Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 05:49 am BST

PDB ID	:	9GD2 / pdb_00009gd2
EMDB ID	:	EMD-51244
Title	:	Structure of Chd1 bound to a dinucleosome with a dyad-to-dyad distance of 103 bp.
Authors	:	Engeholm, M.; Roske, J.J.; Oberbeckmann, E.; Dienemann, C.; Lidschreiber, M.; Cramer, P.; Farnung, L.
Deposited on	:	2024-08-04
Resolution	:	4.20 Å(reported)

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

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

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

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

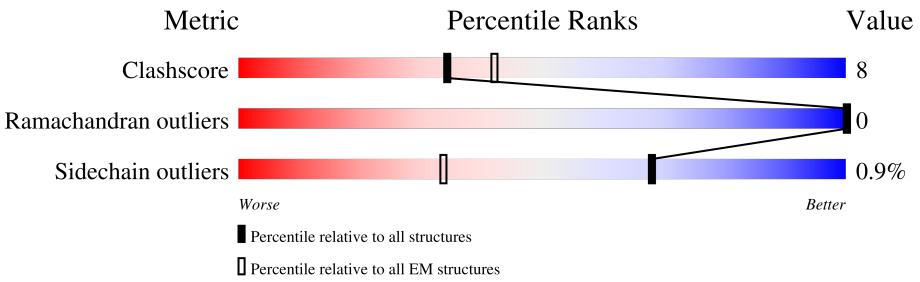
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

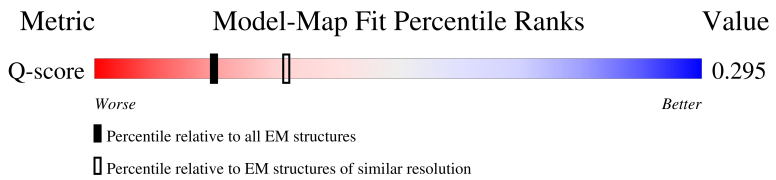
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	136	64% · 32%
1	E	136	65% · 32%
1	K	136	47% 7% 46%
1	O	136	64% 7% 29%

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Mol	Chain	Length	Quality of chain
2	B	103	67% 9% 24%
2	F	103	69% 6% 25%
2	L	103	70% 6% 24%
2	P	103	60% 16% 22%
3	C	130	68% 10% 22%
3	G	130	72% 26%
3	M	130	73% 6% 21%
3	R	130	70% 28%
4	D	123	68% 7% 25%
4	H	123	66% 7% 26%
4	N	123	62% 11% 27%
4	Q	123	69% 5% 26%
5	I	248	30% 65%
6	J	248	43% 52%
7	S	1468	99%
7	T	1468	98%
7	W	1468	35% 9% 56%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 26638 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	93	763	483	143	134	3	0	0
1	E	93	763	483	143	134	3	0	0
1	K	73	592	376	109	104	3	0	0
1	O	96	795	501	154	137	3	0	0

There are 4 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
K	102	ALA	GLY	conflict	UNP P84233
O	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	78	622	393	120	108	1	0	0
2	F	77	614	389	119	105	1	0	0
2	L	78	626	394	124	107	1	0	0
2	P	80	644	408	125	110	1	0	0

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	102	786	495	153	138	0	0
3	G	96	742	465	147	130	0	0
3	M	103	795	501	155	139	0	0
3	R	93	719	450	143	126	0	0

There are 8 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
M	99	ARG	GLY	conflict	UNP P06897
M	123	SER	ALA	conflict	UNP P06897
R	99	ARG	GLY	conflict	UNP P06897
R	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	92	721	454	129	136	2	0	0
4	H	91	708	447	125	134	2	0	0
4	N	90	699	441	123	133	2	0	0
4	Q	91	708	447	125	134	2	0	0

There are 8 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
N	0	MET	-	initiating methionine	UNP P02281
N	29	THR	SER	conflict	UNP P02281
Q	0	MET	-	initiating methionine	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (248-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	237	4828	2293	875	1423	237	0	0

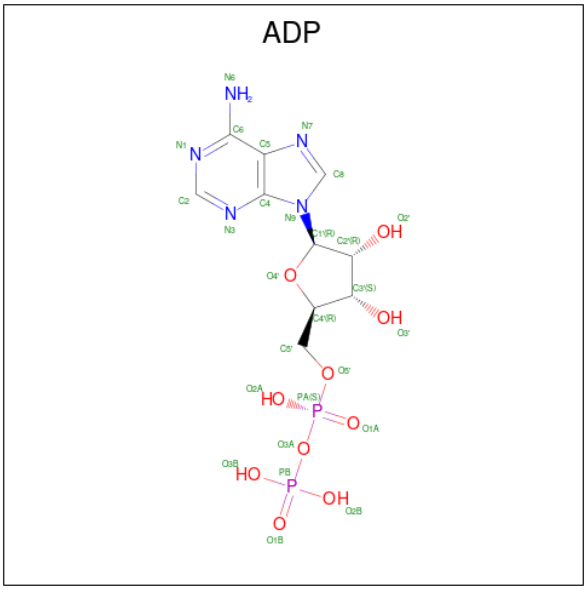
- Molecule 6 is a DNA chain called DNA (248-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	237	4889	2313	918	1421	237	0	0

- Molecule 7 is a protein called Chromo domain-containing protein 1.

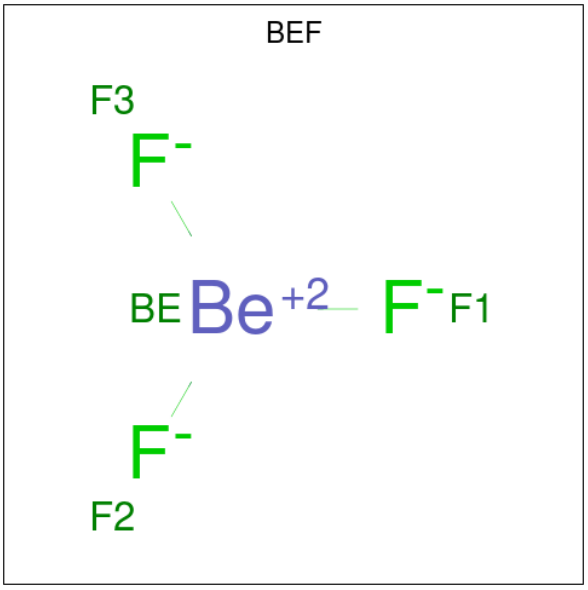
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
7	S	14	122	73	26	23		0	0
			Total	C	N	O			
7	T	23	196	119	35	42		0	0
			Total	C	N	O	S		
7	W	641	5274	3348	920	982	24	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

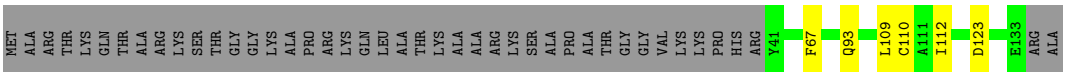
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	W	1	1	1	0

3 Residue-property plots (i)

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

- Molecule 1: Histone H3.2

Chain A:

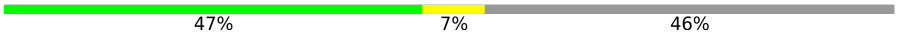


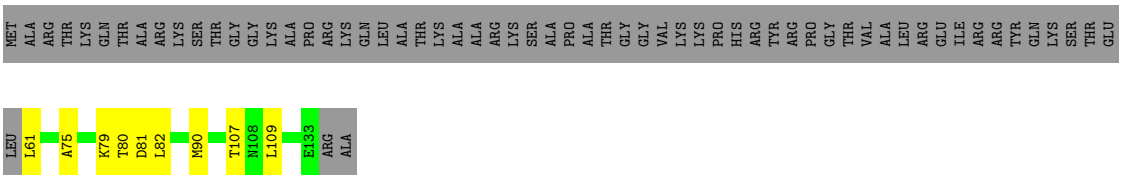
- Molecule 1: Histone H3.2

Chain E:

- Molecule 1: Histone H3.2

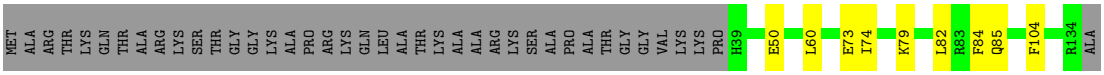
Chain K:





- Molecule 1: Histone H3.2

Chain O:



- Molecule 2: Histone H4

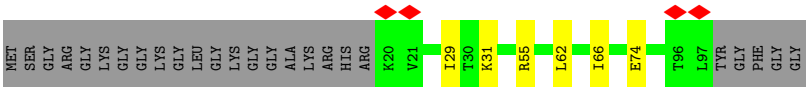
Chain B:

- Molecule 2: Histone H4

Chain F:

- Molecule 2: Histone H4

Chain L:

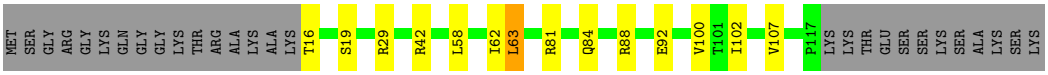


- Molecule 2: Histone H4

Chain P:

- Molecule 3: Histone H2A type 1

Chain C:

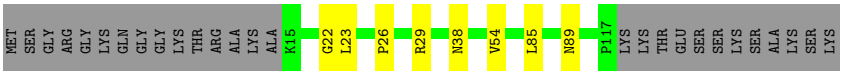


- Molecule 3: Histone H2A type 1

Chain G:

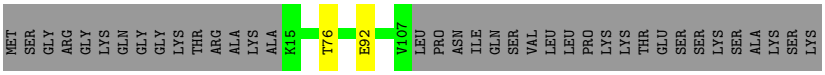
- Molecule 3: Histone H2A type 1

Chain M:



- Molecule 3: Histone H2A type 1

Chain R:

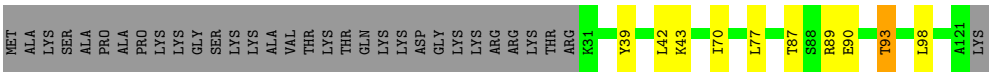


- Molecule 4: Histone H2B 1.1

Chain D: 68% 7% 25%

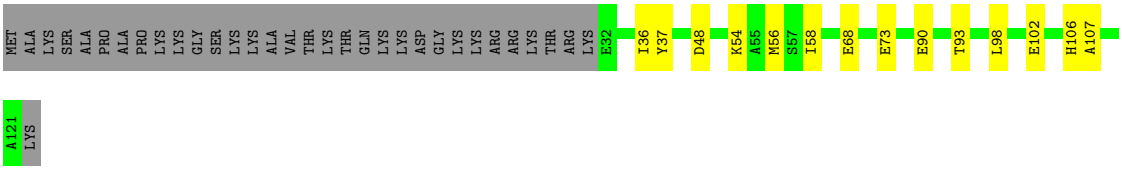
• Molecule 4: Histone H2B 1.1

Chain H: 66% 7% 26%



• Molecule 4: Histone H2B 1.1

Chain N: 62% 11% 27%

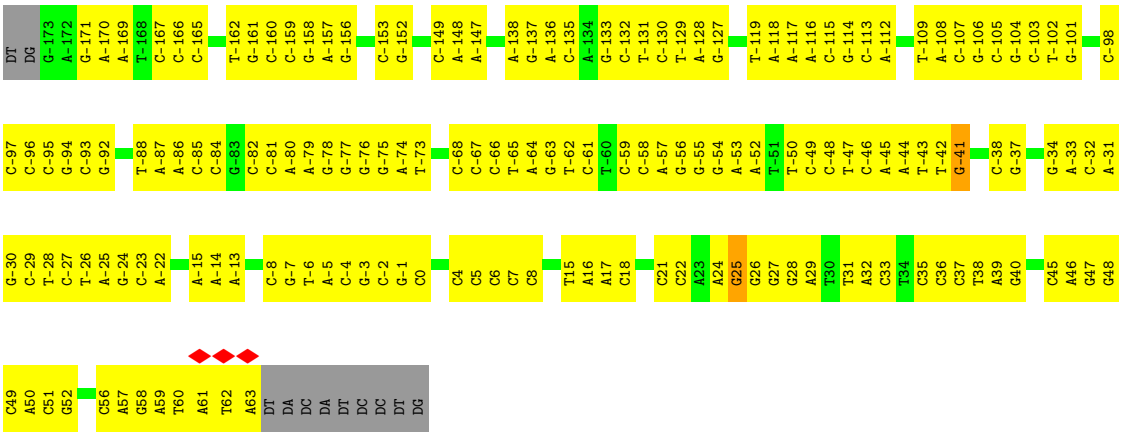


• Molecule 4: Histone H2B 1.1

Chain Q: 69% 5% 26%

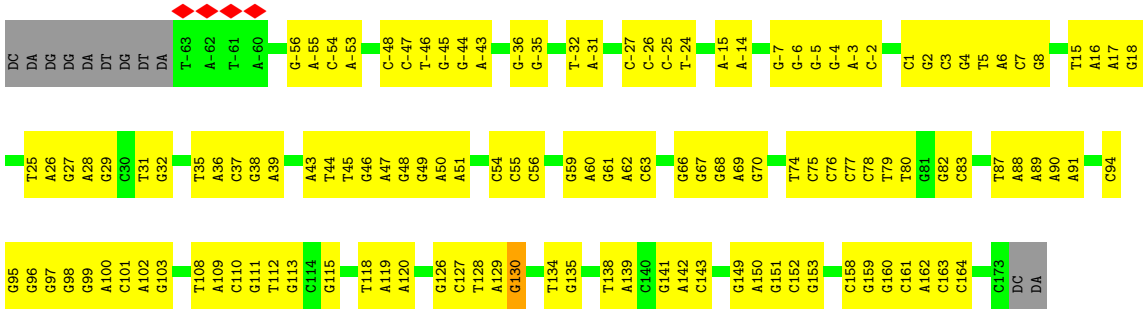
• Molecule 5: DNA (248-MER)

