HD23	2:B:514:LEU:H	1.83	0.43
2:B:837:ASP:OD2	2:B:1016:ALA:HB2	2.19	0.43
1:A:14:VAL:O	1:A:1432:GLN:NE2	2.45	0.43
1:A:1209:MET:HE3	1:A:1236:LEU:HB2	2.00	0.43
9:K:18:LYS:NZ	9:K:38:GLU:OE2	2.46	0.43
17:W:375:GLU:OE1	17:W:377:ARG:NE	2.51	0.43
2:B:299:GLU:OE2	2:B:572:HIS:N	2.51	0.43
2:B:301:ILE:CG2	2:B:314:LEU:HD11	2.44	0.43
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.18	0.43
17:W:400:ALA:HB2	17:W:594:ILE:HD11	2.00	0.43
20:Z:287:ILE:HG21	20:Z:368:LEU:HD22	2.00	0.43
20:Z:334:ARG:HE	20:Z:336:TYR:HE2	1.65	0.43
3:C:146:LYS:C	3:C:147:LEU:HD22	2.44	0.43
13:c:92:GLU:OE1	14:d:103:LEU:HD12	2.19	0.43
14:d:84:SER:OG	15:T:-34:DG:OP1	2.34	0.43
22:G:7:LEU:HD12	22:G:8:SER:N	2.34	0.43
1:A:107:CYS:CB	1:A:110:CYS:SG	3.07	0.43
1:A:571:LEU:HD12	6:H:46:LEU:CD1	2.48	0.43
1:A:775:ILE:HG23	1:A:818:MET:HE1	2.00	0.43
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.54	0.43
2:B:806:THR:HG22	2:B:808:ALA:H	1.83	0.43
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.54	0.43
2:B:868:MET:O	2:B:869:SER:OG	2.29	0.43
5:F:109:VAL:HG21	5:F:123:LYS:HD2	2.00	0.43
1:A:1265:ASN:ND2	1:A:1269:GLU:OE1	2.52	0.42
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.83	0.42
2:B:905:VAL:HG21	2:B:911:ILE:HD11	2.00	0.42
3:C:14:SER:OG	3:C:15:LYS:N	2.52	0.42
10:L:65:VAL:HG23	20:Z:832:HIS:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:62:ILE:HG21	14:h:59:MET:HE1	2.01	0.42
17:W:606:LEU:HD12	17:W:607:PRO:HD2	2.01	0.42
21:D:5:THR:HG21	22:G:7:LEU:HD13	2.01	0.42
21:D:159:THR:O	21:D:163:VAL:HG23	2.19	0.42
1:A:1209:MET:HE3	1:A:1236:LEU:CB	2.49	0.42
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.59	0.42
1:A:729:ALA:HB1	1:A:763:ALA:HB1	2.02	0.42
1:A:1141:THR:OG1	1:A:1274:ARG:N	2.52	0.42
3:C:7:GLN:OE1	9:K:104:ASN:ND2	2.52	0.42
4:E:116:ILE:HG21	4:E:121:MET:SD	2.60	0.42
22:G:122:ASN:ND2	22:G:131:GLN:OE1	2.46	0.42
1:A:783:THR:O	2:B:516:ASN:ND2	2.44	0.42
2:B:437:GLU:OE1	2:B:437:GLU:N	2.47	0.42
5:F:93:ILE:HG23	5:F:132:LEU:HD12	2.02	0.42
13:g:51:LEU:O	13:g:55:LEU:HD13	2.19	0.42
21:D:141:LEU:HD11	22:G:35:GLU:OE2	2.20	0.42
22:G:94:CYS:SG	22:G:95:SER:N	2.92	0.42
1:A:540:PHE:HB3	1:A:571:LEU:HD22	2.02	0.42
2:B:1219:ASP:OD1	2:B:1219:ASP:N	2.53	0.42
12:b:34:ILE:HD12	12:b:54:THR:CG2	2.49	0.42
22:G:51:TYR:O	22:G:54:ILE:HG22	2.20	0.42
1:A:1054:LEU:O	1:A:1057:VAL:HG12	2.19	0.42
17:W:725:ASP:OD1	17:W:740:ARG:NH2	2.52	0.42
3:C:180:TYR:HB3	3:C:228:PHE:HD1	1.85	0.42
1:A:1120:LEU:HD21	1:A:1306:LEU:CD1	2.49	0.42
1:A:1131:ALA:HB1	1:A:1284:MET:HE3	2.02	0.42
4:E:168:TYR:HB3	4:E:170:LEU:HD13	2.01	0.42
21:D:14:ARG:C	21:D:15:LEU:HD12	2.44	0.42
1:A:249:SER:OG	1:A:259:GLU:OE1	2.30	0.42
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.52	0.42
2:B:44:VAL:HG11	2:B:495:LEU:HD23	2.02	0.42
7:I:33:SER:O	7:I:33:SER:OG	2.35	0.42
7:I:85:PHE:CD2	7:I:99:LEU:HD13	2.55	0.42
13:c:62:ILE:HG21	14:d:59:MET:HE1	2.01	0.42
1:A:1198:ASP:OD2	1:A:1200:ALA:N	2.53	0.41
7:I:50:THR:HG22	7:I:92:ARG:NH2	2.35	0.41
13:c:70:ALA:HB1	13:c:75:LYS:O	2.20	0.41
11:e:82:LEU:HD21	12:f:70:VAL:HG12	2.02	0.41
17:W:214:LEU:HD11	17:W:225:ASN:CB	2.50	0.41
17:W:526:TYR:CZ	17:W:558:PHE:HB2	2.55	0.41
1:A:867:ILE:HD11	1:A:1000:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:TYR:OH	7:I:18:GLU:OE1	2.37	0.41
2:B:483:LEU:HD11	2:B:495:LEU:CD1	2.50	0.41
2:B:578:THR:HG21	2:B:593:PRO:HB3	2.02	0.41
4:E:12:LEU:HD21	4:E:55:ARG:HH21	1.85	0.41
9:K:5:ASP:OD2	9:K:6:ARG:N	2.49	0.41
17:W:699:LEU:HD23	17:W:703:LEU:HG	2.01	0.41
1:A:597:LEU:HD13	6:H:103:LYS:HD3	2.03	0.41
1:A:666:ILE:CG2	1:A:670:ILE:HD11	2.50	0.41
1:A:816:HIS:HE2	2:B:763:GLN:HA	1.85	0.41
1:A:1192:LEU:HD11	1:A:1239:ARG:HE	1.85	0.41
4:E:94:LYS:HE3	4:E:94:LYS:HA	2.02	0.41
1:A:471:ASN:O	1:A:474:VAL:HG12	2.21	0.41
1:A:837:ILE:HG23	1:A:1105:LEU:HD12	2.01	0.41
2:B:1112:GLN:N	2:B:1117:GLN:O	2.44	0.41
4:E:2:ASP:OD2	4:E:2:ASP:N	2.51	0.41
12:f:72:TYR:HD1	14:h:77:LEU:HD21	1.84	0.41
19:Y:52:MET:O	19:Y:71:ALA:HB1	2.21	0.41
1:A:30:ILE:HD12	2:B:1170:THR:HG21	2.02	0.41
1:A:381:THR:HG22	5:F:102:SER:O	2.20	0.41
1:A:660:ASN:ND2	1:A:661:GLY:O	2.54	0.41
1:A:709:THR:OG1	1:A:710:LEU:N	2.54	0.41
14:d:87:THR:HG22	14:d:88:SER:N	2.36	0.41
15:T:6:DC:N4	16:N:-7:DG:O6	2.53	0.41
17:W:790:ASP:OD1	17:W:790:ASP:N	2.51	0.41
22:G:27:LYS:NZ	22:G:54:ILE:HD13	2.35	0.41
1:A:269:ILE:HD11	1:A:300:VAL:HA	2.02	0.41
2:B:900:ALA:O	2:B:903:VAL:HG23	2.21	0.41
