Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 04:19 PM EDT

PDB ID	:	9B1E
EMDB ID	:	EMD-44075
Title	:	Cryo-EM structure of native SWR1 bound to nucleosome (composite structure)
Authors	:	Louder, R.K.; Park, G.; Wu, C.
Deposited on	:	2024-03-13
Resolution	:	4.40 Å(reported)
Based on initial models	:	6GEJ, .

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:

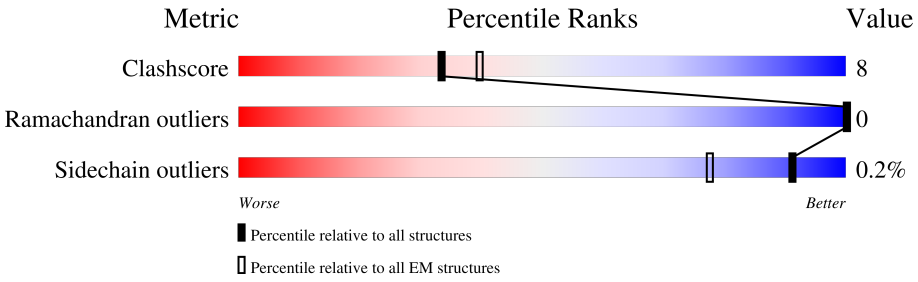
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.40 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.



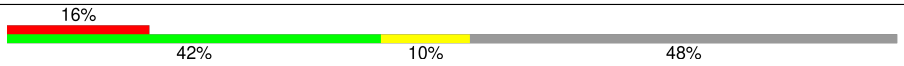
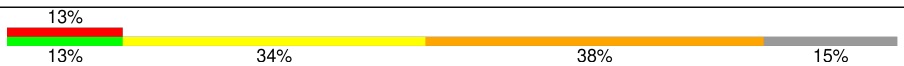
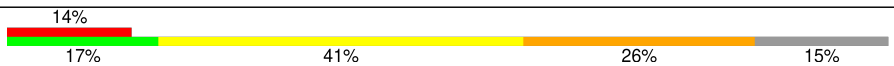
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1544	6% 36% 10% 53%
2	B	795	14% 31% 7% 62%
3	C	438	7% 72% 22% 6%
4	D	280	17% 58% 16% 26%
5	E	837	43% 8% 49%
5	G	837	45% 7% 48%
5	I	837	43% 9% 48%
6	F	471	80% 14% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	471	
6	J	471	
7	K	625	
8	Q	132	
8	S	132	
9	R	131	
9	T	131	
10	U	136	
10	W	136	
11	V	103	
11	X	103	
12	Y	214	
13	Z	214	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49842 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 Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	720	5894	3757	1041	1069	27	0	0

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	303	2513	1598	441	466	8	0	0

- Molecule 3 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	411	3336	2156	544	620	16	0	0

- Molecule 4 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	206	1671	1054	296	311	10	0	0

- Molecule 5 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	426	3281	2072	565	634	10	0	0
5	G	434	3334	2104	575	645	10	0	0
5	I	436	3351	2115	577	649	10	0	0

- Molecule 6 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	443	Total	C	N	O	S	0	0
			3410	2131	591	676	12		
6	H	441	Total	C	N	O	S	0	0
			3393	2119	588	674	12		
6	J	426	Total	C	N	O	S	0	0
			3279	2052	566	650	11		

- Molecule 7 is a protein called SWR1-complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	322	Total	C	N	O	S	0	0
			2671	1699	470	489	13		

- Molecule 8 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	108	Total	C	N	O	0	0
			833	523	164	146		
8	S	106	Total	C	N	O	0	0
			819	514	161	144		

- Molecule 9 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	91	Total	C	N	O	S	0	0
			713	449	125	138	1		
9	T	93	Total	C	N	O	S	0	0
			726	456	127	142	1		

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	107	Total	C	N	O	S	0	0
			864	544	167	150	3		
10	W	98	Total	C	N	O	S	0	0
			807	508	156	140	3		

- Molecule 11 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

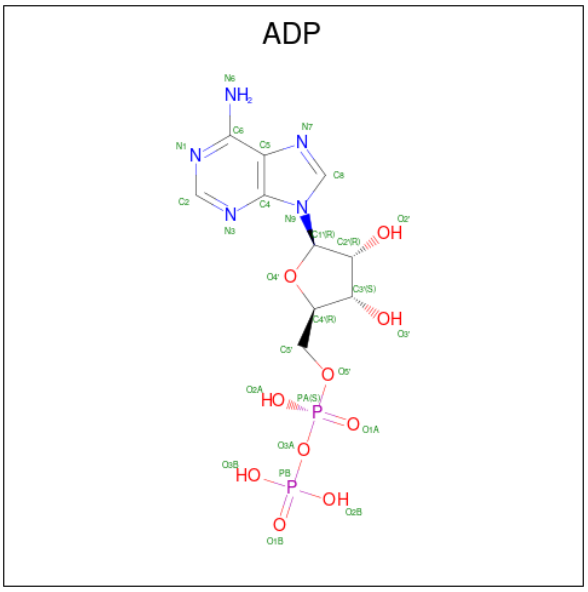
- Molecule 12 is a DNA chain called DNA (214-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	181	Total	C	N	O	P	0	0
			3688	1751	667	1089	181		

- Molecule 13 is a DNA chain called DNA (214-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	181	Total	C	N	O	P	0	0
			3733	1765	704	1083	181		

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



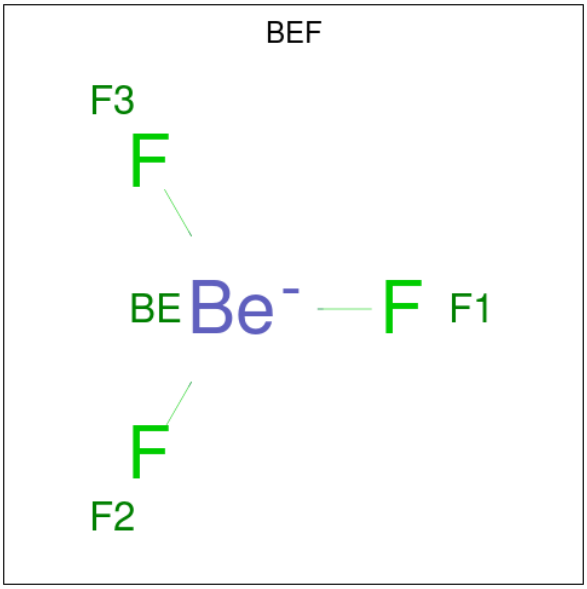
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 15 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Be	F	0
			4	1	3	
15	C	1	Total	Be	F	0
			4	1	3	

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	C	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	E	1	Total Mg 1 1	0
16	F	1	Total Mg 1 1	0
16	G	1	Total Mg 1 1	0
16	H	1	Total Mg 1 1	0
16	I	1	Total Mg 1 1	0
16	J	1	Total Mg 1 1	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

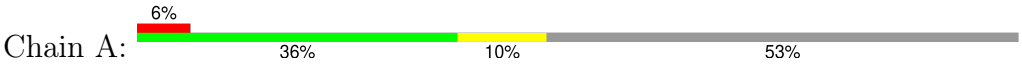
Mol	Chain	Residues	Atoms	AltConf
17	D	2	Total Zn 2 2	0

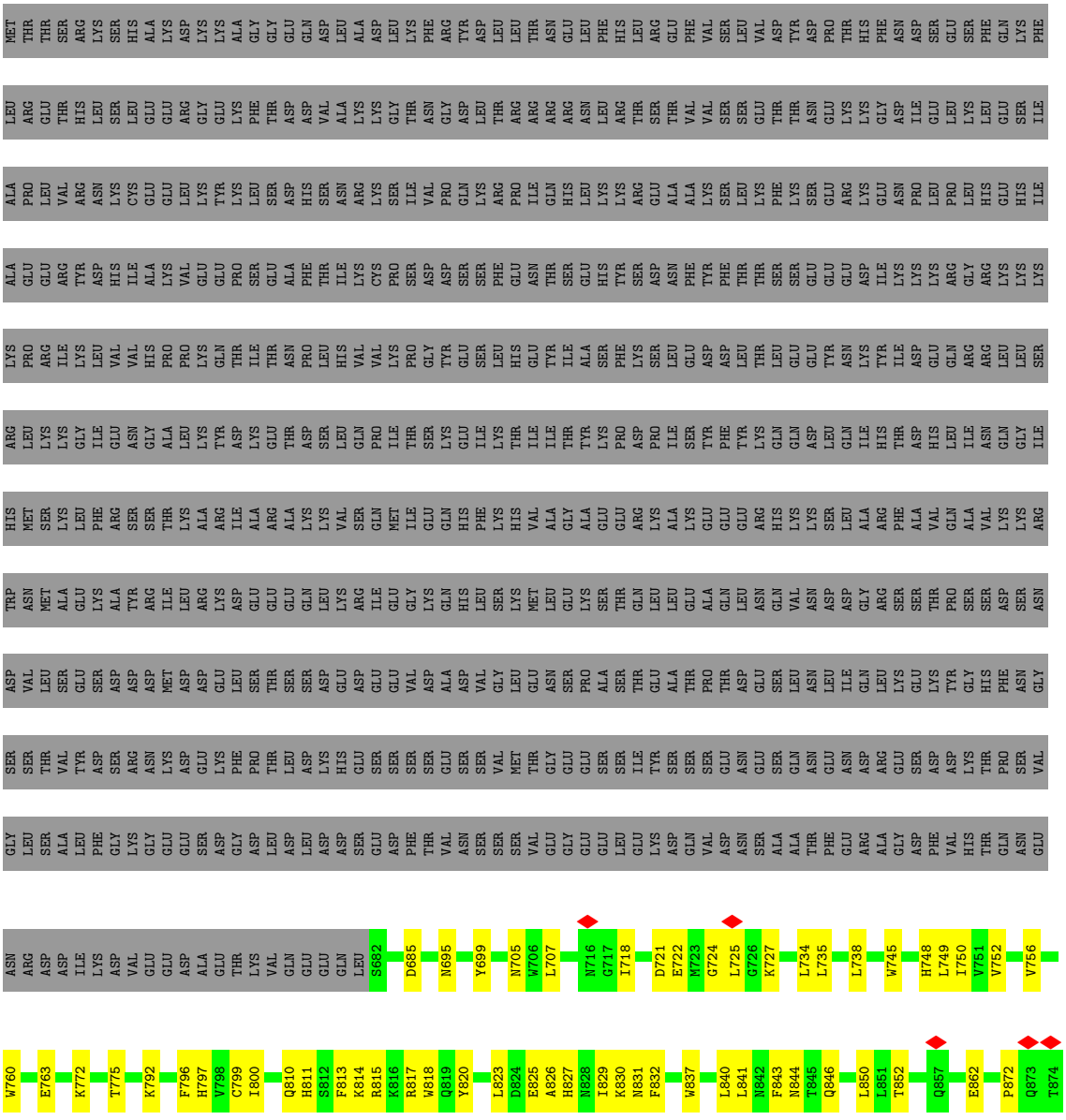
3 Residue-property plots (i)

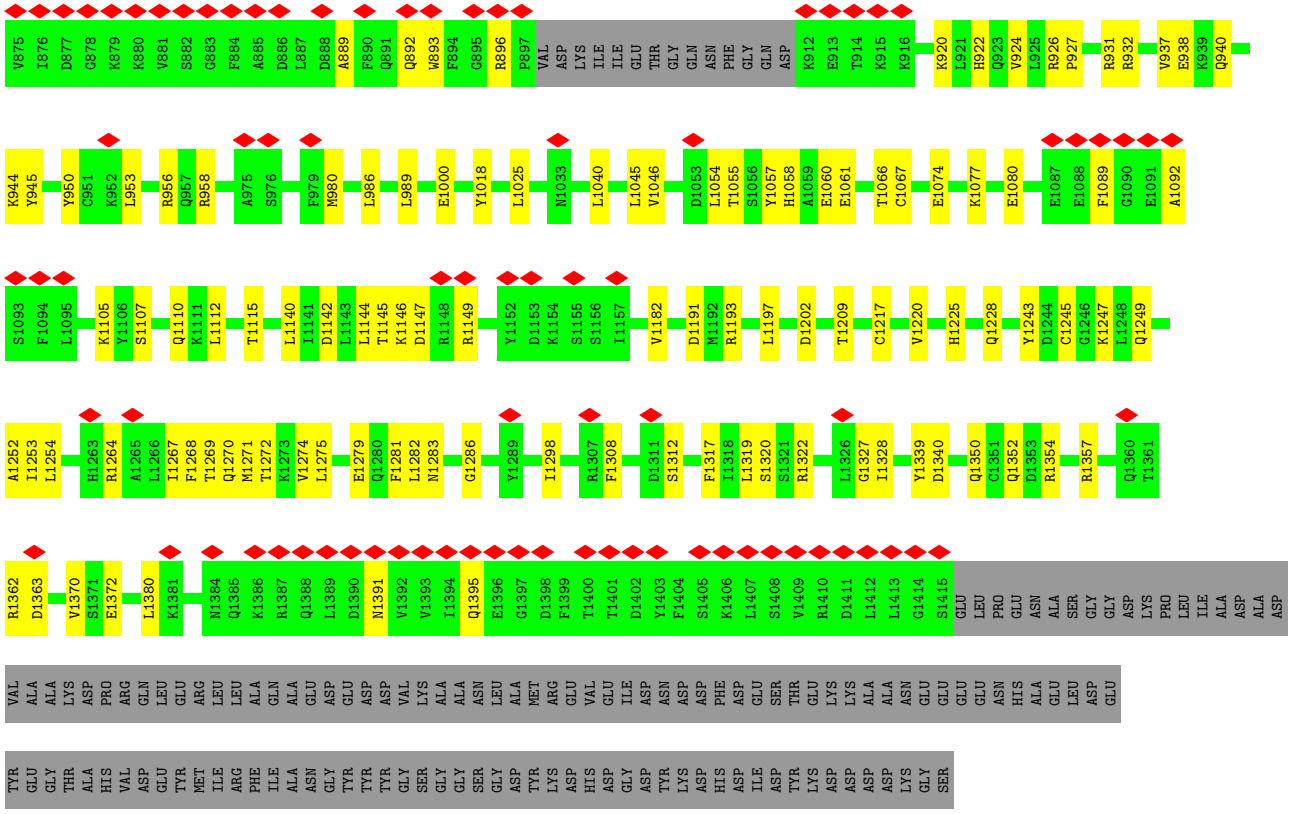
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Helicase SWR1