Chain I: 30% 65%



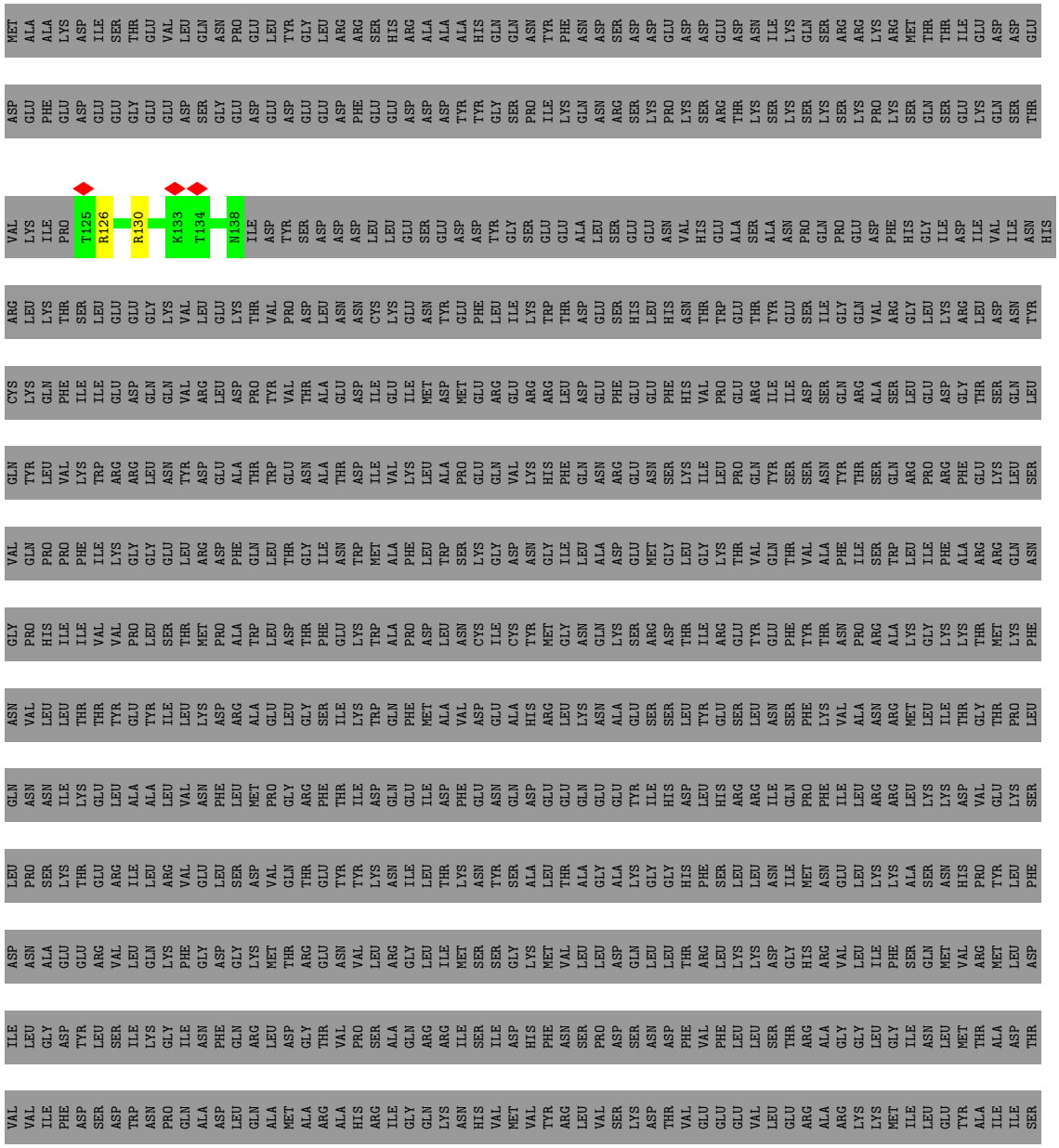
• Molecule 6: DNA (248-MER)