3:C:76:ASP:OD1	3:C:128:ASN:N	2.53	0.41
3:C:239:PRO:O	3:C:242:GLN:N	2.54	0.41
15:T:-48:DC:H2''	15:T:-47:DT:H71	2.01	0.41
20:Z:345:ILE:H	20:Z:345:ILE:HD12	1.85	0.41
1:A:478:TYR:CD1	1:A:487:MET:HE1	2.56	0.41
1:A:590:ARG:NH1	1:A:621:THR:OG1	2.54	0.41
18:P:39:U:H2'	18:P:40:C:C6	2.55	0.41
1:A:351:THR:OG1	1:A:352:VAL:N	2.54	0.41
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.56	0.41
1:A:963:ILE:HD11	1:A:1052:GLN:OE1	2.21	0.41
1:A:1264:GLU:OE2	1:A:1268:LEU:HD22	2.21	0.41
2:B:704:ALA:HB2	2:B:738:PHE:CD1	2.56	0.41
2:B:763:GLN:HB3	2:B:766:ARG:HG2	2.02	0.41
3:C:40:GLU:OE2	3:C:40:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:GLY:HA3	10:L:69:ALA:CB	2.50	0.41
12:b:51:TYR:O	12:b:55:ARG:HG3	2.20	0.41
14:h:34:TYR:CD2	14:h:63:VAL:HG11	2.55	0.41
20:Z:329:ASP:OD1	20:Z:329:ASP:N	2.52	0.41
22:G:25:TYR:O	22:G:28:THR:HG22	2.21	0.41
2:B:952:VAL:HG21	10:L:58:LYS:HE3	2.02	0.41
13:c:88:ARG:HB2	13:c:108:LEU:HD21	2.03	0.41
17:W:826:GLU:OE1	17:W:826:GLU:N	2.48	0.41
21:D:198:LEU:HD12	21:D:201:LYS:HG3	2.03	0.41
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.57	0.40
13:c:81:ARG:HE	13:c:85:LEU:HD21	1.87	0.40
17:W:492:TYR:OH	17:W:513:ASP:O	2.39	0.40
17:W:700:LEU:HD22	17:W:789:PHE:HZ	1.86	0.40
17:W:731:LEU:HD11	17:W:766:VAL:HG11	2.03	0.40
17:W:740:ARG:NH2	17:W:742:ASP:OD1	2.54	0.40
22:G:88:ASP:OD1	22:G:142:ARG:NH1	2.54	0.40
1:A:889:SER:OG	1:A:890:ASP:N	2.54	0.40
1:A:1445:ILE:HD12	22:G:18:PHE:HE2	1.85	0.40
11:a:60:LEU:HD22	11:a:97:GLU:HG3	2.03	0.40
1:A:1120:LEU:HD23	1:A:1304:TRP:O	2.22	0.40
1:A:1341:ILE:CD1	1:A:1376:THR:HG23	2.50	0.40
2:B:336:ARG:HD3	2:B:348:ARG:NH1	2.36	0.40
3:C:143:LEU:HD23	8:J:2:ILE:CG2	2.51	0.40
18:P:36:G:O2'	18:P:37:U:OP2	2.31	0.40
22:G:5:LYS:HD2	22:G:78:VAL:HG21	2.04	0.40
22:G:103:VAL:HG13	22:G:103:VAL:O	2.21	0.40
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	2.04	0.40
17:W:200:THR:OG1	17:W:201:VAL:N	2.55	0.40
17:W:346:ILE:HD11	17:W:419:ILE:HG22	2.03	0.40
20:Z:807:ILE:CD1	20:Z:838:ILE:HD11	2.52	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	A	1399/1733 (81%)	1315 (94%)	84 (6%)	0	100	100
2	B	1102/1224 (90%)	1047 (95%)	55 (5%)	0	100	100
3	C	263/318 (83%)	242 (92%)	21 (8%)	0	100	100
4	E	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
5	F	85/155 (55%)	79 (93%)	6 (7%)	0	100	100
6	H	129/146 (88%)	115 (89%)	14 (11%)	0	100	100
7	I	117/122 (96%)	106 (91%)	11 (9%)	0	100	100
8	J	63/70 (90%)	59 (94%)	4 (6%)	0	100	100
9	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	40 (95%)	2 (5%)	0	100	100
11	a	74/136 (54%)	71 (96%)	3 (4%)	0	100	100
11	e	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
12	b	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
12	f	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
13	c	101/130 (78%)	93 (92%)	8 (8%)	0	100	100
13	g	91/130 (70%)	89 (98%)	2 (2%)	0	100	100
14	d	90/123 (73%)	87 (97%)	3 (3%)	0	100	100
14	h	91/123 (74%)	88 (97%)	3 (3%)	0	100	100
17	W	610/1468 (42%)	584 (96%)	26 (4%)	0	100	100
19	Y	96/102 (94%)	91 (95%)	5 (5%)	0	100	100
20	Z	152/1066 (14%)	142 (93%)	10 (7%)	0	100	100
21	D	176/221 (80%)	159 (90%)	17 (10%)	0	100	100
22	G	169/171 (99%)	159 (94%)	10 (6%)	0	100	100
All	All	5424/8185 (66%)	5125 (94%)	299 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1232/1520 (81%)	1231 (100%)	1 (0%)	88	97
2	B	967/1061 (91%)	966 (100%)	1 (0%)	88	97
3	C	233/274 (85%)	233 (100%)	0	100	100
4	E	196/197 (100%)	196 (100%)	0	100	100
5	F	77/137 (56%)	77 (100%)	0	100	100
6	H	117/128 (91%)	117 (100%)	0	100	100
7	I	113/116 (97%)	113 (100%)	0	100	100
8	J	60/65 (92%)	60 (100%)	0	100	100
9	K	99/102 (97%)	99 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	a	66/111 (60%)	66 (100%)	0	100	100
11	e	84/111 (76%)	84 (100%)	0	100	100
12	b	65/79 (82%)	65 (100%)	0	100	100
12	f	63/79 (80%)	63 (100%)	0	100	100
13	c	82/102 (80%)	82 (100%)	0	100	100
13	g	72/102 (71%)	72 (100%)	0	100	100
14	d	78/103 (76%)	78 (100%)	0	100	100
14	h	79/103 (77%)	79 (100%)	0	100	100
17	W	567/1313 (43%)	565 (100%)	2 (0%)	84	94
19	Y	82/87 (94%)	82 (100%)	0	100	100
20	Z	136/878 (16%)	136 (100%)	0	100	100
21	D	161/200 (80%)	160 (99%)	1 (1%)	78	93
22	G	152/152 (100%)	152 (100%)	0	100	100
All	All	4820/7077 (68%)	4815 (100%)	5 (0%)	87	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	660	ASN
2	B	206	ASN
17	W	323	ASN
17	W	635	SER