Chain A:

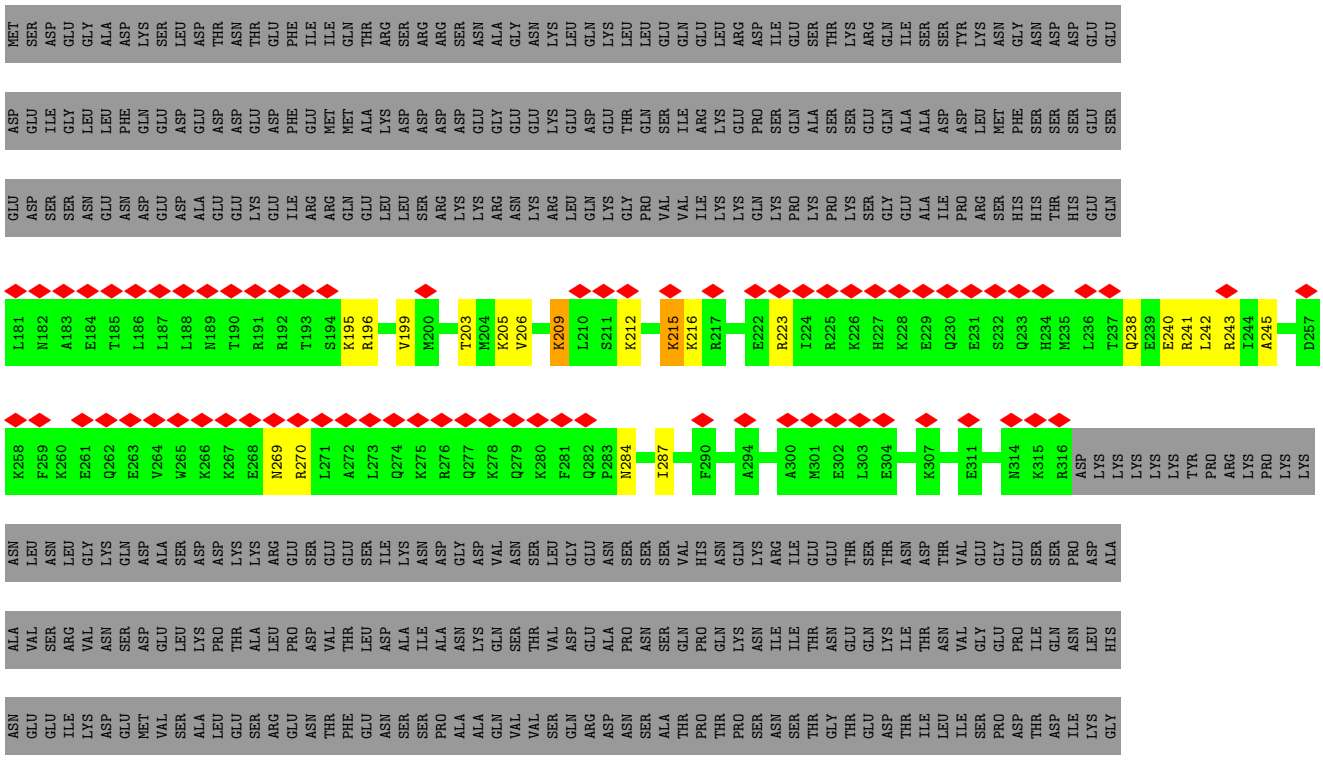


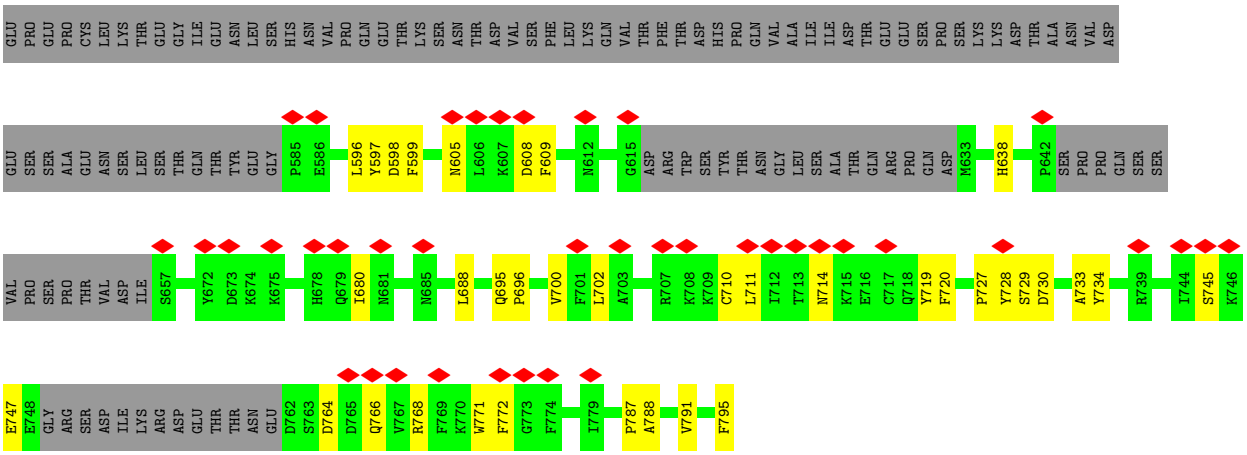




• Molecule 2: Vacuolar protein sorting-associated protein 72

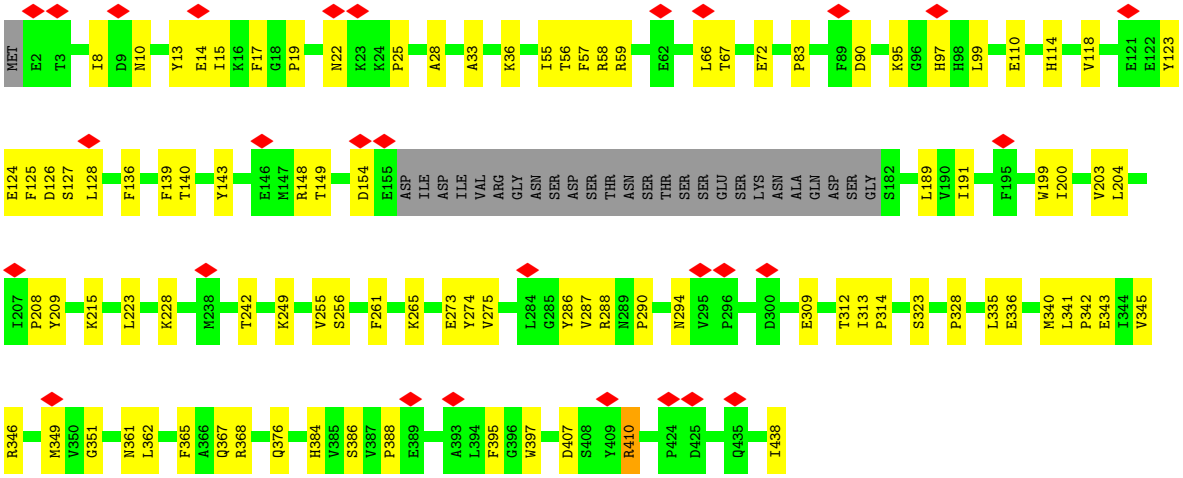
Chain B:





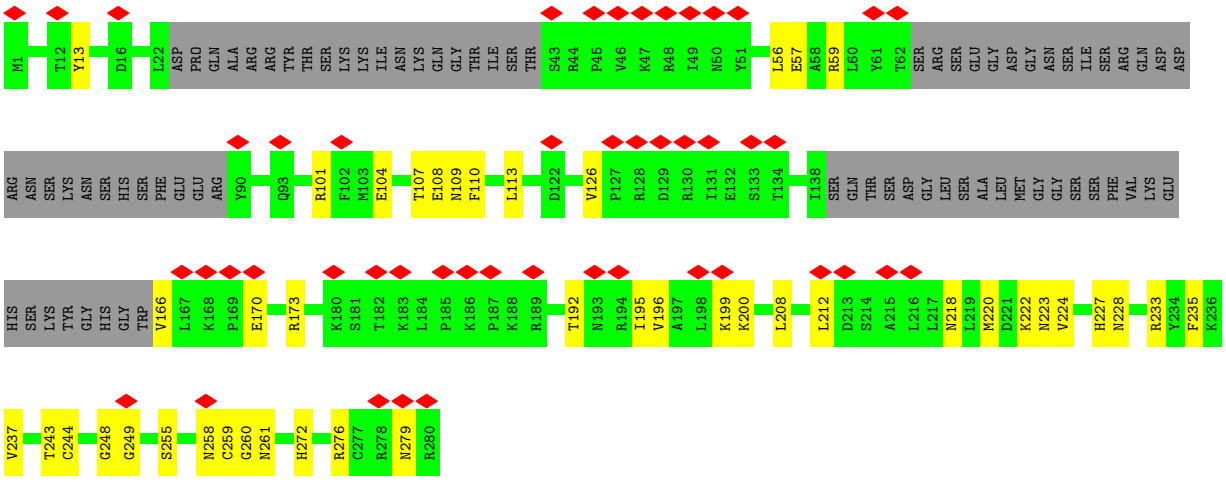
• Molecule 3: Actin-like protein ARP6

Chain C:



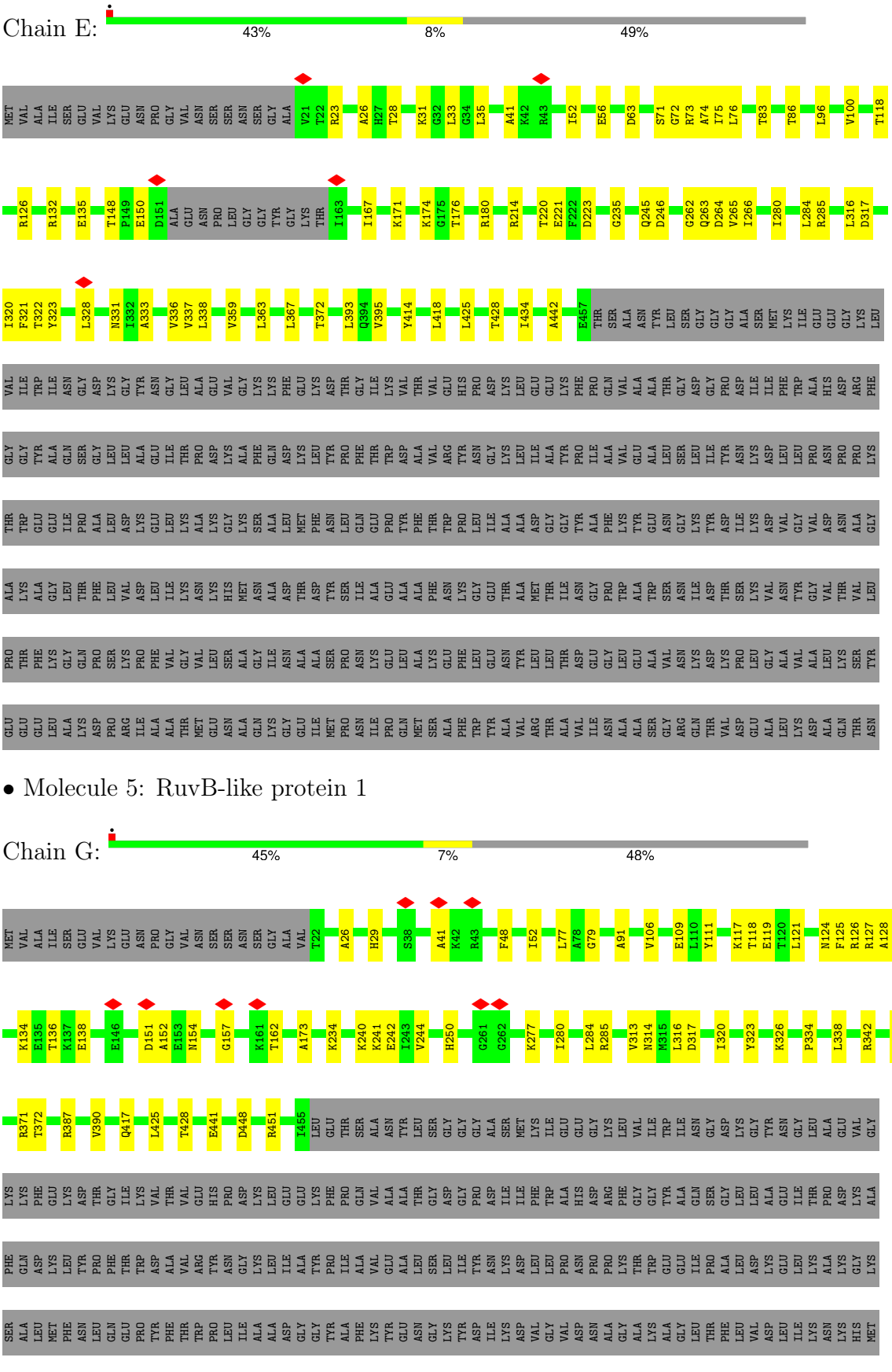
• Molecule 4: Vacuolar protein sorting-associated protein 71

Chain D:



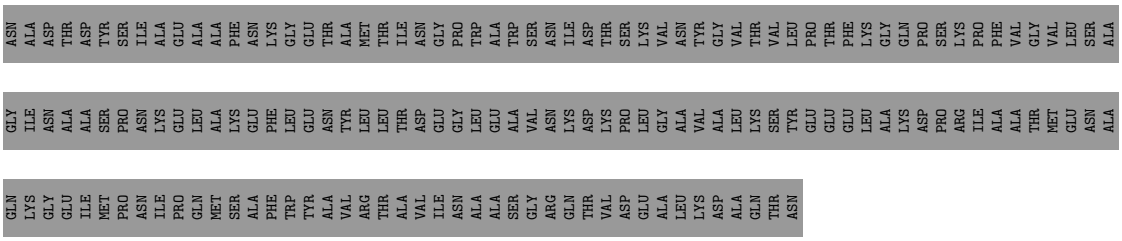
• Molecule 5: RuvB-like protein 1

Chain E:



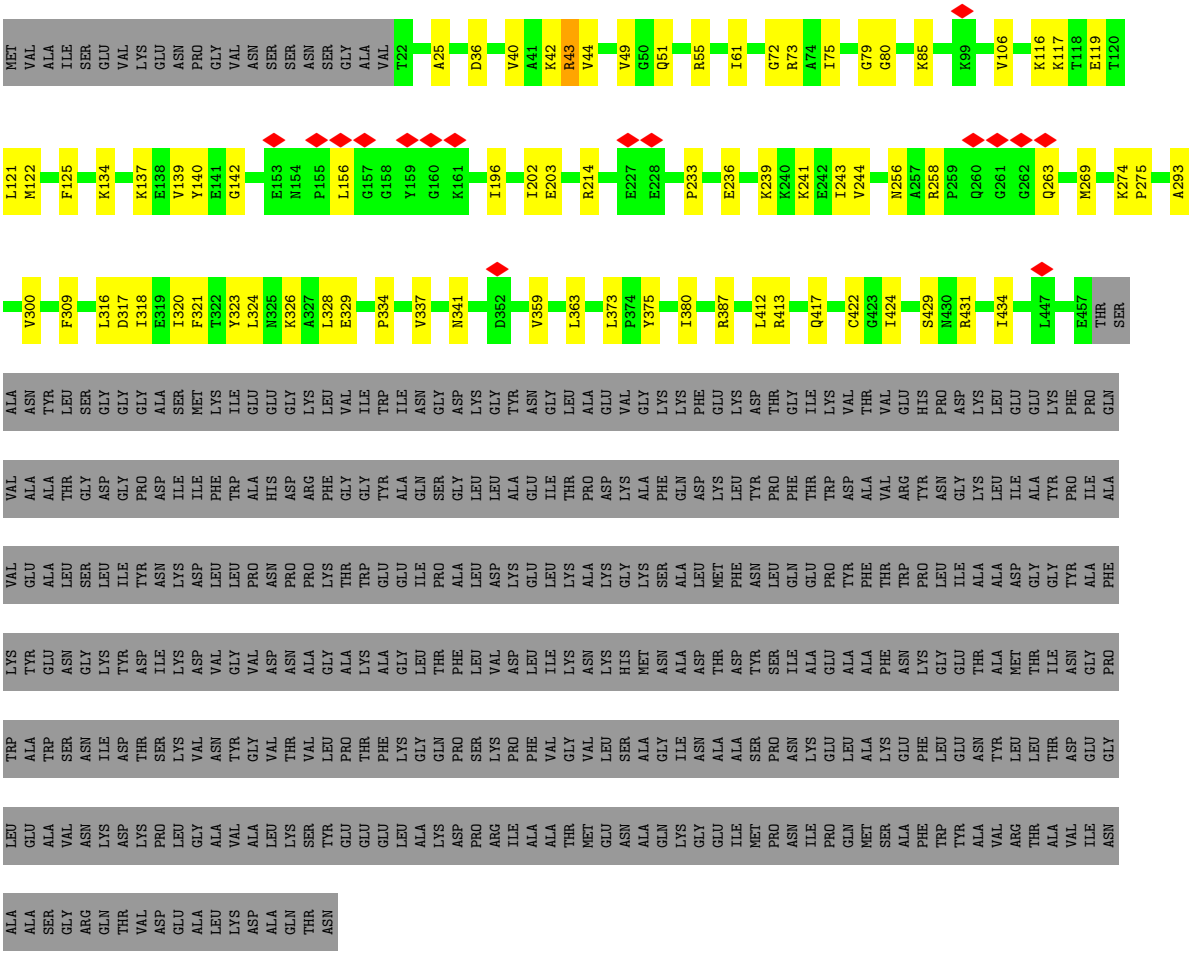
• Molecule 5: RuvB-like protein 1

Chain G:



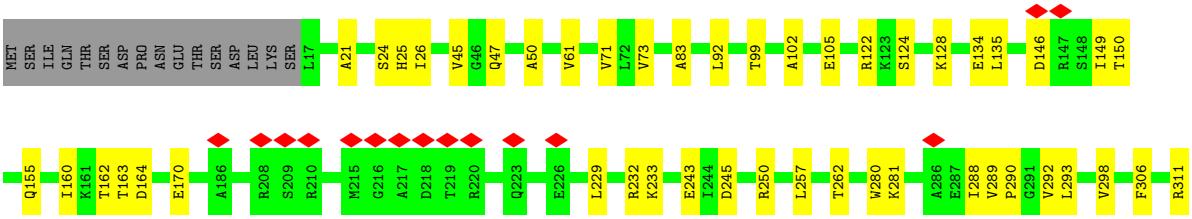
• Molecule 5: RuvB-like protein 1

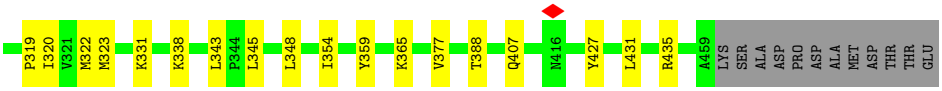
Chain I:



• Molecule 6: RuvB-like protein 2

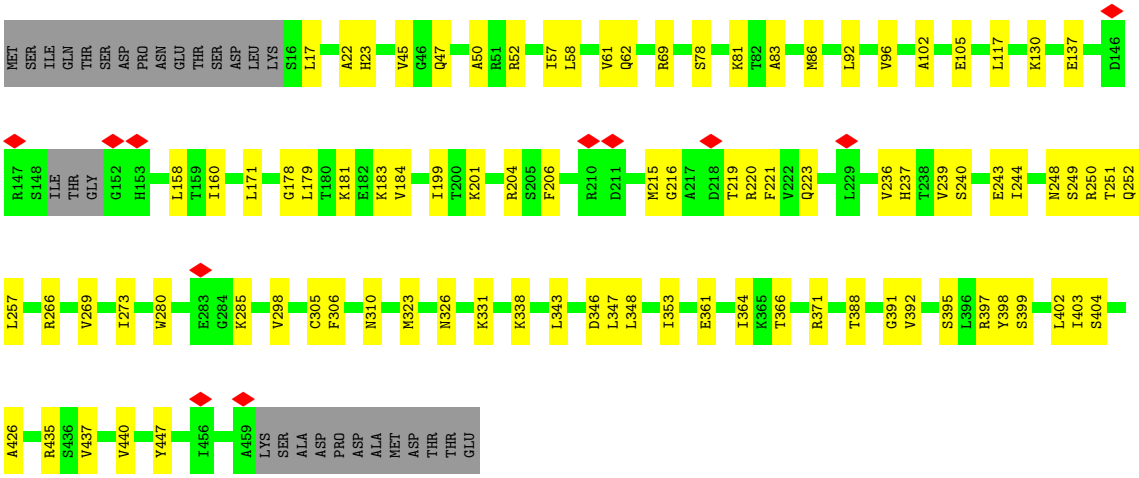
Chain F:





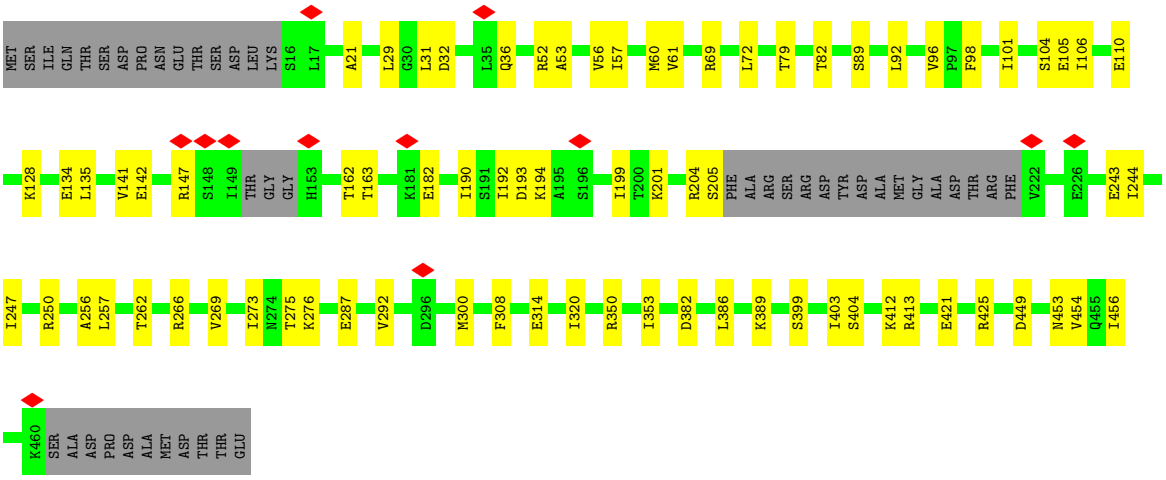
• Molecule 6: RuvB-like protein 2

Chain H:



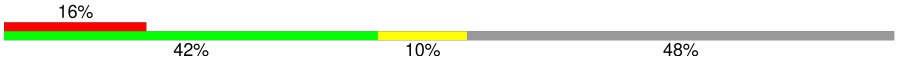
• Molecule 6: RuvB-like protein 2

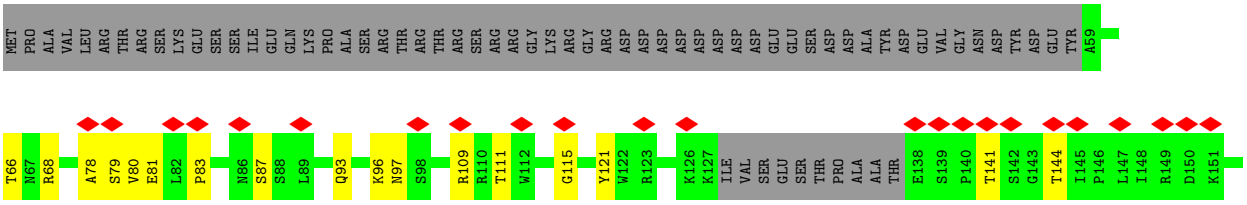
Chain J:

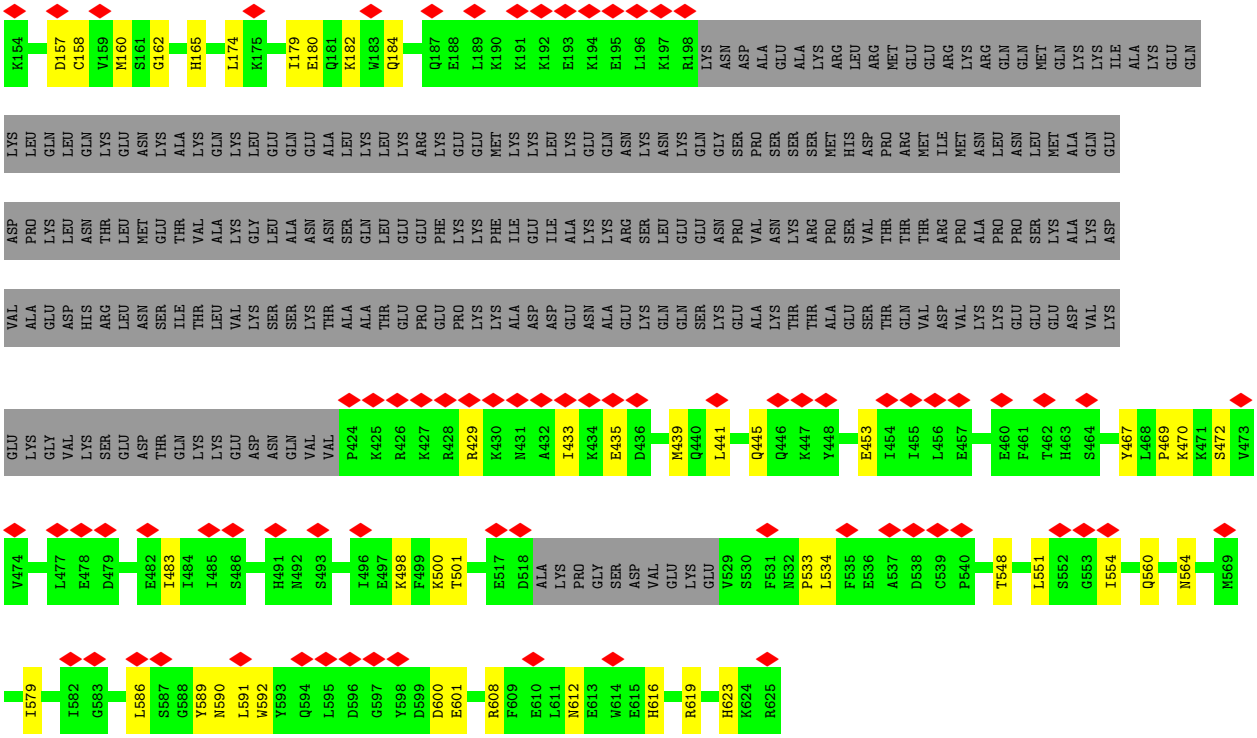


• Molecule 7: SWR1-complex protein 3

Chain K:







• Molecule 8: Histone H2A

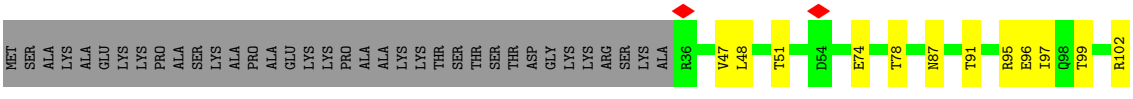
Chain Q:

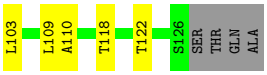
• Molecule 8: Histone H2A

Chain S:

• Molecule 9: Histone H2B

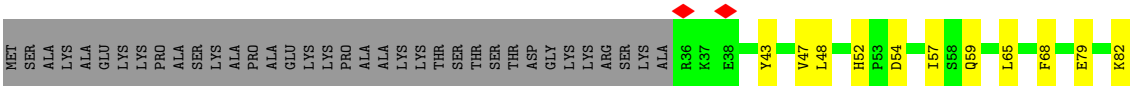
Chain R:

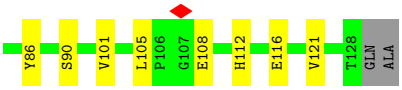




• Molecule 9: Histone H2B

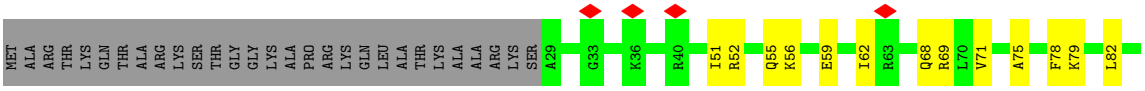
Chain T:

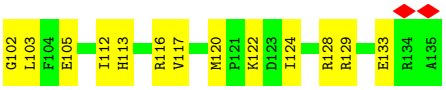




• Molecule 10: Histone H3

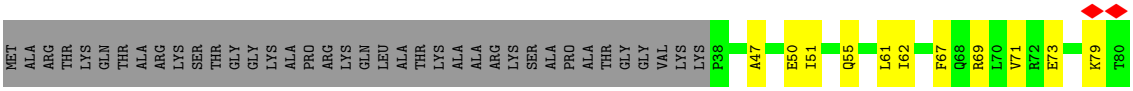
Chain U:





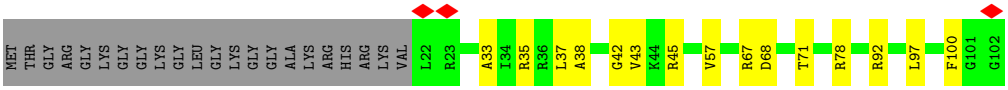
• Molecule 10: Histone H3

Chain W:



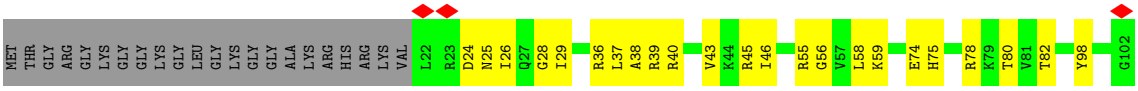
• Molecule 11: Histone H4

Chain V:



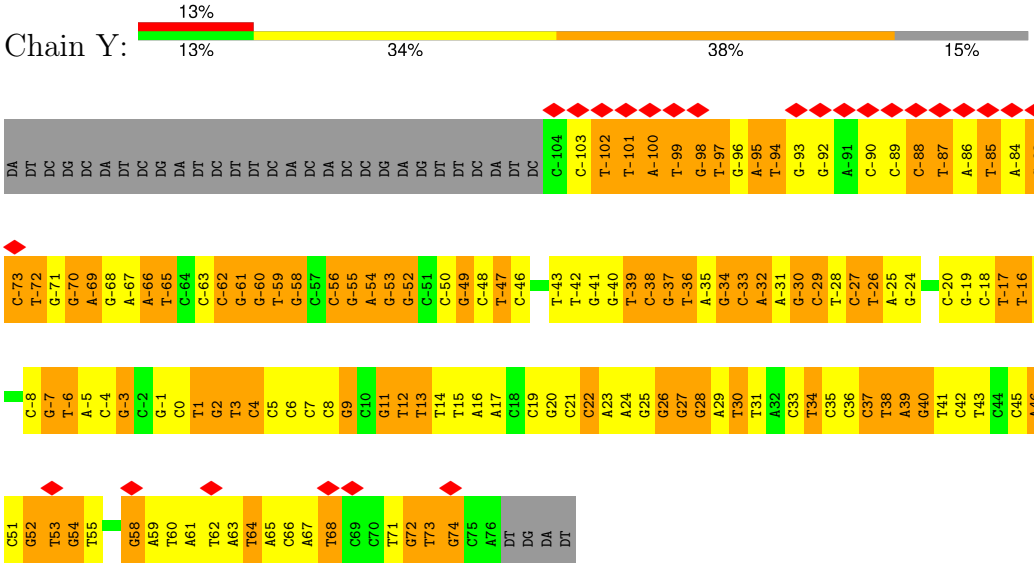
• Molecule 11: Histone H4

Chain X:



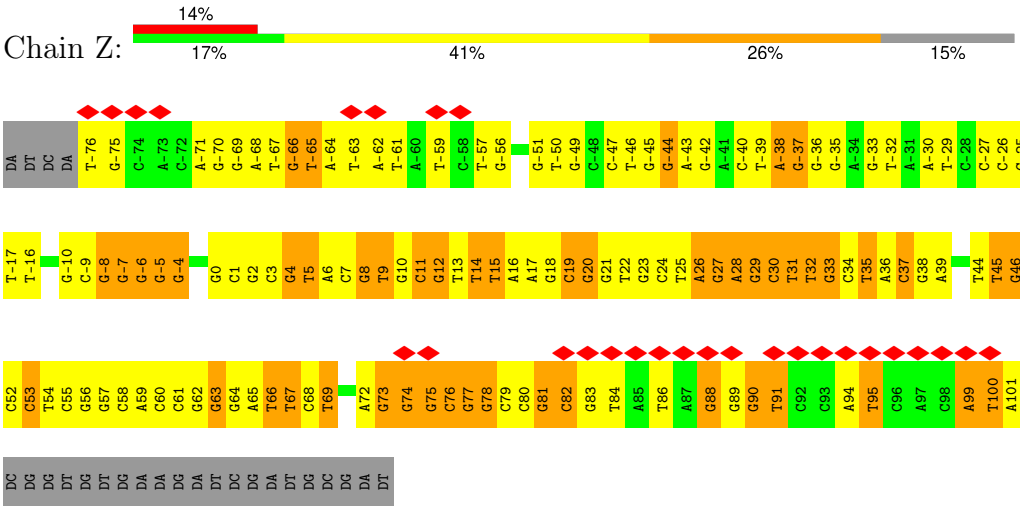
• Molecule 12: DNA (214-MER)

Chain Y:



• Molecule 13: DNA (214-MER)

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16524	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	48543	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.114	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: BEF, ZN, ADP, MG

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	0.25	0/6007	0.48	0/8104
2	B	0.25	0/2559	0.49	0/3432
3	C	0.25	0/3430	0.46	0/4650
4	D	0.24	0/1696	0.52	0/2283
5	E	0.24	0/3319	0.48	0/4487
5	G	0.25	0/3375	0.49	0/4564
5	I	0.25	0/3392	0.47	0/4587
6	F	0.24	0/3448	0.48	0/4648
6	H	0.25	0/3430	0.47	0/4623
6	J	0.24	0/3312	0.48	0/4462
7	K	0.24	0/2724	0.49	0/3650
8	Q	0.24	0/844	0.54	0/1139
8	S	0.26	0/830	0.55	0/1121
9	R	0.25	0/723	0.48	0/973
9	T	0.27	0/736	0.47	0/991
10	U	0.26	0/877	0.56	0/1176
10	W	0.25	0/819	0.57	0/1097
11	V	0.24	0/653	0.59	0/873
11	X	0.26	0/653	0.59	0/873
12	Y	0.67	0/4131	1.48	154/6368 (2.4%)
13	Z	0.65	0/4193	1.47	159/6475 (2.5%)
All	All	0.35	0/51151	0.77	313/70576 (0.4%)

There are no bond length outliers.