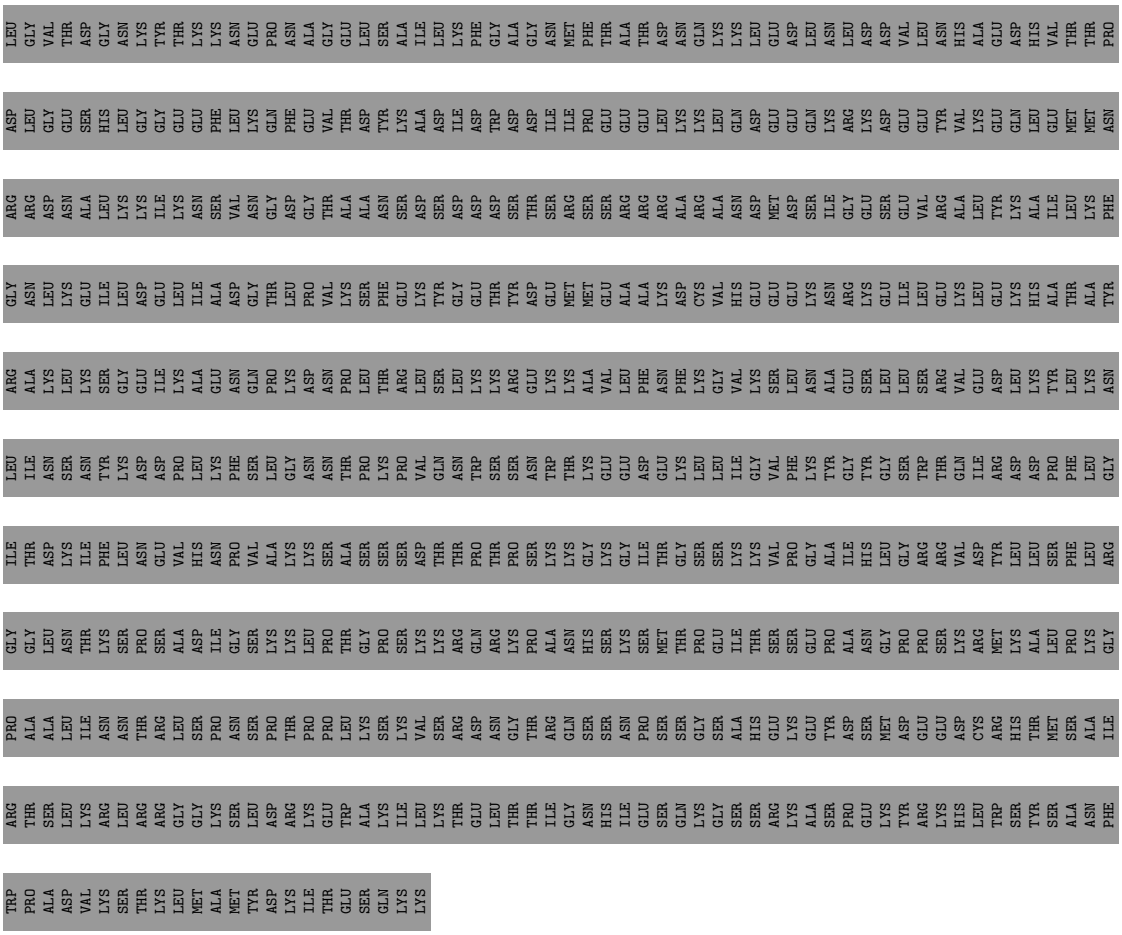
Chain J: 43% 52%



- Molecule 7: Chromo domain-containing protein 1

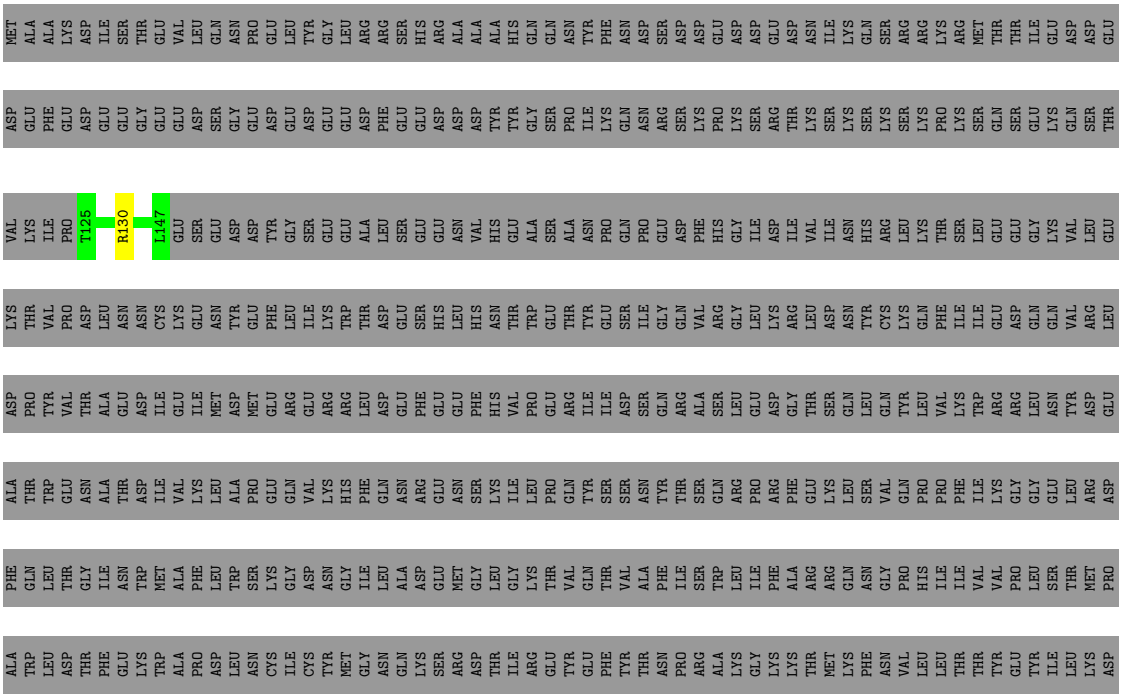
Chain S: 99%

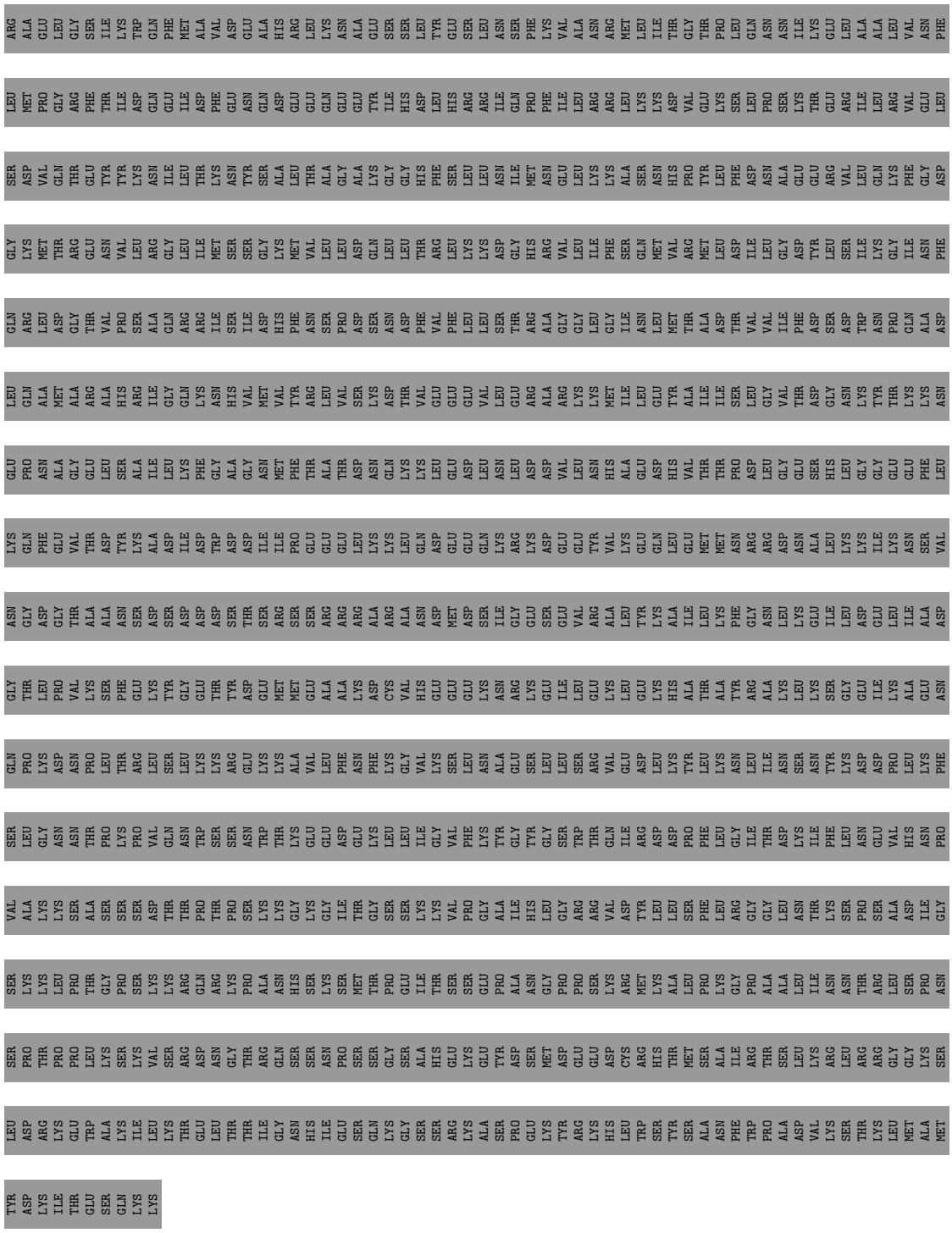




- Molecule 7: Chromo domain-containing protein 1

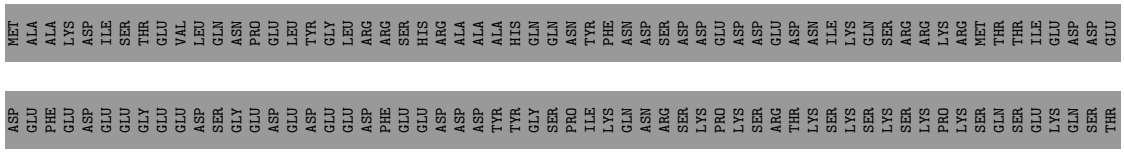
Chain T: 98%

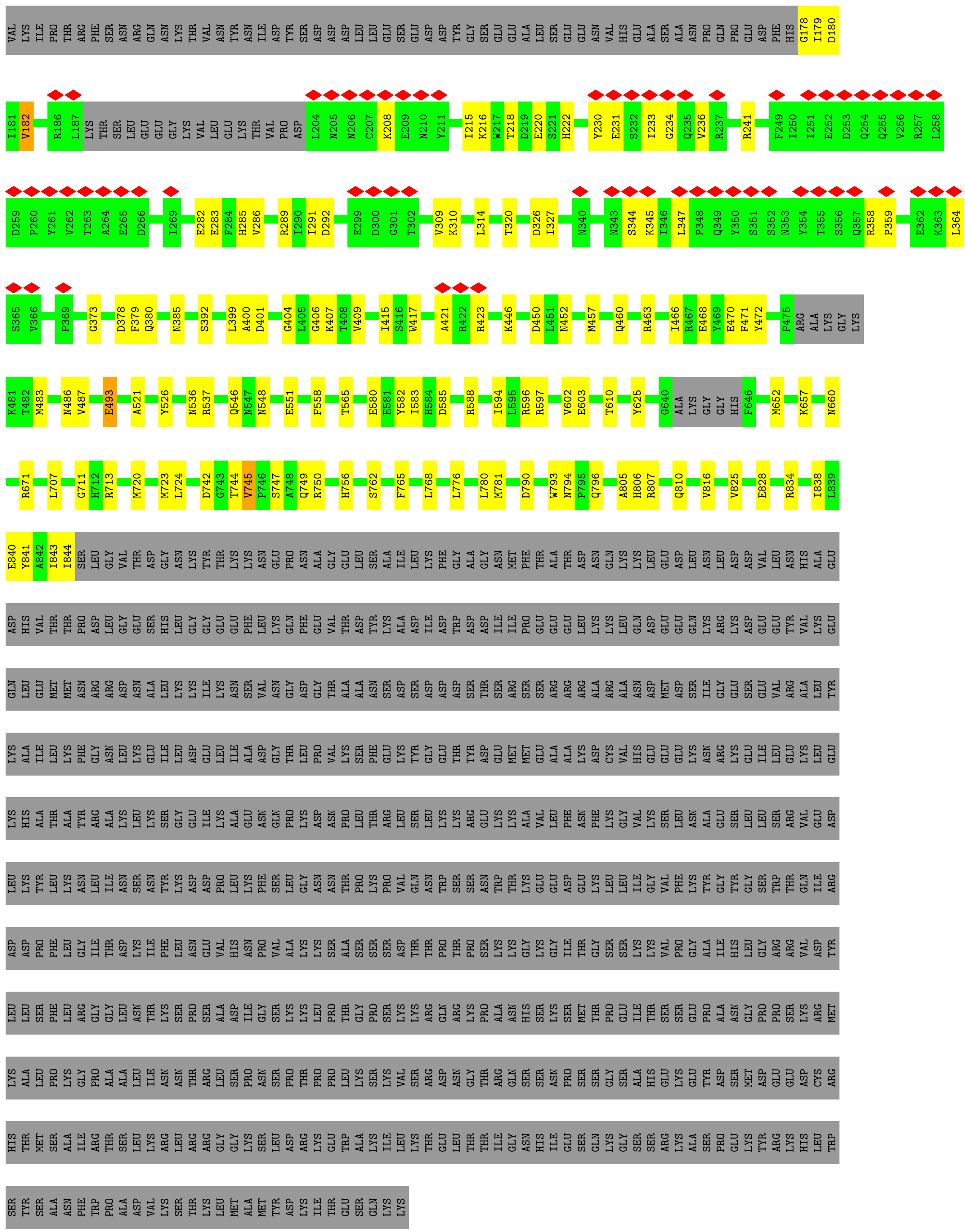




• Molecule 7: Chromo domain-containing protein 1

Chain W:




VAL LYS ILE PRO THR ARG PHE SER ASN ARG GLN ASN LYS THR VAL ASN TYR ASN ILE ASP TYR SER ASP ASP ASP LEU LEU GLU SER GLU ASP ASP TYR GLY SER GLU GLU ALA LEU SER GLU GLU ASN VAL HIS GLU ALA SER ALA ASN PRO GLN PRO GLU ASP PHE HIS G178 I179 D180
I181 V182 R186 L187 LYS THR SER LEU GLU GLU GLY LYS VAL LEU GLU LYS THR VAL PRO ASP L204 N205 N206 C207 K208 E209 N210 Y211 I215 K216 W217 T218 D219 E220 S221 H222 Y230 E231 S232 I233 G234 Q235 V236 R237 R241 F249 I250 I251 E252 D253 Q254 Q255 V256 R257 L258
D259 P260 Y261 V262 T263 A264 E265 D266 I269 E282 E283 F284 H285 V286 R289 I290 I291 D292 E299 D300 G301 T302 V309 K310 L314 T320 D326 I327 N340 N343 S344 K345 I346 L347 P348 Q349 Y350 S351 S352 N353 Y354 T355 S356 Q357 R358 P359 E362 K363 L364
S365 V366 P369 G373 D378 F379 Q380 N385 S392 L399 A400 D401 G404 L405 G406 K407 T408 V409 I415 S416 W417 A421 R422 R423 K446 D450 L451 N452 M457 Q460 R463 I466 R467 E468 Y469 E470 F471 Y472 P475 ARG ALA LYS GLY LYS
K481 T482 M483 N486 V487 E493 A521 Y526 N536 R537 Q546 N547 N548 E551 F558 T565 E580 E581 Y582 I583 H584 D585 R588 I594 L595 R596 R597 V602 E603 T610 Y625 G640 ALA LYS GLY GLY HIS F646 M652 K657 N660
R671 L707 G711 H712 R713 M720 M723 L724 D742 G743 T744 V745 P746 S747 A748 Q749 R750 H756 S762 F765 L768 L776 L780 M781 D790 W793 N794 P795 Q796 A805 H806 R807 Q810 V816 V825 E828 R834 I838 L839
E840 Y841 A842 I843 I844 SER LEU GLY VAL THR ASP GLY ASN LYS TYR THR LYS LYS ASN GLU PRO ASN ALA GLY GLU LEU SER ALA ILE LEU LYS PHE GLY ALA GLY ASN MET PHE THR ALA THR ASP ASN GLN LYS LYS LEU GLU ASP LEU ASN LEU ASP ASP VAL LEU ASN HIS ALA GLU
ASP HIS VAL THR THR PRO ASP LEU GLY GLU SER HIS LEU GLY GLY GLU GLU PHE LEU LYS GLN PHE GLU VAL THR ASP TYR LYS ALA ASP ILE ASP TRP ASP ASP ILE ILE PRO GLU GLU GLU LEU LYS LYS LEU GLN ASP GLU GLU GLN LYS ARG LYS ASP GLU GLU TYR VAL LYS GLU
GLN LEU GLU MET MET ASN ARG ARG ASP ASN ALA LEU LYS LYS ILE LYS ASN SER VAL ASN GLY ASP GLY THR ALA ALA ASN SER ASP SER ASP ASP SER THR SER ARG SER SER ARG ARG ARG ALA ARG ALA ASN ASP MET ASP SER ILE GLY GLU SER GLU VAL ARG ALA LEU TYR
LYS ALA ILE LEU LYS PHE GLY ASN LEU LYS GLU ILE LEU ASP GLU LEU ILE ALA ASP GLY THR LEU PRO VAL LYS SER PHE GLU LYS TYR GLY GLU THR TYR ASP GLU MET MET GLU ALA ALA LYS ASP CYS VAL HIS GLU GLU GLU LYS ASN ARG LYS GLU ILE LEU GLU LYS LEU GLU
LYS HIS ALA THR ALA TYR ARG ALA LYS LEU LYS SER GLY GLU ILE LYS ALA GLU ASN GLN PRO LYS ASP ASN PRO LEU THR ARG LEU SER LEU LYS LYS ARG GLU LYS LYS ALA VAL LEU PHE ASN PHE LYS GLY VAL LYS SER LEU ASN ALA GLU SER LEU LEU SER ARG VAL GLU ASP
LEU LYS TYR LEU LYS ASN LEU ILE ASN SER SER ASN TYR LYS ASP ASP PRO LEU LYS PHE SER LEU GLY ASN ASN THR PRO LYS PRO VAL GLN ASN TRP SER SER ASN TRP THR THR LYS GLU GLU ASP GLU LYS LEU LEU ILE GLY VAL PHE LYS TYR GLY TYR GLY SER TRP THR GLN ILE ARG
ASP ASP PRO PHE LEU GLY ILE THR ASP LYS ILE PHE LEU ASN GLU VAL HIS ASN PRO VAL ALA LYS LYS SER ALA SER SER ASP THR THR PRO THR PRO SER LYS LYS GLY LYS GLY ILE THR GLY SER SER LYS LYS VAL PRO GLY ALA ILE HIS LEU GLY ARG ARG VAL ASP TYR
LEU LEU SER PHE LEU ARG GLY GLY LEU ASN THR LYS SER PRO SER ALA ASP ILE GLY SER LYS LYS LEU PRO THR GLY PRO SER LYS ARG GLN ARG LYS PRO ALA ASN HIS SER LYS SER MET THR PRO GLU ILE THR SER SER GLU PRO ALA ASN GLY PRO PRO SER LYS ARG MET
LYS ALA LEU PRO LYS GLY PRO ALA ALA LEU ILE ASN ASN THR ARG LEU SER PRO ASN SER PRO THR PRO PRO LEU LYS SER LYS VAL SER ARG ASP ASN GLY THR ARG GLN SER SER ASN PRO SER SER GLY SER ALA HIS GLU LYS GLU TYR ASP SER MET ASP GLU GLU ASP CYS ARG
HIS THR MET SER ALA ILE ARG THR SER LEU LYS ARG LEU ARG ARG GLY GLY LYS SER LEU ASP ARG LYS GLU TRP ALA LYS ILE LEU LYS THR GLU LEU THR THR ILE GLY ASN HIS ILE GLU SER GLN LYS GLY SER SER ARG LYS ALA SER PRO GLU LYS TYR ARG LYS HIS LEU TRP
SER TYR SER ALA ASN PHE TRP PRO ALA ASP VAL LYS SER THR LYS LEU MET ALA MET TYR ASP LYS ILE THR GLU SER GLN LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	32.042	Depositor
Minimum map value	-6.536	Depositor
Average map value	0.032	Depositor
Map value standard deviation	1.319	Depositor
Recommended contour level	5	Depositor
Map size (Å)	350.28, 350.28, 350.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.27	0/773	0.43	0/1038
1	E	0.27	0/773	0.42	0/1038
1	K	0.25	0/599	0.41	0/804
1	O	0.24	0/806	0.40	0/1081
2	B	0.32	0/629	0.47	0/843
2	F	0.29	0/621	0.38	0/832
2	L	0.40	0/631	0.59	0/845
2	P	0.26	0/651	0.46	0/873
3	C	0.26	0/796	0.37	0/1077
3	G	0.26	0/751	0.39	0/1013
3	M	0.20	0/805	0.36	0/1088
3	R	0.18	0/727	0.34	0/979
4	D	0.26	0/732	0.35	0/986
4	H	0.28	0/719	0.41	0/969
4	N	0.24	0/710	0.37	0/958
4	Q	0.21	0/719	0.35	0/969
5	I	0.30	0/5409	0.69	3/8338 (0.0%)
6	J	0.31	0/5491	0.68	1/8481 (0.0%)
7	S	0.11	0/123	0.30	0/164
7	T	0.14	0/198	0.48	0/267
7	W	0.19	0/5377	0.45	0/7255
All	All	0.27	0/28040	0.55	4/39898 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	130	DG	C2'-C3'-O3'	-6.08	102.37	111.50
5	I	25	DG	C2'-C3'-O3'	5.83	120.25	111.50
5	I	-41	DG	C2'-C3'-O3'	5.35	119.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	-78	DG	C2'-C3'-O3'	5.29	119.43	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	763	0	800	3	0
1	E	763	0	800	2	0
1	K	592	0	621	6	0
1	O	795	0	833	9	0
2	B	622	0	660	7	0
2	F	614	0	656	5	0
2	L	626	0	682	5	0
2	P	644	0	690	15	0
3	C	786	0	833	11	0
3	G	742	0	784	2	0
3	M	795	0	846	5	0
3	R	719	0	760	2	0
4	D	721	0	742	8	0
4	H	708	0	727	6	0
4	N	699	0	714	10	0
4	Q	708	0	727	6	0
5	I	4828	0	2660	126	0
6	J	4889	0	2659	97	0
7	S	122	0	116	2	0
7	T	196	0	179	1	0
7	W	5274	0	5250	86	0
8	W	27	0	12	3	0
9	W	4	0	0	1	0
10	W	1	0	0	0	0
All	All	26638	0	22751	389	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 8.