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Mol	Chain	Res	Type
21	D	9	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	306	ASN
1	A	515	GLN
1	A	611	GLN
1	A	660	ASN
1	A	767	GLN
1	A	768	GLN
1	A	1011	GLN
1	A	1187	GLN
1	A	1211	GLN
1	A	1354	ASN
2	B	763	GLN
2	B	767	ASN
2	B	770	GLN
2	B	843	GLN
2	B	1093	GLN
2	B	1178	ASN
2	B	1195	HIS
2	B	1205	GLN
3	C	24	ASN
3	C	73	GLN
3	C	188	HIS
3	C	252	GLN
4	E	99	HIS
4	E	146	HIS
7	I	12	ASN
9	K	104	ASN
14	d	60	ASN
17	W	323	ASN
17	W	334	GLN
17	W	508	GLN
17	W	579	GLN
21	D	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	P	15/69 (21%)	4 (26%)	2 (13%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	P	35	U
18	P	36	G
18	P	37	U
18	P	39	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	P	36	G
18	P	38	C

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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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
26	BEF	W	1502	17	0,3,3	-	-	-		
25	ADP	W	1501	-	28,29,29	1.37	5 (17%)	43,45,45	1.91	12 (27%)

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
25	ADP	W	1501	-	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	1501	ADP	C5-C4	4.33	1.46	1.39
25	W	1501	ADP	C5-N7	-2.59	1.34	1.39
25	W	1501	ADP	C5-C6	2.44	1.47	1.41
25	W	1501	ADP	C8-N7	2.19	1.35	1.31
25	W	1501	ADP	C4-N9	-2.12	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	1501	ADP	C5-C4-N3	-5.71	118.85	126.72
25	W	1501	ADP	N3-C4-N9	4.73	135.21	127.17
25	W	1501	ADP	C2-N3-C4	3.87	121.28	111.83
25	W	1501	ADP	N3-C2-N1	-3.84	122.76	128.58
25	W	1501	ADP	C4-C5-N7	-3.22	106.90	110.58
25	W	1501	ADP	C4-N9-C8	3.09	108.99	105.74
25	W	1501	ADP	O5'-C5'-C4'	2.65	118.01	108.99
25	W	1501	ADP	C5-N7-C8	2.52	107.41	103.45
25	W	1501	ADP	C3'-C2'-C1'	2.39	105.98	101.46
25	W	1501	ADP	N9-C8-N7	-2.23	110.77	113.94
25	W	1501	ADP	C6-C5-N7	2.11	136.16	132.09
25	W	1501	ADP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

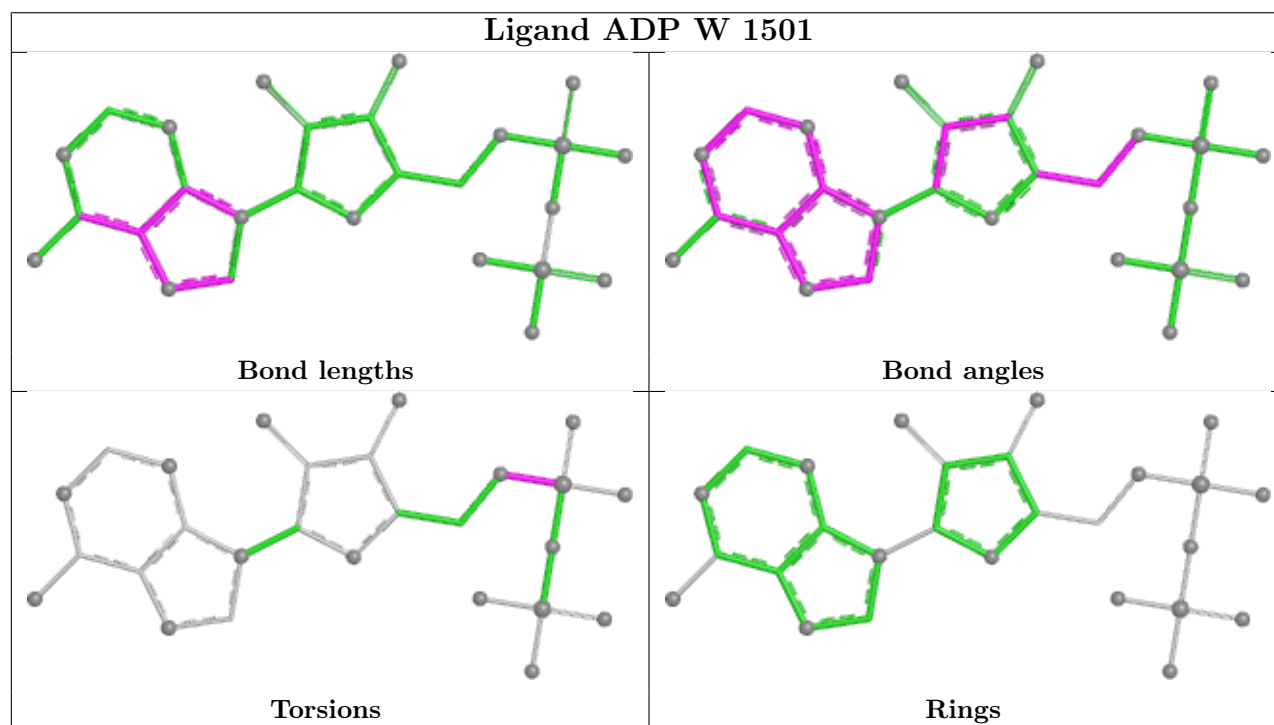
Mol	Chain	Res	Type	Atoms
25	W	1501	ADP	C5'-O5'-PA-O1A
25	W	1501	ADP	C5'-O5'-PA-O2A
25	W	1501	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	W	1502	BEF	3	0
25	W	1501	ADP	3	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.

