Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 03:18 pm BST

PDB ID	:	9Q92 / pdb_00009q92
EMDB ID	:	EMD-52915
Title	:	CryoEM structure of bacterial transcription intermediate complex mediated by activator PspF containing nifH promoter DNA containing mismatch from -11 to -8 - conformation 5
Authors	:	Gao, F.; Zhang, X.
Deposited on	:	2025-02-26
Resolution	:	6.80 Å(reported)

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

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

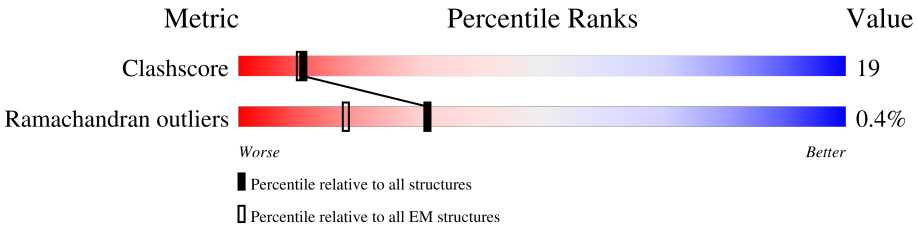
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

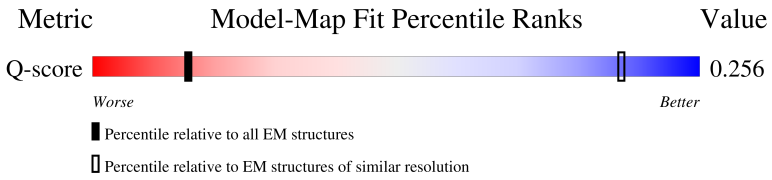
1 Overall quality at a glance

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

The reported resolution of this entry is 6.80 Å.

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





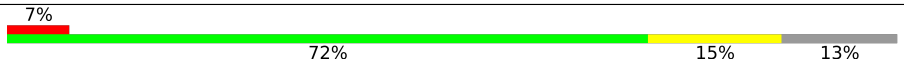
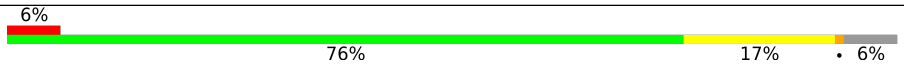
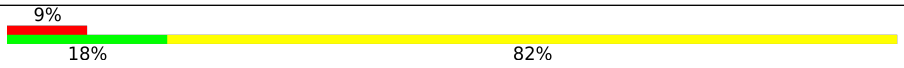
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	503 (6.30 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	T	34	9% 15% 85%
2	1	259	77% 20%
2	2	259	74% 25%
2	3	259	73% 25%
2	4	259	79% 21%

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Mol	Chain	Length	Quality of chain
2	5	259	
2	6	259	
3	M	475	
4	A	329	
4	B	329	
5	C	1341	
6	D	1407	
7	E	91	
8	N	34	

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
10	AF3	2	303	-	-	X	-
10	AF3	3	602	-	-	X	-
10	AF3	5	602	-	-	X	-
9	ADP	3	601	-	-	X	-
9	ADP	4	601	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26767 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 DNA chain called Template DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	34	Total	C	N	O	P	0	0
			700	331	131	204	34		

- Molecule 2 is a protein called Psp operon transcriptional activator.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	6	235	Total	C	N	O	0	0
			1161	691	235	235		
2	1	253	Total	C	N	O	0	0
			1247	741	253	253		
2	2	255	Total	C	N	O	0	0
			1257	747	255	255		
2	3	255	Total	C	N	O	0	0
			1257	747	255	255		
2	4	259	Total	C	N	O	0	0
			1277	759	259	259		
2	5	257	Total	C	N	O	0	0
			1267	753	257	257		

- Molecule 3 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	414	Total	C	N	O	0	0
			2055	1226	414	415		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	initiating methionine	UNP A0A377VEN9
M	2	LYS	-	expression tag	UNP A0A377VEN9
M	3	GLN	-	expression tag	UNP A0A377VEN9
M	4	GLY	-	expression tag	UNP A0A377VEN9
M	5	LEU	-	expression tag	UNP A0A377VEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	6	GLN	-	expression tag	UNP A0A377VEN9
M	7	LEU	-	expression tag	UNP A0A377VEN9
M	8	ARG	-	expression tag	UNP A0A377VEN9
M	9	LEU	-	expression tag	UNP A0A377VEN9
M	10	SER	-	expression tag	UNP A0A377VEN9
M	11	LEU	-	expression tag	UNP A0A377VEN9
M	12	ALA	-	expression tag	UNP A0A377VEN9
M	13	MET	-	expression tag	UNP A0A377VEN9
M	14	THR	-	expression tag	UNP A0A377VEN9
M	15	PRO	-	expression tag	UNP A0A377VEN9
M	16	GLN	-	expression tag	UNP A0A377VEN9
M	17	LEU	-	expression tag	UNP A0A377VEN9
M	18	GLN	-	expression tag	UNP A0A377VEN9
M	19	GLN	-	expression tag	UNP A0A377VEN9
M	20	ALA	-	expression tag	UNP A0A377VEN9
M	21	ILE	-	expression tag	UNP A0A377VEN9
M	22	ARG	-	expression tag	UNP A0A377VEN9
M	23	LEU	-	expression tag	UNP A0A377VEN9

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	229	Total	C	N	O	0	0
			1130	672	229	229		
4	B	217	Total	C	N	O	0	0
			1071	637	217	217		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	1341	Total	C	N	O	0	0
			6599	3917	1341	1341		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	1326	Total	C	N	O	0	0
			6526	3874	1326	1326		

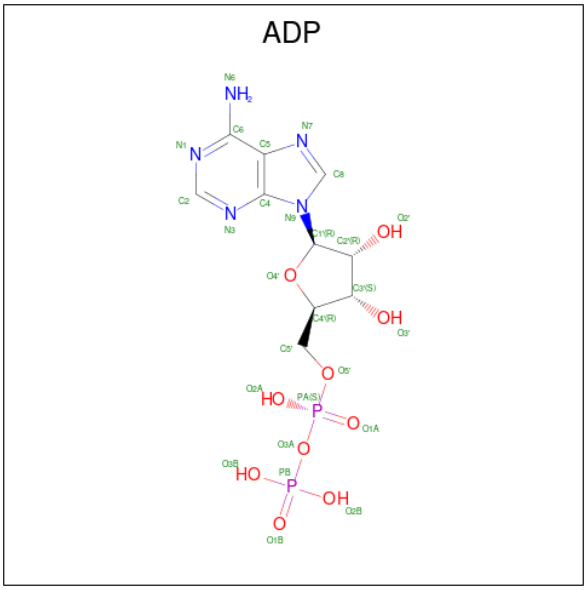
- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	E	74	Total	C	N	O	0	0
			366	218	74	74		

- Molecule 8 is a DNA chain called Non-template DNA (34-MER).

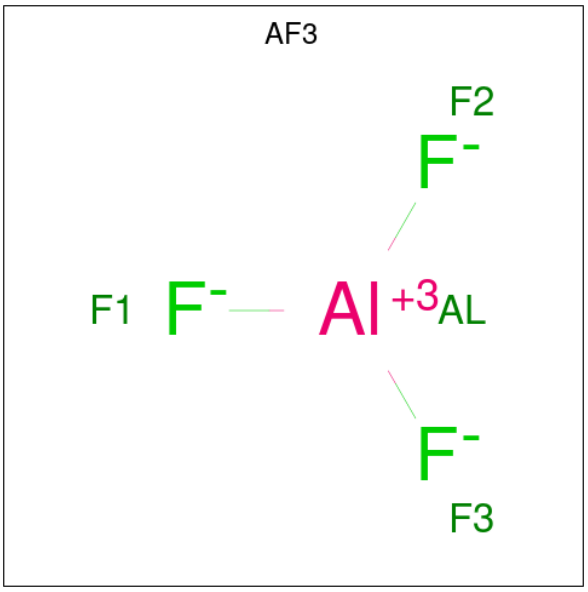
Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	34	Total	C	N	O	P	0	0
			694	329	127	204	34		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
9	1	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	5	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms	AltConf
10	1	1	Total Al F 4 1 3	0
10	2	1	Total Al F 4 1 3	0
10	3	1	Total Al F 4 1 3	0
10	4	1	Total Al F 4 1 3	0
10	5	1	Total Al F 4 1 3	0

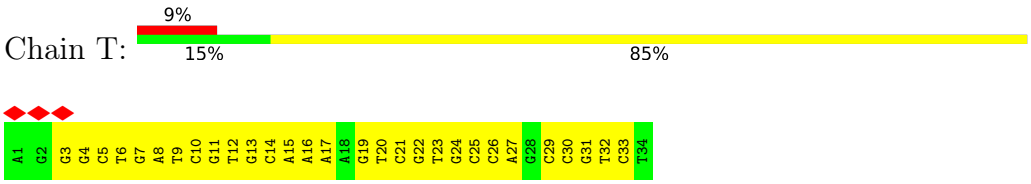
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
11	2	2	Total Mg 2 2	0
11	3	1	Total Mg 1 1	0
11	4	1	Total Mg 1 1	0
11	5	1	Total Mg 1 1	0

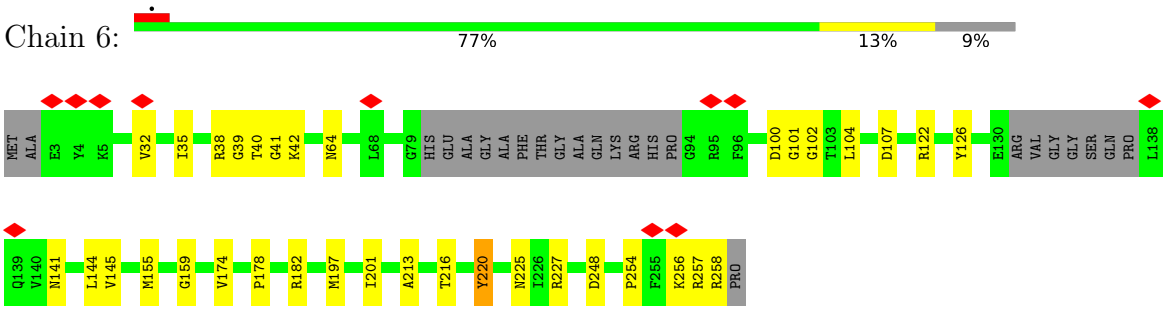
3 Residue-property plots (i)

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.

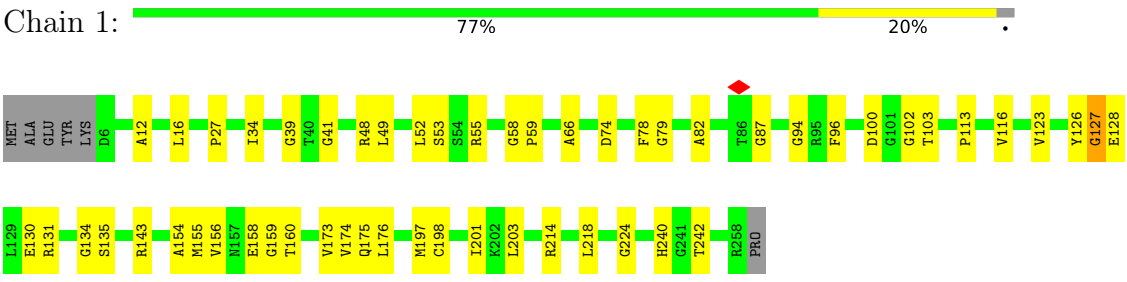
• Molecule 1: Template DNA (34-MER)



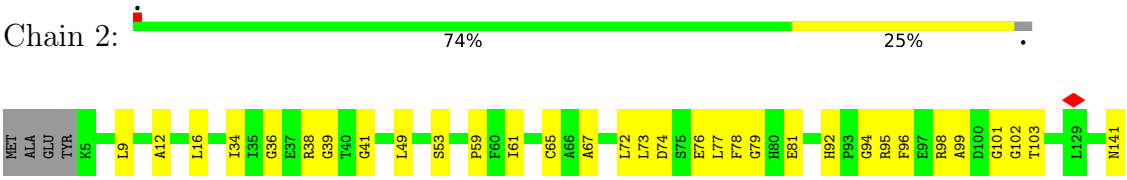
• Molecule 2: Psp operon transcriptional activator

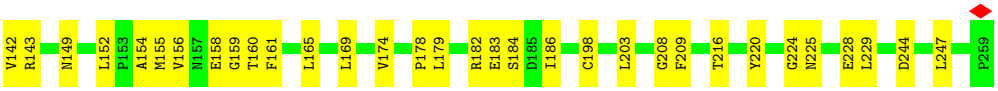


• Molecule 2: Psp operon transcriptional activator



• Molecule 2: Psp operon transcriptional activator

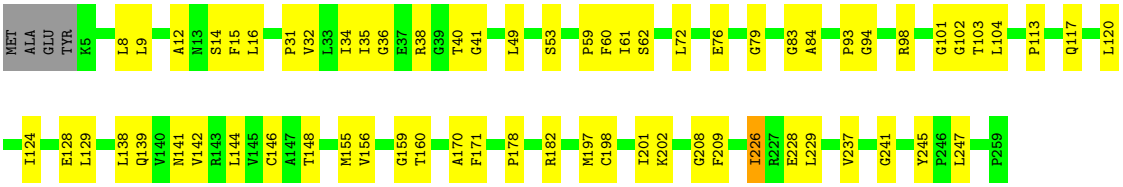




• Molecule 2: Psp operon transcriptional activator

Chain 3:

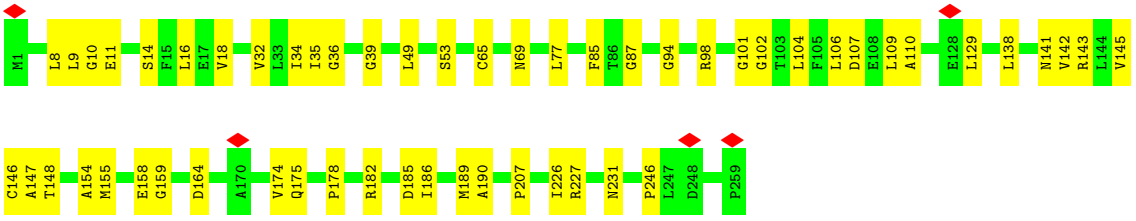




• Molecule 2: Psp operon transcriptional activator

Chain 4:

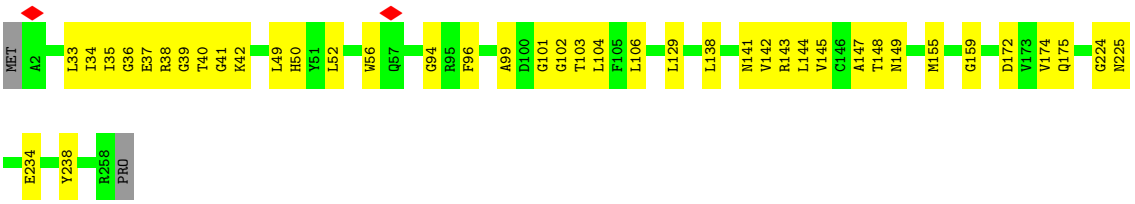




• Molecule 2: Psp operon transcriptional activator

Chain 5:

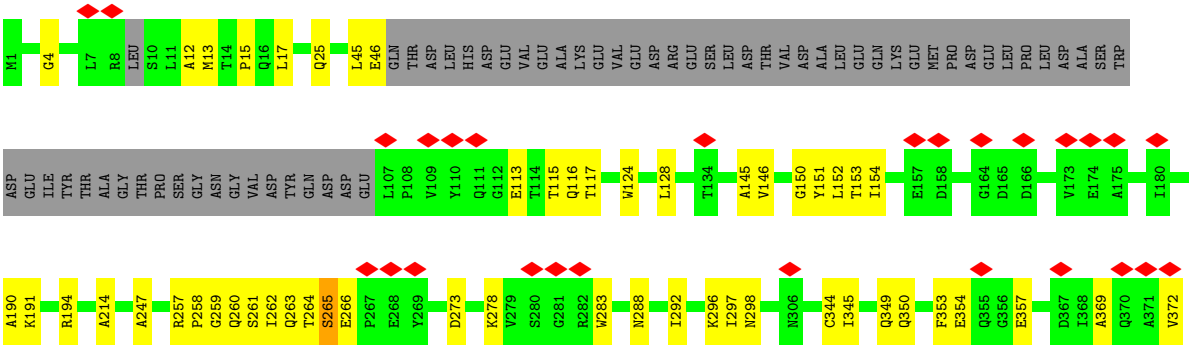


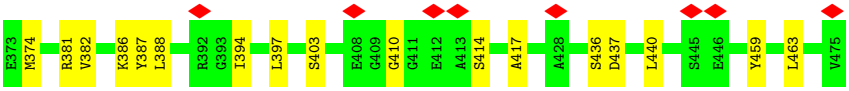


• Molecule 3: RNA polymerase sigma-54 factor

Chain M:



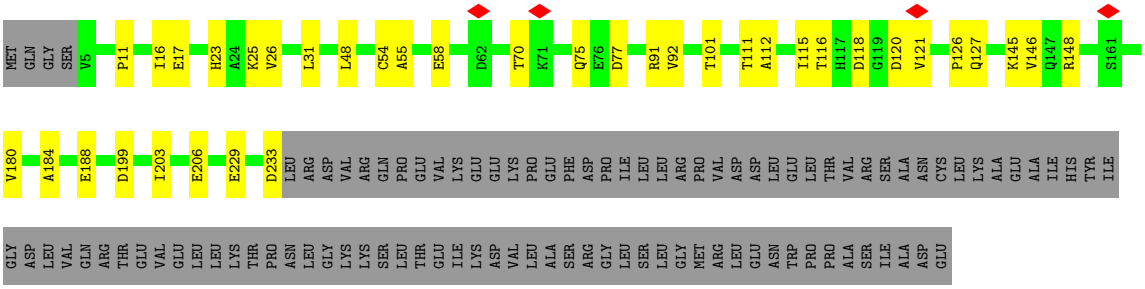




• Molecule 4: DNA-directed RNA polymerase subunit alpha

Chain A:

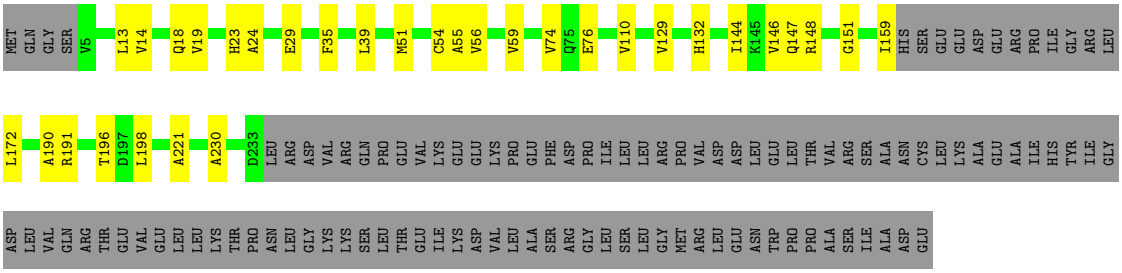




• Molecule 4: DNA-directed RNA polymerase subunit alpha

Chain B:

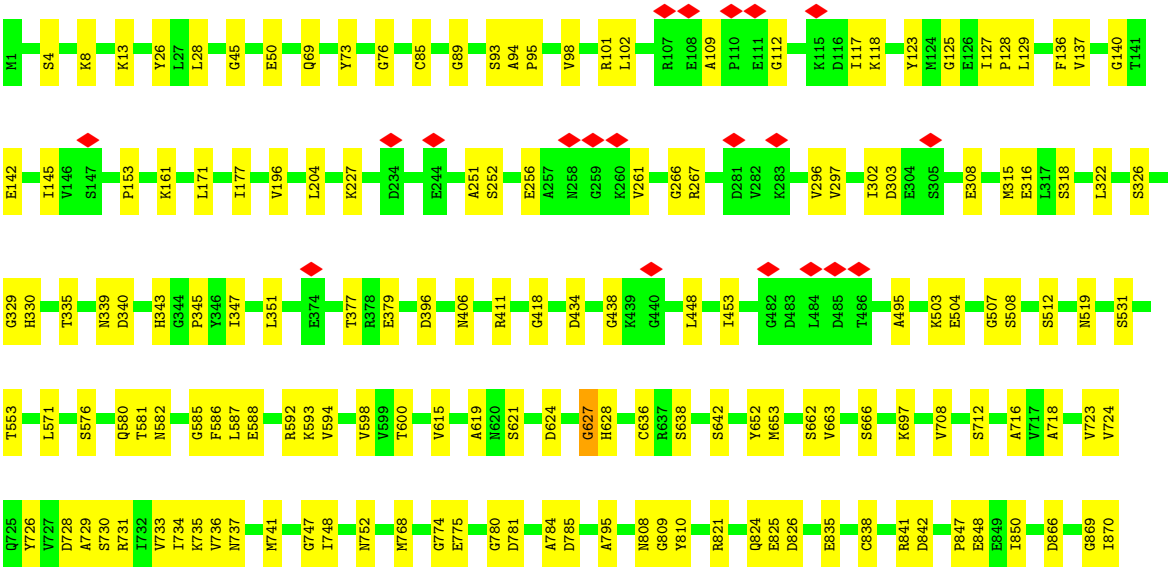


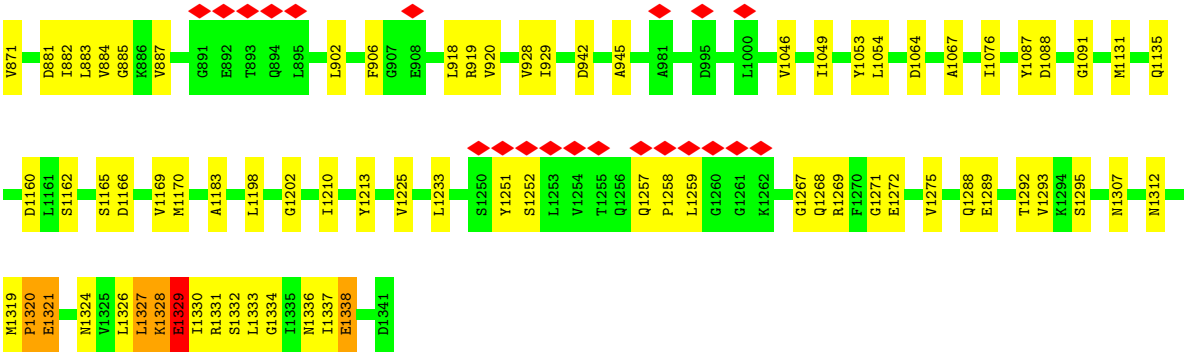


• Molecule 5: DNA-directed RNA polymerase subunit beta

Chain C:



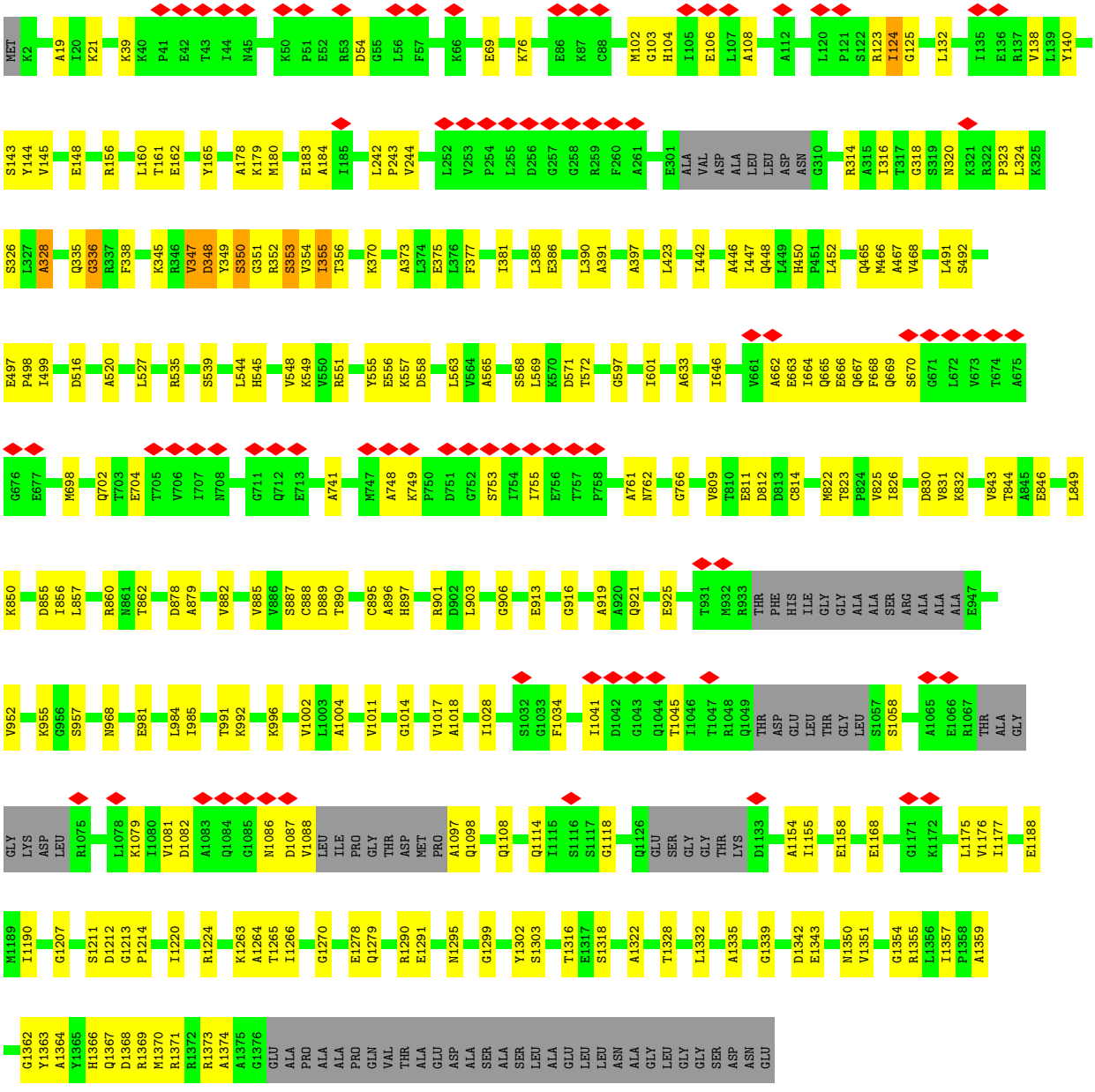




• Molecule 6: DNA-directed RNA polymerase subunit beta'

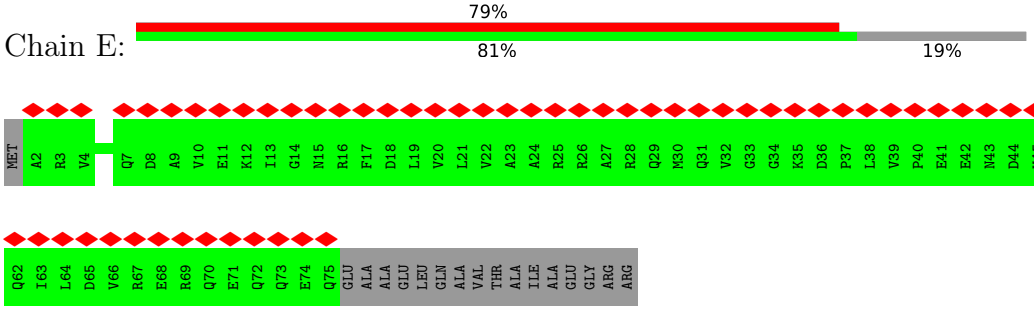
Chain D:





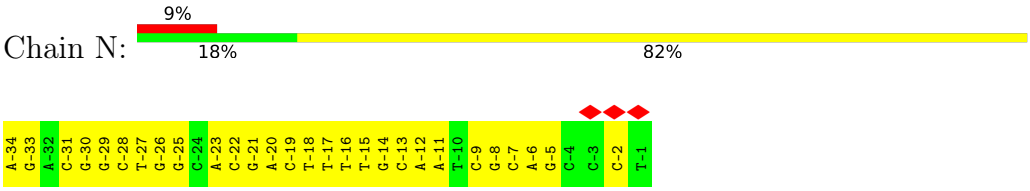
• Molecule 7: DNA-directed RNA polymerase subunit omega

Chain E:



• Molecule 8: Non-template DNA (34-MER)

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23087	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	17.823	Depositor
Minimum map value	-5.571	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	0.935	Depositor
Recommended contour level	3.41	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AF3

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	T	0.39	0/785	0.52	0/1210
2	1	0.41	0/1246	0.64	1/1732 (0.1%)
2	2	0.41	0/1256	0.66	2/1746 (0.1%)
2	3	0.57	0/1256	0.81	2/1746 (0.1%)
2	4	0.65	0/1276	0.88	1/1774 (0.1%)
2	5	0.59	0/1266	0.77	0/1760
2	6	0.38	0/1158	0.63	0/1608
3	M	0.44	0/2052	0.60	1/2857 (0.0%)
4	A	0.42	0/1129	0.63	0/1570
4	B	0.31	0/1069	0.54	0/1485
5	C	0.39	2/6598 (0.0%)	0.59	8/9172 (0.1%)
6	D	0.35	0/6519	0.58	3/9053 (0.0%)
7	E	0.16	0/365	0.48	0/507
8	N	0.40	0/777	0.52	0/1196
All	All	0.42	2/26752 (0.0%)	0.63	18/37416 (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	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1329	GLU	C-O	-6.23	1.16	1.24
5	C	1328	LYS	C-O	6.00	1.31	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1320	PRO	N-CA-C	-10.14	91.59	112.47
2	2	244	ASP	CA-C-N	-8.59	109.18	121.20
2	2	244	ASP	C-N-CA	-8.59	109.18	121.20
5	C	1324	ASN	N-CA-C	-8.44	102.03	111.82
5	C	1327	LEU	N-CA-C	-8.28	102.19	111.14
3	M	258	PRO	N-CA-C	-7.12	103.14	113.75
2	3	226	ILE	N-CA-C	-6.41	107.25	113.53
5	C	1331	ARG	N-CA-C	-6.33	102.65	111.39
2	1	66	ALA	N-CA-C	-6.24	106.64	114.56
2	4	69	ASN	CB-CA-C	-6.00	109.67	116.63
5	C	1321	GLU	N-CA-C	-5.97	104.84	111.71
6	D	906	GLY	N-CA-C	-5.89	107.03	114.16
5	C	1326	LEU	N-CA-C	-5.83	105.66	112.89
5	C	627	GLY	N-CA-C	-5.71	107.90	114.69
6	D	328	ALA	N-CA-C	-5.42	106.71	113.55
6	D	527	LEU	N-CA-C	5.39	115.14	108.19
5	C	519	ASN	N-CA-C	-5.18	101.14	109.58
2	3	14	SER	N-CA-C	-5.16	105.56	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	115	THR	Peptide

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	T	700	0	382	50	0
2	1	1247	0	566	37	0
2	2	1257	0	569	52	0
2	3	1257	0	569	46	0
2	4	1277	0	583	45	0
2	5	1267	0	576	41	0
2	6	1161	0	517	26	0
3	M	2055	0	920	43	0
4	A	1130	0	514	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1071	0	489	20	0
5	C	6599	0	2971	145	0
6	D	6526	0	3019	174	0
7	E	366	0	167	0	0
8	N	694	0	382	55	0
9	1	27	0	12	6	0
9	2	27	0	12	8	0
9	3	27	0	12	9	0
9	4	27	0	12	11	0
9	5	27	0	12	6	0
10	1	4	0	0	0	0
10	2	4	0	0	4	0
10	3	4	0	0	2	0
10	4	4	0	0	1	0
10	5	4	0	0	5	0
11	2	2	0	0	0	0
11	3	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
All	All	26767	0	12284	722	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 19.