All (389) 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:C:16:THR:N	3:C:19:SER:HG	1.88	0.71
7:W:486:ASN:OD1	7:W:487:VAL:N	2.24	0.71
7:W:724:LEU:HB3	7:W:768:LEU:HD21	1.73	0.70
6:J:150:DA:H2"	6:J:151:DG:C8	2.31	0.66
1:O:50:GLU:OE2	2:P:39:ARG:NE	2.30	0.65
5:I:-148:DA:H2"	5:I:-147:DA:C8	2.32	0.64
5:I:-159:DC:H2"	5:I:-158:DG:C8	2.33	0.64
5:I:-107:DC:H2"	5:I:-106:DG:C8	2.33	0.64
6:J:-45:DG:H2"	6:J:-44:DG:C8	2.33	0.64
5:I:46:DA:H2"	5:I:47:DG:C8	2.34	0.63
5:I:47:DG:H2"	5:I:48:DG:C8	2.33	0.63
1:O:79:LYS:HB3	1:O:82:LEU:HD21	1.81	0.62
5:I:-137:DG:H2"	5:I:-136:DA:C8	2.35	0.62
6:J:98:DG:H2"	6:J:99:DG:C8	2.35	0.61
5:I:-46:DC:H2"	5:I:-45:DA:C8	2.36	0.61
5:I:-77:DG:H2"	5:I:-76:DG:C8	2.36	0.61
5:I:-87:DA:H2"	5:I:-86:DA:C8	2.36	0.61
5:I:16:DA:H2"	5:I:17:DA:C8	2.36	0.60
5:I:-75:DG:H2"	5:I:-74:DA:C8	2.37	0.60
5:I:-56:DG:H2"	5:I:-55:DG:C8	2.35	0.60
6:J:7:DC:H2"	6:J:8:DG:C8	2.37	0.59
7:W:231:GLU:OE1	7:W:231:GLU:N	2.34	0.59
6:J:37:DC:H2"	6:J:38:DG:C8	2.36	0.59
6:J:128:DT:H2"	6:J:129:DA:C8	2.37	0.59
5:I:-14:DA:H2"	5:I:-13:DA:C8	2.38	0.59
5:I:-4:DC:H2"	5:I:-3:DG:C8	2.36	0.59
6:J:141:DG:H2"	6:J:142:DA:C8	2.38	0.59
5:I:-117:DA:H2"	5:I:-116:DA:C8	2.38	0.59
5:I:-57:DA:H2"	5:I:-56:DG:C8	2.38	0.58
5:I:49:DC:H2"	5:I:50:DA:C8	2.37	0.58
6:J:47:DA:H2"	6:J:48:DG:C8	2.39	0.58
5:I:-158:DG:H2"	5:I:-157:DA:C8	2.39	0.58
6:J:108:DT:H2"	6:J:109:DA:C8	2.39	0.58
5:I:-23:DC:H2"	5:I:-22:DA:C8	2.39	0.57
6:J:89:DA:H2"	6:J:90:DA:C8	2.39	0.57
7:W:546:GLN:N	7:W:551:GLU:OE2	2.33	0.57
6:J:88:DA:H2"	6:J:89:DA:C8	2.39	0.57
5:I:-26:DT:H2"	5:I:-25:DA:C8	2.40	0.57
5:I:56:DC:H2"	5:I:57:DA:C8	2.39	0.57
6:J:68:DG:H2"	6:J:69:DA:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-109:DT:H2"	5:I:-108:DA:C8	2.39	0.57
3:R:92:GLU:OE1	7:S:130:ARG:NH2	2.36	0.57
7:W:406:GLY:N	8:W:1501:ADP:O2A	2.38	0.57
2:P:23:ARG:O	2:P:26:ILE:HG22	2.04	0.57
5:I:-88:DT:H2"	5:I:-87:DA:C8	2.39	0.57
3:C:92:GLU:OE1	7:T:130:ARG:NH2	2.38	0.56
5:I:-115:DC:H2"	5:I:-114:DG:C8	2.40	0.56
5:I:38:DT:H2"	5:I:39:DA:C8	2.40	0.56
5:I:57:DA:H2"	5:I:58:DG:C8	2.41	0.56
6:J:79:DT:OP1	1:O:85:GLN:NE2	2.38	0.56
7:W:794:ASN:OD1	7:W:796:GLN:N	2.39	0.56
5:I:58:DG:H2"	5:I:59:DA:C8	2.41	0.56
6:J:3:DC:H2"	6:J:4:DG:C8	2.41	0.56
5:I:28:DG:H2"	5:I:29:DA:C8	2.40	0.55
6:J:161:DC:H2"	6:J:162:DA:C8	2.42	0.55
5:I:-53:DA:H2"	5:I:-52:DA:C8	2.41	0.55
5:I:27:DG:H2"	5:I:28:DG:C8	2.41	0.55
5:I:36:DC:H2"	5:I:37:DC:C5	2.42	0.55
6:J:26:DA:H2"	6:J:27:DG:C8	2.42	0.55
5:I:-105:DC:H2"	5:I:-104:DG:C8	2.42	0.55
7:W:768:LEU:C	7:W:768:LEU:HD23	2.32	0.55
6:J:69:DA:H2"	6:J:70:DG:C8	2.42	0.54
6:J:149:DG:H2"	6:J:150:DA:C8	2.42	0.54
5:I:-15:DA:H2"	5:I:-14:DA:C8	2.42	0.54
5:I:-149:DC:H2"	5:I:-148:DA:C8	2.43	0.54
6:J:-5:DG:H2"	6:J:-4:DG:C8	2.43	0.54
6:J:-46:DT:H2"	6:J:-45:DG:C8	2.43	0.54
7:W:745:VAL:O	7:W:750:ARG:NH2	2.40	0.54
3:C:42:ARG:HD3	6:J:39:DA:H5"	1.90	0.54
7:W:364:LEU:O	7:W:385:ASN:ND2	2.41	0.54
5:I:-93:DC:H2"	5:I:-92:DG:C8	2.43	0.54
6:J:67:DG:H2"	6:J:68:DG:C8	2.43	0.54
5:I:-45:DA:H2"	5:I:-44:DA:C8	2.43	0.54
7:W:326:ASP:OD1	7:W:327:ILE:N	2.41	0.54
5:I:-6:DT:H2"	5:I:-5:DA:C8	2.42	0.53
5:I:-55:DG:H2"	5:I:-54:DG:C8	2.42	0.53
5:I:-118:DA:H2"	5:I:-117:DA:C8	2.43	0.53
5:I:-25:DA:H2"	5:I:-24:DG:C8	2.43	0.53
6:J:5:DT:H2"	6:J:6:DA:C8	2.44	0.53
5:I:-86:DA:H2"	5:I:-85:DC:C6	2.44	0.53
6:J:6:DA:H2"	6:J:7:DC:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:84:MET:HE3	2:P:84:MET:HA	1.90	0.53
6:J:99:DG:H2"	6:J:100:DA:C8	2.44	0.53
6:J:-36:DG:H2"	6:J:-35:DG:C8	2.43	0.52
5:I:-2:DC:H2"	5:I:-1:DG:C8	2.45	0.52
6:J:79:DT:H2"	6:J:80:DT:C6	2.43	0.52
6:J:160:DG:H2"	6:J:161:DC:C6	2.43	0.52
7:W:468:GLU:HA	7:W:472:TYR:CD2	2.44	0.52
7:W:834:ARG:O	7:W:838:ILE:HG12	2.10	0.52
6:J:59:DG:H2"	6:J:60:DA:C8	2.45	0.52
4:N:48:ASP:OD1	4:N:48:ASP:N	2.43	0.52
6:J:78:DC:H2"	6:J:79:DT:C6	2.44	0.52
6:J:109:DA:H2"	6:J:110:DC:C6	2.45	0.52
7:W:794:ASN:OD1	7:W:794:ASN:C	2.52	0.52
5:I:-97:DC:H2"	5:I:-96:DC:C5	2.45	0.52
6:J:16:DA:H2"	6:J:17:DA:C8	2.45	0.52
6:J:110:DC:H2"	6:J:111:DG:C8	2.45	0.52
6:J:115:DG:H3'	7:W:241:ARG:NE	2.25	0.52
5:I:-54:DG:H2"	5:I:-53:DA:C8	2.46	0.51
6:J:82:DG:H2"	6:J:83:DC:C6	2.46	0.51
6:J:129:DA:H2"	6:J:130:DG:C8	2.46	0.51
3:C:42:ARG:HB2	4:D:85:THR:HA	1.92	0.51
6:J:36:DA:H2"	6:J:37:DC:C6	2.46	0.51
7:W:720:MET:HG3	7:W:723:MET:H	1.73	0.51
5:I:-58:DC:H2"	5:I:-57:DA:C8	2.46	0.51
5:I:-38:DC:H2"	5:I:-37:DG:C8	2.45	0.51
7:W:657:LYS:HA	7:W:660:ASN:ND2	2.26	0.50
6:J:-55:DA:H2"	6:J:-54:DC:C6	2.45	0.50
6:J:152:DC:H2"	6:J:153:DG:C8	2.47	0.50
2:L:29:ILE:O	2:L:55:ARG:NH2	2.40	0.50
7:W:806:HIS:ND1	7:W:810:GLN:OE1	2.45	0.50
6:J:-15:DA:H2"	6:J:-14:DA:C8	2.46	0.50
5:I:21:DC:H2"	5:I:22:DC:C6	2.47	0.50
7:W:602:VAL:HG12	7:W:603:GLU:HG3	1.93	0.50
6:J:48:DG:H2"	6:J:49:DG:C8	2.46	0.50
6:J:90:DA:H2"	6:J:91:DA:C8	2.47	0.50
5:I:-157:DA:H2"	5:I:-156:DG:C8	2.46	0.50
5:I:15:DT:H2"	5:I:16:DA:C8	2.47	0.50
7:W:781:MET:HA	7:W:781:MET:HE2	1.92	0.50
5:I:-171:DG:H2"	5:I:-170:DA:C8	2.47	0.50
6:J:-4:DG:H2"	6:J:-3:DA:C8	2.47	0.50
6:J:159:DG:H2"	6:J:160:DG:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:82:LEU:N	1:O:82:LEU:HD22	2.27	0.50
5:I:-82:DC:H2"	5:I:-81:DC:C6	2.46	0.49
6:J:162:DA:H2"	6:J:163:DC:C6	2.47	0.49
7:W:401:ASP:HA	7:W:597:ARG:H	1.76	0.49
5:I:-34:DG:H2"	5:I:-33:DA:C8	2.47	0.49
5:I:5:DC:H2"	5:I:6:DC:C6	2.47	0.49
6:J:97:DG:H2"	6:J:98:DG:C8	2.47	0.49
3:C:42:ARG:CD	6:J:39:DA:H5"	2.42	0.49
7:W:400:ALA:HB3	7:W:594:ILE:HD11	1.95	0.49
4:H:87:THR:HG22	4:H:90:GLU:OE1	2.13	0.49
7:W:222:HIS:HB3	7:W:285:HIS:ND1	2.28	0.49
5:I:60:DT:H2"	5:I:61:DA:C8	2.48	0.49
6:J:-54:DC:H2"	6:J:-53:DA:C8	2.48	0.49
6:J:96:DG:H2"	6:J:97:DG:C8	2.48	0.49
1:K:79:LYS:O	1:K:80:THR:OG1	2.25	0.49
5:I:-44:DA:H2"	5:I:-43:DT:C6	2.48	0.49
5:I:39:DA:H2"	5:I:40:DG:C8	2.48	0.49
3:C:62:ILE:HD11	4:D:59:MET:HE1	1.95	0.49
5:I:-119:DT:H2"	5:I:-118:DA:C8	2.48	0.49
5:I:-113:DC:H2"	5:I:-112:DA:C8	2.48	0.49
7:W:790:ASP:OD1	7:W:790:ASP:N	2.42	0.49
5:I:-170:DA:H2"	5:I:-169:DA:C8	2.48	0.49
6:J:-26:DC:H2"	6:J:-25:DC:C6	2.48	0.49
7:W:625:TYR:OH	7:W:671:ARG:NH2	2.46	0.49
5:I:-161:DG:H2"	5:I:-160:DC:C6	2.48	0.48
5:I:-129:DT:H2"	5:I:-128:DA:C8	2.48	0.48
5:I:-87:DA:C2	6:J:88:DA:C2	3.01	0.48
6:J:151:DG:H2"	6:J:152:DC:C6	2.48	0.48
4:D:87:THR:N	4:D:90:GLU:OE1	2.46	0.48
6:J:-7:DG:H2"	6:J:-6:DG:C8	2.49	0.48
7:W:400:ALA:O	7:W:596:ARG:NH1	2.39	0.48
5:I:-153:DC:H2"	5:I:-152:DG:C8	2.48	0.48
2:B:29:ILE:N	2:B:29:ILE:HD12	2.29	0.48
7:W:182:VAL:HG12	7:W:215:ILE:HD12	1.96	0.48
5:I:-42:DT:H2"	5:I:-41:DG:C8	2.48	0.48
5:I:35:DC:H2"	5:I:36:DC:C6	2.49	0.48
5:I:36:DC:H2"	5:I:37:DC:C6	2.48	0.48
4:Q:45:VAL:O	4:Q:46:HIS:ND1	2.46	0.48
7:W:466:ILE:O	7:W:470:GLU:HB2	2.13	0.48
5:I:-68:DC:H2"	5:I:-67:DC:C6	2.48	0.48
6:J:43:DA:H2"	6:J:44:DT:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:101:DC:H2"	6:J:102:DA:C8	2.49	0.48
2:F:25:ASN:OD1	2:F:27:GLN:N	2.40	0.48
5:I:17:DA:H2"	5:I:18:DC:C6	2.49	0.47
6:J:17:DA:H2"	6:J:18:DG:C8	2.48	0.47
2:P:75:HIS:NE2	4:Q:77:LEU:HD21	2.29	0.47
6:J:66:DG:H2"	6:J:67:DG:C8	2.48	0.47
6:J:75:DC:H2"	6:J:76:DC:C6	2.49	0.47
7:W:471:PHE:O	7:W:483:MET:HA	2.14	0.47
7:W:216:LYS:NZ	7:W:220:GLU:O	2.48	0.47
5:I:-138:DA:H2"	5:I:-137:DG:C8	2.50	0.47
5:I:-95:DC:H2"	5:I:-94:DG:C8	2.49	0.47
5:I:35:DC:H2"	5:I:36:DC:C5	2.49	0.47
7:W:358:ARG:NH2	7:W:536:ASN:OD1	2.38	0.47
6:J:45:DT:H2"	6:J:46:DG:C8	2.50	0.47
7:W:282:GLU:HA	7:W:285:HIS:CD2	2.50	0.47
5:I:-167:DC:H2"	5:I:-166:DC:C6	2.49	0.47
5:I:-64:DA:H2"	5:I:-63:DG:C8	2.48	0.47
5:I:-62:DT:H2"	5:I:-61:DC:C6	2.50	0.47
3:C:29:ARG:NE	4:D:32:GLU:OE2	2.48	0.47
5:I:-32:DC:H2"	5:I:-31:DA:C8	2.50	0.47
7:W:781:MET:HE1	7:W:805:ALA:O	2.15	0.47
5:I:26:DG:H2"	5:I:27:DG:C8	2.50	0.47
4:N:90:GLU:O	4:N:93:THR:HG22	2.15	0.47
7:W:283:GLU:O	7:W:286:VAL:HG12	2.14	0.47
7:W:537:ARG:NH1	7:W:558:PHE:O	2.45	0.47
5:I:-66:DC:H2"	5:I:-65:DT:C6	2.50	0.46
5:I:-14:DA:H2"	5:I:-13:DA:H8	1.79	0.46
5:I:-3:DG:H2"	5:I:-2:DC:C6	2.49	0.46
7:W:406:GLY:O	7:W:409:VAL:HG22	2.15	0.46
6:J:25:DT:H2"	6:J:26:DA:C8	2.50	0.46
5:I:-136:DA:H2"	5:I:-135:DC:C6	2.50	0.46
5:I:24:DA:H2"	5:I:25:DG:C8	2.50	0.46
1:K:75:ALA:HB2	2:L:66:ILE:HD11	1.97	0.46
2:B:92:ARG:HA	2:B:92:ARG:NH1	2.31	0.46
5:I:-133:DG:H2"	5:I:-132:DC:C6	2.51	0.46
4:N:73:GLU:HG3	4:N:98:LEU:HD21	1.97	0.46
2:P:49:LEU:HD22	2:P:49:LEU:H	1.81	0.46
6:J:74:DT:H2"	6:J:75:DC:C6	2.51	0.46
7:W:406:GLY:O	7:W:407:LYS:C	2.56	0.46
7:W:471:PHE:CD1	7:W:471:PHE:N	2.84	0.46
6:J:-44:DG:H2"	6:J:-43:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-3:DA:H2"	6:J:-2:DC:C6	2.51	0.46
3:C:84:GLN:HB2	3:C:102:ILE:HD11	1.98	0.45
5:I:-33:DA:H2"	5:I:-32:DC:C6	2.51	0.45
5:I:-108:DA:H2"	5:I:-107:DC:C6	2.52	0.45
7:W:310:LYS:NZ	7:W:314:LEU:O	2.42	0.45
7:W:378:ASP:OD1	7:W:379:PHE:N	2.49	0.45
6:J:112:DT:H2"	6:J:113:DG:C8	2.51	0.45
7:W:407:LYS:N	8:W:1501:ADP:O3B	2.49	0.45
5:I:-28:DT:H2"	5:I:-27:DC:C6	2.52	0.45
6:J:138:DT:H2"	6:J:139:DA:C8	2.51	0.45
4:N:73:GLU:HA	4:N:73:GLU:OE1	2.17	0.45
4:Q:77:LEU:C	4:Q:77:LEU:HD23	2.41	0.45