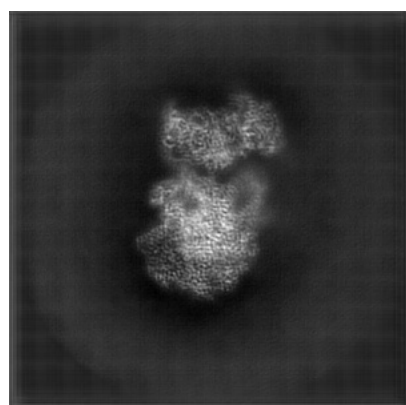
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12449. These allow visual inspection of the internal detail of the map and identification of artifacts.

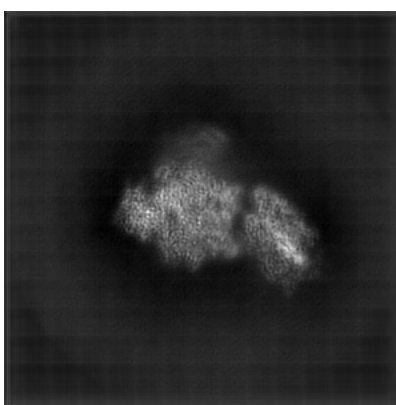
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

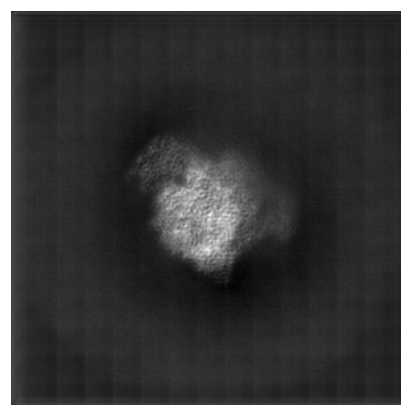
6.1.1 Primary map



X



Y

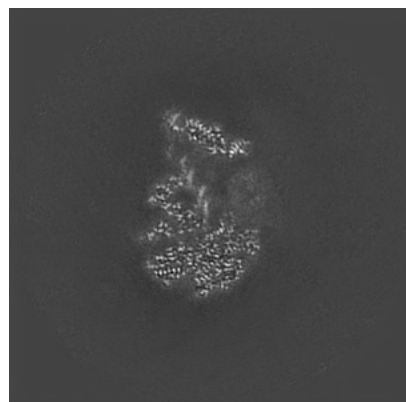


Z

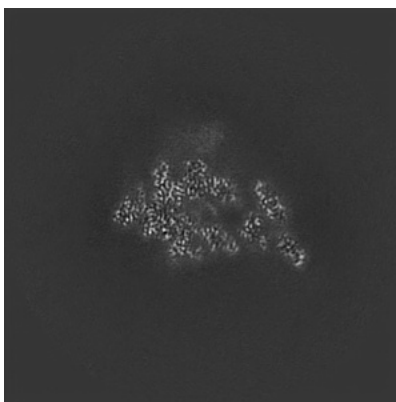
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

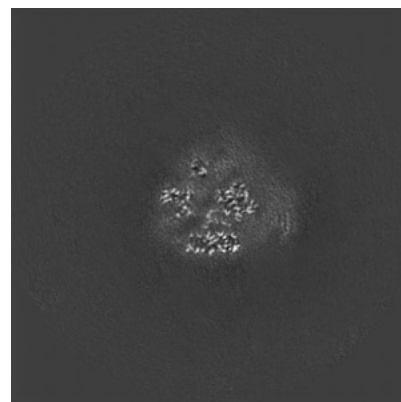
6.2.1 Primary map



X Index: 200



Y Index: 200

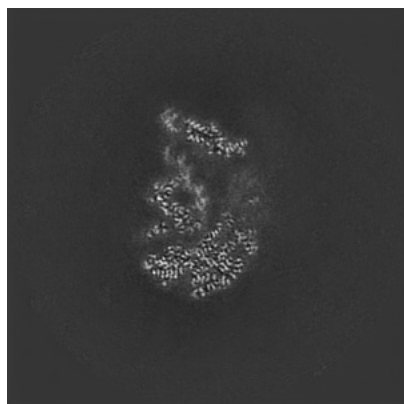


Z Index: 200

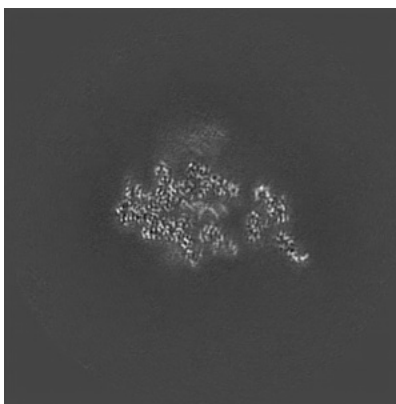
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