All (722) 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)
2:2:9:LEU:CB	9:2:302:ADP:C2	1.80	1.60
5:C:1332:SER:CB	6:D:243:PRO:CB	1.92	1.47
2:2:9:LEU:CB	9:2:302:ADP:N1	1.77	1.40
6:D:353:SER:HA	6:D:466:MET:N	1.44	1.32
2:5:38:ARG:CA	10:5:602:AF3:F1	1.72	1.25
6:D:353:SER:CB	6:D:465:GLN:CB	2.16	1.24
2:5:38:ARG:HA	10:5:602:AF3:F1	1.18	1.23
2:5:40:THR:N	9:5:601:ADP:O2A	1.72	1.20
2:2:9:LEU:CB	9:2:302:ADP:H2	1.36	1.16
2:5:42:LYS:N	9:5:601:ADP:O1A	1.79	1.15
2:4:9:LEU:CB	9:4:601:ADP:HN61	1.66	1.07
2:5:38:ARG:N	10:5:602:AF3:F1	1.81	1.04
2:5:37:GLU:C	10:5:602:AF3:F1	1.91	1.04
6:D:352:ARG:CB	6:D:468:VAL:CB	2.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:264:THR:C	3:M:266:GLU:H	1.68	1.01
6:D:353:SER:CA	6:D:466:MET:N	2.25	0.99
6:D:826:ILE:HA	6:D:831:VAL:HA	1.46	0.97
6:D:353:SER:CA	6:D:466:MET:H	1.78	0.97
6:D:354:VAL:CB	6:D:447:ILE:H	1.79	0.95
6:D:353:SER:HA	6:D:466:MET:H	1.16	0.95
6:D:822:MET:O	6:D:879:ALA:HA	1.66	0.94
1:T:9:DT:O4	8:N:-9:DC:N3	2.00	0.94
6:D:354:VAL:CB	6:D:447:ILE:CB	2.44	0.94
5:C:1251:TYR:HA	5:C:1258:PRO:HA	1.55	0.89
5:C:882:ILE:HA	5:C:919:ARG:HA	1.51	0.89
2:2:41:GLY:HA3	9:2:302:ADP:C8	2.08	0.88
2:4:129:LEU:HA	2:4:138:LEU:HA	1.54	0.88
2:4:9:LEU:CB	9:4:601:ADP:N6	2.37	0.88
2:2:41:GLY:HA3	9:2:302:ADP:H8	1.38	0.87
5:C:866:ASP:H	5:C:871:VAL:HA	1.40	0.87
2:4:39:GLY:HA2	9:4:601:ADP:O3A	1.76	0.86
4:A:11:PRO:O	4:B:230:ALA:HB1	1.76	0.86
2:2:81:GLU:HA	2:2:92:HIS:H	1.38	0.85
5:C:296:VAL:HA	5:C:316:GLU:HA	1.56	0.85
2:2:38:ARG:HA	10:2:303:AF3:F1	1.67	0.85
4:A:188:GLU:O	4:A:199:ASP:HA	1.77	0.85
2:1:49:LEU:O	2:1:53:SER:N	2.10	0.84
6:D:316:ILE:HA	6:D:323:PRO:HA	1.60	0.83
6:D:665:GLN:O	6:D:669:GLN:N	2.11	0.83
4:A:31:LEU:O	4:A:199:ASP:N	2.11	0.83
6:D:1328:THR:O	6:D:1332:LEU:N	2.11	0.83
5:C:718:ALA:O	5:C:780:GLY:N	2.12	0.82
3:M:278:LYS:HA	3:M:283:TRP:HA	1.61	0.82
6:D:662:ALA:O	6:D:666:GLU:N	2.10	0.81
2:5:33:LEU:N	2:5:172:ASP:O	2.14	0.80
5:C:1319:MET:O	5:C:1320:PRO:C	2.21	0.80
6:D:551:ARG:HA	6:D:568:SER:O	1.81	0.80
4:A:118:ASP:N	4:A:121:VAL:O	2.15	0.80
4:B:191:ARG:HA	4:B:196:THR:HA	1.62	0.80
6:D:1034:PHE:HA	6:D:1114:GLN:H	1.46	0.80
2:4:39:GLY:HA2	9:4:601:ADP:PB	2.22	0.80
6:D:352:ARG:CB	6:D:468:VAL:N	2.45	0.79
5:C:1336:ASN:C	5:C:1338:GLU:H	1.89	0.79
6:D:138:VAL:HA	6:D:184:ALA:H	1.44	0.79
4:A:70:THR:HA	4:A:77:ASP:HA	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:491:LEU:HA	6:D:499:ILE:H	1.48	0.78
2:3:79:GLY:HA3	2:3:93:PRO:C	2.08	0.78
5:C:1327:LEU:O	5:C:1328:LYS:C	2.26	0.78
2:1:154:ALA:O	2:1:158:GLU:N	2.17	0.78
2:5:104:LEU:H	2:5:144:LEU:HA	1.49	0.78
3:M:264:THR:C	3:M:266:GLU:N	2.38	0.78
6:D:492:SER:N	6:D:497:GLU:O	2.16	0.77
2:4:178:PRO:O	2:4:182:ARG:N	2.15	0.77
6:D:1357:ILE:O	6:D:1359:ALA:N	2.17	0.77
6:D:104:HIS:HA	6:D:242:LEU:O	1.84	0.77
2:5:37:GLU:O	10:5:602:AF3:F1	1.92	0.77
3:M:273:ASP:N	3:M:387:TYR:O	2.16	0.77
4:A:233:ASP:O	4:B:14:VAL:CB	2.33	0.76
6:D:1364:ALA:O	6:D:1368:ASP:N	2.16	0.76
6:D:1168:GLU:HA	6:D:1175:LEU:H	1.50	0.76
2:2:225:ASN:O	2:2:229:LEU:N	2.18	0.76
6:D:664:ILE:O	6:D:668:PHE:N	2.17	0.76
2:2:72:LEU:O	2:2:76:GLU:N	2.19	0.76
6:D:1350:ASN:O	6:D:1355:ARG:N	2.18	0.76
1:T:9:DT:N3	8:N:-9:DC:O2	2.18	0.75
6:D:846:GLU:HA	6:D:860:ARG:HA	1.68	0.75
2:5:41:GLY:C	9:5:601:ADP:O1A	2.00	0.75
5:C:884:VAL:O	5:C:918:LEU:N	2.18	0.75
2:4:186:ILE:O	2:4:190:ALA:HB2	1.87	0.75
2:3:209:PHE:O	2:3:247:LEU:N	2.19	0.74
2:6:104:LEU:O	2:6:145:VAL:N	2.20	0.74
4:B:51:MET:H	4:B:151:GLY:HA2	1.52	0.74
5:C:1330:ILE:O	5:C:1334:GLY:N	2.20	0.74
5:C:942:ASP:HA	5:C:945:ALA:HB3	1.70	0.74
6:D:549:LYS:HA	6:D:571:ASP:HA	1.71	0.73
6:D:809:VAL:N	6:D:913:GLU:O	2.18	0.73
6:D:1028:ILE:HA	6:D:1118:GLY:HA2	1.70	0.73
6:D:1176:VAL:O	6:D:1190:ILE:N	2.21	0.73
2:4:226:ILE:CB	9:4:601:ADP:H5'2	2.19	0.73
5:C:1087:TYR:N	5:C:1213:TYR:O	2.22	0.73
2:2:208:GLY:O	2:2:247:LEU:N	2.21	0.73
4:A:229:GLU:HA	4:B:221:ALA:HB1	1.71	0.72
6:D:811:GLU:O	6:D:896:ALA:N	2.22	0.72
1:T:9:DT:C4	8:N:-9:DC:N3	2.57	0.72
6:D:1265:THR:O	6:D:1303:SER:N	2.20	0.72
8:N:-21:DG:H2"	8:N:-20:DA:C8	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:35:ILE:N	2:4:174:VAL:O	2.23	0.72
2:4:129:LEU:HA	2:4:138:LEU:CA	2.20	0.72
2:1:197:MET:O	2:1:201:ILE:N	2.17	0.71
6:D:353:SER:HA	6:D:466:MET:CA	2.00	0.71
5:C:724:VAL:HA	5:C:734:ILE:HA	1.72	0.71
2:5:39:GLY:HA3	2:5:224:GLY:CA	2.21	0.71
3:M:145:ALA:O	3:M:153:THR:N	2.23	0.71
6:D:370:LYS:N	6:D:442:ILE:O	2.18	0.71
5:C:737:ASN:O	5:C:741:MET:N	2.23	0.70
4:A:91:ARG:O	4:A:121:VAL:HA	1.91	0.70
2:5:36:GLY:HA3	2:5:148:THR:C	2.16	0.70
4:A:16:ILE:HA	4:A:26:VAL:HA	1.74	0.70
5:C:347:ILE:O	5:C:351:LEU:N	2.23	0.70
6:D:353:SER:CB	6:D:465:GLN:CA	2.70	0.70
5:C:581:THR:HA	5:C:587:LEU:HA	1.74	0.70
4:A:112:ALA:HB3	4:A:126:PRO:HA	1.74	0.69
5:C:153:PRO:HA	5:C:177:ILE:O	1.92	0.69
6:D:762:ASN:O	6:D:766:GLY:N	2.25	0.69
3:M:349:GLN:O	3:M:353:PHE:N	2.26	0.69
4:A:11:PRO:O	4:B:230:ALA:CB	2.40	0.69
6:D:354:VAL:N	6:D:466:MET:H	1.90	0.69
3:M:25:GLN:HA	3:M:382:VAL:HA	1.73	0.69
5:C:928:VAL:HA	5:C:1054:LEU:HA	1.73	0.69
5:C:736:VAL:N	5:C:747:GLY:O	2.24	0.69
5:C:624:ASP:N	5:C:628:HIS:O	2.23	0.69
6:D:825:VAL:O	6:D:832:LYS:N	2.26	0.68
6:D:355:ILE:H	6:D:446:ALA:HB1	1.56	0.68
5:C:883:LEU:N	5:C:918:LEU:O	2.26	0.68
2:5:35:ILE:O	2:5:149:ASN:HA	1.93	0.68
1:T:9:DT:N3	8:N:-9:DC:C2	2.62	0.68
2:2:73:LEU:HA	2:2:77:LEU:H	1.57	0.68
2:4:227:ARG:O	2:4:231:ASN:N	2.25	0.68
3:M:146:VAL:HA	3:M:153:THR:H	1.59	0.68
5:C:1198:LEU:O	5:C:1202:GLY:N	2.26	0.68
6:D:354:VAL:CB	6:D:447:ILE:N	2.56	0.68
5:C:1289:GLU:O	5:C:1293:VAL:N	2.26	0.68
5:C:4:SER:O	5:C:8:LYS:N	2.26	0.67
6:D:1266:ILE:HA	6:D:1302:TYR:HA	1.76	0.67
2:2:155:MET:O	2:2:160:THR:N	2.24	0.67
5:C:716:ALA:HB3	5:C:784:ALA:H	1.59	0.67
2:6:40:THR:HA	2:6:225:ASN:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:152:LEU:H	3:M:191:LYS:H	1.43	0.67
6:D:1264:ALA:N	6:D:1278:GLU:O	2.28	0.67
1:T:6:DT:H2'	1:T:7:DG:C4	2.29	0.67
2:1:74:ASP:CB	2:1:79:GLY:HA3	2.24	0.67
5:C:256:GLU:HA	5:C:261:VAL:HA	1.76	0.67
5:C:580:GLN:O	5:C:588:GLU:N	2.22	0.66
6:D:39:LYS:N	6:D:54:ASP:O	2.25	0.66
3:M:345:ILE:O	3:M:349:GLN:N	2.26	0.66
4:B:56:VAL:HA	4:B:146:VAL:HA	1.76	0.66
2:3:41:GLY:HA3	9:3:601:ADP:C8	2.30	0.66
2:1:12:ALA:O	2:1:16:LEU:N	2.26	0.66
5:C:303:ASP:HA	5:C:329:GLY:HA2	1.77	0.66
5:C:592:ARG:O	5:C:653:MET:N	2.20	0.66
1:T:25:DC:N4	8:N:-26:DG:O6	2.28	0.66
2:1:102:GLY:O	2:1:143:ARG:N	2.29	0.66
2:3:178:PRO:O	2:3:182:ARG:N	2.28	0.66
2:4:129:LEU:CA	2:4:138:LEU:HA	2.26	0.65
6:D:952:VAL:O	6:D:1014:GLY:N	2.25	0.65
5:C:13:LYS:O	5:C:1183:ALA:N	2.27	0.65
5:C:881:ASP:O	5:C:920:VAL:N	2.30	0.65
2:2:178:PRO:O	2:2:182:ARG:N	2.29	0.65
5:C:1319:MET:O	5:C:1321:GLU:N	2.30	0.65
6:D:354:VAL:H	6:D:466:MET:H	1.43	0.65
8:N:-7:DC:H2"	8:N:-6:DA:C8	2.32	0.65
5:C:1271:GLY:O	5:C:1275:VAL:N	2.27	0.65
2:2:38:ARG:HA	10:2:303:AF3:F3	1.86	0.64
6:D:161:THR:O	6:D:165:TYR:N	2.24	0.64
2:5:35:ILE:N	2:5:174:VAL:O	2.26	0.64
5:C:842:ASP:HA	5:C:847:PRO:HA	1.79	0.64
2:6:257:ARG:HA	2:1:175:GLN:HA	1.78	0.64
5:C:1165:SER:O	5:C:1169:VAL:N	2.23	0.64
5:C:76:GLY:N	5:C:95:PRO:O	2.31	0.64
4:A:17:GLU:N	4:A:25:LYS:O	2.26	0.64
6:D:1318:SER:HA	6:D:1342:ASP:HA	1.79	0.64
3:M:264:THR:O	3:M:266:GLU:N	2.29	0.64
6:D:180:MET:HA	6:D:183:GLU:HA	1.79	0.64
6:D:385:LEU:O	6:D:390:LEU:N	2.31	0.64
5:C:318:SER:O	5:C:322:LEU:N	2.31	0.64
5:C:1288:GLN:O	5:C:1292:THR:CB	2.46	0.64
6:D:981:GLU:HA	6:D:996:LYS:HA	1.80	0.64
6:D:1082:ASP:H	6:D:1087:ASP:HA	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:40:THR:CA	9:5:601:ADP:O2A	2.40	0.63
5:C:125:GLY:H	5:C:495:ALA:HB1	1.63	0.63
2:5:99:ALA:HB1	2:5:102:GLY:HA3	1.80	0.63
4:A:31:LEU:N	4:A:199:ASP:O	2.31	0.63
6:D:666:GLU:O	6:D:670:SER:N	2.32	0.63
2:6:35:ILE:N	2:6:174:VAL:O	2.32	0.63
5:C:593:LYS:O	5:C:600:THR:N	2.31	0.63
2:2:179:LEU:O	2:2:183:GLU:N	2.23	0.62
2:3:129:LEU:N	2:3:138:LEU:O	2.30	0.62
5:C:1336:ASN:C	5:C:1338:GLU:N	2.50	0.62
6:D:377:PHE:O	6:D:381:ILE:N	2.31	0.62
6:D:663:GLU:O	6:D:667:GLN:N	2.21	0.62
3:M:151:TYR:HA	3:M:190:ALA:H	1.64	0.62
2:6:38:ARG:HA	2:6:42:LYS:HA	1.81	0.62
2:6:64:ASN:O	2:6:107:ASP:N	2.32	0.62
6:D:103:GLY:O	6:D:243:PRO:HA	1.98	0.62
1:T:10:DC:H2'	8:N:-11:DA:N7	2.14	0.62
5:C:636:CYS:O	5:C:642:SER:HA	1.99	0.62
2:5:39:GLY:HA3	2:5:224:GLY:HA2	1.82	0.62
6:D:1220:ILE:O	6:D:1224:ARG:N	2.32	0.62
2:5:104:LEU:O	2:5:145:VAL:N	2.32	0.62
2:5:155:MET:O	2:5:159:GLY:N	2.33	0.62
2:6:178:PRO:O	2:6:182:ARG:N	2.25	0.62
2:3:101:GLY:H	2:3:142:VAL:HA	1.64	0.61
5:C:723:VAL:O	5:C:735:LYS:N	2.33	0.61
5:C:1307:ASN:O	5:C:1312:ASN:N	2.34	0.61
2:4:185:ASP:O	2:4:189:MET:N	2.31	0.61
2:2:77:LEU:O	2:2:95:ARG:N	2.34	0.61
5:C:866:ASP:N	5:C:871:VAL:HA	2.15	0.61
2:5:39:GLY:HA3	2:5:224:GLY:HA3	1.81	0.61
5:C:821:ARG:O	5:C:825:GLU:N	2.34	0.61
6:D:698:MET:O	6:D:702:GLN:N	2.34	0.61
5:C:1067:ALA:N	5:C:1233:LEU:O	2.34	0.60
6:D:1079:LYS:HA	6:D:1098:GLN:HA	1.82	0.60
6:D:1154:ALA:N	6:D:1214:PRO:O	2.34	0.60
2:2:61:ILE:N	2:2:103:THR:O	2.34	0.60
4:B:13:LEU:H	4:B:29:GLU:CB	2.15	0.60
5:C:406:ASN:O	5:C:411:ARG:N	2.32	0.60
4:B:55:ALA:O	4:B:147:GLN:N	2.33	0.60
5:C:1327:LEU:O	5:C:1329:GLU:O	2.19	0.60
2:2:38:ARG:CA	10:2:303:AF3:F3	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:602:AF3:F2	2:4:164:ASP:CB	2.39	0.60
3:M:45:LEU:HA	3:M:297:ILE:HA	1.84	0.60
5:C:93:SER:HA	5:C:128:PRO:HA	1.84	0.60
2:1:41:GLY:CA	9:1:601:ADP:PB	2.90	0.60
2:3:61:ILE:N	2:3:103:THR:O	2.26	0.60
6:D:748:ALA:HB1	6:D:755:ILE:H	1.66	0.60
6:D:1367:GLN:O	6:D:1371:ARG:N	2.30	0.60
2:3:34:ILE:O	2:3:148:THR:N	2.33	0.60
4:B:159:ILE:HA	4:B:172:LEU:HA	1.83	0.60
5:C:297:VAL:N	5:C:315:MET:O	2.26	0.59
6:D:555:TYR:HA	6:D:565:ALA:HA	1.84	0.59
1:T:8:DA:N3	1:T:8:DA:H2'	2.16	0.59
2:4:104:LEU:O	2:4:145:VAL:N	2.27	0.59
4:B:59:VAL:HA	4:B:144:ILE:HA	1.83	0.59
6:D:516:ASP:HA	6:D:544:LEU:HA	1.83	0.59
2:2:73:LEU:CA	2:2:77:LEU:H	2.15	0.59
2:3:101:GLY:N	2:3:141:ASN:O	2.36	0.59
4:A:75:GLN:HA	5:C:729:ALA:HB2	1.84	0.59
6:D:356:THR:C	6:D:448:GLN:HA	2.28	0.59
2:2:77:LEU:O	2:2:96:PHE:N	2.36	0.59
5:C:598:VAL:HA	5:C:627:GLY:C	2.27	0.59
6:D:1081:VAL:HA	6:D:1087:ASP:HA	1.83	0.59
8:N:-22:DC:H2"	8:N:-21:DG:C8	2.38	0.59
3:M:13:MET:CB	8:N:-12:DA:C2	2.86	0.59