5:I:-65:DT:H2"	5:I:-64:DA:C8	2.52	0.45
5:I:-59:DC:H2"	5:I:-58:DC:C6	2.51	0.45
5:I:-5:DA:H2"	5:I:-4:DC:C6	2.52	0.45
6:J:95:DG:H2"	6:J:96:DG:C8	2.52	0.45
6:J:158:DC:H2"	6:J:159:DG:C8	2.52	0.45
6:J:-6:DG:H2"	6:J:-5:DG:C8	2.52	0.45
1:O:82:LEU:HB2	1:O:84:PHE:CE1	2.51	0.45
4:N:68:GLU:OE1	2:P:91:LYS:NZ	2.49	0.45
3:M:54:VAL:HG23	4:N:107:ALA:HB1	1.98	0.45
6:J:44:DT:H2"	6:J:45:DT:C6	2.52	0.45
7:W:742:ASP:OD1	7:W:744:THR:OG1	2.33	0.45
7:W:460:GLN:OE1	7:W:463:ARG:NH2	2.43	0.44
6:J:94:DC:H2"	6:J:95:DG:C8	2.52	0.44
2:P:22:LEU:HA	2:P:25:ASN:HB2	1.99	0.44
7:W:309:VAL:HG12	7:W:320:THR:O	2.17	0.44
7:W:749:GLN:H	7:W:749:GLN:CD	2.25	0.44
5:I:-85:DC:H2"	5:I:-84:DC:C6	2.52	0.44
6:J:87:DT:H2"	6:J:88:DA:C8	2.53	0.44
6:J:119:DA:H2"	6:J:120:DA:C8	2.51	0.44
7:W:780:LEU:C	7:W:781:MET:HE2	2.42	0.44
5:I:-98:DC:H2"	5:I:-97:DC:C6	2.52	0.44
5:I:48:DG:H2"	5:I:49:DC:C6	2.53	0.44
3:M:38:ASN:O	3:M:38:ASN:ND2	2.48	0.44
5:I:-97:DC:H2"	5:I:-96:DC:C6	2.52	0.44
6:J:60:DA:H2"	6:J:61:DG:C8	2.52	0.44
2:L:29:ILE:N	2:L:29:ILE:HD12	2.33	0.44
7:W:379:PHE:CD1	7:W:602:VAL:HG13	2.51	0.44
5:I:31:DT:H2"	5:I:32:DA:C8	2.52	0.44
4:N:36:ILE:HG23	4:N:37:TYR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-76:DG:H2"	5:I:-75:DG:C8	2.51	0.44
5:I:-30:DG:H2"	5:I:-29:DC:C6	2.53	0.44
5:I:7:DC:H2"	5:I:8:DC:C6	2.53	0.44
2:F:29:ILE:HD12	2:F:29:ILE:N	2.33	0.44
6:J:134:DT:H2"	6:J:135:DG:C8	2.53	0.44
5:I:-67:DC:H2"	5:I:-66:DC:C6	2.52	0.44
6:J:100:DA:H2"	6:J:101:DC:C6	2.53	0.44
6:J:126:DG:H4'	7:W:793:TRP:CD1	2.53	0.44
7:W:548:ASN:N	7:W:551:GLU:OE1	2.37	0.44
6:J:127:DC:H2"	6:J:128:DT:C6	2.53	0.43
2:B:38:ALA:HB1	2:B:43:VAL:HB	1.99	0.43
4:H:77:LEU:HD13	4:H:93:THR:CG2	2.48	0.43
6:J:28:DA:H2"	6:J:29:DG:C8	2.53	0.43
1:E:68:GLN:HA	1:E:71:VAL:HG12	1.99	0.43
5:I:-74:DA:H2"	5:I:-73:DT:C6	2.53	0.43
6:J:-56:DG:H2"	6:J:-55:DA:C8	2.53	0.43
3:M:85:LEU:O	3:M:89:ASN:ND2	2.41	0.43
2:P:67:ARG:O	2:P:70:VAL:HG12	2.18	0.43
7:W:580:GLU:HA	7:W:583:ILE:HG22	2.00	0.43
2:F:78:ARG:NH1	2:F:80:THR:O	2.51	0.43
3:G:71:ARG:HH11	3:G:71:ARG:HG2	1.83	0.43
5:I:51:DC:H2"	5:I:52:DG:C8	2.53	0.43
3:M:22:GLY:C	3:M:23:LEU:HD12	2.44	0.43
7:W:179:ILE:HD11	7:W:236:VAL:HB	2.01	0.43
7:W:399:LEU:N	7:W:399:LEU:HD22	2.33	0.43
5:I:-24:DG:H2"	5:I:-23:DC:C6	2.54	0.43
2:P:38:ALA:HB1	2:P:43:VAL:HG22	2.00	0.43
7:W:373:GLY:O	7:W:446:LYS:NZ	2.46	0.43
7:W:417:TRP:O	7:W:421:ALA:N	2.36	0.43
7:W:756:HIS:O	7:W:762:SER:HB3	2.18	0.43
7:W:781:MET:HE2	7:W:781:MET:CA	2.48	0.43
1:A:123:ASP:OD1	1:A:123:ASP:N	2.51	0.43
4:D:83:ARG:HH22	5:I:-33:DA:P	2.41	0.43
7:W:652:MET:SD	7:W:652:MET:C	3.01	0.43
3:C:63:LEU:HD21	4:D:59:MET:HE2	2.01	0.43
4:H:42:LEU:HD23	4:H:42:LEU:C	2.43	0.43
6:J:-48:DC:H2"	6:J:-47:DC:C6	2.54	0.43
2:P:29:ILE:O	2:P:29:ILE:HG13	2.18	0.43
7:W:233:ILE:HG13	7:W:234:GLY:N	2.34	0.43
2:L:62:LEU:HD23	2:L:62:LEU:C	2.44	0.43
1:E:62:ILE:HD11	1:E:93:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-106:DG:H2"	5:I:-105:DC:C6	2.54	0.43
1:K:79:LYS:HB3	1:K:82:LEU:HD21	1.99	0.43
1:K:81:ASP:C	1:K:82:LEU:HD22	2.44	0.43
2:B:88:TYR:CD1	4:D:80:TYR:CE2	3.07	0.42
5:I:-162:DT:H2"	5:I:-161:DG:C8	2.54	0.42
5:I:-49:DC:H2"	5:I:-48:DC:C6	2.54	0.42
5:I:-8:DC:H2"	5:I:-7:DG:C8	2.54	0.42
4:N:102:GLU:OE1	4:N:106:HIS:CE1	2.72	0.42
7:W:807:ARG:NH2	9:W:1502:BEF:F1	2.42	0.42
5:I:45:DC:H2"	5:I:46:DA:C8	2.54	0.42
6:J:62:DA:H2"	6:J:63:DC:C6	2.54	0.42
7:W:713:ARG:HD2	7:W:765:PHE:HB2	2.00	0.42
6:J:15:DT:H2"	6:J:16:DA:C8	2.54	0.42
7:W:466:ILE:HG22	7:W:471:PHE:CE1	2.54	0.42
6:J:1:DC:H2"	6:J:2:DG:C8	2.55	0.42
2:P:24:ASP:O	2:P:28:GLY:N	2.50	0.42
7:W:521:ALA:HA	7:W:526:TYR:CD1	2.55	0.42
3:C:81:ARG:NH2	3:C:107:VAL:O	2.49	0.42
5:I:-81:DC:H2"	5:I:-80:DA:C8	2.54	0.42
6:J:35:DT:H2"	6:J:36:DA:C8	2.54	0.42
6:J:90:DA:H2"	6:J:91:DA:H8	1.83	0.42
1:K:61:LEU:C	1:K:61:LEU:HD23	2.44	0.42
7:W:208:LYS:O	7:W:230:TYR:CD1	2.73	0.42
2:F:25:ASN:OD1	2:F:25:ASN:C	2.63	0.42
5:I:-23:DC:H2"	5:I:-22:DA:H8	1.84	0.42
4:Q:59:MET:HE2	4:Q:59:MET:HA	2.01	0.42
4:D:56:MET:SD	4:D:56:MET:C	3.03	0.42
5:I:-128:DA:H2"	5:I:-127:DG:C8	2.53	0.42
5:I:-116:DA:H2"	5:I:-115:DC:C6	2.54	0.42
6:J:-27:DC:H2"	6:J:-26:DC:C6	2.54	0.42
4:N:56:MET:C	4:N:56:MET:SD	3.02	0.42
7:W:404:GLY:HA2	7:W:807:ARG:CZ	2.49	0.42
7:W:493:GLU:H	7:W:493:GLU:CD	2.28	0.42
3:C:88:ARG:NH2	3:C:100:VAL:O	2.47	0.42
6:J:54:DC:H2"	6:J:55:DC:C6	2.54	0.42
7:W:409:VAL:HG21	8:W:1501:ADP:N7	2.35	0.42
6:J:77:DC:H2"	6:J:78:DC:C6	2.54	0.42
7:W:291:ILE:N	7:W:291:ILE:HD12	2.34	0.42
1:K:90:MET:SD	1:K:90:MET:C	3.03	0.41
7:W:585:ASP:O	7:W:588:ARG:HG3	2.20	0.41
5:I:-48:DC:H2"	5:I:-47:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:50:DA:H2"	6:J:51:DA:C8	2.55	0.41
7:W:359:PRO:O	7:W:392:SER:HB3	2.20	0.41
7:W:580:GLU:O	7:W:583:ILE:HG22	2.20	0.41
6:J:-25:DC:H2"	6:J:-24:DT:C6	2.55	0.41
2:P:38:ALA:HB1	2:P:43:VAL:CG2	2.50	0.41
4:Q:50:GLY:N	3:R:76:THR:O	2.53	0.41
7:W:292:ASP:OD1	7:W:292:ASP:C	2.62	0.41
7:W:610:THR:O	7:W:816:VAL:N	2.54	0.41
7:W:840:GLU:O	7:W:843:ILE:HG22	2.20	0.41
5:I:4:DC:H2"	5:I:5:DC:C6	2.55	0.41
6:J:102:DA:H2"	6:J:103:DG:C8	2.55	0.41
6:J:163:DC:H2"	6:J:164:DC:C6	2.55	0.41
1:O:104:PHE:CE2	2:P:38:ALA:HB2	2.55	0.41
4:H:70:ILE:HD13	4:H:98:LEU:HD12	2.02	0.41
4:H:39:TYR:OH	4:H:43:LYS:HE3	2.20	0.41
1:A:109:LEU:HD12	1:A:112:ILE:HD11	2.02	0.41
2:B:49:LEU:HD12	2:B:49:LEU:N	2.35	0.41
6:J:118:DT:H2"	6:J:119:DA:C8	2.55	0.41
6:J:142:DA:H2"	6:J:143:DC:C6	2.55	0.41
7:W:450:ASP:OD1	7:W:450:ASP:N	2.43	0.41
7:W:807:ARG:HH11	7:W:807:ARG:HG2	1.84	0.41
3:G:15:LYS:HG3	3:G:16:THR:H	1.84	0.41
5:I:-166:DC:H2"	5:I:-165:DC:C6	2.55	0.41
5:I:-131:DT:H2"	5:I:-130:DC:C6	2.55	0.41
5:I:-50:DT:H2"	5:I:-49:DC:C6	2.56	0.41
7:W:180:ASP:HB3	7:W:216:LYS:C	2.46	0.41
7:W:452:ASN:O	7:W:486:ASN:OD1	2.39	0.41
7:W:457:MET:HE2	7:W:457:MET:HB2	1.98	0.41
7:W:841:TYR:HA	7:W:844:ILE:HG12	2.03	0.41
2:B:74:GLU:CD	2:B:74:GLU:C	2.89	0.41
5:I:-47:DT:H2"	5:I:-46:DC:C6	2.56	0.41
5:I:37:DC:H2"	5:I:38:DT:C6	2.55	0.41
5:I:62:DT:H2"	5:I:63:DA:C8	2.56	0.41
6:J:31:DT:H2"	6:J:32:DG:C8	2.56	0.41
7:W:178:GLY:N	7:W:218:THR:OG1	2.53	0.41
7:W:379:PHE:CZ	7:W:380:GLN:CD	2.99	0.41
7:W:565:THR:O	7:W:582:TYR:OH	2.32	0.41
7:W:825:VAL:O	7:W:828:GLU:N	2.54	0.41
5:I:-117:DA:H2"	5:I:-116:DA:H8	1.82	0.41
5:I:-102:DT:H2"	5:I:-101:DG:C8	2.56	0.41
5:I:-80:DA:H2"	5:I:-79:DA:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-32:DT:H2"	6:J:-31:DA:C8	2.56	0.41
3:M:26:PRO:HG2	3:M:29:ARG:HB3	2.03	0.41
1:O:73:GLU:HB2	2:P:22:LEU:HD23	2.02	0.41
2:F:77:LYS:HE2	4:H:89:ARG:NH1	2.36	0.40
5:I:-104:DG:H2"	5:I:-103:DC:C6	2.55	0.40
2:L:74:GLU:CD	2:L:74:GLU:C	2.89	0.40
5:I:-93:DC:H2"	5:I:-92:DG:H8	1.85	0.40
7:W:707:LEU:O	7:W:711:GLY:N	2.55	0.40
1:A:67:PHE:CZ	1:A:93:GLN:HA	2.56	0.40
5:I:-1:DG:H2"	5:I:0:DC:C6	2.56	0.40
1:O:60:LEU:N	1:O:60:LEU:HD22	2.37	0.40
1:O:74:ILE:HG13	2:P:66:ILE:HD11	2.03	0.40
4:Q:110:GLU:OE2	7:S:126:ARG:NH1	2.52	0.40
7:W:747:SER:O	7:W:750:ARG:HG2	2.22	0.40
2:B:31:LYS:HD3	2:B:51:TYR:CE2	2.57	0.40
5:I:-7:DG:H2"	5:I:-6:DT:C6	2.57	0.40
5:I:32:DA:H2"	5:I:33:DC:C6	2.57	0.40
6:J:55:DC:H2"	6:J:56:DC:C6	2.55	0.40
4:N:54:LYS:O	4:N:58:ILE:HG12	2.20	0.40
7:W:344:SER:O	7:W:345:LYS:HG2	2.22	0.40
7:W:776:LEU:N	7:W:776:LEU:HD22	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	91/136 (67%)	87 (96%)	4 (4%)	0	100	100
1	E	91/136 (67%)	91 (100%)	0	0	100	100
1	K	71/136 (52%)	70 (99%)	1 (1%)	0	100	100
1	O	94/136 (69%)	93 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
2	F	75/103 (73%)	75 (100%)	0	0	100	100
2	L	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
2	P	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
3	C	100/130 (77%)	99 (99%)	1 (1%)	0	100	100
3	G	94/130 (72%)	93 (99%)	1 (1%)	0	100	100
3	M	101/130 (78%)	99 (98%)	2 (2%)	0	100	100
3	R	91/130 (70%)	89 (98%)	2 (2%)	0	100	100
4	D	90/123 (73%)	90 (100%)	0	0	100	100
4	H	89/123 (72%)	89 (100%)	0	0	100	100
4	N	88/123 (72%)	88 (100%)	0	0	100	100
4	Q	89/123 (72%)	87 (98%)	2 (2%)	0	100	100
7	S	12/1468 (1%)	12 (100%)	0	0	100	100
7	T	21/1468 (1%)	20 (95%)	1 (5%)	0	100	100
7	W	633/1468 (43%)	616 (97%)	17 (3%)	0	100	100
All	All	2060/6372 (32%)	2025 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/111 (73%)	80 (99%)	1 (1%)	63	73
1	E	81/111 (73%)	81 (100%)	0	100	100
1	K	63/111 (57%)	61 (97%)	2 (3%)	34	56
1	O	84/111 (76%)	84 (100%)	0	100	100
2	B	64/79 (81%)	64 (100%)	0	100	100
2	F	63/79 (80%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	66/79 (84%)	65 (98%)	1 (2%)	57	70
2	P	67/79 (85%)	64 (96%)	3 (4%)	24	47
3	C	81/102 (79%)	79 (98%)	2 (2%)	42	62
3	G	75/102 (74%)	75 (100%)	0	100	100
3	M	82/102 (80%)	82 (100%)	0	100	100
3	R	72/102 (71%)	72 (100%)	0	100	100
4	D	79/103 (77%)	79 (100%)	0	100	100
4	H	77/103 (75%)	76 (99%)	1 (1%)	61	71
4	N	76/103 (74%)	76 (100%)	0	100	100
4	Q	77/103 (75%)	77 (100%)	0	100	100
7	S	14/1313 (1%)	14 (100%)	0	100	100
7	T	23/1313 (2%)	23 (100%)	0	100	100
7	W	581/1313 (44%)	574 (99%)	7 (1%)	63	73
All	All	1806/5519 (33%)	1789 (99%)	17 (1%)	68	75