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Y	-72	DT	OP1-P-OP2	-8.04	107.54	119.60
12	Y	-85	DT	OP1-P-OP2	-7.89	107.76	119.60
12	Y	-87	DT	OP1-P-OP2	-7.85	107.83	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	61	DC	OP1-P-O3'	7.76	122.28	105.20
13	Z	-18	DG	OP1-P-OP2	-7.68	108.08	119.60
13	Z	32	DT	OP1-P-O3'	7.68	122.09	105.20
12	Y	39	DA	OP1-P-O3'	7.57	121.85	105.20
13	Z	-5	DG	OP1-P-O3'	7.54	121.80	105.20
12	Y	38	DT	OP1-P-OP2	-7.54	108.29	119.60
13	Z	99	DA	O4'-C1'-N9	7.49	113.24	108.00
12	Y	-102	DT	OP1-P-OP2	-7.49	108.37	119.60
12	Y	40	DG	OP1-P-OP2	-7.42	108.47	119.60
12	Y	-94	DT	OP1-P-OP2	-7.39	108.51	119.60
12	Y	48	DG	OP1-P-OP2	-7.36	108.56	119.60
13	Z	33	DG	OP1-P-OP2	-7.35	108.57	119.60
13	Z	62	DG	OP1-P-OP2	-7.33	108.60	119.60
12	Y	-73	DC	OP1-P-O3'	7.30	121.25	105.20
12	Y	-97	DT	OP1-P-OP2	-7.22	108.77	119.60
13	Z	-6	DG	OP1-P-OP2	-7.20	108.80	119.60
13	Z	5	DT	OP1-P-OP2	-7.16	108.86	119.60
12	Y	-34	DG	OP1-P-OP2	-7.14	108.89	119.60
13	Z	-10	DG	OP1-P-OP2	-7.14	108.89	119.60
12	Y	-16	DT	OP1-P-OP2	-7.14	108.89	119.60
12	Y	72	DG	OP1-P-OP2	-7.11	108.93	119.60
13	Z	-44	DG	OP1-P-OP2	-7.11	108.93	119.60
12	Y	-86	DA	OP1-P-O3'	7.10	120.81	105.20
12	Y	-101	DT	OP1-P-OP2	-7.08	108.98	119.60
12	Y	-65	DT	OP1-P-OP2	-7.07	109.00	119.60
13	Z	-37	DG	OP1-P-OP2	-7.05	109.02	119.60
13	Z	20	DG	OP1-P-OP2	-7.04	109.05	119.60
13	Z	27	DG	OP1-P-OP2	-7.02	109.08	119.60
12	Y	-88	DC	OP1-P-O3'	7.01	120.62	105.20
12	Y	-33	DC	OP1-P-OP2	-7.01	109.09	119.60
13	Z	-4	DG	OP1-P-OP2	-7.00	109.10	119.60
12	Y	47	DG	OP1-P-O3'	7.00	120.59	105.20
13	Z	56	DG	OP1-P-OP2	-6.98	109.12	119.60
13	Z	10	DG	OP1-P-OP2	-6.98	109.14	119.60
12	Y	-79	DG	OP1-P-OP2	-6.95	109.18	119.60
13	Z	86	DT	OP1-P-OP2	-6.94	109.19	119.60
13	Z	84	DT	OP1-P-OP2	-6.93	109.21	119.60
12	Y	20	DG	OP1-P-OP2	-6.91	109.23	119.60
13	Z	-46	DT	OP1-P-OP2	-6.91	109.23	119.60
12	Y	-26	DT	OP1-P-OP2	-6.91	109.24	119.60
12	Y	64	DT	OP1-P-OP2	-6.90	109.25	119.60
12	Y	-7	DG	OP1-P-OP2	-6.90	109.25	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Y	-59	DT	OP1-P-OP2	-6.89	109.27	119.60
12	Y	-1	DG	OP1-P-OP2	-6.88	109.28	119.60
13	Z	18	DG	OP1-P-OP2	-6.88	109.28	119.60
12	Y	-61	DG	OP1-P-OP2	-6.87	109.30	119.60
13	Z	35	DT	OP1-P-OP2	-6.87	109.30	119.60
12	Y	-49	DG	OP1-P-OP2	-6.87	109.30	119.60
13	Z	19	DC	OP1-P-O3'	6.86	120.28	105.20
13	Z	4	DG	OP1-P-OP2	-6.85	109.32	119.60
12	Y	-39	DT	OP1-P-OP2	-6.85	109.33	119.60
13	Z	21	DG	OP1-P-OP2	-6.85	109.33	119.60
13	Z	57	DG	OP1-P-OP2	-6.84	109.34	119.60
12	Y	27	DG	OP1-P-OP2	-6.84	109.34	119.60
13	Z	4	DG	OP2-P-O3'	6.84	120.24	105.20
12	Y	3	DT	OP1-P-OP2	-6.84	109.35	119.60
13	Z	-19	DG	OP1-P-OP2	-6.83	109.35	119.60
12	Y	58	DG	OP1-P-OP2	-6.83	109.36	119.60
13	Z	0	DG	OP1-P-OP2	-6.83	109.36	119.60
13	Z	-51	DG	OP1-P-OP2	-6.83	109.36	119.60
12	Y	-55	DG	OP1-P-OP2	-6.82	109.37	119.60
12	Y	-99	DT	OP1-P-OP2	-6.82	109.37	119.60
12	Y	-19	DG	OP1-P-OP2	-6.82	109.38	119.60
12	Y	37	DC	OP2-P-O3'	6.82	120.20	105.20
12	Y	52	DG	OP1-P-OP2	-6.82	109.37	119.60
13	Z	74	DG	OP1-P-OP2	-6.82	109.38	119.60
12	Y	-80	DG	OP1-P-OP2	-6.81	109.38	119.60
12	Y	-32	DA	OP1-P-OP2	-6.81	109.39	119.60
12	Y	-98	DG	OP1-P-OP2	-6.81	109.39	119.60
12	Y	-76	DG	OP1-P-OP2	-6.81	109.39	119.60
12	Y	2	DG	OP1-P-OP2	-6.81	109.39	119.60
13	Z	-32	DT	OP1-P-OP2	-6.80	109.39	119.60
12	Y	26	DG	OP1-P-OP2	-6.80	109.39	119.60
12	Y	1	DT	OP1-P-OP2	-6.80	109.40	119.60
13	Z	-23	DT	OP1-P-OP2	-6.80	109.40	119.60
12	Y	-37	DG	OP1-P-OP2	-6.80	109.40	119.60
13	Z	44	DT	OP1-P-OP2	-6.80	109.40	119.60
12	Y	-17	DT	OP1-P-OP2	-6.80	109.41	119.60
13	Z	-50	DT	OP1-P-OP2	-6.79	109.41	119.60
13	Z	91	DT	OP1-P-OP2	-6.79	109.41	119.60
12	Y	28	DG	OP1-P-OP2	-6.79	109.41	119.60
12	Y	-52	DG	OP1-P-OP2	-6.79	109.42	119.60
13	Z	51	DG	OP1-P-OP2	-6.79	109.42	119.60
12	Y	60	DT	OP1-P-OP2	-6.78	109.43	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	-8	DG	OP1-P-OP2	-6.78	109.43	119.60
13	Z	32	DT	OP1-P-OP2	-6.78	109.43	119.60
13	Z	22	DT	OP1-P-OP2	-6.78	109.43	119.60
13	Z	75	DG	OP1-P-OP2	-6.78	109.44	119.60
12	Y	43	DT	OP1-P-OP2	-6.77	109.44	119.60
13	Z	-33	DG	OP1-P-OP2	-6.77	109.44	119.60
13	Z	-49	DG	OP1-P-OP2	-6.77	109.44	119.60
13	Z	12	DG	OP1-P-OP2	-6.77	109.45	119.60
13	Z	25	DT	OP1-P-OP2	-6.76	109.45	119.60
13	Z	31	DT	OP1-P-OP2	-6.76	109.45	119.60
12	Y	74	DG	OP1-P-OP2	-6.76	109.46	119.60
13	Z	-24	DT	OP1-P-OP2	-6.76	109.46	119.60
12	Y	30	DT	OP1-P-OP2	-6.75	109.47	119.60
13	Z	-75	DG	OP1-P-OP2	-6.75	109.47	119.60
13	Z	78	DG	OP1-P-OP2	-6.75	109.47	119.60
12	Y	-60	DG	OP1-P-OP2	-6.75	109.48	119.60
12	Y	-58	DG	OP1-P-OP2	-6.75	109.48	119.60
13	Z	-67	DT	OP1-P-OP2	-6.75	109.48	119.60
13	Z	-59	DT	OP1-P-OP2	-6.75	109.48	119.60
13	Z	29	DG	OP1-P-OP2	-6.75	109.48	119.60
13	Z	73	DG	OP1-P-OP2	-6.75	109.48	119.60
13	Z	38	DG	OP1-P-OP2	-6.75	109.48	119.60
13	Z	66	DT	OP1-P-OP2	-6.75	109.48	119.60
13	Z	103	DG	OP1-P-OP2	-6.74	109.49	119.60
13	Z	-17	DT	OP1-P-OP2	-6.74	109.49	119.60
13	Z	-61	DT	OP1-P-OP2	-6.73	109.50	119.60
13	Z	15	DT	OP1-P-OP2	-6.73	109.51	119.60
12	Y	-40	DG	OP1-P-OP2	-6.73	109.51	119.60
13	Z	-39	DT	OP1-P-OP2	-6.73	109.51	119.60
12	Y	-93	DG	OP1-P-OP2	-6.73	109.51	119.60
12	Y	-28	DT	OP1-P-OP2	-6.73	109.51	119.60
12	Y	13	DT	OP1-P-OP2	-6.73	109.51	119.60
12	Y	53	DT	OP1-P-OP2	-6.72	109.51	119.60
13	Z	67	DT	OP1-P-OP2	-6.72	109.51	119.60
12	Y	-47	DT	OP1-P-OP2	-6.72	109.52	119.60
12	Y	-82	DG	OP1-P-OP2	-6.72	109.52	119.60
12	Y	62	DT	OP1-P-OP2	-6.72	109.53	119.60
12	Y	12	DT	OP1-P-OP2	-6.71	109.53	119.60
13	Z	-22	DG	OP1-P-OP2	-6.71	109.53	119.60
12	Y	25	DG	OP1-P-OP2	-6.71	109.53	119.60
13	Z	-65	DT	OP1-P-OP2	-6.71	109.54	119.60
13	Z	95	DT	OP1-P-OP2	-6.71	109.54	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	-7	DG	OP1-P-OP2	-6.70	109.55	119.60
13	Z	-42	DG	OP1-P-OP2	-6.70	109.55	119.60
12	Y	-30	DG	OP1-P-OP2	-6.70	109.56	119.60
12	Y	55	DT	OP1-P-OP2	-6.69	109.56	119.60
13	Z	-57	DT	OP1-P-OP2	-6.69	109.56	119.60
13	Z	-56	DG	OP1-P-OP2	-6.69	109.56	119.60
13	Z	14	DT	OP1-P-OP2	-6.69	109.57	119.60
12	Y	-92	DG	OP1-P-OP2	-6.68	109.58	119.60
13	Z	-70	DG	OP1-P-OP2	-6.68	109.59	119.60
13	Z	-69	DG	OP1-P-OP2	-6.67	109.59	119.60
13	Z	-76	DT	OP1-P-OP2	-6.67	109.59	119.60
12	Y	73	DT	OP1-P-OP2	-6.67	109.59	119.60
13	Z	-36	DG	OP1-P-OP2	-6.67	109.59	119.60
13	Z	100	DT	OP1-P-OP2	-6.67	109.60	119.60
12	Y	54	DG	OP1-P-OP2	-6.67	109.60	119.60
13	Z	8	DG	OP1-P-OP2	-6.67	109.60	119.60
13	Z	64	DG	OP1-P-OP2	-6.67	109.60	119.60
13	Z	77	DG	OP1-P-OP2	-6.67	109.60	119.60
13	Z	104	DG	OP1-P-OP2	-6.66	109.60	119.60
12	Y	-71	DG	OP1-P-OP2	-6.66	109.61	119.60
13	Z	-29	DT	OP1-P-OP2	-6.66	109.61	119.60
13	Z	23	DG	OP1-P-OP2	-6.66	109.61	119.60
12	Y	11	DG	OP1-P-OP2	-6.66	109.61	119.60
12	Y	31	DT	OP1-P-OP2	-6.66	109.61	119.60
12	Y	-103	DC	OP1-P-O3'	6.65	119.84	105.20
12	Y	-68	DG	OP1-P-OP2	-6.65	109.63	119.60