2:2:102:GLY:H	2:2:142:VAL:HA	1.66	0.58
2:3:72:LEU:O	2:3:76:GLU:N	2.35	0.58
2:4:39:GLY:N	9:4:601:ADP:O1B	2.36	0.58
6:D:353:SER:C	6:D:466:MET:H	2.11	0.58
2:1:123:VAL:HA	2:1:127:GLY:HA2	1.84	0.58
5:C:252:SER:O	5:C:266:GLY:N	2.37	0.58
2:3:113:PRO:O	2:3:117:GLN:N	2.29	0.58
2:4:35:ILE:HA	2:4:148:THR:H	1.68	0.58
3:M:437:ASP:N	8:N:-28:DC:OP1	2.23	0.58
2:3:237:VAL:O	2:3:241:GLY:N	2.33	0.58
5:C:453:ILE:N	5:C:585:GLY:O	2.22	0.58
5:C:1328:LYS:O	5:C:1329:GLU:O	2.22	0.58
2:2:9:LEU:CA	9:2:302:ADP:N1	2.65	0.58
2:3:31:PRO:O	2:3:171:PHE:N	2.37	0.58
5:C:434:ASP:O	5:C:438:GLY:N	2.37	0.58
5:C:1330:ILE:CB	5:C:1333:LEU:HA	2.34	0.58
2:3:128:GLU:H	2:3:139:GLN:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:594:VAL:H	5:C:652:TYR:HA	1.69	0.58
2:1:198:CYS:O	2:1:203:LEU:N	2.36	0.57
6:D:551:ARG:HA	6:D:569:LEU:HA	1.85	0.57
6:D:968:ASN:HA	6:D:1118:GLY:HA3	1.86	0.57
2:2:102:GLY:O	2:2:143:ARG:N	2.35	0.57
6:D:1034:PHE:N	6:D:1081:VAL:O	2.38	0.57
2:3:155:MET:O	2:3:160:THR:N	2.33	0.57
6:D:123:ARG:O	6:D:124:ILE:C	2.47	0.57
6:D:1290:ARG:O	6:D:1295:ASN:N	2.29	0.57
2:2:198:CYS:O	2:2:203:LEU:N	2.35	0.57
5:C:339:ASN:O	5:C:343:HIS:N	2.37	0.57
8:N:-21:DG:H2"	8:N:-20:DA:N7	2.20	0.57
2:1:27:PRO:HA	2:1:53:SER:HA	1.87	0.57
3:M:124:TRP:O	3:M:128:LEU:N	2.37	0.57
6:D:353:SER:CB	6:D:465:GLN:C	2.78	0.57
6:D:353:SER:CB	6:D:466:MET:N	2.68	0.57
1:T:5:DC:H2"	1:T:6:DT:C7	2.35	0.57
6:D:749:LYS:HA	6:D:753:SER:O	2.04	0.57
2:4:104:LEU:N	2:4:143:ARG:O	2.38	0.57
2:4:129:LEU:HA	2:4:138:LEU:C	2.30	0.57
5:C:396:ASP:HA	5:C:418:GLY:HA3	1.87	0.57
2:1:34:ILE:HA	2:1:174:VAL:CB	2.35	0.56
2:5:102:GLY:O	2:5:143:ARG:N	2.36	0.56
2:5:129:LEU:H	2:5:138:LEU:H	1.53	0.56
3:M:150:GLY:HA3	3:M:259:GLY:HA3	1.87	0.56
5:C:1336:ASN:O	5:C:1338:GLU:N	2.38	0.56
6:D:1369:ARG:O	6:D:1373:ARG:N	2.33	0.56
8:N:-23:DA:H2'	8:N:-22:DC:C6	2.40	0.56
2:6:32:VAL:O	2:6:145:VAL:HA	2.05	0.56
2:1:214:ARG:O	2:1:218:LEU:N	2.36	0.56
9:1:601:ADP:O2A	9:1:601:ADP:H3'	2.04	0.56
5:C:841:ARG:H	5:C:1046:VAL:HA	1.70	0.56
6:D:349:TYR:O	6:D:350:SER:C	2.48	0.56
2:6:122:ARG:O	2:6:126:TYR:N	2.39	0.56
2:2:165:LEU:O	2:2:169:LEU:N	2.39	0.56
6:D:812:ASP:O	6:D:897:HIS:N	2.39	0.56
6:D:916:GLY:HA2	6:D:919:ALA:HB3	1.86	0.56
6:D:1366:HIS:O	6:D:1370:MET:N	2.30	0.56
5:C:136:PHE:O	5:C:142:GLU:HA	2.05	0.56
2:4:207:PRO:C	2:4:246:PRO:HA	2.30	0.56
5:C:504:GLU:O	5:C:508:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1338:GLU:HA	6:D:21:LYS:H	1.70	0.56
6:D:335:GLN:O	6:D:336:GLY:C	2.49	0.55
2:1:82:ALA:HA	2:1:87:GLY:HA2	1.88	0.55
1:T:4:DG:H1'	1:T:5:DC:H5'	1.89	0.55
2:4:154:ALA:O	2:4:158:GLU:N	2.30	0.55
5:C:94:ALA:N	5:C:127:ILE:O	2.40	0.55
8:N:-9:DC:H5"	8:N:-9:DC:H6	1.71	0.55
2:4:14:SER:O	2:4:18:VAL:N	2.34	0.55
5:C:592:ARG:N	5:C:653:MET:O	2.39	0.55
4:A:188:GLU:O	4:A:199:ASP:CA	2.53	0.55
6:D:761:ALA:HB1	6:D:766:GLY:O	2.08	0.54
1:T:8:DA:N6	8:N:-9:DC:O2	2.40	0.54
6:D:888:CYS:CB	6:D:895:CYS:H	2.19	0.54
1:T:11:DG:H21	3:M:17:LEU:HA	1.72	0.54
2:1:155:MET:O	2:1:159:GLY:N	2.40	0.54
2:2:154:ALA:O	2:2:158:GLU:N	2.31	0.54
2:3:94:GLY:O	2:3:98:ARG:N	2.40	0.54
6:D:556:GLU:O	6:D:563:LEU:HA	2.07	0.54
6:D:849:LEU:HA	6:D:856:ILE:HA	1.89	0.54
1:T:16:DA:H1'	1:T:17:DA:C8	2.43	0.54
1:T:31:DG:O6	8:N:-30:DG:N1	2.40	0.54
6:D:1155:ILE:O	6:D:1211:SER:N	2.39	0.54
2:3:208:GLY:HA3	2:3:245:TYR:C	2.33	0.54
2:6:32:VAL:N	2:6:144:LEU:O	2.40	0.54
2:3:226:ILE:CB	9:3:601:ADP:H1'	2.38	0.54
3:M:436:SER:O	3:M:440:LEU:N	2.35	0.54
4:A:101:THR:O	4:A:115:ILE:HA	2.08	0.54
5:C:728:ASP:N	5:C:731:ARG:O	2.26	0.54
6:D:335:GLN:O	6:D:338:PHE:N	2.41	0.53
2:2:156:VAL:HA	2:2:161:PHE:H	1.73	0.53
3:M:260:GLN:O	3:M:261:SER:C	2.49	0.53
5:C:902:LEU:O	5:C:906:PHE:N	2.36	0.53
5:C:1252:SER:N	5:C:1257:GLN:O	2.25	0.53
6:D:324:LEU:O	6:D:326:SER:N	2.42	0.53
6:D:352:ARG:CB	6:D:468:VAL:H	2.20	0.53
2:6:258:ARG:N	2:1:176:LEU:H	2.06	0.53
5:C:724:VAL:O	5:C:774:GLY:N	2.42	0.53
5:C:835:GLU:HA	5:C:1053:TYR:HA	1.90	0.53
6:D:1058:SER:HA	6:D:1108:GLN:HA	1.90	0.53
2:4:8:LEU:O	2:4:10:GLY:N	2.42	0.53
2:4:94:GLY:O	2:4:98:ARG:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:39:GLY:N	10:2:303:AF3:F3	2.32	0.53
6:D:144:TYR:HA	6:D:179:LYS:C	2.34	0.53
6:D:849:LEU:HA	6:D:857:LEU:H	1.72	0.53
8:N:-23:DA:H2"	8:N:-22:DC:H5'	1.91	0.53
1:T:6:DT:H2'	1:T:7:DG:N9	2.24	0.53
2:5:35:ILE:CB	2:5:175:GLN:HA	2.39	0.53
2:5:56:TRP:N	3:M:410:GLY:O	2.42	0.53
5:C:448:LEU:H	5:C:553:THR:CB	2.21	0.53
6:D:491:LEU:HA	6:D:498:PRO:HA	1.91	0.52
6:D:822:MET:O	6:D:879:ALA:CA	2.51	0.52
2:6:155:MET:O	2:6:159:GLY:N	2.42	0.52
3:M:257:ARG:O	3:M:261:SER:N	2.36	0.52
5:C:808:ASN:C	5:C:810:TYR:N	2.67	0.52
2:4:186:ILE:O	2:4:190:ALA:CB	2.57	0.52
6:D:1363:TYR:O	6:D:1367:GLN:N	2.31	0.52
1:T:26:DC:H2'	1:T:26:DC:OP2	2.10	0.52
6:D:391:ALA:HB1	6:D:397:ALA:HB2	1.90	0.52
8:N:-8:DG:N7	8:N:-7:DC:N4	2.56	0.52
1:T:13:DG:C5	1:T:14:DC:C4	2.97	0.52
2:2:49:LEU:O	2:2:53:SER:N	2.43	0.52
5:C:102:LEU:O	5:C:117:ILE:N	2.31	0.52
5:C:808:ASN:O	5:C:810:TYR:N	2.43	0.52
2:5:101:GLY:HA2	2:5:141:ASN:O	2.10	0.52
8:N:-14:DG:H2"	8:N:-13:DC:O5'	2.10	0.52
5:C:94:ALA:O	5:C:127:ILE:N	2.35	0.52
5:C:1272:GLU:N	6:D:345:LYS:CB	2.72	0.52
6:D:520:ALA:H	6:D:545:HIS:HA	1.74	0.52
2:1:48:ARG:O	2:1:52:LEU:N	2.31	0.52
2:5:94:GLY:C	2:5:96:PHE:H	2.17	0.52
5:C:73:TYR:HA	5:C:98:VAL:HA	1.92	0.52
5:C:137:VAL:O	5:C:140:GLY:N	2.42	0.52
4:B:190:ALA:O	4:B:198:LEU:CB	2.58	0.52
2:1:55:ARG:C	2:1:58:GLY:H	2.18	0.51
6:D:957:SER:H	6:D:985:ILE:H	1.58	0.51
8:N:-30:DG:OP2	8:N:-30:DG:H2'	2.10	0.51
2:4:39:GLY:HA2	9:4:601:ADP:O1B	2.10	0.51
4:B:19:VAL:N	4:B:23:HIS:O	2.43	0.51
1:T:29:DC:H2"	1:T:30:DC:C5	2.45	0.51
2:4:102:GLY:O	2:4:143:ARG:N	2.43	0.51
2:3:49:LEU:O	2:3:53:SER:N	2.43	0.51
2:5:41:GLY:HA3	9:5:601:ADP:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:356:THR:N	6:D:447:ILE:O	2.43	0.51
5:C:1269:ARG:CB	6:D:347:VAL:H	2.24	0.51
2:1:59:PRO:O	2:1:103:THR:N	2.32	0.51
4:B:35:PHE:O	4:B:39:LEU:CB	2.59	0.51
6:D:597:GLY:O	6:D:601:ILE:N	2.36	0.51
3:M:46:GLU:N	3:M:296:LYS:O	2.22	0.51
2:4:49:LEU:O	2:4:53:SER:N	2.44	0.51
5:C:768:MET:N	5:C:785:ASP:O	2.29	0.51
5:C:726:TYR:O	5:C:733:VAL:N	2.31	0.51
6:D:347:VAL:O	6:D:348:ASP:CB	2.58	0.51
6:D:1154:ALA:HA	6:D:1212:ASP:O	2.11	0.51
8:N:-27:DT:H2"	8:N:-26:DG:C8	2.46	0.51
2:6:258:ARG:H	2:1:176:LEU:H	1.59	0.50
5:C:503:LYS:O	5:C:507:GLY:N	2.34	0.50
5:C:1088:ASP:C	5:C:1091:GLY:H	2.18	0.50
6:D:1177:ILE:HA	6:D:1188:GLU:O	2.12	0.50
2:1:39:GLY:HA3	2:1:224:GLY:O	2.10	0.50
4:B:74:VAL:C	4:B:76:GLU:H	2.20	0.50
6:D:144:TYR:O	6:D:178:ALA:HB1	2.12	0.50
1:T:31:DG:H5'	1:T:31:DG:C8	2.47	0.50
2:1:130:GLU:HA	2:1:135:SER:HA	1.92	0.50
2:2:156:VAL:C	2:2:159:GLY:H	2.18	0.50
6:D:355:ILE:N	6:D:446:ALA:HB1	2.26	0.50
2:6:100:ASP:C	2:6:102:GLY:H	2.19	0.50
2:1:131:ARG:N	2:1:134:GLY:O	2.32	0.50
5:C:85:CYS:O	5:C:89:GLY:N	2.45	0.50
6:D:1158:GLU:HA	6:D:1207:GLY:O	2.11	0.50
2:2:216:THR:O	2:2:220:TYR:N	2.44	0.50
5:C:93:SER:HA	5:C:129:LEU:H	1.76	0.50
5:C:1210:ILE:N	5:C:1225:VAL:O	2.42	0.50
6:D:557:LYS:HA	6:D:563:LEU:HA	1.94	0.50
2:6:197:MET:O	2:6:201:ILE:N	2.27	0.50
2:2:36:GLY:O	2:2:149:ASN:HA	2.12	0.50
2:2:73:LEU:O	2:2:77:LEU:N	2.45	0.50
2:4:36:GLY:N	2:4:148:THR:O	2.43	0.49
6:D:535:ARG:O	6:D:539:SER:N	2.44	0.49
6:D:830:ASP:HA	6:D:992:LYS:O	2.11	0.49
1:T:29:DC:OP2	1:T:29:DC:H2'	2.12	0.49
4:B:18:GLN:HA	4:B:24:ALA:HA	1.94	0.49
2:2:12:ALA:O	2:2:16:LEU:N	2.39	0.49
2:3:83:GLY:O	2:3:84:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:102:MET:HA	6:D:244:VAL:O	2.12	0.49
1:T:32:DT:H2"	1:T:33:DC:C4	2.47	0.49
6:D:326:SER:C	6:D:328:ALA:H	2.19	0.49
2:6:39:GLY:H	2:6:42:LYS:CB	2.25	0.49
2:6:213:ALA:N	2:6:248:ASP:O	2.45	0.49
2:2:73:LEU:C	2:2:76:GLU:H	2.20	0.49
2:2:102:GLY:N	2:2:142:VAL:HA	2.28	0.49
2:4:109:LEU:O	2:4:110:ALA:HB3	2.12	0.49
1:T:13:DG:C8	1:T:13:DG:H5'	2.47	0.49
2:4:227:ARG:CB	9:4:601:ADP:H4'	2.42	0.49
9:2:302:ADP:H8	9:2:302:ADP:H5'2	1.78	0.49
2:3:12:ALA:HB3	2:3:15:PHE:CB	2.42	0.49
2:5:106:LEU:N	2:5:145:VAL:O	2.42	0.49
6:D:386:GLU:N	6:D:391:ALA:HB3	2.28	0.49
5:C:619:ALA:C	5:C:621:SER:H	2.20	0.48
5:C:850:ILE:HA	5:C:885:GLY:O	2.13	0.48
2:3:35:ILE:HA	2:3:148:THR:O	2.14	0.48
4:A:23:HIS:HA	4:A:206:GLU:HA	1.94	0.48
6:D:19:ALA:HA	6:D:1343:GLU:HA	1.95	0.48
2:3:198:CYS:O	2:3:202:LYS:N	2.45	0.48
3:M:350:GLN:O	3:M:354:GLU:N	2.44	0.48
3:M:459:TYR:O	3:M:463:LEU:N	2.40	0.48
6:D:888:CYS:O	6:D:890:THR:N	2.46	0.48
2:5:102:GLY:H	2:5:142:VAL:CB	2.26	0.48
5:C:1332:SER:CB	6:D:243:PRO:CA	2.85	0.48
2:4:39:GLY:CA	9:4:601:ADP:PB	2.99	0.48
5:C:808:ASN:C	5:C:810:TYR:H	2.21	0.48
2:3:38:ARG:HA	9:3:601:ADP:O3B	2.13	0.48
2:3:41:GLY:CA	9:3:601:ADP:C8	2.96	0.48
3:M:381:ARG:HA	8:N:-16:DT:H72	1.95	0.48
5:C:251:ALA:O	5:C:266:GLY:N	2.47	0.48
5:C:768:MET:O	5:C:785:ASP:N	2.40	0.48
6:D:984:LEU:O	6:D:991:THR:HA	2.13	0.48
8:N:-19:DC:H2'	8:N:-18:DT:H71	1.95	0.48
1:T:12:DT:OP1	3:M:12:ALA:HB1	2.14	0.48
3:M:288:ASN:O	3:M:292:ILE:N	2.47	0.48
5:C:101:ARG:HA	5:C:118:LYS:HA	1.95	0.48
5:C:1327:LEU:C	5:C:1329:GLU:N	2.72	0.48
6:D:106:GLU:C	6:D:108:ALA:H	2.21	0.48
2:2:41:GLY:HA2	9:2:302:ADP:O1A	2.12	0.48
2:4:32:VAL:O	2:4:146:CYS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4:601:ADP:O1B	10:4:602:AF3:F3	2.21	0.48
2:5:39:GLY:O	2:5:225:ASN:N	2.47	0.48
3:M:214:ALA:HB2	3:M:247:ALA:HB1	1.96	0.48
4:A:58:GLU:O	4:A:145:LYS:N	2.44	0.48
4:B:110:VAL:O	4:B:129:VAL:HA	2.14	0.48
1:T:7:DG:C4	8:N:-8:DG:N2	2.81	0.48
2:1:126:TYR:O	2:1:128:GLU:N	2.46	0.48
2:4:155:MET:O	2:4:159:GLY:N	2.47	0.48
2:5:34:ILE:CB	2:5:147:ALA:HA	2.44	0.48
3:M:386:LYS:O	3:M:397:LEU:N	2.46	0.48
6:D:1362:GLY:O	6:D:1366:HIS:N	2.24	0.48
5:C:251:ALA:N	5:C:267:ARG:O	2.47	0.47
5:C:734:ILE:O	5:C:748:ILE:HA	2.13	0.47
5:C:866:ASP:N	5:C:870:ILE:O	2.48	0.47
6:D:1082:ASP:N	6:D:1086:ASN:O	2.48	0.47
2:6:256:LYS:O	2:1:175:GLN:HA	2.14	0.47
2:2:224:GLY:C	2:2:228:GLU:H	2.21	0.47
6:D:844:THR:HA	6:D:882:VAL:HA	1.97	0.47
6:D:952:VAL:C	6:D:1014:GLY:H	2.18	0.47
8:N:-26:DG:H2”	8:N:-25:DG:C8	2.50	0.47
5:C:1267:GLY:O	5:C:1268:GLN:C	2.58	0.47
6:D:352:ARG:CB	6:D:468:VAL:CA	2.92	0.47
2:1:41:GLY:N	9:1:601:ADP:O2B	2.47	0.47
5:C:1160:ASP:C	5:C:1162:SER:H	2.21	0.47
6:D:1041:ILE:H	6:D:1045:THR:CB	2.28	0.47