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	CYS
3	C	58	LEU
3	C	63	LEU
4	H	93	THR
1	K	107	THR
1	K	109	LEU
2	L	31	LYS
2	P	25	ASN
2	P	43	VAL
2	P	78	ARG
7	W	182	VAL
7	W	289	ARG
7	W	347	LEU
7	W	415	ILE
7	W	423	ARG
7	W	493	GLU
7	W	745	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	31	HIS
3	C	82	HIS
4	D	81	ASN
2	F	75	HIS
3	G	24	GLN
4	H	44	GLN
4	H	92	GLN
1	K	93	GLN
4	N	81	ASN
4	Q	44	GLN
7	T	136	ASN
7	W	210	ASN
7	W	222	HIS
7	W	224	HIS
7	W	285	HIS
7	W	340	ASN
7	W	353	ASN
7	W	459	ASN
7	W	546	GLN
7	W	547	ASN
7	W	574	ASN
7	W	667	ASN
7	W	737	ASN
7	W	810	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
9	BEF	W	1502	8	0,3,3	-	-	-		
8	ADP	W	1501	9,10	27,29,29	1.33	4 (14%)	42,45,45	2.16	13 (30%)

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
8	ADP	W	1501	9,10	-	4/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1501	ADP	C5-C4	4.28	1.47	1.39
8	W	1501	ADP	C5-C6	2.49	1.48	1.41
8	W	1501	ADP	C5-N7	-2.29	1.34	1.39
8	W	1501	ADP	C8-N7	2.15	1.35	1.31

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	1501	ADP	C5-C4-N3	-5.90	119.06	126.75
8	W	1501	ADP	PA-O3A-PB	-5.16	115.11	132.83
8	W	1501	ADP	N3-C4-N9	4.99	135.31	127.08
8	W	1501	ADP	C2-N3-C4	3.91	120.99	111.75
8	W	1501	ADP	N3-C2-N1	-3.59	122.99	128.60
8	W	1501	ADP	C4-N9-C8	3.33	109.33	105.73
8	W	1501	ADP	C4-C5-N7	-2.99	106.98	110.62
8	W	1501	ADP	C5-N7-C8	2.84	107.54	103.51
8	W	1501	ADP	N9-C8-N7	-2.49	110.51	113.91
8	W	1501	ADP	C2'-C1'-N9	-2.36	107.32	113.30
8	W	1501	ADP	O3B-PB-O2B	2.24	116.21	107.64
8	W	1501	ADP	C3'-C2'-C1'	2.20	105.61	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	1501	ADP	C6-C5-N7	2.10	135.93	132.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

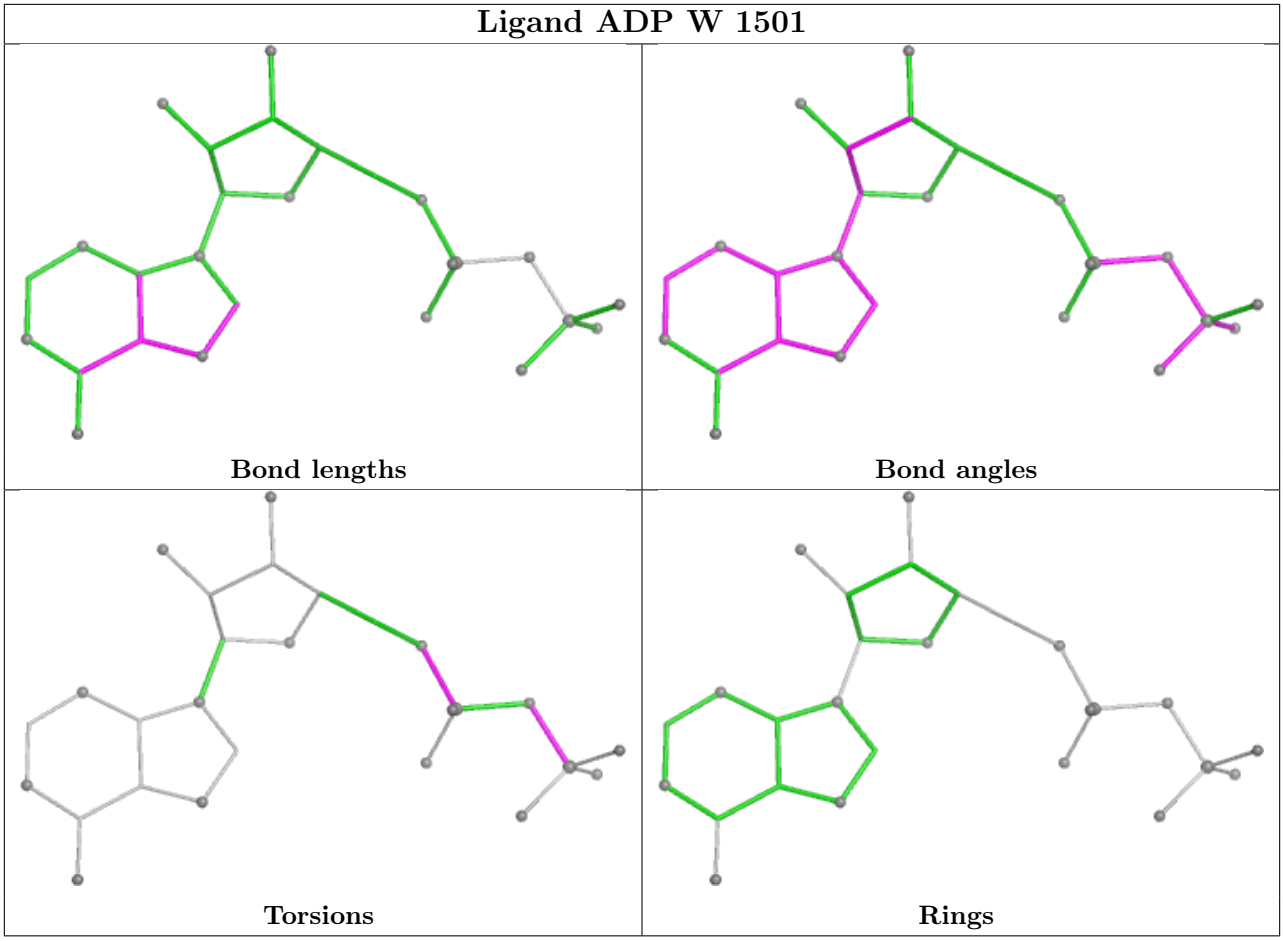
Mol	Chain	Res	Type	Atoms
8	W	1501	ADP	PA-O3A-PB-O3B
8	W	1501	ADP	C5'-O5'-PA-O2A
8	W	1501	ADP	C5'-O5'-PA-O3A
8	W	1501	ADP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	1502	BEF	1	0
8	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

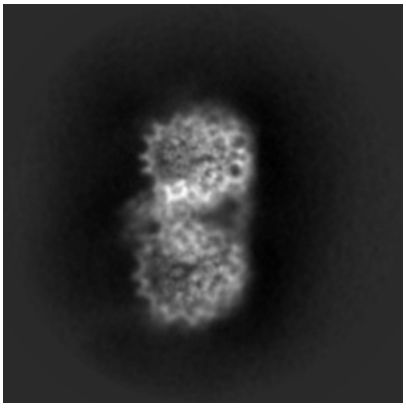
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-51244. These allow visual inspection of the internal detail of the map and identification of artifacts.