13	Z	-63	DT	OP1-P-OP2	-6.65	109.63	119.60
12	Y	47	DG	OP1-P-OP2	-6.64	109.63	119.60
13	Z	46	DG	OP1-P-OP2	-6.64	109.64	119.60
13	Z	89	DG	OP1-P-OP2	-6.63	109.65	119.60
12	Y	-6	DT	OP1-P-OP2	-6.63	109.65	119.60
13	Z	90	DG	OP1-P-OP2	-6.63	109.65	119.60
12	Y	-41	DG	OP1-P-OP2	-6.63	109.66	119.60
13	Z	81	DG	OP1-P-OP2	-6.62	109.67	119.60
13	Z	50	DG	OP1-P-OP2	-6.61	109.69	119.60
12	Y	14	DT	OP1-P-OP2	-6.60	109.70	119.60
12	Y	68	DT	OP1-P-OP2	-6.60	109.70	119.60
12	Y	-53	DG	OP1-P-OP2	-6.59	109.71	119.60
13	Z	54	DT	OP1-P-OP2	-6.59	109.71	119.60
12	Y	71	DT	OP1-P-O3'	6.59	119.69	105.20
13	Z	83	DG	OP1-P-OP2	-6.58	109.73	119.60
12	Y	-96	DG	OP1-P-OP2	-6.58	109.73	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	-21	DG	OP1-P-OP2	-6.58	109.73	119.60
13	Z	45	DT	OP1-P-OP2	-6.58	109.74	119.60
12	Y	71	DT	OP1-P-OP2	-6.57	109.75	119.60
13	Z	88	DG	OP1-P-OP2	-6.56	109.75	119.60
12	Y	-70	DG	OP1-P-OP2	-6.56	109.76	119.60
12	Y	-36	DT	OP1-P-OP2	-6.56	109.76	119.60
13	Z	-66	DG	OP1-P-OP2	-6.55	109.77	119.60
12	Y	34	DT	OP1-P-OP2	-6.54	109.79	119.60
12	Y	15	DT	OP1-P-OP2	-6.53	109.80	119.60
13	Z	2	DG	OP1-P-OP2	-6.53	109.80	119.60
12	Y	-42	DT	OP1-P-OP2	-6.51	109.83	119.60
13	Z	-38	DA	OP1-P-O3'	6.51	119.53	105.20
13	Z	-5	DG	OP1-P-OP2	-6.50	109.85	119.60
12	Y	41	DT	OP1-P-OP2	-6.49	109.86	119.60
12	Y	-11	DG	OP1-P-OP2	-6.48	109.88	119.60
12	Y	-100	DA	OP1-P-O3'	6.46	119.42	105.20
12	Y	1	DT	OP1-P-O3'	6.46	119.42	105.20
13	Z	24	DC	OP2-P-O3'	6.42	119.33	105.20
12	Y	-97	DT	O4'-C1'-N1	-6.42	103.50	108.00
12	Y	-38	DC	OP1-P-O3'	6.42	119.32	105.20
12	Y	-102	DT	OP1-P-O3'	6.41	119.29	105.20
13	Z	69	DT	OP1-P-OP2	-6.39	110.02	119.60
13	Z	-19	DG	OP1-P-O3'	6.36	119.19	105.20
12	Y	-24	DG	OP1-P-OP2	-6.33	110.10	119.60
13	Z	77	DG	O4'-C1'-N9	6.33	112.43	108.00
13	Z	13	DT	OP1-P-OP2	-6.32	110.12	119.60
12	Y	-43	DT	OP1-P-OP2	-6.31	110.14	119.60
13	Z	-16	DT	OP1-P-OP2	-6.30	110.14	119.60
13	Z	73	DG	O4'-C1'-N9	6.26	112.38	108.00
13	Z	56	DG	OP1-P-O3'	6.18	118.79	105.20
12	Y	-53	DG	OP1-P-O3'	6.15	118.73	105.20
13	Z	-35	DG	OP1-P-OP2	-6.14	110.38	119.60
13	Z	-7	DG	OP1-P-O3'	6.14	118.71	105.20
12	Y	-50	DC	OP1-P-O3'	6.12	118.65	105.20
12	Y	26	DG	OP1-P-O3'	6.09	118.61	105.20
12	Y	-35	DA	OP1-P-O3'	6.08	118.58	105.20
13	Z	3	DC	OP1-P-O3'	6.08	118.56	105.20
13	Z	-40	DC	OP1-P-O3'	6.07	118.55	105.20
12	Y	-20	DC	OP1-P-O3'	6.05	118.51	105.20
12	Y	-69	DA	OP1-P-O3'	6.03	118.47	105.20
12	Y	-54	DA	O4'-C1'-N9	-6.03	103.78	108.00
13	Z	-37	DG	OP1-P-O3'	6.03	118.46	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	26	DA	OP1-P-O3'	5.99	118.38	105.20
12	Y	9	DG	OP1-P-OP2	-5.95	110.68	119.60
13	Z	-25	DC	OP1-P-O3'	5.95	118.28	105.20
12	Y	-61	DG	OP1-P-O3'	5.92	118.22	105.20
13	Z	77	DG	OP1-P-O3'	5.91	118.20	105.20
12	Y	-17	DT	OP1-P-O3'	5.91	118.19	105.20
12	Y	24	DA	OP1-P-O3'	5.89	118.16	105.20
12	Y	-29	DC	OP1-P-O3'	5.88	118.13	105.20
12	Y	-59	DT	OP1-P-O3'	5.86	118.10	105.20
13	Z	1	DC	O4'-C1'-N1	5.83	112.08	108.00
12	Y	19	DC	OP1-P-O3'	5.83	118.03	105.20
13	Z	73	DG	OP1-P-O3'	5.80	117.96	105.20
12	Y	-3	DG	OP1-P-OP2	-5.79	110.91	119.60
13	Z	48	DG	OP1-P-OP2	-5.78	110.92	119.60
12	Y	-66	DA	OP1-P-O3'	5.78	117.91	105.20
13	Z	31	DT	OP1-P-O3'	5.74	117.84	105.20
12	Y	-99	DT	OP1-P-O3'	5.73	117.80	105.20
13	Z	11	DC	OP1-P-O3'	5.72	117.78	105.20
13	Z	34	DC	OP2-P-O3'	5.71	117.75	105.20
12	Y	33	DC	OP1-P-O3'	5.69	117.72	105.20
13	Z	45	DT	OP1-P-O3'	5.68	117.70	105.20
12	Y	-89	DC	O4'-C1'-N1	-5.68	104.02	108.00
13	Z	55	DC	OP1-P-O3'	5.68	117.69	105.20
12	Y	-71	DG	OP1-P-O3'	5.65	117.63	105.20
13	Z	-66	DG	OP1-P-O3'	5.64	117.62	105.20
12	Y	-83	DC	OP1-P-O3'	5.64	117.61	105.20
13	Z	9	DT	OP1-P-O3'	5.63	117.59	105.20
13	Z	37	DC	OP1-P-O3'	5.63	117.58	105.20
12	Y	-33	DC	OP1-P-O3'	5.62	117.55	105.20
13	Z	66	DT	OP1-P-O3'	5.59	117.50	105.20
13	Z	-50	DT	OP1-P-O3'	5.59	117.50	105.20
13	Z	63	DG	OP1-P-O3'	5.58	117.49	105.20
12	Y	-40	DG	OP1-P-O3'	5.58	117.48	105.20
13	Z	72	DA	OP1-P-O3'	5.58	117.47	105.20
13	Z	-9	DC	OP1-P-O3'	5.57	117.45	105.20
12	Y	-72	DT	OP1-P-O3'	5.56	117.43	105.20
13	Z	83	DG	OP2-P-O3'	5.55	117.42	105.20
13	Z	1	DC	OP1-P-O3'	5.54	117.39	105.20
13	Z	67	DT	O4'-C1'-N1	5.53	111.87	108.00
13	Z	-45	DG	OP1-P-OP2	-5.52	111.32	119.60
13	Z	7	DC	OP1-P-O3'	5.52	117.34	105.20
13	Z	73	DG	C1'-O4'-C4'	-5.49	104.61	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Y	-81	DC	OP1-P-O3'	5.47	117.24	105.20
13	Z	-8	DG	OP1-P-O3'	5.47	117.23	105.20
12	Y	27	DG	O4'-C1'-N9	5.46	111.82	108.00
13	Z	-43	DA	OP1-P-O3'	5.45	117.20	105.20
12	Y	27	DG	OP1-P-O3'	5.44	117.17	105.20
12	Y	22	DC	O4'-C1'-N1	5.43	111.80	108.00
13	Z	-33	DG	OP1-P-O3'	5.42	117.12	105.20
12	Y	-95	DA	OP1-P-O3'	5.40	117.08	105.20
13	Z	9	DT	OP1-P-OP2	-5.38	111.53	119.60
12	Y	-98	DG	OP1-P-O3'	5.37	117.01	105.20
12	Y	-62	DC	OP1-P-O3'	5.34	116.95	105.20
12	Y	46	DA	OP1-P-O3'	5.34	116.95	105.20
13	Z	76	DC	OP1-P-O3'	5.34	116.94	105.20
12	Y	73	DT	OP1-P-O3'	5.33	116.94	105.20
12	Y	-14	DA	O4'-C1'-N9	-5.31	104.28	108.00
12	Y	42	DC	OP1-P-O3'	5.29	116.84	105.20
12	Y	51	DC	OP1-P-O3'	5.29	116.83	105.20
13	Z	-47	DC	OP1-P-O3'	5.28	116.81	105.20
12	Y	-80	DG	OP1-P-O3'	5.26	116.77	105.20
12	Y	-68	DG	O4'-C1'-N9	5.26	111.68	108.00
12	Y	-8	DC	OP1-P-O3'	5.26	116.77	105.20
13	Z	-46	DT	O4'-C1'-N1	5.26	111.68	108.00
13	Z	38	DG	O4'-C1'-N9	5.25	111.68	108.00
12	Y	-55	DG	O4'-C1'-N9	-5.25	104.33	108.00
12	Y	-27	DC	OP2-P-O3'	5.24	116.73	105.20
13	Z	44	DT	OP1-P-O3'	5.24	116.72	105.20
12	Y	-97	DT	OP1-P-O3'	5.23	116.70	105.20
12	Y	-54	DA	OP1-P-O3'	5.22	116.69	105.20
13	Z	-18	DG	O4'-C1'-N9	-5.22	104.34	108.00
13	Z	30	DC	OP1-P-O3'	5.22	116.69	105.20
12	Y	-42	DT	OP1-P-O3'	5.22	116.68	105.20
13	Z	-76	DT	OP1-P-O3'	5.21	116.65	105.20
13	Z	-71	DA	OP1-P-O3'	5.21	116.65	105.20
12	Y	-90	DC	O4'-C1'-N1	-5.19	104.37	108.00
12	Y	52	DG	OP1-P-O3'	5.19	116.62	105.20
13	Z	83	DG	O4'-C1'-N9	5.18	111.63	108.00
12	Y	-93	DG	OP1-P-O3'	5.17	116.58	105.20
12	Y	40	DG	OP1-P-O3'	5.17	116.57	105.20
13	Z	12	DG	OP1-P-O3'	5.17	116.57	105.20
12	Y	61	DA	OP1-P-O3'	5.16	116.56	105.20
13	Z	24	DC	O4'-C1'-N1	-5.14	104.40	108.00
13	Z	74	DG	OP1-P-O3'	5.14	116.52	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	-46	DT	OP1-P-O3'	5.12	116.47	105.20
12	Y	-34	DG	OP1-P-O3'	5.11	116.45	105.20
13	Z	53	DC	OP1-P-O3'	5.11	116.45	105.20
13	Z	-30	DA	OP1-P-O3'	5.11	116.44	105.20
13	Z	-62	DA	OP1-P-O3'	5.11	116.43	105.20
13	Z	-68	DA	OP1-P-O3'	5.10	116.42	105.20
13	Z	102	DA	OP1-P-O3'	5.09	116.40	105.20
12	Y	-73	DC	O4'-C4'-C3'	-5.08	102.47	104.50
12	Y	-56	DC	OP1-P-O3'	5.07	116.36	105.20
12	Y	-71	DG	C1'-O4'-C4'	-5.05	105.05	110.10
12	Y	-77	DC	OP1-P-O3'	5.05	116.31	105.20
12	Y	4	DC	C1'-O4'-C4'	-5.05	105.05	110.10
13	Z	82	DC	OP1-P-O3'	5.03	116.28	105.20
13	Z	28	DA	OP1-P-O3'	5.03	116.25	105.20
12	Y	-43	DT	OP1-P-O3'	5.02	116.25	105.20
13	Z	88	DG	OP1-P-O3'	5.00	116.21	105.20