2:2:94:GLY:O	2:2:98:ARG:N	2.37	0.47
2:4:101:GLY:C	2:4:142:VAL:HA	2.40	0.47
4:B:54:CYS:HA	4:B:148:ARG:HA	1.96	0.47
2:1:96:PHE:O	2:1:100:ASP:N	2.47	0.47
2:2:209:PHE:HA	2:2:247:LEU:O	2.14	0.47
5:C:1329:GLU:O	5:C:1333:LEU:N	2.42	0.47
6:D:69:GLU:HA	6:D:76:LYS:HA	1.96	0.47
6:D:1088:VAL:C	6:D:1097:ALA:HB3	2.39	0.47
6:D:1168:GLU:HA	6:D:1175:LEU:N	2.25	0.47
8:N:-12:DA:H2’	8:N:-11:DA:N3	2.30	0.47
2:2:34:ILE:HA	2:2:174:VAL:O	2.15	0.47
2:2:74:ASP:HA	2:2:79:GLY:N	2.30	0.47
8:N:-12:DA:H2”	8:N:-11:DA:O5’	2.15	0.47
1:T:7:DG:H2”	1:T:8:DA:C8	2.50	0.47
2:2:184:SER:C	2:2:186:ILE:H	2.23	0.47
2:4:65:CYS:H	2:4:107:ASP:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1328:LYS:C	5:C:1329:GLU:O	2.58	0.47
6:D:812:ASP:HA	6:D:896:ALA:HB3	1.96	0.46
1:T:14:DC:H2"	1:T:15:DA:C8	2.50	0.46
1:T:21:DC:H2"	1:T:22:DG:C8	2.50	0.46
2:2:73:LEU:O	2:2:78:PHE:N	2.48	0.46
2:2:101:GLY:H	2:2:142:VAL:N	2.13	0.46
5:C:723:VAL:HA	5:C:775:GLU:O	2.15	0.46
6:D:423:LEU:HA	6:D:467:ALA:O	2.15	0.46
2:3:62:SER:HA	2:3:104:LEU:HA	1.97	0.46
2:5:38:ARG:O	2:5:39:GLY:C	2.58	0.46
6:D:885:VAL:O	6:D:887:SER:N	2.46	0.46
6:D:1004:ALA:N	6:D:1017:VAL:O	2.48	0.46
2:3:79:GLY:HA3	2:3:94:GLY:N	2.31	0.46
2:3:197:MET:O	2:3:201:ILE:N	2.26	0.46
5:C:848:GLU:HA	5:C:887:VAL:O	2.16	0.46
4:B:76:GLU:CB	4:B:132:HIS:H	2.28	0.46
6:D:125:GLY:HA2	6:D:132:LEU:HA	1.96	0.46
1:T:12:DT:H4'	1:T:13:DG:OP1	2.15	0.46
2:4:34:ILE:H	2:4:147:ALA:HA	1.81	0.46
5:C:1327:LEU:O	5:C:1329:GLU:C	2.59	0.46
2:2:59:PRO:O	2:2:103:THR:N	2.49	0.46
2:2:101:GLY:H	2:2:141:ASN:C	2.24	0.46
3:M:145:ALA:HB1	3:M:154:ILE:H	1.80	0.46
3:M:263:GLN:C	3:M:265:SER:H	2.24	0.46
6:D:1176:VAL:HA	6:D:1190:ILE:O	2.16	0.46
8:N:-16:DT:OP2	8:N:-16:DT:H2'	2.16	0.46
5:C:697:LYS:HA	5:C:795:ALA:HB2	1.98	0.45
1:T:26:DC:H2"	1:T:27:DA:C8	2.51	0.45
1:T:23:DT:C2	1:T:24:DG:C8	3.04	0.45
2:3:12:ALA:O	2:3:16:LEU:N	2.48	0.45
2:5:49:LEU:O	2:5:50:HIS:C	2.58	0.45
5:C:26:TYR:C	5:C:28:LEU:H	2.25	0.45
8:N:-9:DC:H2'	8:N:-8:DG:C4	2.51	0.45
6:D:551:ARG:CA	6:D:568:SER:O	2.60	0.45
1:T:9:DT:O4	8:N:-9:DC:C4	2.68	0.45
5:C:145:ILE:HA	5:C:512:SER:HA	1.99	0.45
6:D:1263:LYS:HA	6:D:1279:GLN:HA	1.99	0.45
1:T:6:DT:H2'	1:T:7:DG:C8	2.52	0.45
2:2:152:LEU:HA	2:2:155:MET:CB	2.47	0.45
5:C:1166:ASP:O	5:C:1170:MET:N	2.40	0.45
8:N:-31:DC:H2"	8:N:-30:DG:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:5:DC:H2"	1:T:6:DT:C5	2.52	0.45
2:3:40:THR:N	9:3:601:ADP:O1A	2.50	0.45
2:4:39:GLY:CA	9:4:601:ADP:O1B	2.65	0.45
2:5:36:GLY:HA3	2:5:148:THR:CA	2.47	0.45
6:D:349:TYR:O	6:D:351:GLY:N	2.50	0.45
8:N:-17:DT:H2"	8:N:-16:DT:C7	2.47	0.44
6:D:548:VAL:O	6:D:572:THR:N	2.45	0.44
8:N:-28:DC:H1'	8:N:-27:DT:H5'	1.99	0.44
4:B:191:ARG:CA	4:B:196:THR:HA	2.41	0.44
5:C:838:CYS:O	5:C:1049:ILE:HA	2.17	0.44
6:D:702:GLN:O	6:D:704:GLU:N	2.46	0.44
6:D:921:GLN:O	6:D:925:GLU:N	2.51	0.44
8:N:-15:DT:H2"	8:N:-14:DG:C8	2.53	0.44
5:C:1064:ASP:O	5:C:1076:ILE:N	2.31	0.44
1:T:20:DT:OP2	1:T:20:DT:H2'	2.17	0.44
5:C:718:ALA:HB3	5:C:781:ASP:H	1.83	0.44
6:D:919:ALA:C	6:D:921:GLN:H	2.24	0.44
1:T:11:DG:O4'	3:M:13:MET:CB	2.64	0.44
5:C:123:TYR:O	5:C:495:ALA:HB2	2.18	0.44
5:C:716:ALA:HB3	5:C:784:ALA:N	2.30	0.44
6:D:356:THR:O	6:D:448:GLN:HA	2.18	0.44
1:T:8:DA:H5"	1:T:9:DT:C7	2.48	0.44
2:3:60:PHE:HA	2:3:103:THR:H	1.83	0.44
2:3:156:VAL:C	2:3:159:GLY:H	2.26	0.44
2:6:101:GLY:CA	2:6:141:ASN:HA	2.48	0.44
5:C:252:SER:C	5:C:266:GLY:H	2.26	0.44
5:C:619:ALA:O	5:C:621:SER:N	2.43	0.44
6:D:1270:GLY:HA3	6:D:1299:GLY:C	2.43	0.44
2:1:155:MET:O	2:1:160:THR:N	2.31	0.43
2:4:11:GLU:O	2:4:16:LEU:N	2.51	0.43
4:A:55:ALA:O	4:A:146:VAL:HA	2.18	0.43
5:C:1327:LEU:O	5:C:1329:GLU:N	2.49	0.43
8:N:-28:DC:H6	8:N:-28:DC:O5'	2.02	0.43
8:N:-19:DC:C2'	8:N:-18:DT:H71	2.48	0.43
6:D:145:VAL:HA	6:D:160:LEU:O	2.18	0.43
6:D:491:LEU:HA	6:D:499:ILE:N	2.26	0.43
8:N:-8:DG:C8	8:N:-7:DC:C4	3.05	0.43
2:5:34:ILE:HA	2:5:174:VAL:H	1.82	0.43
2:5:41:GLY:HA3	9:5:601:ADP:C8	2.53	0.43
3:M:344:CYS:CB	3:M:372:VAL:CB	2.96	0.43
3:M:403:SER:O	3:M:414:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1335:ALA:O	6:D:1339:GLY:N	2.46	0.43
8:N:-29:DG:H8	8:N:-29:DG:OP2	2.01	0.43
5:C:69:GLN:O	5:C:101:ARG:N	2.51	0.43
5:C:576:SER:HA	5:C:662:SER:HA	2.00	0.43
8:N:-9:DC:C5	8:N:-8:DG:N1	2.86	0.43
2:6:39:GLY:C	2:6:41:GLY:H	2.26	0.43
2:6:40:THR:CB	2:6:225:ASN:H	2.31	0.43
2:3:61:ILE:O	2:3:104:LEU:HA	2.18	0.43
2:3:155:MET:O	2:3:159:GLY:N	2.51	0.43
8:N:-6:DA:H1'	8:N:-5:DG:C8	2.53	0.43
1:T:19:DG:H2"	1:T:20:DT:C6	2.54	0.43
2:5:234:GLU:O	2:5:238:TYR:N	2.51	0.43
8:N:-34:DA:H1'	8:N:-33:DG:C5	2.54	0.43
2:5:103:THR:HA	2:5:143:ARG:C	2.42	0.43
4:A:111:THR:CB	4:A:127:GLN:HA	2.49	0.43
5:C:808:ASN:H	6:D:633:ALA:HB2	1.83	0.43
6:D:1370:MET:O	6:D:1374:ALA:N	2.52	0.43
8:N:-14:DG:C5	8:N:-13:DC:C4	3.07	0.43
2:3:41:GLY:CA	9:3:601:ADP:H8	2.32	0.43
2:3:36:GLY:N	2:3:148:THR:O	2.52	0.43
9:3:601:ADP:O3B	10:3:602:AF3:F3	2.27	0.43
6:D:450:HIS:C	6:D:452:LEU:N	2.77	0.43
8:N:-15:DT:C2	8:N:-14:DG:C6	3.06	0.43
3:M:45:LEU:HA	3:M:298:ASN:H	1.83	0.43
5:C:196:VAL:O	5:C:204:LEU:N	2.52	0.43
2:3:31:PRO:HA	2:3:144:LEU:O	2.19	0.42
2:3:120:LEU:O	2:3:124:ILE:N	2.50	0.42
5:C:1272:GLU:CA	6:D:345:LYS:CB	2.97	0.42
6:D:556:GLU:O	6:D:558:ASP:N	2.47	0.42
2:3:31:PRO:O	2:3:170:ALA:HB3	2.19	0.42
5:C:109:ALA:HB1	5:C:112:GLY:HA3	2.01	0.42
8:N:-30:DG:H1'	8:N:-29:DG:C8	2.54	0.42
2:3:41:GLY:HA3	9:3:601:ADP:N7	2.35	0.42
2:4:34:ILE:C	2:4:147:ALA:HA	2.44	0.42
8:N:-8:DG:C5	8:N:-7:DC:N4	2.88	0.42
1:T:14:DC:C4	1:T:15:DA:N6	2.87	0.42
1:T:31:DG:N1	8:N:-30:DG:C2	2.87	0.42
5:C:377:THR:C	5:C:379:GLU:H	2.26	0.42
1:T:3:DG:N2	8:N:-2:DC:O2	2.52	0.42
1:T:7:DG:C5	8:N:-8:DG:C2	3.07	0.42
4:A:48:LEU:HA	4:A:180:VAL:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:101:THR:O	4:A:116:THR:N	2.52	0.42
5:C:326:SER:HA	5:C:330:HIS:O	2.20	0.42
5:C:615:VAL:HA	5:C:638:SER:HA	2.00	0.42
5:C:1269:ARG:HA	6:D:347:VAL:CB	2.50	0.42
1:T:23:DT:H2"	1:T:24:DG:O5'	2.20	0.42
1:T:26:DC:OP2	1:T:26:DC:H6	2.01	0.42
3:M:113:GLU:O	3:M:117:THR:HA	2.19	0.42
3:M:388:LEU:O	3:M:394:ILE:HA	2.19	0.42
6:D:103:GLY:H	6:D:244:VAL:H	1.67	0.42
2:6:40:THR:CA	2:6:225:ASN:H	2.28	0.42
2:6:216:THR:O	2:6:220:TYR:N	2.51	0.42
5:C:45:GLY:HA2	5:C:50:GLU:CB	2.49	0.42
5:C:730:SER:O	5:C:752:ASN:HA	2.19	0.42
6:D:352:ARG:O	6:D:353:SER:CB	2.67	0.42
8:N:-17:DT:H2"	8:N:-16:DT:H73	2.02	0.42
2:3:41:GLY:N	9:3:601:ADP:O1A	2.42	0.42
4:A:54:CYS:HA	4:A:148:ARG:HA	2.01	0.42
5:C:929:ILE:H	5:C:1054:LEU:HA	1.84	0.42
6:D:318:GLY:C	6:D:320:ASN:H	2.28	0.42
6:D:1291:GLU:HA	6:D:1295:ASN:O	2.20	0.42
1:T:13:DG:H1'	1:T:14:DC:O4'	2.20	0.42
6:D:354:VAL:H	6:D:466:MET:N	2.16	0.42
6:D:814:CYS:CB	6:D:889:ASP:H	2.33	0.42
2:1:41:GLY:HA3	9:1:601:ADP:O3A	2.20	0.42
2:4:101:GLY:N	2:4:141:ASN:O	2.34	0.42
4:A:92:VAL:HA	4:A:120:ASP:O	2.20	0.42
1:T:9:DT:C4	8:N:-9:DC:C2	3.08	0.41
2:3:8:LEU:O	2:3:9:LEU:C	2.63	0.41
2:3:32:VAL:O	2:3:146:CYS:N	2.52	0.41
2:4:35:ILE:CB	2:4:175:GLN:HA	2.50	0.41
1:T:29:DC:H1'	1:T:30:DC:C2	2.55	0.41
2:1:41:GLY:HA2	9:1:601:ADP:PB	2.59	0.41
4:A:184:ALA:O	4:A:203:ILE:HA	2.20	0.41
6:D:1154:ALA:HB2	6:D:1213:GLY:O	2.20	0.41
2:1:78:PHE:HA	2:1:94:GLY:HA3	2.03	0.41
2:1:240:HIS:O	2:1:242:THR:N	2.53	0.41
2:4:85:PHE:C	2:4:87:GLY:N	2.77	0.41
5:C:302:ILE:HA	5:C:308:GLU:O	2.20	0.41
5:C:582:ASN:N	5:C:586:PHE:O	2.40	0.41
2:2:95:ARG:O	2:2:99:ALA:N	2.40	0.41
5:C:345:PRO:C	5:C:347:ILE:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:39:GLY:O	2:6:227:ARG:N	2.28	0.41
5:C:663:VAL:O	5:C:666:SER:N	2.53	0.41
5:C:869:GLY:O	5:C:884:VAL:HA	2.20	0.41
6:D:1264:ALA:O	6:D:1278:GLU:N	2.53	0.41
2:1:41:GLY:HA2	9:1:601:ADP:O3B	2.20	0.41
2:3:128:GLU:N	2:3:139:GLN:HA	2.35	0.41
5:C:227:LYS:HA	5:C:335:THR:O	2.20	0.41
6:D:850:LYS:N	6:D:855:ASP:O	2.53	0.41
6:D:1002:VAL:O	6:D:1018:ALA:HA	2.20	0.41
2:3:228:GLU:O	2:3:229:LEU:C	2.63	0.41
8:N:-26:DG:OP2	8:N:-26:DG:H8	2.04	0.41
5:C:531:SER:HA	5:C:571:LEU:O	2.21	0.41
5:C:1131:MET:O	5:C:1135:GLN:N	2.53	0.41
6:D:143:SER:HA	6:D:162:GLU:N	2.35	0.41
6:D:373:ALA:C	6:D:375:GLU:H	2.28	0.41
1:T:8:DA:H5"	1:T:9:DT:H73	2.03	0.41
1:T:11:DG:C4'	3:M:13:MET:CB	2.98	0.41
2:1:240:HIS:C	2:1:242:THR:N	2.78	0.41
2:2:65:CYS:O	2:2:67:ALA:N	2.54	0.41
2:3:59:PRO:O	2:3:102:GLY:HA3	2.21	0.41
2:5:94:GLY:O	2:5:96:PHE:N	2.54	0.41
3:M:260:GLN:C	3:M:262:ILE:N	2.78	0.41
3:M:263:GLN:C	3:M:265:SER:N	2.79	0.41
6:D:646:ILE:CB	6:D:741:ALA:HB1	2.51	0.41
2:1:113:PRO:O	2:1:116:VAL:N	2.53	0.41
2:1:156:VAL:C	2:1:159:GLY:H	2.29	0.41
2:4:77:LEU:O	2:4:94:GLY:HA3	2.21	0.41
5:C:340:ASP:HA	5:C:343:HIS:O	2.21	0.41
5:C:708:VAL:O	5:C:712:SER:N	2.54	0.41
6:D:823:THR:HA	6:D:878:ASP:O	2.21	0.41
6:D:1316:THR:CB	6:D:1322:ALA:HB2	2.51	0.41
8:N:-14:DG:C8	8:N:-13:DC:C5	3.09	0.41
8:N:-12:DA:H2'	8:N:-11:DA:C2	2.56	0.41
1:T:16:DA:H1'	1:T:17:DA:N9	2.36	0.40
2:6:254:PRO:C	2:1:173:VAL:HA	2.46	0.40
2:5:36:GLY:HA3	2:5:149:ASN:N	2.35	0.40
2:5:49:LEU:O	2:5:52:LEU:N	2.54	0.40
5:C:824:GLN:C	5:C:826:ASP:H	2.29	0.40
6:D:148:GLU:HA	6:D:156:ARG:HA	2.03	0.40
6:D:901:ARG:O	6:D:903:LEU:N	2.54	0.40
6:D:1351:VAL:C	6:D:1354:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:38:ARG:C	2:6:40:THR:H	2.29	0.40
2:2:59:PRO:CB	2:2:102:GLY:HA3	2.52	0.40
2:2:78:PHE:O	2:2:94:GLY:HA3	2.21	0.40
2:4:106:LEU:N	2:4:145:VAL:O	2.46	0.40
1:T:9:DT:C2	8:N:-9:DC:O2	2.75	0.40
5:C:161:LYS:CB	5:C:171:LEU:H	2.34	0.40
3:M:357:GLU:O	3:M:417:ALA:HA	2.21	0.40
6:D:955:LYS:HA	6:D:1011:VAL:O	2.21	0.40
3:M:369:ALA:HA	3:M:374:MET:CB	2.51	0.40
6:D:843:VAL:HA	6:D:862:THR:O	2.21	0.40
8:N:-26:DG:C2	8:N:-25:DG:C5	3.10	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
2	1	251/259 (97%)	217 (86%)	33 (13%)	1 (0%)	30 67
2	2	253/259 (98%)	213 (84%)	40 (16%)	0	100 100
2	3	253/259 (98%)	215 (85%)	38 (15%)	0	100 100
2	4	257/259 (99%)	205 (80%)	52 (20%)	0	100 100
2	5	255/259 (98%)	217 (85%)	38 (15%)	0	100 100
2	6	229/259 (88%)	181 (79%)	47 (20%)	1 (0%)	30 67
3	M	408/475 (86%)	364 (89%)	39 (10%)	5 (1%)	10 44
4	A	227/329 (69%)	198 (87%)	29 (13%)	0	100 100
4	B	213/329 (65%)	188 (88%)	25 (12%)	0	100 100
5	C	1339/1341 (100%)	1220 (91%)	113 (8%)	6 (0%)	30 67
6	D	1312/1407 (93%)	1117 (85%)	186 (14%)	9 (1%)	18 56