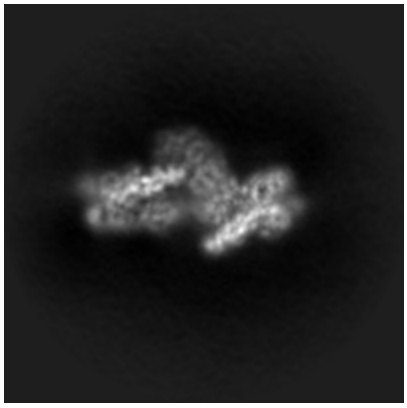
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

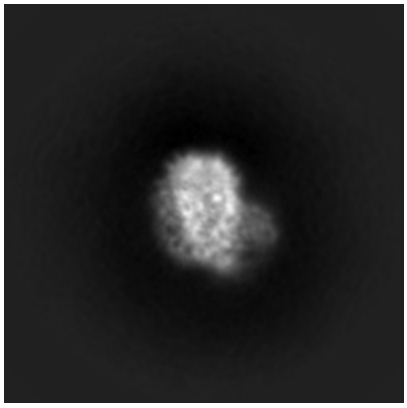
6.1.1 Primary map



X



Y

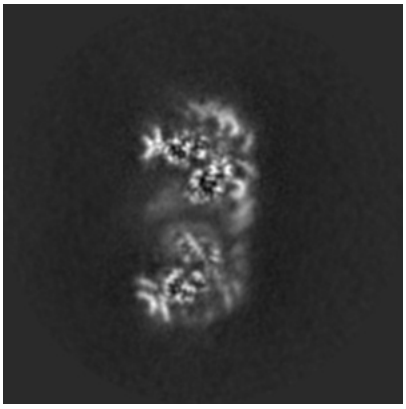


Z

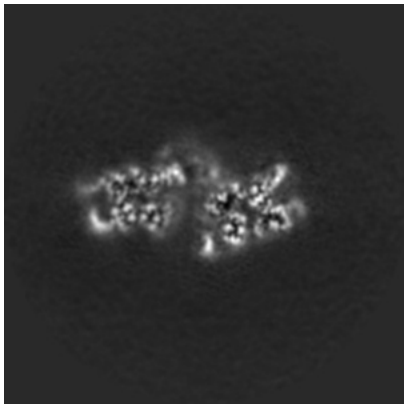
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

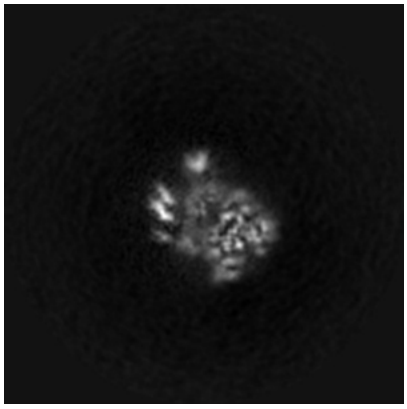
6.2.1 Primary map



X Index: 210



Y Index: 210

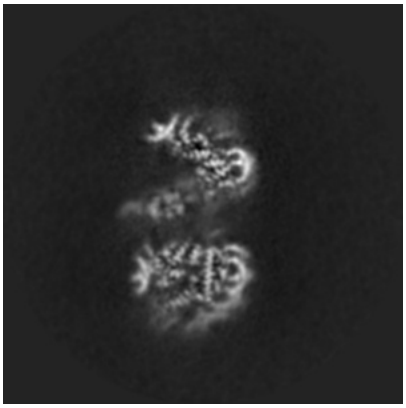


Z Index: 210

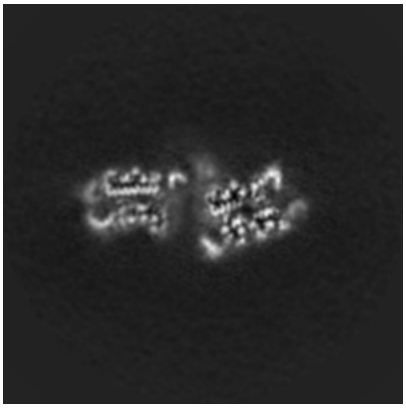
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

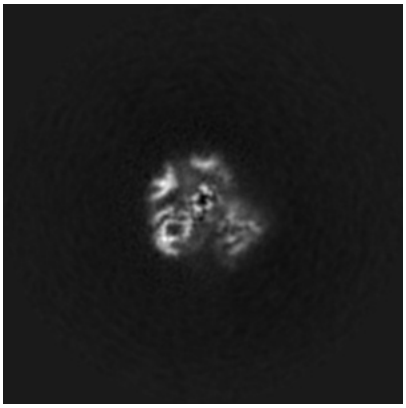
6.3.1 Primary map



X Index: 224



Y Index: 216

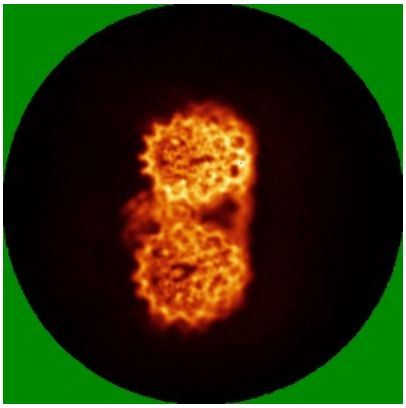


Z Index: 225

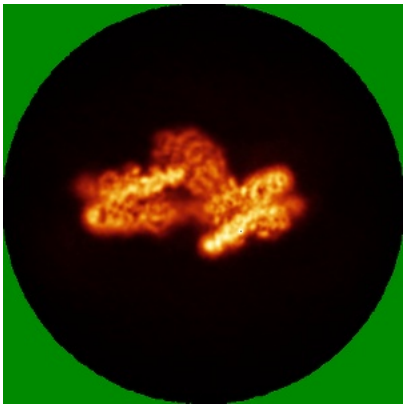
The images above show the largest variance slices of the map in three orthogonal directions.

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

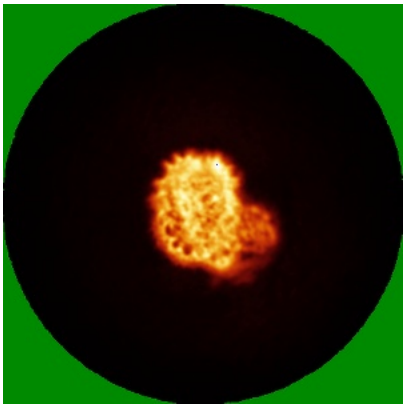
6.4.1 Primary map



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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

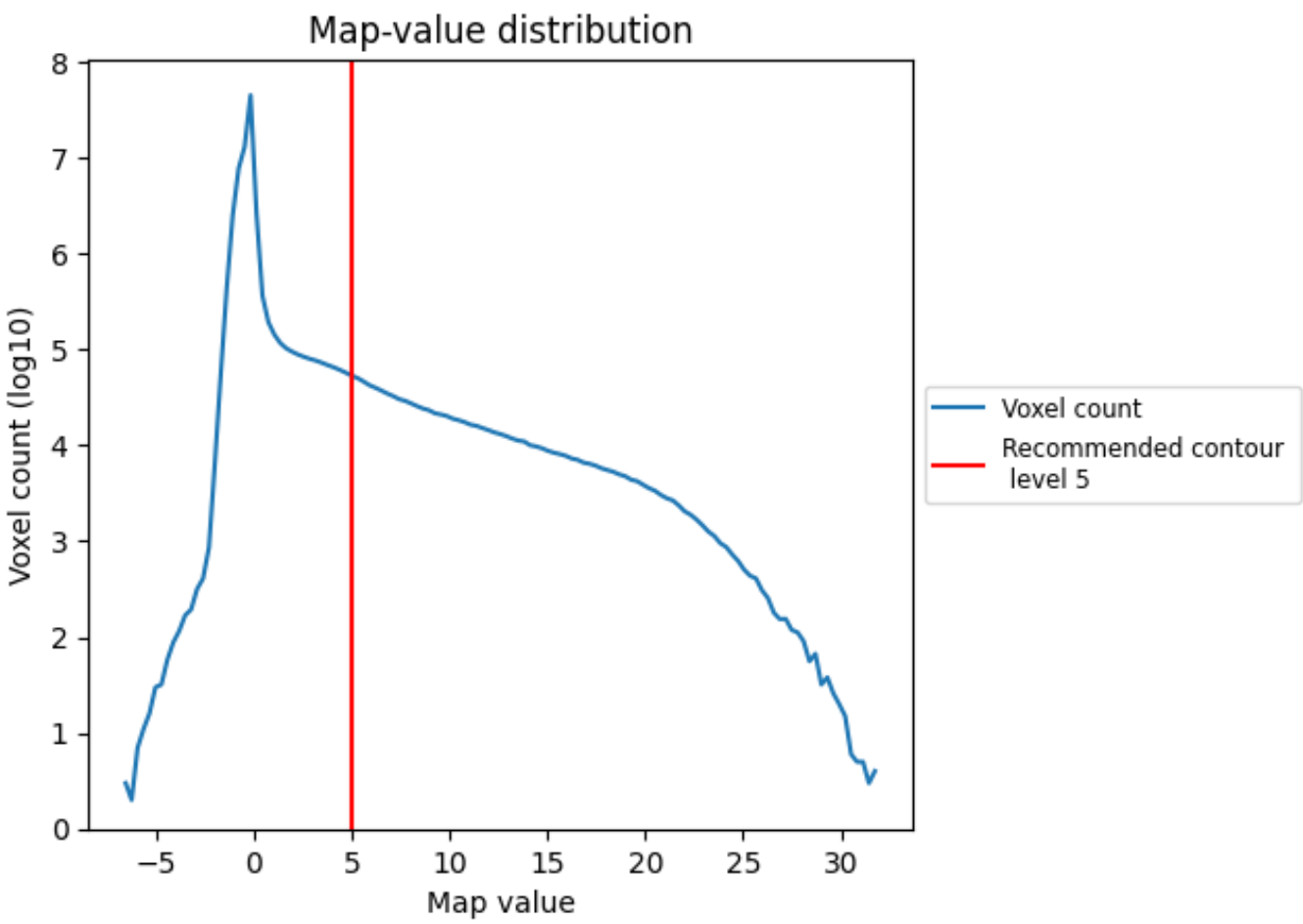
6.6 Mask visualisation (i)

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

7 Map analysis (i)

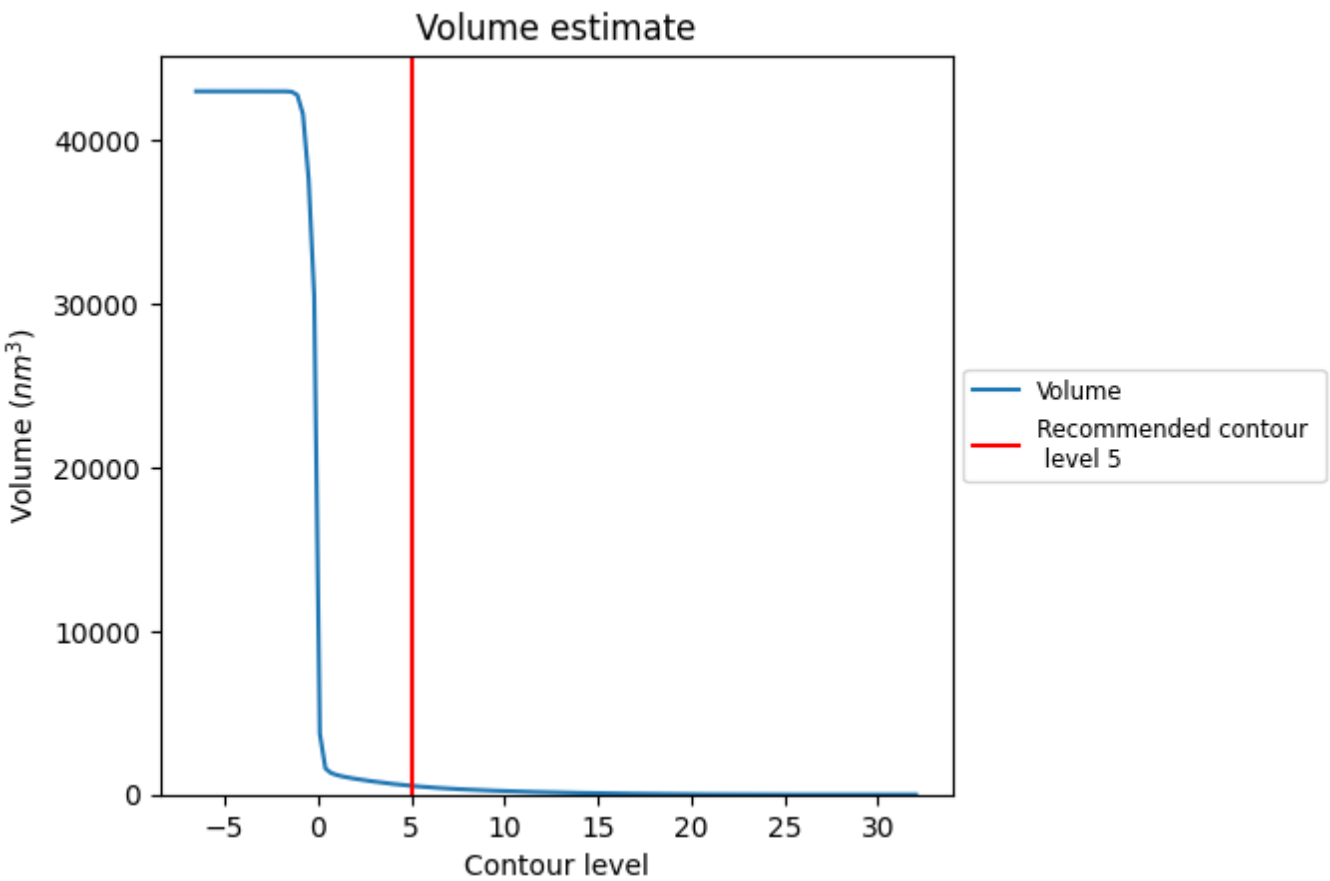
This section contains the results of statistical analysis of the map.