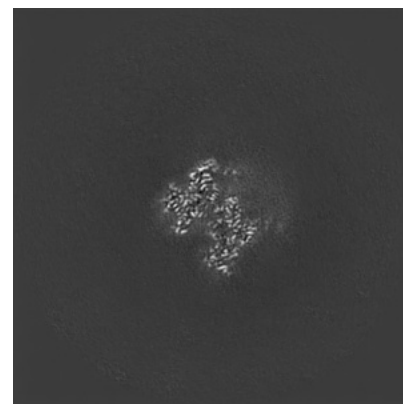
6.3.1 Primary map



X Index: 198



Y Index: 195

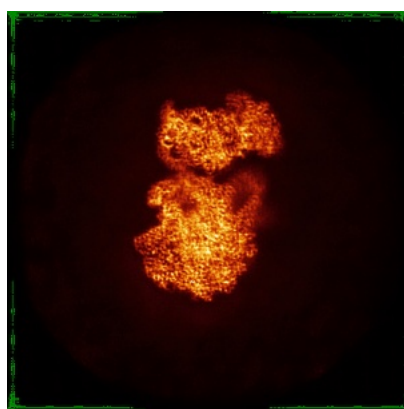


Z Index: 176

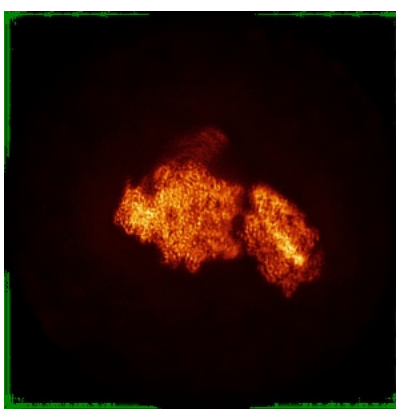
The images above show the largest variance slices of the map in three orthogonal directions.

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

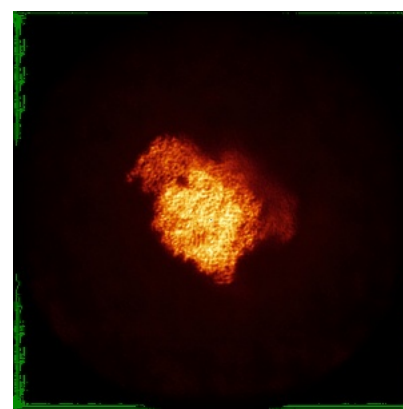
6.4.1 Primary map



X



Y

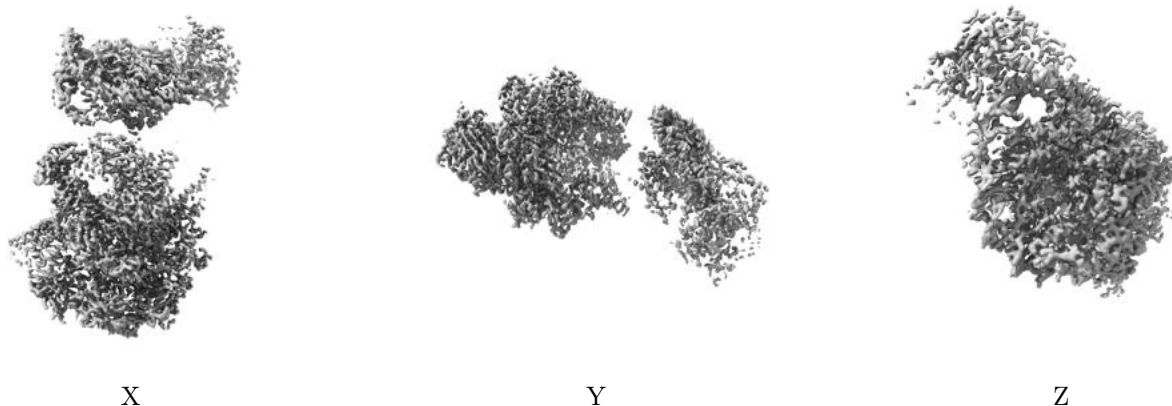


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

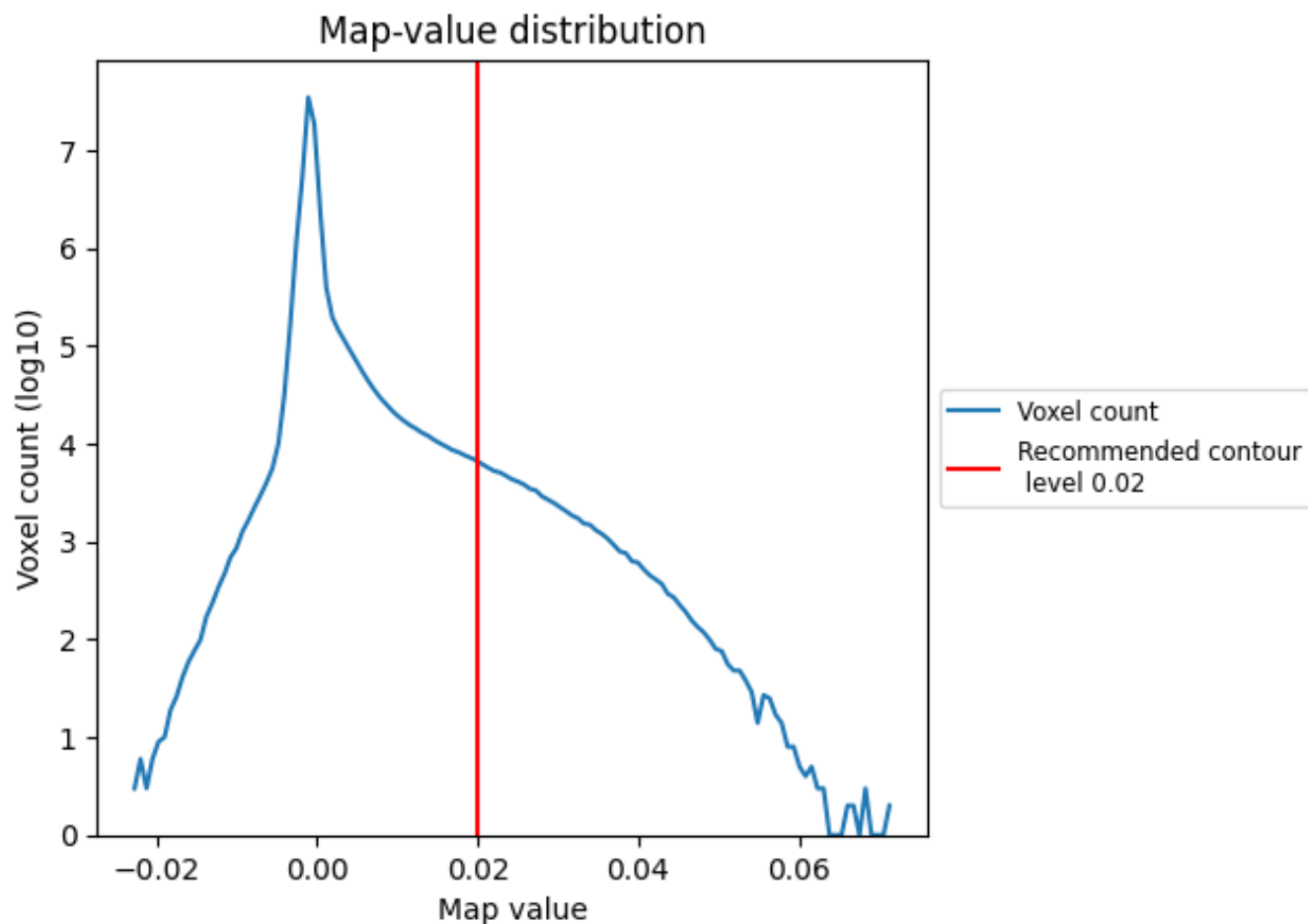
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