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	E	72/91 (79%)	70 (97%)	2 (3%)	0	100 100
All	All	5069/5526 (92%)	4405 (87%)	642 (13%)	22 (0%)	31 67

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	15	PRO
3	M	116	GLN
3	M	265	SER
5	C	1295	SER
5	C	1329	GLU
6	D	124	ILE
6	D	348	ASP
2	1	127	GLY
3	M	194	ARG
5	C	1337	ILE
6	D	336	GLY
6	D	347	VAL
6	D	350	SER
6	D	353	SER
6	D	355	ILE
2	6	220	TYR
5	C	809	GLY
5	C	1259	LEU
5	C	1338	GLU
6	D	140	TYR
6	D	314	ARG
3	M	4	GLY

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	ADP	5	601	11	27,29,29	1.35	4 (14%)	42,45,45	2.03	12 (28%)
9	ADP	4	601	11,10	27,29,29	0.40	0	42,45,45	0.45	0
10	AF3	5	602	-	0,3,3	-	-	-		
10	AF3	1	602	9	0,3,3	-	-	-		
9	ADP	1	601	11,10	27,29,29	0.41	0	42,45,45	0.52	0
9	ADP	3	601	11,10	27,29,29	1.35	4 (14%)	42,45,45	2.06	11 (26%)
9	ADP	2	302	10	27,29,29	0.39	0	42,45,45	0.47	0
10	AF3	3	602	9	0,3,3	-	-	-		
10	AF3	4	602	9	0,3,3	-	-	-		
10	AF3	2	303	9	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	5	601	11	-	5/16/32/32	0/3/3/3
9	ADP	4	601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	1	601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	3	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	2	302	10	-	8/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	601	ADP	C5-C4	4.43	1.47	1.39
9	3	601	ADP	C5-C4	4.43	1.47	1.39
9	5	601	ADP	C5-C6	2.74	1.48	1.41
9	3	601	ADP	C5-C6	2.62	1.48	1.41
9	5	601	ADP	C8-N7	2.47	1.36	1.31
9	3	601	ADP	C8-N7	2.40	1.36	1.31
9	3	601	ADP	C5-N7	-2.25	1.34	1.39
9	5	601	ADP	C5-N7	-2.01	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	601	ADP	C5-C4-N3	-6.24	118.61	126.75
9	5	601	ADP	C5-C4-N3	-6.08	118.82	126.75
9	3	601	ADP	N3-C4-N9	4.87	135.10	127.08
9	5	601	ADP	N3-C4-N9	4.50	134.50	127.08
9	3	601	ADP	PA-O3A-PB	-4.49	117.41	132.83
9	5	601	ADP	PA-O3A-PB	-4.21	118.39	132.83
9	3	601	ADP	C2-N3-C4	3.97	121.12	111.75
9	5	601	ADP	C2-N3-C4	3.77	120.66	111.75
9	5	601	ADP	C4-C5-N7	-3.76	106.04	110.62
9	3	601	ADP	N3-C2-N1	-3.30	123.44	128.60
9	3	601	ADP	C4-C5-N7	-3.30	106.60	110.62
9	5	601	ADP	C5-N7-C8	3.09	107.89	103.51
9	5	601	ADP	N3-C2-N1	-2.93	124.02	128.60
9	3	601	ADP	C5-N7-C8	2.82	107.51	103.51
9	5	601	ADP	C4-N9-C8	2.70	108.65	105.73
9	3	601	ADP	C4-N9-C8	2.62	108.57	105.73
9	5	601	ADP	C6-C5-N7	2.53	136.74	132.02
9	5	601	ADP	N9-C8-N7	-2.32	110.74	113.91
9	5	601	ADP	O4'-C1'-N9	2.22	112.44	108.06
9	3	601	ADP	C6-C5-N7	2.21	136.14	132.02
9	3	601	ADP	N9-C8-N7	-2.11	111.02	113.91
9	5	601	ADP	C3'-C2'-C1'	2.07	105.35	101.43
9	3	601	ADP	C3'-C2'-C1'	2.06	105.34	101.43

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	2	302	ADP	PA-O3A-PB-O2B
9	2	302	ADP	C5'-O5'-PA-O1A

Continued on next page...

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Mol	Chain	Res	Type	Atoms
9	2	302	ADP	O4'-C4'-C5'-O5'
9	2	302	ADP	C3'-C4'-C5'-O5'
9	3	601	ADP	C5'-O5'-PA-O3A
9	4	601	ADP	C5'-O5'-PA-O1A
9	5	601	ADP	C5'-O5'-PA-O3A
9	4	601	ADP	O4'-C4'-C5'-O5'
9	4	601	ADP	C3'-C4'-C5'-O5'
9	5	601	ADP	O4'-C4'-C5'-O5'
9	5	601	ADP	C3'-C4'-C5'-O5'
9	1	601	ADP	C4'-C5'-O5'-PA
9	1	601	ADP	O4'-C4'-C5'-O5'
9	2	302	ADP	C5'-O5'-PA-O3A
9	1	601	ADP	C2'-C1'-N9-C8
9	4	601	ADP	C4'-C5'-O5'-PA
9	2	302	ADP	C5'-O5'-PA-O2A
9	3	601	ADP	C5'-O5'-PA-O1A
9	5	601	ADP	C5'-O5'-PA-O1A
9	5	601	ADP	C5'-O5'-PA-O2A
9	4	601	ADP	C2'-C1'-N9-C8
9	1	601	ADP	C2'-C1'-N9-C4
9	4	601	ADP	C2'-C1'-N9-C4
9	1	601	ADP	O4'-C1'-N9-C8
9	2	302	ADP	PA-O3A-PB-O3B
9	1	601	ADP	C3'-C4'-C5'-O5'
9	2	302	ADP	PA-O3A-PB-O1B

There are no ring outliers.

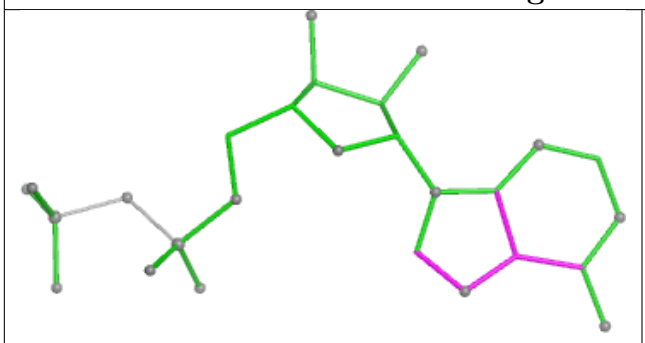
9 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	5	601	ADP	6	0
9	4	601	ADP	11	0
10	5	602	AF3	5	0
9	1	601	ADP	6	0
9	3	601	ADP	9	0
9	2	302	ADP	8	0
10	3	602	AF3	2	0
10	4	602	AF3	1	0
10	2	303	AF3	4	0

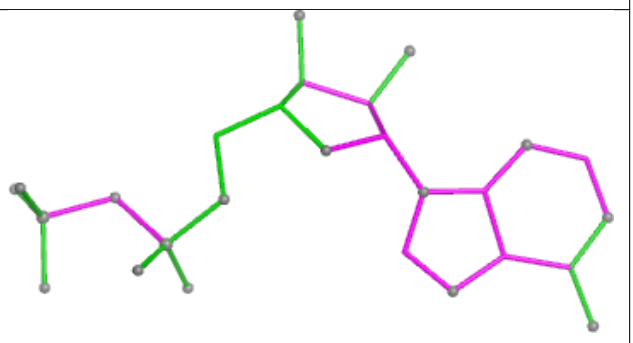
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