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	5894	0	5984	115	0
2	B	2513	0	2547	46	0
3	C	3336	0	3256	62	0
4	D	1671	0	1722	29	0
5	E	3281	0	3425	47	0
5	G	3334	0	3472	39	0
5	I	3351	0	3490	53	0
6	F	3410	0	3484	41	0
6	H	3393	0	3456	62	0
6	J	3279	0	3371	58	0
7	K	2671	0	2721	50	0
8	Q	833	0	883	21	0
8	S	819	0	865	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	R	713	0	736	13	0
9	T	726	0	748	21	0
10	U	864	0	908	27	0
10	W	807	0	844	24	0
11	V	646	0	687	15	0
11	X	646	0	687	28	0
12	Y	3688	0	2032	96	0
13	Z	3733	0	2029	67	0
14	A	27	0	12	3	0
14	C	27	0	12	1	0
14	E	27	0	12	1	0
14	F	27	0	12	4	0
14	G	27	0	12	0	0
14	H	27	0	12	4	0
14	I	27	0	12	2	0
14	J	27	0	12	1	0
15	A	4	0	0	1	0
15	C	4	0	0	1	0
16	A	1	0	0	0	0
16	C	1	0	0	0	0
16	E	1	0	0	0	0
16	F	1	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
17	D	2	0	0	0	0
All	All	49842	0	47443	787	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 (787) 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)
6:H:17:LEU:HB2	5:I:293:ALA:HB2	1.57	0.84
4:D:259:CYS:SG	4:D:261:ASN:ND2	2.55	0.80
8:Q:64:LEU:HD22	9:R:48:LEU:HD13	1.65	0.78
2:B:688:LEU:HD12	4:D:233:ARG:HE	1.49	0.77
3:C:15:ILE:HB	3:C:28:ALA:HB3	1.66	0.75
11:X:29:ILE:HD11	11:X:55:ARG:HG2	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:130:LYS:HG2	6:H:236:VAL:HG12	1.69	0.73
3:C:288:ARG:NH1	3:C:294:ASN:OD1	2.22	0.72
6:F:281:LYS:HD2	6:F:288:ILE:HD12	1.71	0.72
8:S:113:HIS:HB3	8:S:116:LEU:HD23	1.71	0.72
7:K:79:SER:HG	7:K:592:TRP:HE1	1.38	0.72
9:T:59:GLN:NE2	12:Y:-54:DA:OP2	2.23	0.71
10:U:120:MET:SD	10:U:122:LYS:NZ	2.63	0.71
12:Y:-73:DC:H2'	12:Y:-72:DT:H71	1.72	0.71
12:Y:-59:DT:H2'	12:Y:-58:DG:C8	2.26	0.71
10:W:61:LEU:HD21	11:X:36:ARG:HB2	1.73	0.71
12:Y:36:DC:H2"	12:Y:37:DC:C5	2.26	0.70
5:I:42:LYS:O	5:I:55:ARG:NH2	2.25	0.69
13:Z:99:DA:H2"	13:Z:100:DT:H72	1.74	0.69
6:F:427:TYR:O	6:F:435:ARG:NH2	2.23	0.69
8:Q:69:ASN:OD1	8:Q:72:ARG:NH2	2.25	0.69
6:H:201:LYS:O	6:H:220:ARG:NH2	2.26	0.69
6:F:47:GLN:HG3	6:F:50:ALA:HB3	1.75	0.68
1:A:745:TRP:HB2	2:B:241:ARG:HH22	1.57	0.68
3:C:341:LEU:HD21	3:C:349:MET:HE3	1.76	0.68
10:W:107:THR:HG21	10:W:124:ILE:HD13	1.76	0.68
5:E:393:LEU:HD23	5:E:434:ILE:HD11	1.76	0.68
5:E:76:LEU:HB2	5:E:367:LEU:HD23	1.76	0.68
5:I:122:MET:SD	5:I:323:TYR:OH	2.52	0.67
2:B:695:GLN:O	7:K:608:ARG:NH1	2.28	0.67
2:B:787:PRO:HB2	2:B:791:VAL:HG11	1.76	0.67
6:J:413:ARG:NH1	6:J:421:GLU:OE2	2.27	0.67
12:Y:6:DC:H2"	12:Y:7:DC:C5	2.29	0.67
11:V:45:ARG:HH11	13:Z:8:DG:H5'	1.60	0.67
10:U:128:ARG:NH1	10:U:133:GLU:OE1	2.28	0.66
3:C:203:VAL:HA	3:C:208:PRO:HA	1.77	0.66
5:I:49:VAL:N	14:I:901:ADP:N1	2.42	0.66
13:Z:-38:DA:H2"	13:Z:-37:DG:C8	2.31	0.66
9:T:79:GLU:OE2	11:V:92:ARG:NH1	2.27	0.66
12:Y:16:DA:C8	12:Y:16:DA:H5'	2.31	0.66
5:G:117:LYS:HD2	5:G:320:ILE:HD11	1.77	0.66
6:H:102:ALA:HB3	6:H:105:GLU:HG3	1.78	0.66
5:G:154:ASN:ND2	5:G:157:GLY:O	2.29	0.66
1:A:1267:ILE:HD11	1:A:1339:TYR:HB2	1.77	0.66
5:I:275:PRO:HD3	6:J:250:ARG:HD3	1.77	0.66
3:C:256:SER:OG	3:C:368:ARG:NH1	2.29	0.65
5:E:135:GLU:OE1	5:E:245:GLN:NE2	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1354:ARG:HD3	1:A:1357:ARG:HH12	1.62	0.65
2:B:787:PRO:HA	7:K:548:THR:HG21	1.77	0.65
5:G:138:GLU:HG2	5:G:240:LYS:HG2	1.76	0.65
7:K:78:ALA:HB2	7:K:591:LEU:HD23	1.77	0.65
5:I:196:ILE:O	5:I:214:ARG:NH1	2.30	0.65
2:B:787:PRO:HG2	2:B:791:VAL:HG21	1.79	0.65
1:A:1279:GLU:O	1:A:1283:ASN:ND2	2.29	0.65
12:Y:-37:DG:H2"	12:Y:-36:DT:C5	2.32	0.65
10:W:62:ILE:HB	10:W:93:GLN:HE21	1.62	0.65
10:W:93:GLN:NE2	10:W:97:GLU:OE2	2.27	0.65
3:C:58:ARG:NH2	4:D:166:VAL:O	2.29	0.64
5:G:29:HIS:HB3	5:G:390:VAL:HG21	1.80	0.64
12:Y:-39:DT:H2"	12:Y:-38:DC:C6	2.32	0.64
5:I:43:ARG:HD3	5:I:44:VAL:HG23	1.79	0.64
13:Z:19:DC:H2'	13:Z:20:DG:C8	2.32	0.64
13:Z:30:DC:H2"	13:Z:31:DT:H72	1.79	0.64
5:I:51:GLN:NE2	5:I:373:LEU:O	2.30	0.64
8:S:50:VAL:HG13	9:T:121:VAL:HG22	1.80	0.64
1:A:1370:VAL:HG21	1:A:1380:LEU:HD22	1.80	0.63
6:F:134:GLU:OE2	6:F:232:ARG:NH1	2.32	0.63
6:H:251:THR:HG23	6:H:252:GLN:HG2	1.80	0.63
1:A:1066:THR:O	6:H:223:GLN:NE2	2.30	0.63
7:K:174:LEU:HB3	7:K:453:GLU:HB2	1.81	0.63
2:B:711:LEU:O	7:K:109:ARG:NH1	2.29	0.63
3:C:323:SER:O	4:D:101:ARG:NH1	2.31	0.63
2:B:747:GLU:HG3	2:B:766:GLN:HE22	1.64	0.62
6:F:431:LEU:HD11	5:G:371:ARG:HE	1.64	0.62
6:J:72:LEU:HD23	6:J:353:ILE:HG12	1.82	0.62
6:F:298:VAL:HG21	6:F:323:MET:HB3	1.80	0.62
1:A:817:ARG:NH1	1:A:844:ASN:O	2.33	0.62
1:A:721:ASP:H	1:A:727:LYS:HE2	1.64	0.62
12:Y:39:DA:H1'	12:Y:40:DG:N7	2.15	0.62
1:A:792:LYS:NZ	13:Z:63:DG:OP1	2.32	0.62
8:Q:108:VAL:HG23	10:U:55:GLN:HE21	1.65	0.62
3:C:341:LEU:O	3:C:346:ARG:NH2	2.33	0.62
5:E:331:ASN:HA	6:J:21:ALA:HB2	1.82	0.62
12:Y:-61:DG:H2'	12:Y:-60:DG:C8	2.35	0.62
6:H:179:LEU:HD22	6:H:184:VAL:HG11	1.81	0.61
6:H:331:LYS:HA	6:H:338:LYS:HA	1.80	0.61
1:A:1391:ASN:O	1:A:1395:GLN:NE2	2.32	0.61
6:J:269:VAL:O	6:J:273:ILE:HG12	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:52:LEU:HD22	9:R:97:ILE:HG21	1.81	0.61
1:A:1268:PHE:HE1	1:A:1319:LEU:HD13	1.66	0.61
5:G:317:ASP:OD1	5:G:348:ARG:NH1	2.34	0.61
6:J:250:ARG:HH22	6:J:256:ALA:HB2	1.64	0.61
3:C:126:ASP:OD1	3:C:127:SER:N	2.34	0.61
5:G:134:LYS:HG2	5:G:244:VAL:HG12	1.82	0.61
12:Y:1:DT:H2'	12:Y:2:DG:C8	2.36	0.60
2:B:196:ARG:NH2	8:S:93:GLU:OE2	2.33	0.60
5:G:317:ASP:H	5:G:320:ILE:HD12	1.66	0.60
7:K:111:THR:O	7:K:115:GLY:N	2.32	0.60
12:Y:-102:DT:H2"	12:Y:-101:DT:H71	1.82	0.60
6:H:83:ALA:N	14:H:501:ADP:O1A	2.31	0.60
12:Y:-15:DA:H1'	12:Y:-14:DA:C8	2.37	0.60
6:J:92:LEU:HG	6:J:96:VAL:HG11	1.83	0.60
7:K:483:ILE:O	7:K:551:LEU:N	2.27	0.60
12:Y:37:DC:H2"	12:Y:38:DT:C5	2.36	0.60
2:B:240:GLU:HA	2:B:243:ARG:HG2	1.82	0.60
6:H:398:TYR:OH	6:H:435:ARG:NH2	2.34	0.60
5:I:380:ILE:HG12	5:I:412:LEU:HD13	1.84	0.60
9:R:74:GLU:O	9:R:78:THR:HG23	2.02	0.60
13:Z:35:DT:H2"	13:Z:36:DA:C8	2.37	0.60
5:I:241:LYS:HE2	5:I:243:ILE:HD11	1.84	0.60
4:D:110:PHE:HA	4:D:113:LEU:HD23	1.83	0.59
12:Y:4:DC:H2"	12:Y:5:DC:C5	2.37	0.59
13:Z:15:DT:H5'	13:Z:15:DT:C6	2.36	0.59
5:I:413:ARG:NH2	14:I:901:ADP:O2A	2.29	0.59
6:H:158:LEU:HB2	6:H:171:LEU:HD11	1.83	0.59
3:C:110:GLU:O	3:C:114:HIS:ND1	2.28	0.59
5:G:111:TYR:OH	5:G:348:ARG:NH1	2.35	0.59
1:A:735:LEU:HA	1:A:738:LEU:HD12	1.84	0.59
5:E:83:THR:HG22	5:E:372:THR:HG22	1.84	0.59
6:H:298:VAL:HG21	6:H:323:MET:HB3	1.84	0.59
6:J:399:SER:O	6:J:403:ILE:HG13	2.03	0.59
3:C:309:GLU:HA	3:C:312:THR:HG22	1.84	0.59
5:E:132:ARG:NH2	5:E:246:ASP:OD2	2.36	0.59
13:Z:-8:DG:H5'	13:Z:-8:DG:C8	2.37	0.59
1:A:846:GLN:N	1:A:846:GLN:OE1	2.36	0.58
2:B:680:ILE:HG23	3:C:209:TYR:CZ	2.38	0.58
6:J:32:ASP:OD1	6:J:36:GLN:N	2.36	0.58
12:Y:26:DG:C8	12:Y:26:DG:H5'	2.39	0.58
5:E:33:LEU:HB3	5:E:35:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:173:ALA:HB3	5:G:234:LYS:HA	1.86	0.58
12:Y:37:DC:H2"	12:Y:38:DT:C6	2.38	0.58
13:Z:26:DA:H2"	13:Z:27:DG:C8	2.39	0.58
5:E:280:ILE:HG23	5:E:284:LEU:HD23	1.84	0.58
3:C:67:THR:HG21	4:D:208:LEU:HB2	1.86	0.58
12:Y:46:DA:H1'	12:Y:47:DG:C8	2.38	0.58
1:A:823:LEU:HB2	1:A:850:LEU:HD23	1.85	0.57
6:H:306:PHE:O	6:H:310:ASN:ND2	2.37	0.57
6:J:256:ALA:HB1	6:J:262:THR:HG22	1.86	0.57
13:Z:-7:DG:H2"	13:Z:-6:DG:C8	2.39	0.57
1:A:1264:ARG:HD3	1:A:1362:ARG:HH22	1.69	0.57
10:W:85:GLN:HE22	11:X:82:THR:HA	1.69	0.57
6:F:134:GLU:HG3	6:F:232:ARG:HG2	1.86	0.57
1:A:841:LEU:HD11	1:A:872:PRO:HB3	1.86	0.57
6:J:182:GLU:OE1	6:J:201:LYS:NZ	2.38	0.57
13:Z:-65:DT:H1'	13:Z:-64:DA:C5	2.40	0.57
1:A:810:GLN:N	1:A:810:GLN:OE1	2.36	0.57
1:A:825:GLU:OE1	1:A:827:HIS:NE2	2.35	0.57
1:A:1197:LEU:HD12	5:E:266:ILE:HG23	1.86	0.57
1:A:815:ARG:NH1	13:Z:60:DC:O2	2.37	0.57
12:Y:-34:DG:C8	12:Y:-34:DG:H5'	2.40	0.57
1:A:1191:ASP:OD1	1:A:1191:ASP:N	2.38	0.57
6:H:81:LYS:NZ	6:H:326:ASN:HB3	2.20	0.57
6:H:243:GLU:HA	6:H:257:LEU:HD21	1.87	0.56
5:I:25:ALA:O	5:I:387:ARG:NH2	2.31	0.56
5:I:121:LEU:HD21	5:I:324:LEU:HG	1.87	0.56
1:A:1298:ILE:H	1:A:1298:ILE:HD12	1.70	0.56
7:K:483:ILE:HD12	7:K:554:ILE:HD12	1.87	0.56
11:V:45:ARG:NH1	13:Z:8:DG:H5'	2.19	0.56
5:E:118:THR:HG21	6:J:105:GLU:HG2	1.86	0.56
5:E:338:LEU:HD12	5:E:367:LEU:HD21	1.86	0.56
6:F:45:VAL:O	14:F:501:ADP:N6	2.34	0.56
1:A:938:GLU:OE1	1:A:940:GLN:N	2.36	0.56
1:A:1089:PHE:HD1	1:A:1105:LYS:HD2	1.71	0.56
2:B:710:CYS:HB2	2:B:729:SER:HB3	1.86	0.56
3:C:25:PRO:HB3	3:C:397:TRP:CE2	2.41	0.56
6:J:82:THR:HG23	14:J:501:ADP:O2B	2.06	0.56
5:I:121:LEU:HD23	5:I:323:TYR:HD2	1.71	0.56
1:A:1228:GLN:NE2	5:E:262:GLY:O	2.38	0.56
10:W:61:LEU:HD22	11:X:37:LEU:HG	1.88	0.56
6:J:192:ILE:HG12	6:J:199:ILE:HG23	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:0:DC:H2'	12:Y:1:DT:H71	1.89	0.55
4:D:56:LEU:HA	4:D:59:ARG:HE	1.70	0.55
8:S:114:GLN:HA	8:S:117:LEU:HD23	1.88	0.55
1:A:1354:ARG:HA	1:A:1357:ARG:NH1	2.22	0.55
6:H:361:GLU:HG2	6:H:392:VAL:HG11	1.88	0.55
1:A:1040:LEU:HD22	1:A:1045:LEU:HD12	1.89	0.55
2:B:714:ASN:HB2	7:K:109:ARG:NH2	2.22	0.55
6:H:92:LEU:HD22	6:H:96:VAL:HG11	1.87	0.55
1:A:986:LEU:HA	1:A:989:LEU:HD12	1.89	0.55
5:E:223:ASP:HB2	6:F:170:GLU:H	1.72	0.55
12:Y:-100:DA:H2"	12:Y:-99:DT:H71	1.87	0.55
12:Y:5:DC:H2"	12:Y:6:DC:C5	2.42	0.55
3:C:10:ASN:ND2	3:C:72:GLU:OE2	2.40	0.55
5:I:139:VAL:HG12	5:I:203:GLU:HG2	1.89	0.55
10:W:47:ALA:HA	11:X:39:ARG:NH2	2.21	0.55
10:W:47:ALA:O	10:W:51:ILE:HG12	2.07	0.55
7:K:93:GLN:HB3	7:K:97:ASN:HB2	1.89	0.54
10:U:52:ARG:HG2	10:U:56:LYS:NZ	2.22	0.54
1:A:1055:THR:HB	1:A:1058:HIS:HB2	1.88	0.54
13:Z:35:DT:H2"	13:Z:36:DA:N7	2.23	0.54
1:A:772:LYS:HB2	1:A:797:HIS:H	1.72	0.54
1:A:1144:LEU:HD11	6:H:239:VAL:HG21	1.89	0.54
3:C:223:LEU:HD23	3:C:249:LYS:HE2	1.88	0.54
5:I:125:PHE:CE2	5:I:334:PRO:HD2	2.42	0.54
7:K:601:GLU:N	7:K:601:GLU:OE1	2.40	0.54
9:R:118:THR:O	9:R:122:THR:HG23	2.07	0.54
3:C:204:LEU:HD23	3:C:209:TYR:HB2	1.90	0.54
5:I:142:GLY:HA2	5:I:233:PRO:HG2	1.89	0.54
5:I:274:LYS:HA	6:J:250:ARG:HD3	1.89	0.54
7:K:141:THR:O	7:K:144:THR:OG1	2.25	0.54
9:R:99:THR:HG21	11:X:75:HIS:ND1	2.23	0.54
1:A:722:GLU:N	1:A:931:ARG:HH12	2.06	0.54
1:A:945:TYR:HE2	1:A:1363:ASP:HB3	1.73	0.54
14:A:1601:ADP:O1B	15:A:1602:BEF:F2	2.15	0.54