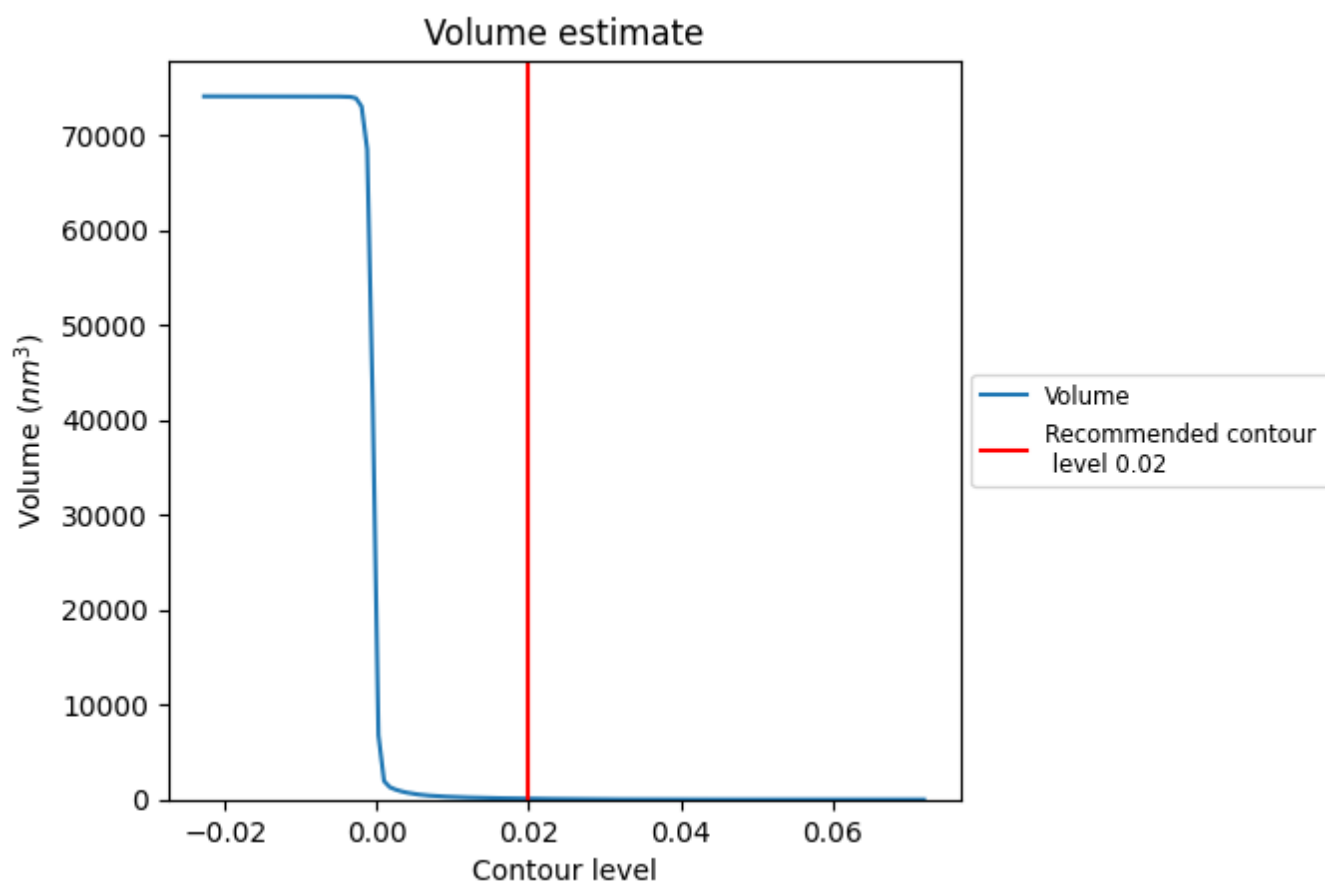
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