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.

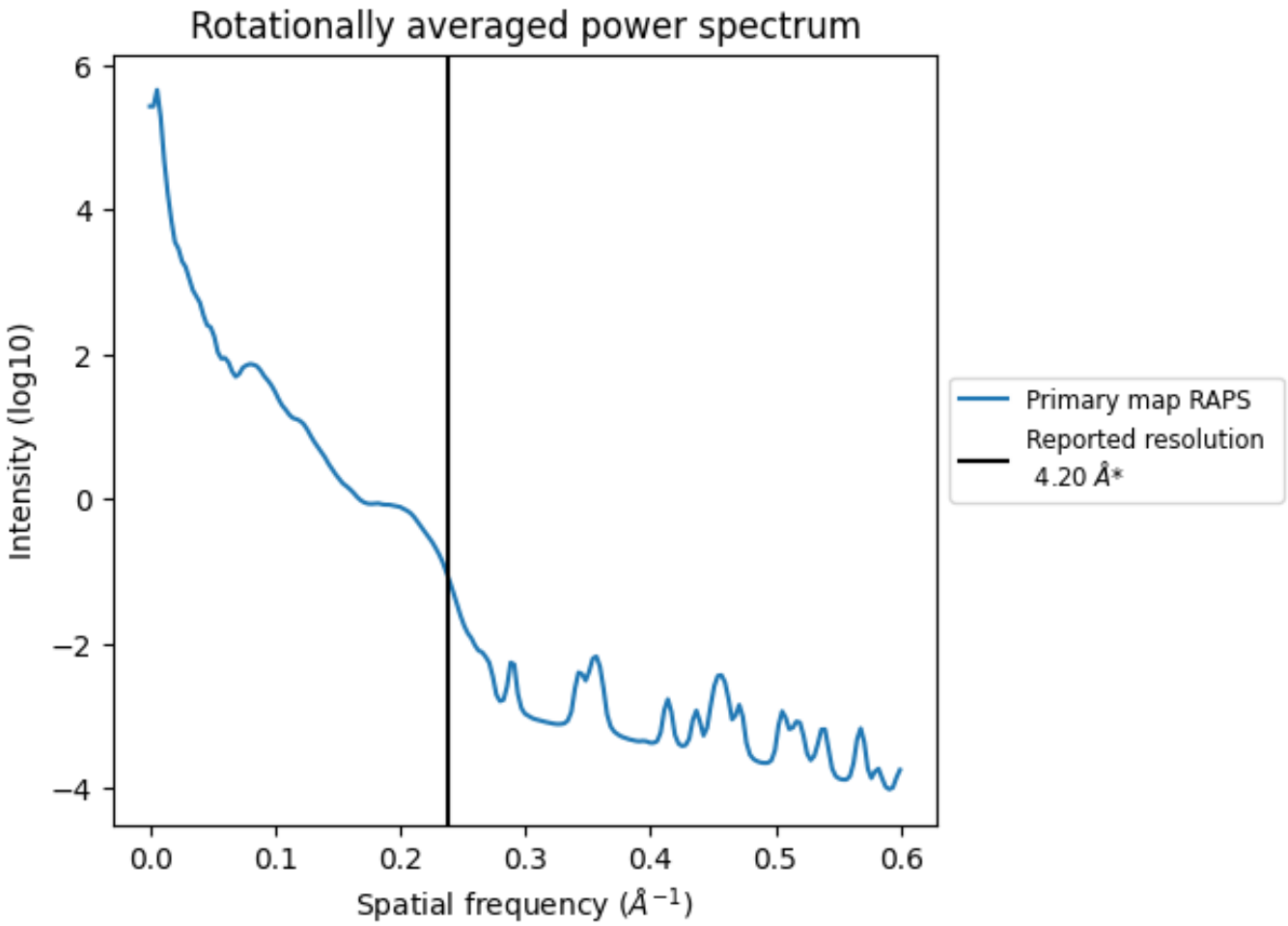
7.2 Volume estimate (i)



The volume at the recommended contour level is 534 nm^3; this corresponds to an approximate mass of 482 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

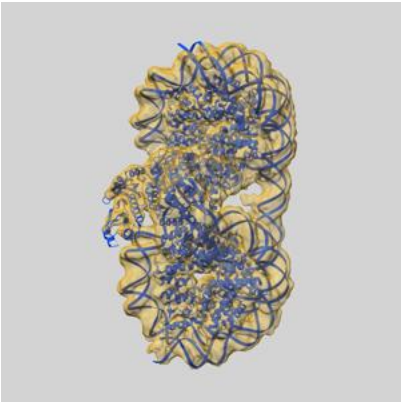
8 Fourier-Shell correlation (i)

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

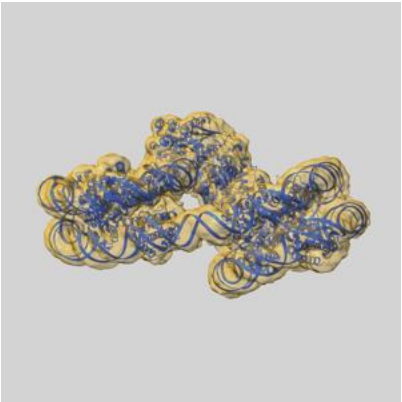
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-51244 and PDB model 9GD2. Per-residue inclusion information can be found in section 3 on page 8.

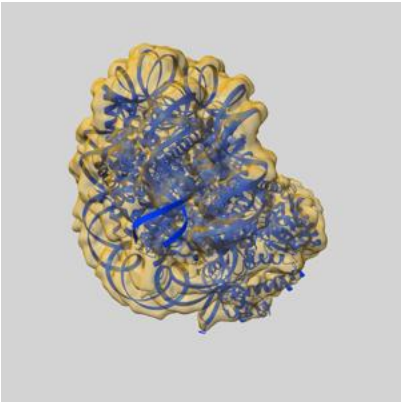
9.1 Map-model overlay (i)



X



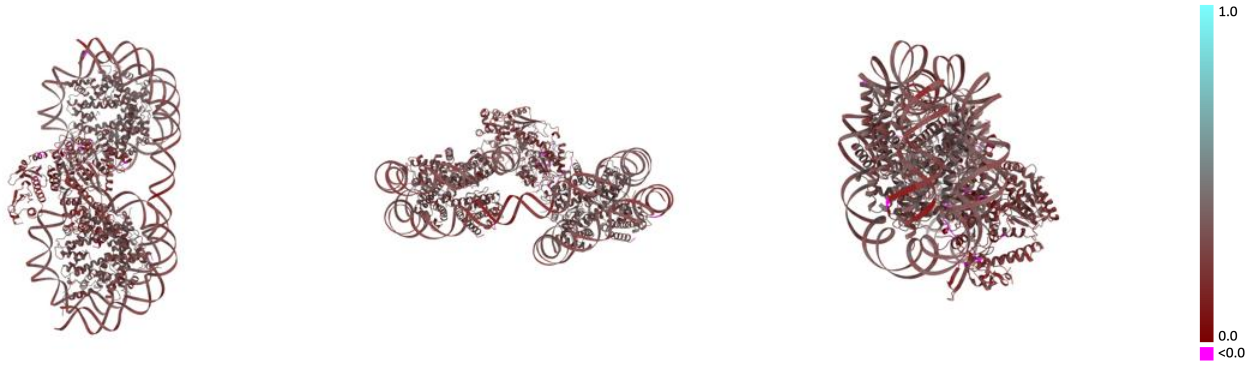
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

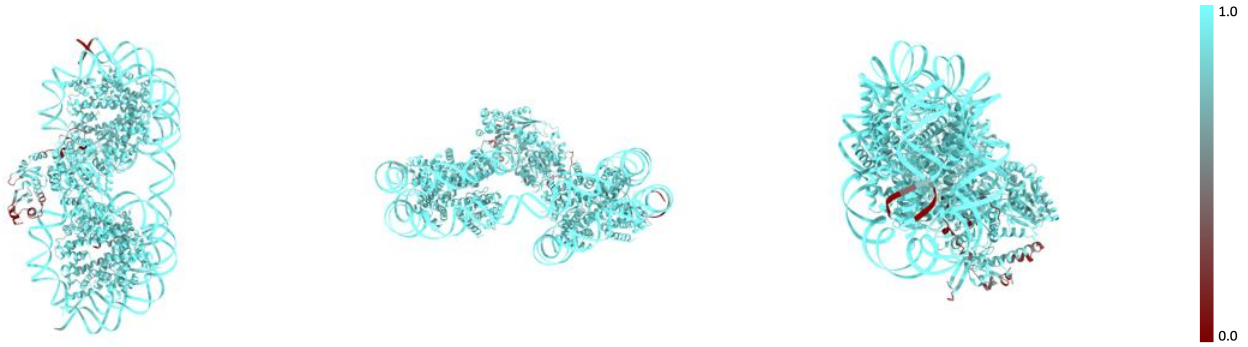
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

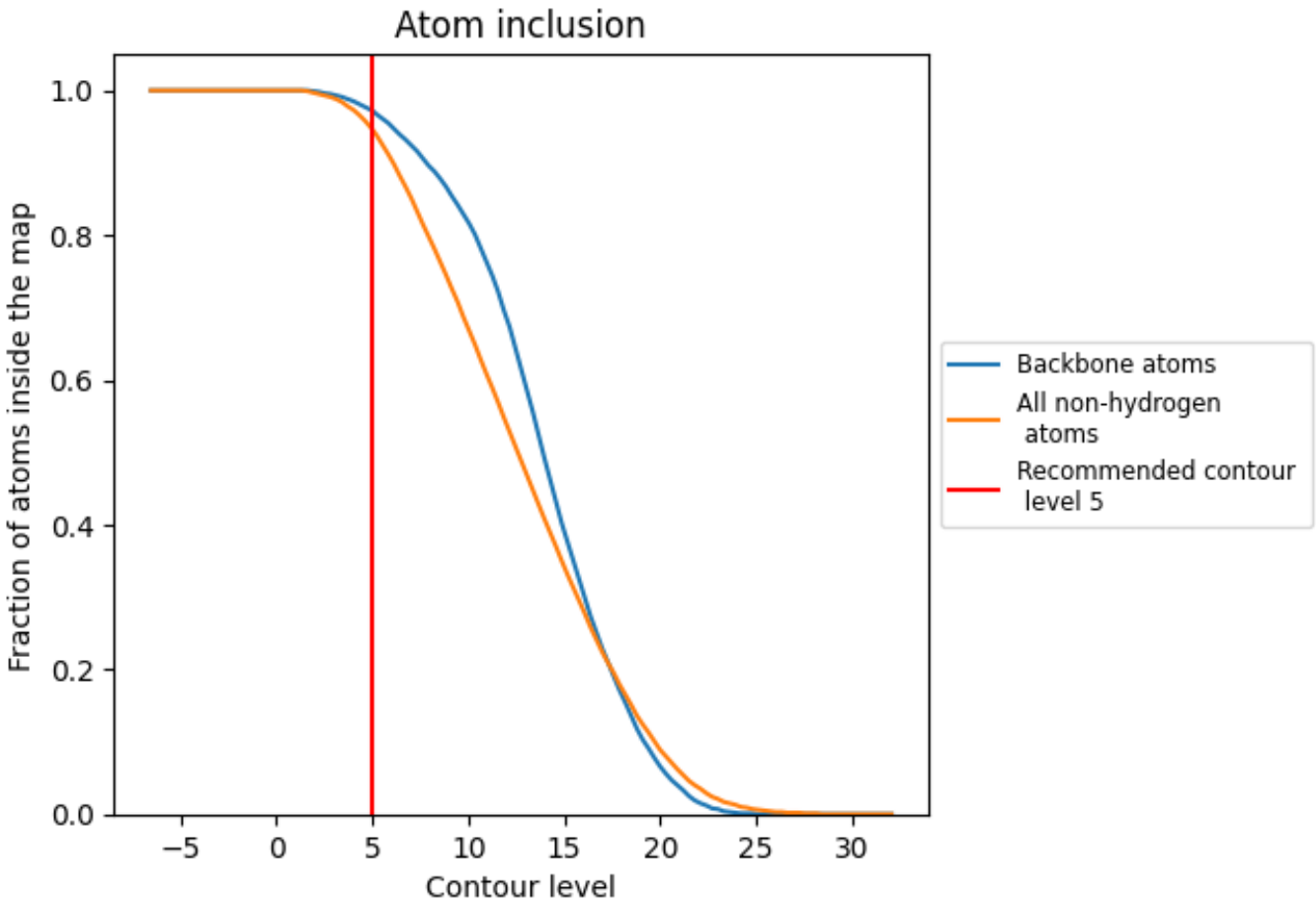
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.2950
A	0.9840	0.3460
B	0.9870	0.3730
C	0.9670	0.3490
D	0.9800	0.3420
E	0.9840	0.3410
F	0.9920	0.3640
G	0.9820	0.3540
H	0.9900	0.3400
I	0.9760	0.2950
J	0.9750	0.2950
K	0.9760	0.3080
L	0.9180	0.2820
M	0.9600	0.3350
N	0.9770	0.3130
O	0.9620	0.2990
P	0.9560	0.3100
Q	0.9730	0.2830
R	0.9580	0.2800
S	0.6840	0.1570
T	0.9840	0.2930
W	0.8430	0.2330