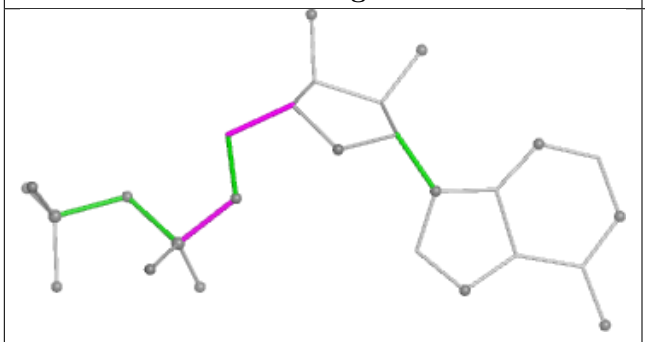
Ligand ADP 5 601



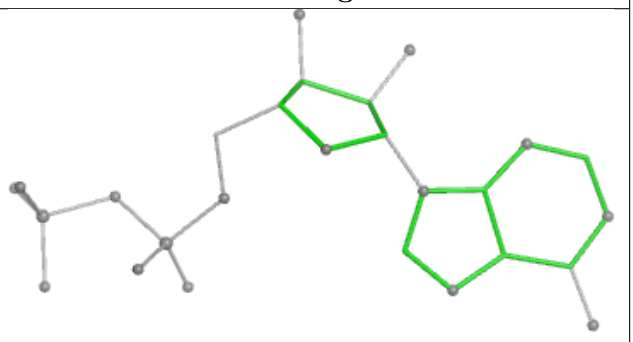
Bond lengths



Bond angles

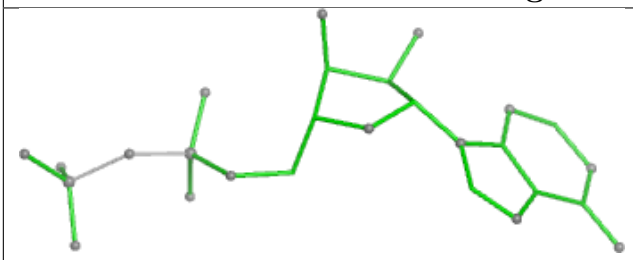


Torsions

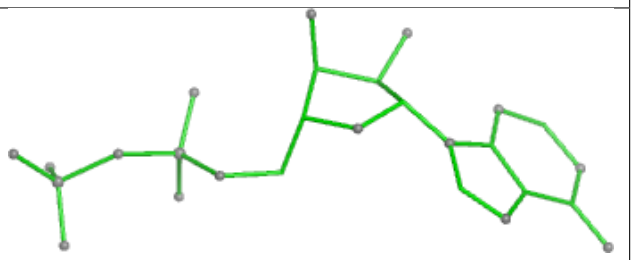


Rings

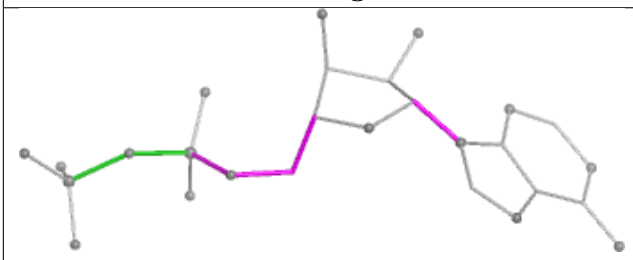
Ligand ADP 4 601



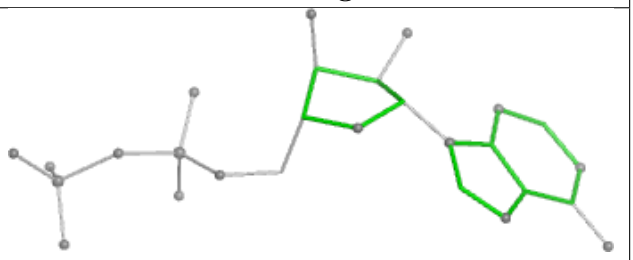
Bond lengths



Bond angles

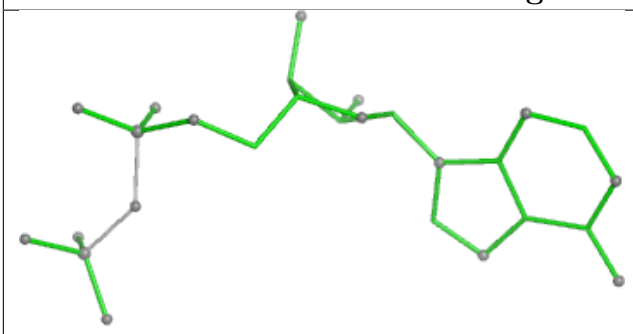


Torsions

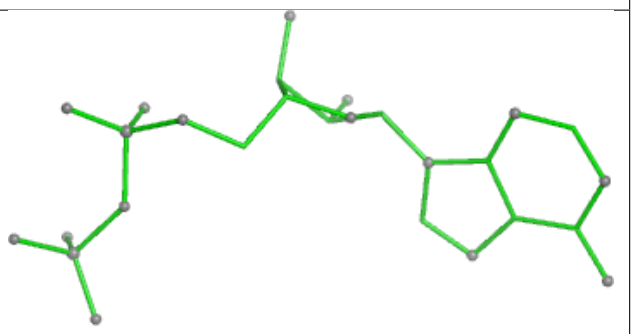


Rings

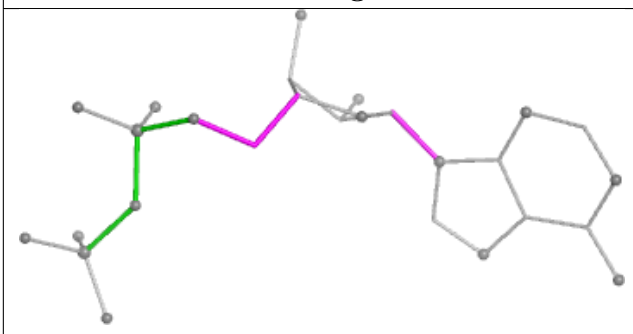
Ligand ADP 1 601



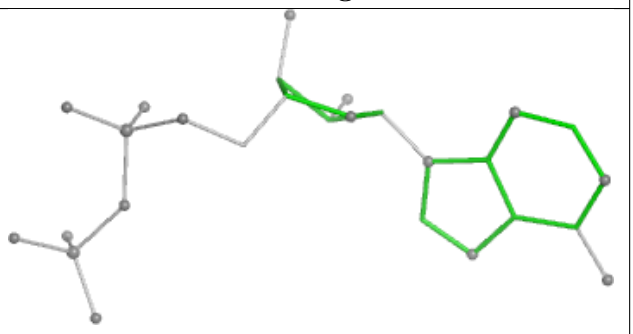
Bond lengths



Bond angles

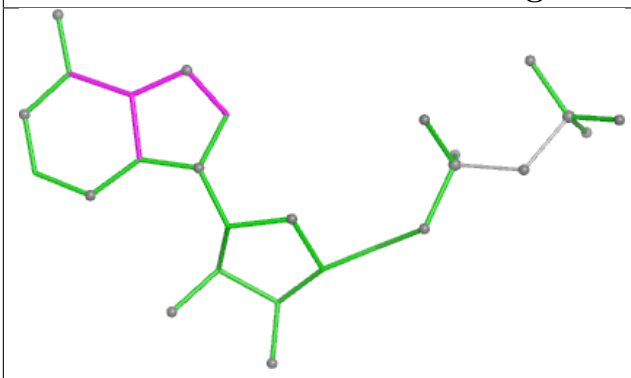


Torsions

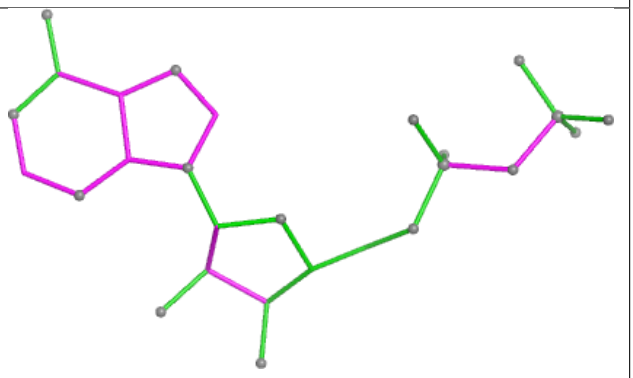


Rings

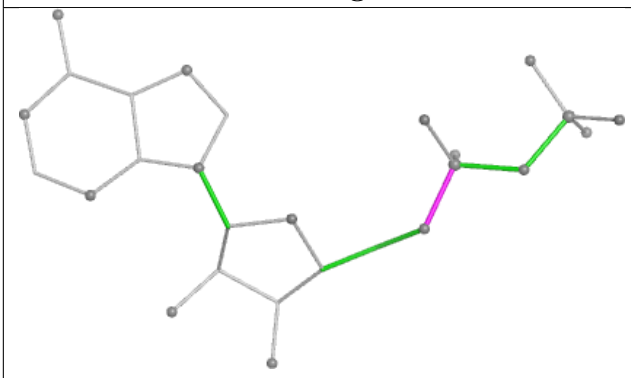
Ligand ADP 3 601



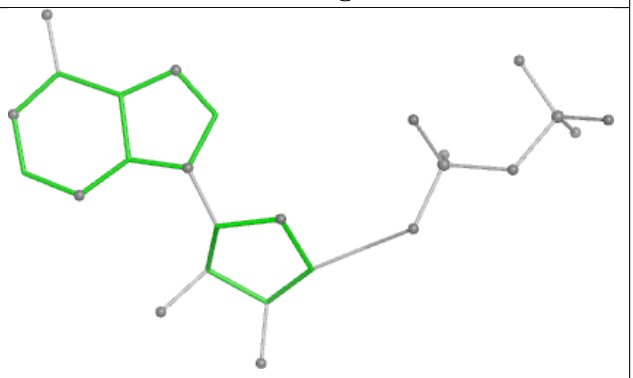
Bond lengths



Bond angles

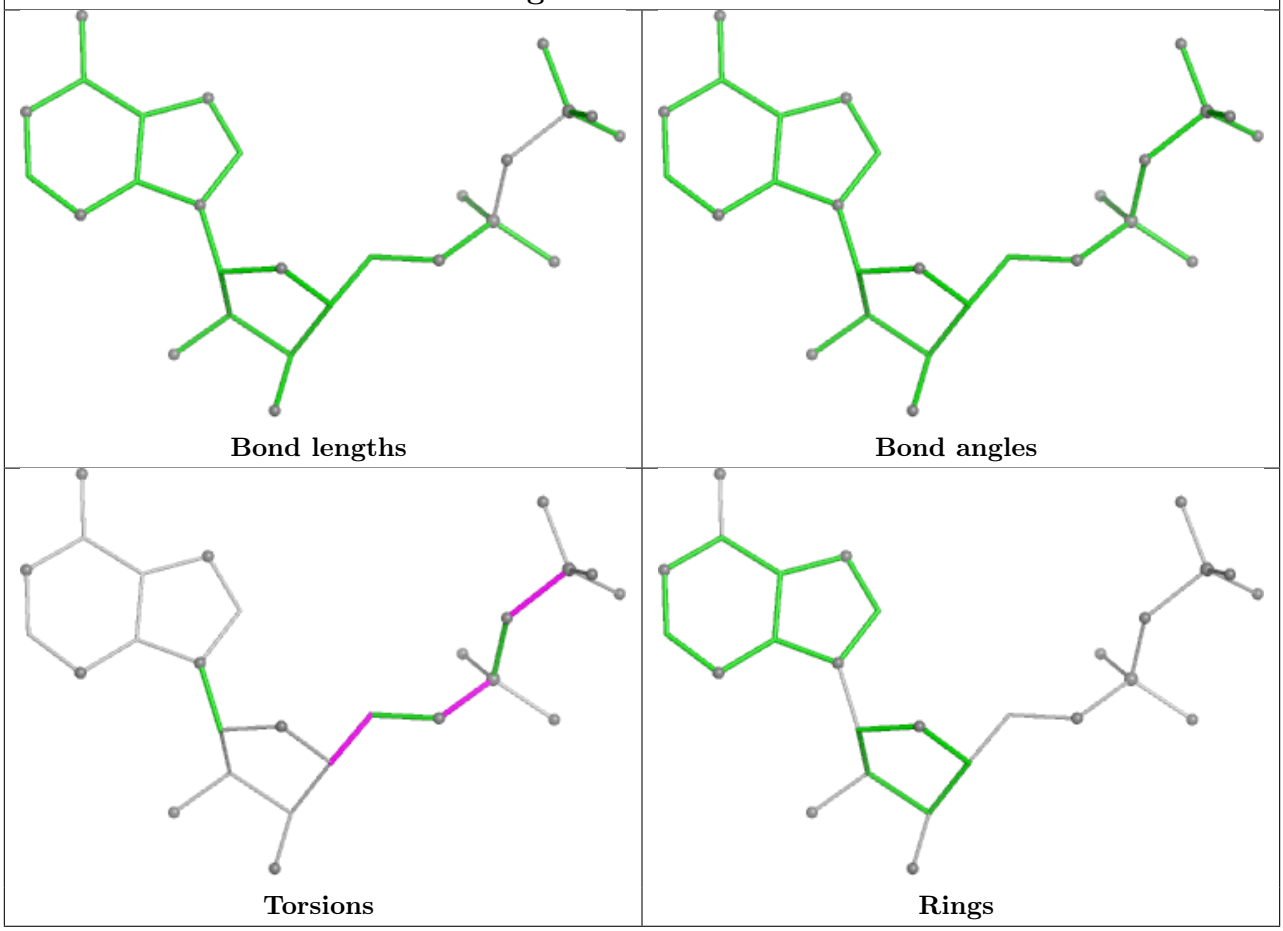


Torsions



Rings

Ligand ADP 2 302



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.

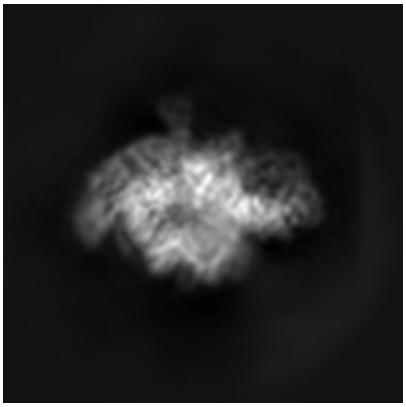
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52915. These allow visual inspection of the internal detail of the map and identification of artifacts.

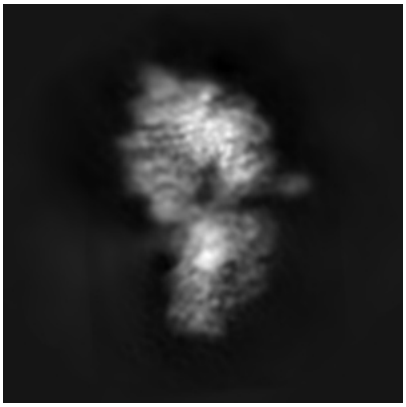
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

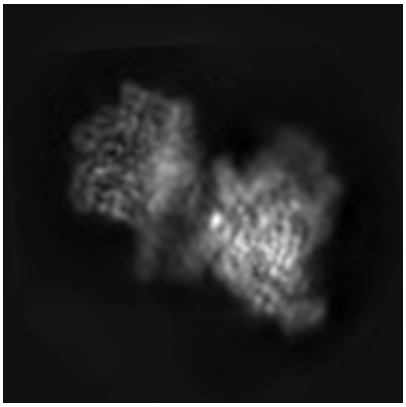
6.1.1 Primary map



X



Y

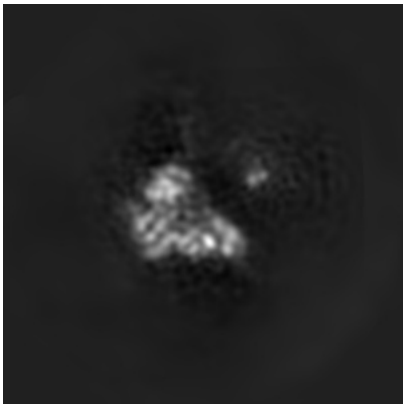


Z

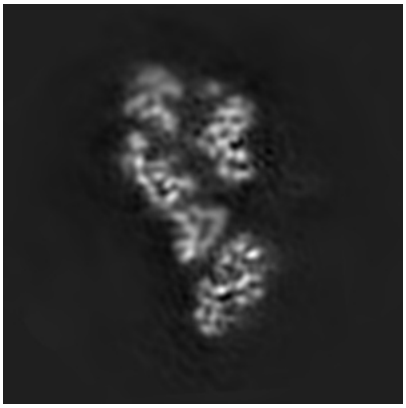
The images above show the map projected in three orthogonal directions.

6.2 Central slices

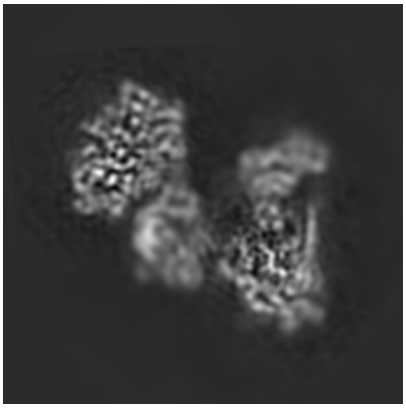
6.2.1 Primary map



X Index: 140



Y Index: 140

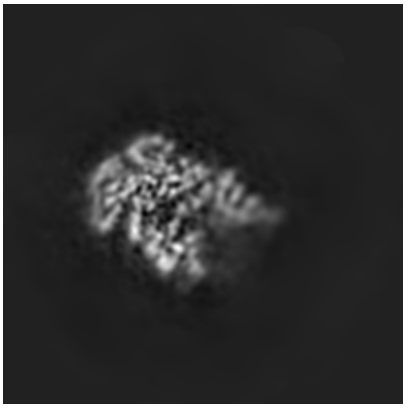


Z Index: 140

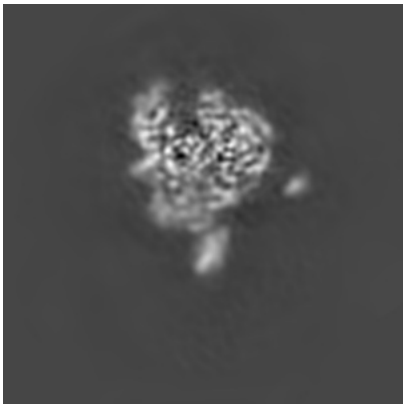
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

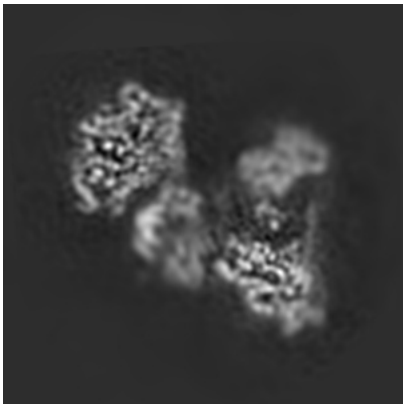
6.3.1 Primary map



X Index: 189



Y Index: 110

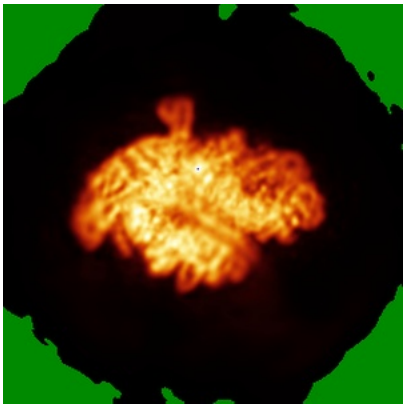


Z Index: 137

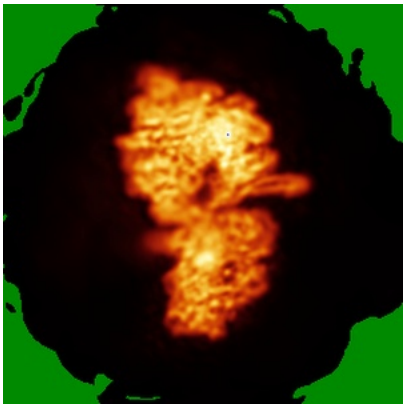
The images above show the largest variance slices of the map in three orthogonal directions.

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

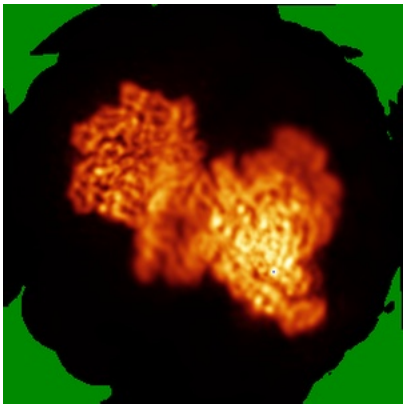
6.4.1 Primary map



X



Y

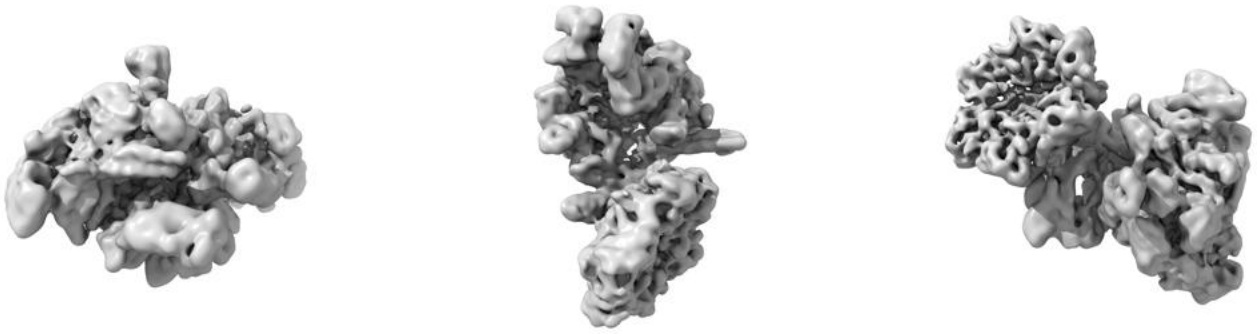


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

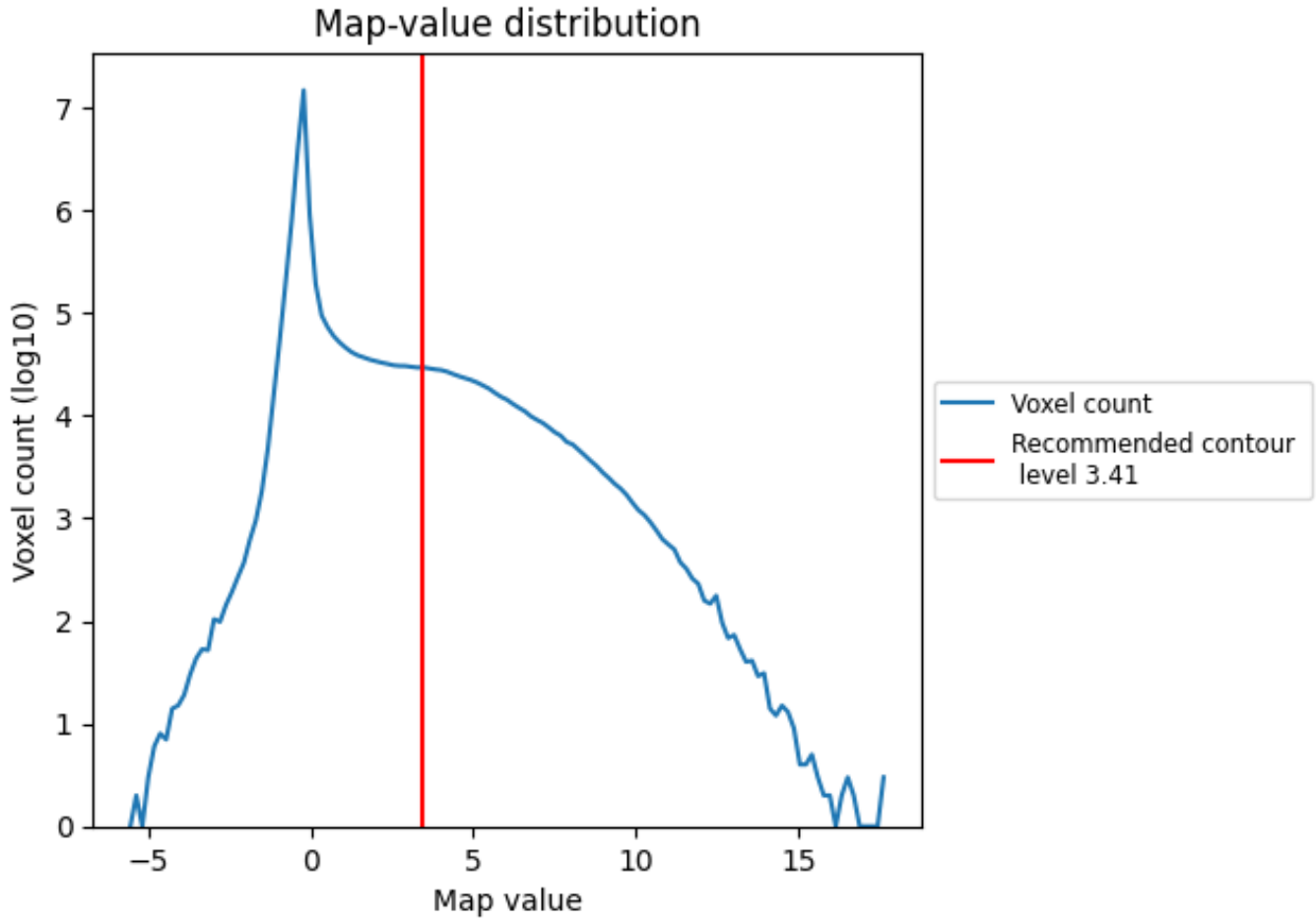
6.6 Mask visualisation (i)