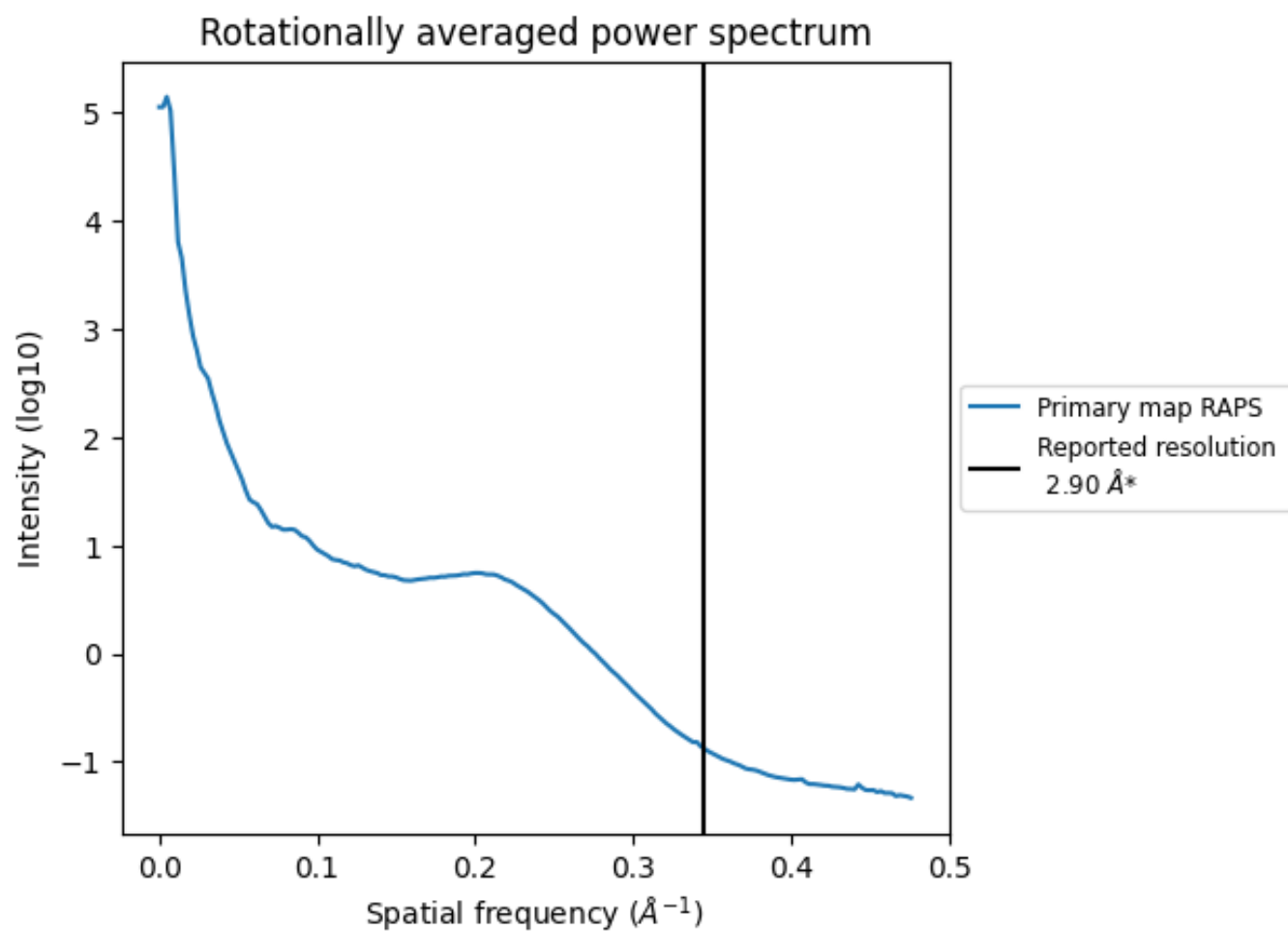
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm³; this corresponds to an approximate mass of 85 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 0.345 $\text{\AA}^{-1}$

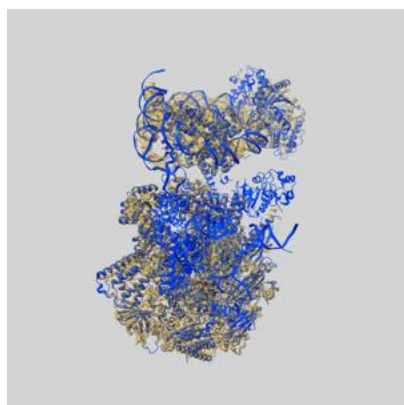
8 Fourier-Shell correlation

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

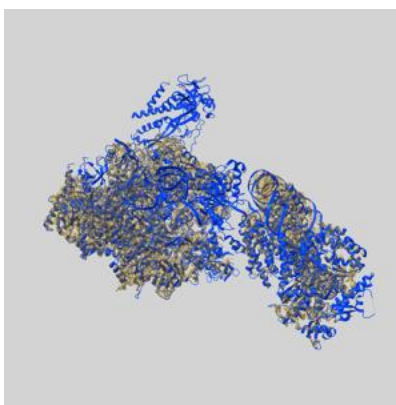
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12449 and PDB model 7NKX. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

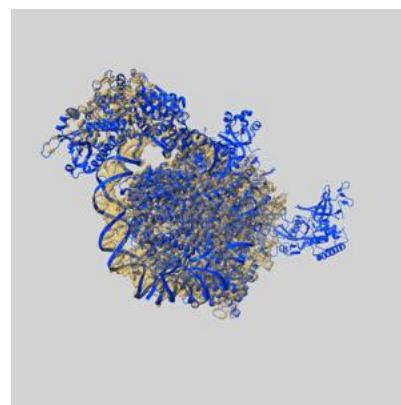
9.1 Map-model overlay [i](#)



X



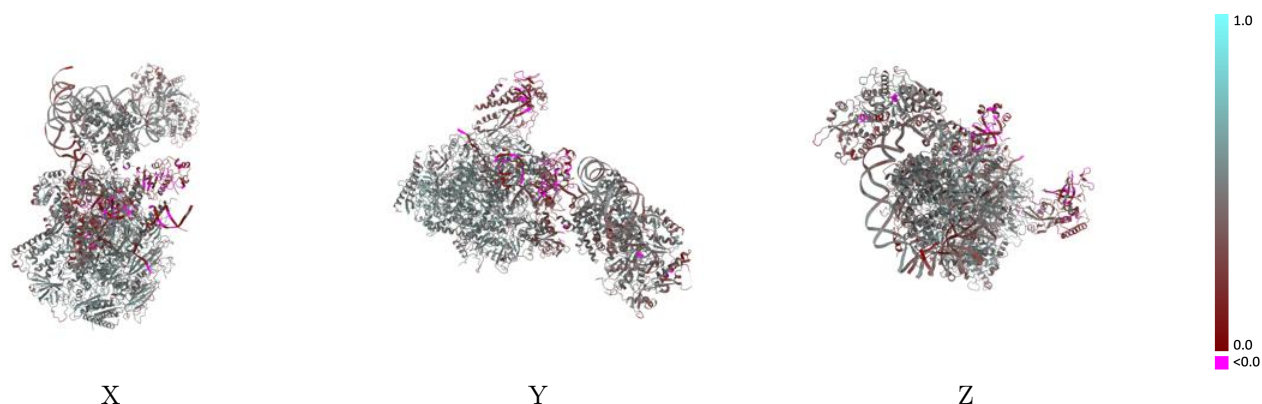
Y



Z

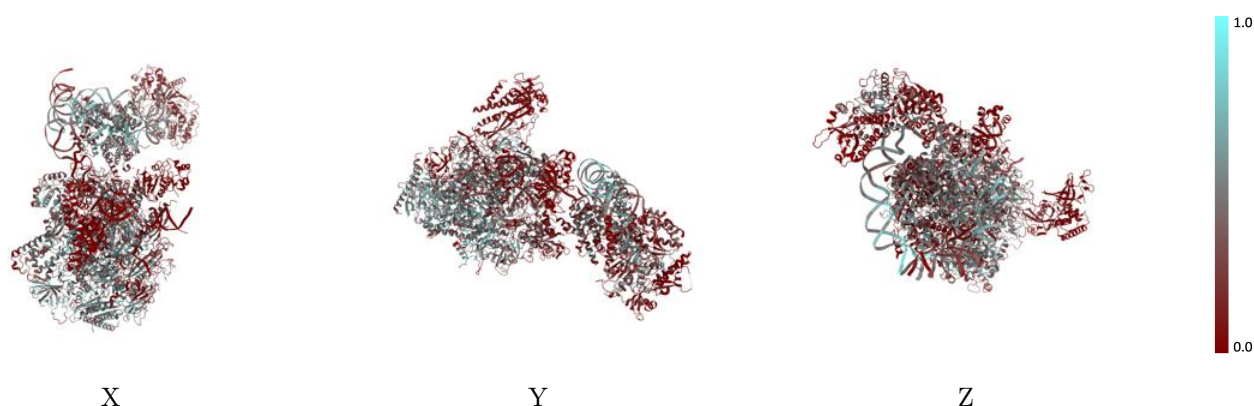
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



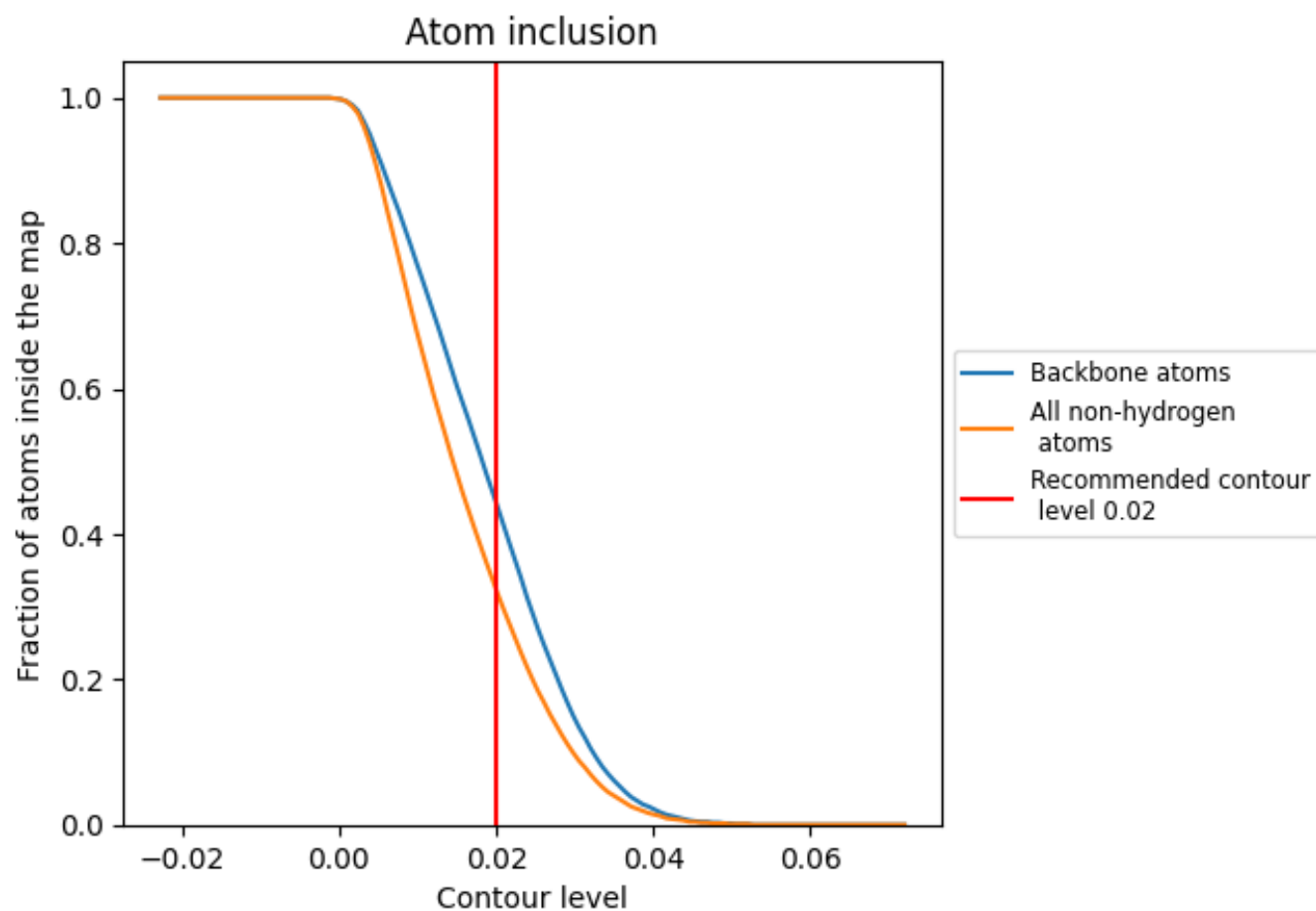
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 32% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3240	 0.4440
A	 0.3640	 0.4840
B	 0.3900	 0.5010
C	 0.4920	 0.5190
D	 0.0000	 0.2480
E	 0.4530	 0.4830
F	 0.3920	 0.4980
G	 0.0030	 0.2450
H	 0.4640	 0.4980
I	 0.1930	 0.3710
J	 0.5510	 0.5330
K	 0.4150	 0.5120
L	 0.2740	 0.4640
N	 0.3920	 0.3710
P	 0.3180	 0.3410
T	 0.3880	 0.3770
W	 0.1680	 0.4200
Y	 0.0000	 0.1590
Z	 0.0010	 0.2830
a	 0.3660	 0.4880
b	 0.3970	 0.5000
c	 0.4130	 0.4830
d	 0.4330	 0.4630
e	 0.3120	 0.4710
f	 0.4120	 0.4980
g	 0.1890	 0.4410
h	 0.2780	 0.4460