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

7 Map analysis

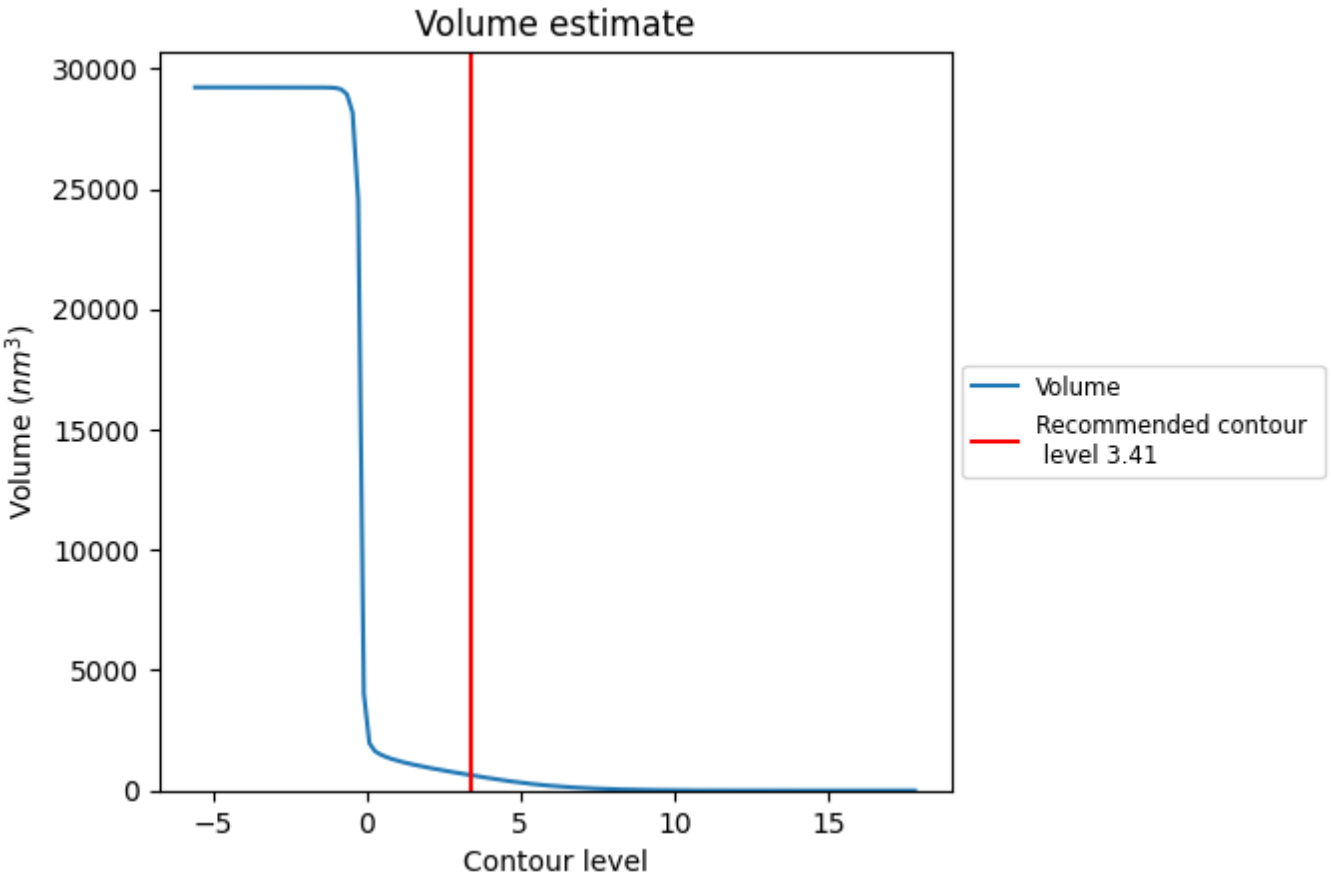
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

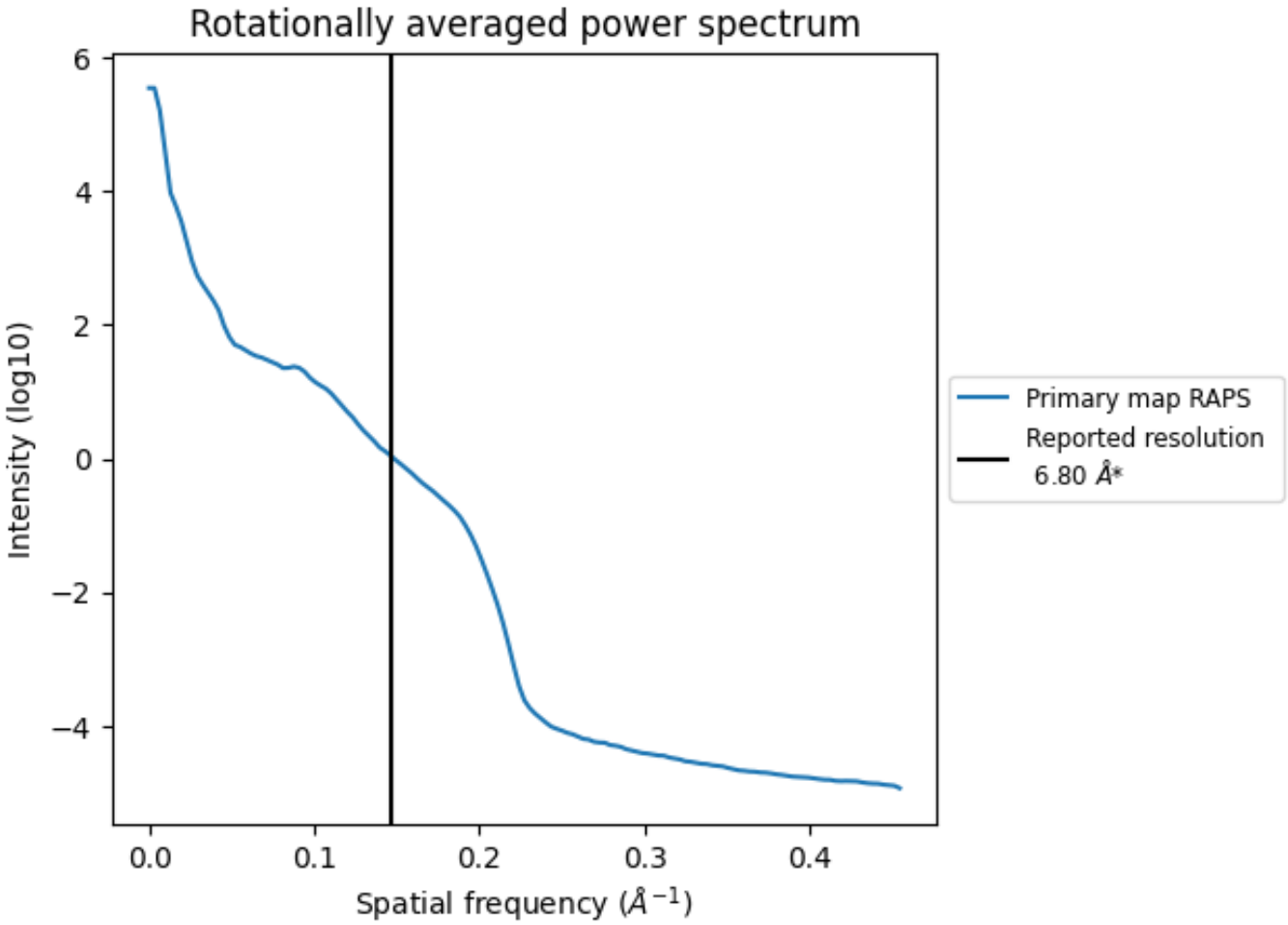
7.2 Volume estimate



The volume at the recommended contour level is 636 nm^3; this corresponds to an approximate mass of 575 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 0.147 $Å^{-1}$

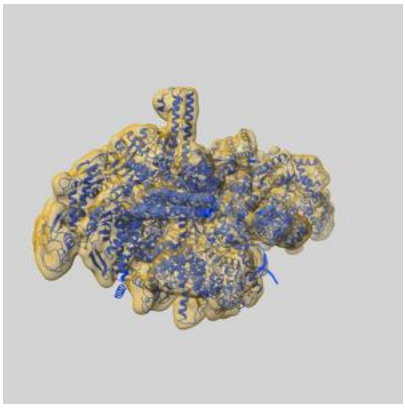
8 Fourier-Shell correlation (i)

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

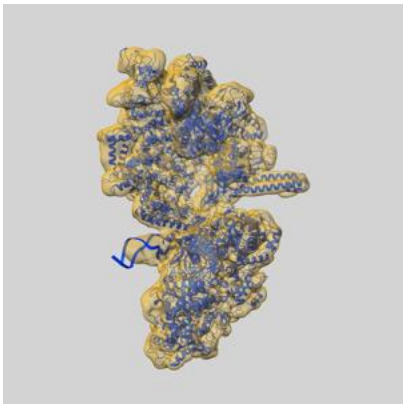
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52915 and PDB model 9Q92. Per-residue inclusion information can be found in section 3 on page 8.

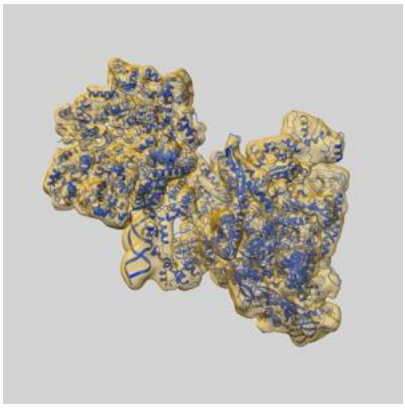
9.1 Map-model overlay



X



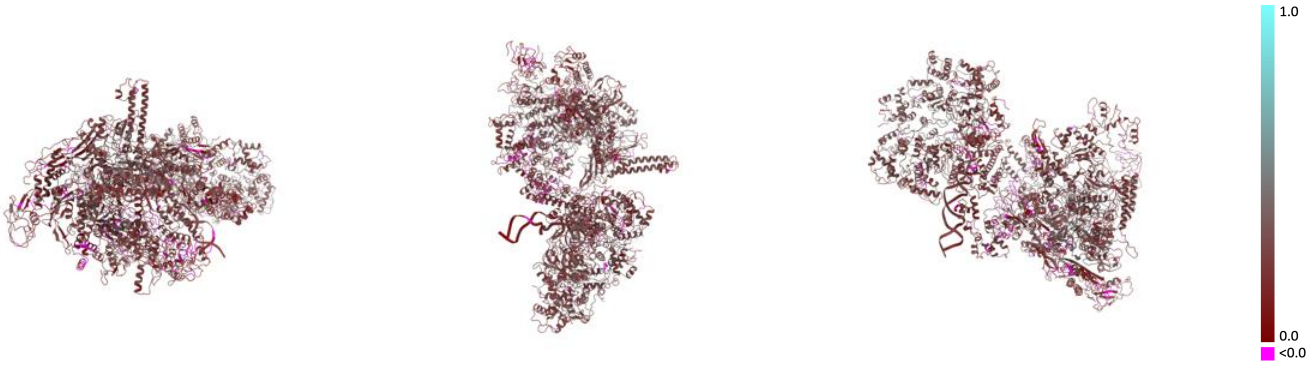
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.41 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.

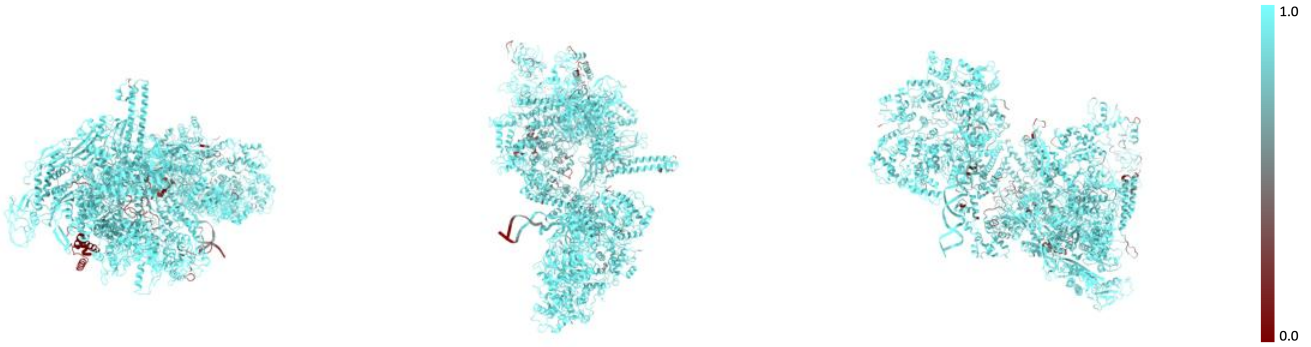
9.2 Q-score mapped to coordinate model (i)



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.

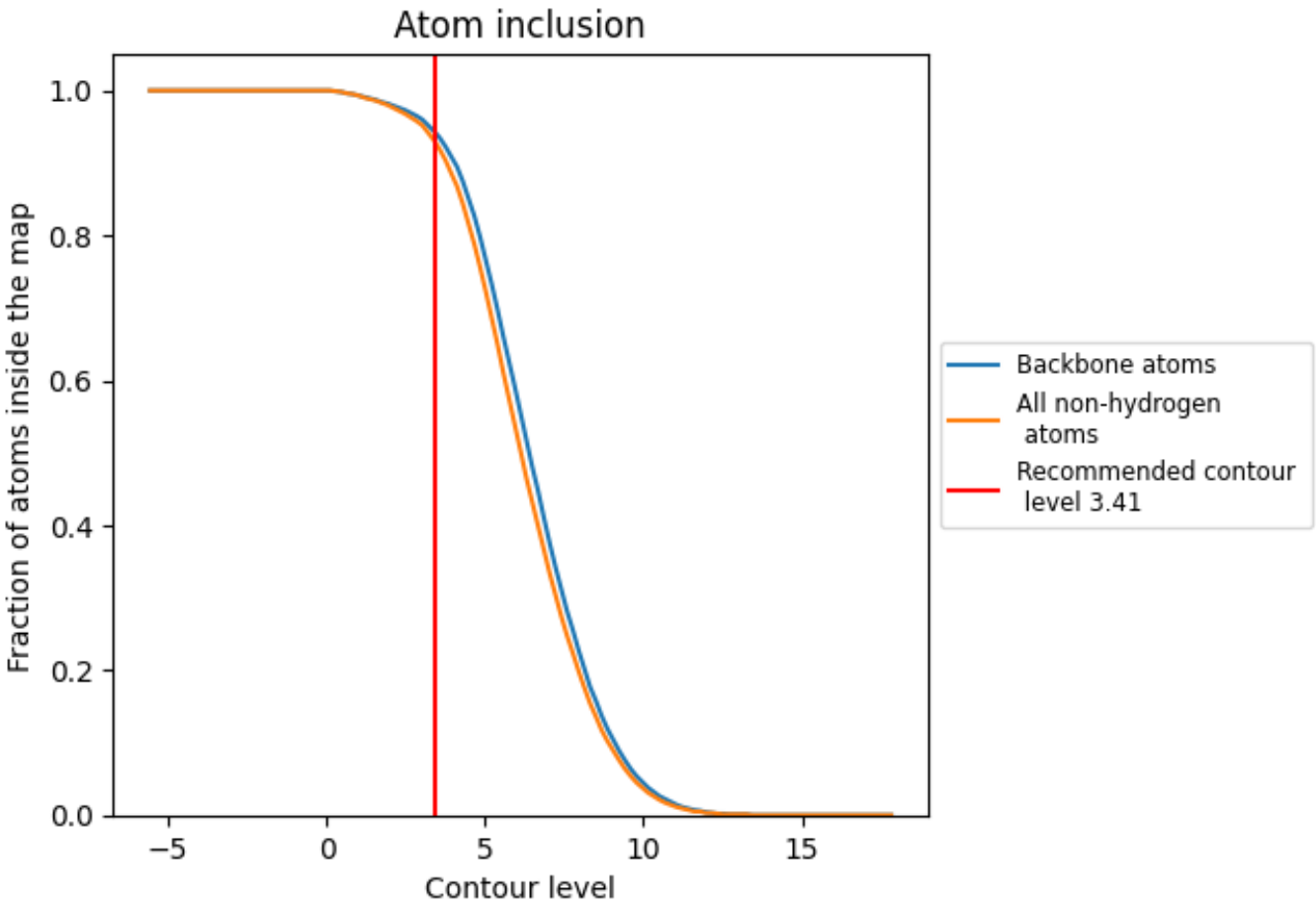
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.41).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (3.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.2560
1	0.9710	0.3080
2	0.9760	0.3100
3	0.9740	0.3130
4	0.9580	0.2980
5	0.9490	0.2720
6	0.9220	0.2700
A	0.9640	0.2100
B	0.9800	0.2040
C	0.9590	0.2770
D	0.9290	0.2460
E	0.0330	0.0600
M	0.8980	0.2000
N	0.8490	0.2050
T	0.8690	0.1880