4:D:57:GLU:HG3	10:U:52:ARG:HD2	1.90	0.54
6:F:377:VAL:HG22	6:F:407:GLN:HG3	1.89	0.54
7:K:500:LYS:HD2	7:K:533:PRO:HG3	1.90	0.54
1:A:1317:PHE:CD2	1:A:1319:LEU:HD11	2.43	0.54
5:I:424:ILE:HG13	6:J:60:MET:HG2	1.89	0.54
2:B:702:LEU:HD13	7:K:619:ARG:HG3	1.90	0.53
5:E:126:ARG:HD2	5:E:285:ARG:HD3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:429:ARG:NE	13:Z:102:DA:OP2	2.39	0.53
8:Q:71:ALA:HA	8:Q:83:HIS:HD2	1.74	0.53
12:Y:3:DT:H2"	12:Y:4:DC:C6	2.44	0.53
7:K:608:ARG:CZ	7:K:612:ASN:HD21	2.22	0.53
11:X:78:ARG:NH1	11:X:80:THR:O	2.41	0.53
2:B:719:TYR:HB2	2:B:728:TYR:CZ	2.44	0.53
5:G:316:LEU:HD22	5:G:320:ILE:HG21	1.89	0.53
6:H:117:LEU:HD11	6:H:305:CYS:HB3	1.89	0.53
10:W:100:LEU:HD11	11:X:58:LEU:HD13	1.91	0.53
12:Y:64:DT:H2"	12:Y:65:DA:N7	2.24	0.53
1:A:1202:ASP:OD1	1:A:1202:ASP:N	2.42	0.53
12:Y:-47:DT:H2"	12:Y:-46:DC:C5	2.43	0.53
2:B:702:LEU:HD22	7:K:619:ARG:HD2	1.90	0.53
7:K:616:HIS:HA	7:K:619:ARG:HH21	1.72	0.53
8:S:65:GLU:OE1	9:T:52:HIS:NE2	2.40	0.53
12:Y:-62:DC:H2"	12:Y:-61:DG:C8	2.44	0.53
9:T:65:LEU:HA	9:T:68:PHE:HD1	1.74	0.52
5:I:316:LEU:HB2	5:I:321:PHE:CZ	2.44	0.52
7:K:433:ILE:HD11	13:Z:101:DA:H5"	1.91	0.52
6:H:343:LEU:HD23	6:H:347:LEU:HD23	1.91	0.52
4:D:192:THR:HG22	4:D:195:ILE:HG12	1.92	0.52
5:E:28:THR:O	5:E:31:LYS:NZ	2.42	0.52
6:H:23:HIS:HE1	5:I:329:GLU:HG2	1.73	0.52
1:A:1271:MET:HB3	1:A:1274:VAL:HG22	1.92	0.52
12:Y:8:DC:H2"	12:Y:9:DG:C8	2.45	0.52
8:Q:110:PRO:HD3	10:U:55:GLN:HE22	1.75	0.52
12:Y:47:DG:H2"	12:Y:48:DG:C5	2.44	0.52
12:Y:58:DG:H2"	12:Y:59:DA:C8	2.44	0.52
1:A:1140:LEU:HD13	6:H:237:HIS:ND1	2.24	0.52
1:A:1272:THR:HA	1:A:1275:LEU:HD12	1.92	0.52
7:K:469:PRO:HB2	7:K:472:SER:HB3	1.92	0.52
12:Y:-85:DT:H2"	12:Y:-84:DA:C8	2.45	0.52
13:Z:8:DG:H2'	13:Z:9:DT:H71	1.92	0.52
1:A:695:ASN:O	14:A:1601:ADP:N6	2.43	0.52
4:D:13:TYR:OH	5:E:150:GLU:OE2	2.23	0.52
4:D:258:ASN:HB3	4:D:279:ASN:ND2	2.24	0.52
6:J:449:ASP:OD1	6:J:453:ASN:N	2.36	0.52
9:T:108:GLU:O	9:T:112:HIS:ND1	2.43	0.51
2:B:238:GLN:OE1	2:B:238:GLN:N	2.39	0.51
3:C:341:LEU:HG	3:C:342:PRO:HD2	1.92	0.51
4:D:223:ASN:HA	4:D:227:HIS:HD2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:534:LEU:HD13	7:K:579:ILE:HD11	1.92	0.51
8:S:63:ILE:HG21	9:T:68:PHE:CZ	2.45	0.51
12:Y:-56:DC:H1'	12:Y:-55:DG:C5	2.46	0.51
2:B:212:LYS:O	2:B:215:LYS:HG3	2.11	0.51
6:F:128:LYS:HE2	6:F:289:VAL:HG11	1.92	0.51
5:G:425:LEU:O	5:G:428:THR:OG1	2.28	0.51
3:C:95:LYS:HA	3:C:124:GLU:O	2.10	0.51
6:F:149:ILE:HG22	6:F:150:THR:HG23	1.91	0.51
11:X:26:ILE:O	11:X:29:ILE:HG12	2.10	0.51
1:A:956:ARG:NH2	1:A:1000:GLU:OE1	2.33	0.51
6:F:102:ALA:HB2	5:G:326:LYS:HD2	1.92	0.51
6:F:250:ARG:NH2	6:F:262:THR:O	2.41	0.51
7:K:608:ARG:NE	7:K:612:ASN:OD1	2.44	0.51
6:F:160:ILE:HG23	6:F:229:LEU:HD11	1.93	0.51
5:I:309:PHE:HD1	5:I:337:VAL:HG23	1.75	0.51
1:A:1282:LEU:O	1:A:1286:GLY:N	2.43	0.51
6:J:141:VAL:HG12	6:J:142:GLU:H	1.76	0.51
6:F:365:LYS:HB2	6:F:388:THR:HG21	1.93	0.51
5:G:313:VAL:HG21	5:G:338:LEU:HD13	1.92	0.51
5:I:258:ARG:HH22	6:J:266:ARG:HD3	1.76	0.51
6:H:81:LYS:HZ1	6:H:326:ASN:HB3	1.76	0.51
6:H:179:LEU:HD23	6:H:199:ILE:HD13	1.93	0.51
1:A:685:ASP:OD1	1:A:705:ASN:ND2	2.43	0.51
4:D:104:GLU:HG3	4:D:113:LEU:HD11	1.93	0.51
5:E:214:ARG:NH2	5:E:221:GLU:OE1	2.40	0.51
5:E:73:ARG:HH12	6:J:404:SER:HB2	1.77	0.50
5:E:171:LYS:HA	5:E:176:THR:HA	1.93	0.50
5:I:80:GLY:O	5:I:85:LYS:NZ	2.45	0.50
11:X:43:VAL:HG21	11:X:46:ILE:HD11	1.93	0.50
14:C:501:ADP:O3B	15:C:502:BEF:F2	2.20	0.50
10:U:117:VAL:HG23	11:V:45:ARG:HG2	1.93	0.50
5:E:41:ALA:HB3	5:E:52:ILE:HG23	1.93	0.50
6:H:440:VAL:HG23	6:H:447:TYR:HD2	1.76	0.50
3:C:19:PRO:HG2	3:C:22:ASN:HB2	1.94	0.50
6:F:25:HIS:CE1	6:F:26:ILE:HG23	2.47	0.50
7:K:179:ILE:HA	7:K:182:LYS:HE3	1.94	0.50
10:U:113:HIS:NE2	10:W:123:ASP:OD1	2.45	0.50
1:A:892:GLN:O	1:A:896:ARG:NE	2.41	0.50
4:D:243:THR:HB	4:D:248:GLY:HA2	1.94	0.50
5:G:125:PHE:HD1	5:G:334:PRO:HD2	1.76	0.50
10:U:102:GLY:O	10:U:105:GLU:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:PRO:HB3	4:D:235:PHE:HA	1.92	0.50
12:Y:-18:DC:H2”	12:Y:-17:DT:H5’	1.93	0.50
1:A:813:PHE:O	1:A:818:TRP:NE1	2.42	0.50
2:B:284:ASN:HA	2:B:599:PHE:HB3	1.94	0.50
5:E:316:LEU:HB2	5:E:321:PHE:CZ	2.47	0.50
5:G:124:ASN:OD1	5:G:127:ARG:NH1	2.44	0.50
12:Y:-15:DA:H1’	12:Y:-14:DA:N7	2.26	0.50
13:Z:-23:DT:H2’	13:Z:-22:DG:C8	2.47	0.50
13:Z:5:DT:H2”	13:Z:6:DA:N7	2.27	0.50
1:A:1089:PHE:HE2	1:A:1092:ALA:HA	1.77	0.49
9:R:96:GLU:O	9:R:99:THR:HG22	2.11	0.49
12:Y:-27:DC:H2”	12:Y:-26:DT:C7	2.42	0.49
12:Y:73:DT:H1’	12:Y:74:DG:C8	2.47	0.49
1:A:817:ARG:HA	1:A:817:ARG:HH11	1.77	0.49
1:A:1067:CYS:HA	6:H:223:GLN:HE21	1.76	0.49
6:F:61:VAL:HG22	6:F:320:ILE:HD12	1.95	0.49
5:G:119:GLU:OE2	5:G:285:ARG:NH2	2.46	0.49
5:G:151:ASP:N	5:G:151:ASP:OD1	2.44	0.49
10:U:124:ILE:H	10:U:124:ILE:HD12	1.77	0.49
5:I:413:ARG:HH12	6:J:350:ARG:NH2	2.11	0.49
13:Z:30:DC:H2”	13:Z:31:DT:C7	2.42	0.49
1:A:980:MET:HE3	13:Z:-23:DT:H2”	1.94	0.49
1:A:1328:ILE:HD12	1:A:1328:ILE:H	1.78	0.49
5:G:41:ALA:HB3	5:G:52:ILE:HG23	1.94	0.49
6:J:128:LYS:HB2	6:J:287:GLU:HG2	1.94	0.49
10:W:85:GLN:NE2	11:X:82:THR:HA	2.26	0.49
11:X:45:ARG:HH12	13:Z:-4:DG:H5”	1.78	0.49
1:A:1018:TYR:HE2	6:J:247:ILE:HD11	1.77	0.49
12:Y:-77:DC:H2”	12:Y:-76:DG:C8	2.48	0.49
5:E:317:ASP:H	5:E:320:ILE:HD12	1.78	0.49
8:S:51:TYR:HD1	9:T:121:VAL:HG21	1.77	0.49
8:S:58:TYR:CE1	9:T:116:GLU:HG3	2.47	0.49
10:U:117:VAL:N	12:Y:-3:DG:OP1	2.44	0.49
12:Y:-53:DG:H1’	12:Y:-52:DG:C8	2.47	0.49
3:C:255:VAL:HG21	3:C:365:PHE:HD1	1.77	0.49
5:I:317:ASP:OD1	5:I:318:ILE:N	2.44	0.49
8:S:115:ASN:HB2	10:W:112:ILE:HD11	1.95	0.49
3:C:388:PRO:HG3	3:C:395:PHE:CG	2.48	0.49
3:C:149:THR:HA	3:C:386:SER:HA	1.95	0.49
6:F:359:TYR:OH	14:F:501:ADP:N7	2.34	0.49
7:K:83:PRO:HB3	7:K:592:TRP:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:87:ASN:HD21	11:X:75:HIS:HD2	1.61	0.49
1:A:760:TRP:HA	1:A:763:GLU:HG3	1.94	0.48
3:C:114:HIS:O	3:C:118:VAL:HG12	2.13	0.48
6:J:250:ARG:NH2	6:J:256:ALA:HB2	2.27	0.48
8:Q:116:LEU:HD21	10:U:112:ILE:HD11	1.93	0.48
6:J:243:GLU:HA	6:J:257:LEU:HD21	1.95	0.48
12:Y:-33:DC:H2"	12:Y:-32:DA:C8	2.48	0.48
3:C:438:ILE:HG22	7:K:87:SER:HB2	1.96	0.48
5:G:48:PHE:HE2	5:G:91:ALA:HB2	1.76	0.48
12:Y:-67:DA:H2"	12:Y:-66:DA:H8	1.78	0.48
3:C:13:TYR:CD1	3:C:14:GLU:HG3	2.48	0.48
6:F:73:VAL:HG22	6:F:354:ILE:HD11	1.94	0.48
7:K:68:ARG:NE	7:K:600:ASP:OD1	2.46	0.48
9:T:101:VAL:HG13	9:T:105:LEU:HD12	1.94	0.48
10:U:51:ILE:HD12	11:V:42:GLY:HA2	1.95	0.48
6:F:105:GLU:HG2	5:G:118:THR:HG21	1.96	0.48
10:U:52:ARG:HG2	10:U:56:LYS:HZ3	1.78	0.48
1:A:817:ARG:NH1	1:A:817:ARG:HA	2.28	0.48
5:G:417:GLN:HG2	6:H:69:ARG:HD3	1.95	0.48
6:H:215:MET:HB3	6:H:219:THR:HG21	1.95	0.48
9:T:82:LYS:O	9:T:86:TYR:HD1	1.96	0.48
12:Y:-83:DC:H1'	12:Y:-82:DG:N7	2.28	0.48
1:A:748:HIS:ND1	1:A:820:TYR:HB3	2.29	0.48
1:A:924:VAL:O	1:A:927:PRO:HD2	2.14	0.48
3:C:313:ILE:HB	3:C:314:PRO:HD3	1.95	0.48
5:E:74:ALA:HA	5:E:336:VAL:O	2.14	0.48
6:H:346:ASP:OD1	6:H:347:LEU:N	2.47	0.48
13:Z:-6:DG:H2"	13:Z:-5:DG:C8	2.49	0.48
13:Z:52:DC:H2"	13:Z:53:DC:C6	2.48	0.48
3:C:59:ARG:NH1	4:D:108:GLU:OE1	2.36	0.48
6:J:29:LEU:HD23	6:J:31:LEU:HD11	1.95	0.48
7:K:435:GLU:O	7:K:439:MET:HG3	2.13	0.48
1:A:840:LEU:HA	1:A:843:PHE:CD2	2.49	0.48
6:J:61:VAL:HG22	6:J:320:ILE:HD12	1.95	0.48
8:Q:80:ILE:HG12	8:Q:83:HIS:ND1	2.28	0.48
1:A:752:VAL:HG22	1:A:756:VAL:HG23	1.95	0.47
5:E:86:THR:HG23	6:F:311:ARG:HH22	1.79	0.47
6:H:348:LEU:HD22	6:H:353:ILE:HD11	1.95	0.47
12:Y:47:DG:H2"	12:Y:48:DG:C8	2.49	0.47
5:I:72:GLY:O	5:I:328:LEU:HD22	2.14	0.47
13:Z:-38:DA:H2"	13:Z:-37:DG:N7	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:323:TYR:HB2	6:J:104:SER:OG	2.13	0.47
5:E:425:LEU:O	5:E:428:THR:OG1	2.29	0.47
5:G:152:ALA:O	5:G:162:THR:OG1	2.32	0.47
6:J:53:ALA:O	6:J:57:ILE:HG12	2.14	0.47
7:K:162:GLY:N	7:K:165:HIS:O	2.39	0.47
10:U:59:GLU:OE1	10:U:59:GLU:N	2.44	0.47
12:Y:72:DG:H2"	12:Y:73:DT:H5'	1.95	0.47
1:A:750:ILE:HB	1:A:800:ILE:HG22	1.95	0.47
8:S:64:LEU:HD22	9:T:48:LEU:HD13	1.96	0.47
6:H:178:GLY:HA2	6:H:181:LYS:HG2	1.96	0.47
6:J:89:SER:HB2	6:J:98:PHE:CE1	2.49	0.47
1:A:1243:TYR:O	1:A:1249:GLN:NE2	2.45	0.47
6:F:21:ALA:H	6:F:24:SER:HB3	1.77	0.47
6:J:52:ARG:O	6:J:56:VAL:HG23	2.15	0.47
8:Q:59:LEU:HD11	9:R:109:LEU:HD21	1.97	0.47
8:Q:71:ALA:HA	8:Q:83:HIS:CD2	2.49	0.47
8:S:113:HIS:CD2	10:W:112:ILE:HD13	2.49	0.47
11:V:38:ALA:HB1	11:V:43:VAL:HG21	1.97	0.47
10:W:83:ARG:HB2	11:X:80:THR:HG22	1.97	0.47
12:Y:34:DT:H2"	12:Y:35:DC:C6	2.49	0.47
13:Z:73:DG:H1'	13:Z:74:DG:N7	2.30	0.47
5:E:71:SER:HB2	5:E:333:ALA:H	1.79	0.47
5:E:148:THR:O	5:E:167:ILE:N	2.32	0.47
6:F:92:LEU:HD21	6:F:292:VAL:HG23	1.96	0.47
6:H:102:ALA:HB2	5:I:326:LYS:HD3	1.97	0.47
6:H:437:VAL:HA	6:H:440:VAL:HG12	1.97	0.47
6:J:204:ARG:NH1	6:J:205:SER:O	2.46	0.47
11:V:78:ARG:NH2	13:Z:29:DG:OP2	2.39	0.47
2:B:287:ILE:N	2:B:597:TYR:O	2.43	0.47
9:T:65:LEU:HA	9:T:68:PHE:CD1	2.49	0.47
11:X:45:ARG:HG2	12:Y:8:DC:H5'	1.96	0.47
3:C:66:LEU:HD11	3:C:72:GLU:CD	2.35	0.47
12:Y:-15:DA:H1'	12:Y:-14:DA:C5	2.50	0.47
13:Z:27:DG:H2"	13:Z:28:DA:C8	2.49	0.47
1:A:832:PHE:HA	1:A:837:TRP:CG	2.49	0.46
3:C:8:ILE:HG13	3:C:17:PHE:HB3	1.97	0.46
3:C:275:VAL:N	3:C:286:TYR:O	2.44	0.46
4:D:218:ASN:ND2	7:K:81:GLU:OE1	2.49	0.46
12:Y:65:DA:H1'	12:Y:66:DC:O4'	2.15	0.46
1:A:1264:ARG:CZ	1:A:1312:SER:HA	2.45	0.46
3:C:148:ARG:HH12	3:C:367:GLN:HE22	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:119:LYS:HG3	8:Q:120:LYS:H	1.80	0.46
8:S:26:PHE:HB2	8:S:53:THR:HG23	1.96	0.46
13:Z:14:DT:H5'	13:Z:14:DT:C6	2.50	0.46
2:B:772:PHE:HD2	7:K:586:LEU:HD23	1.80	0.46
4:D:244:CYS:HB3	4:D:249:GLY:H	1.81	0.46
5:I:61:ILE:HG13	5:I:75:ILE:HD13	1.98	0.46
5:I:422:CYS:HB3	5:I:434:ILE:HG21	1.96	0.46
9:T:90:SER:N	12:Y:-34:DG:OP1	2.47	0.46
13:Z:31:DT:H2'	13:Z:32:DT:C6	2.49	0.46
1:A:1272:THR:O	1:A:1275:LEU:HB2	2.15	0.46
5:I:236:GLU:O	5:I:239:LYS:NZ	2.41	0.46
8:Q:108:VAL:O	10:U:55:GLN:NE2	2.48	0.46
12:Y:-49:DG:C8	12:Y:-49:DG:H5'	2.51	0.46
1:A:1077:LYS:O	1:A:1080:GLU:HG3	2.15	0.46
1:A:1197:LEU:HD13	5:I:269:MET:HE1	1.98	0.46
1:A:1327:GLY:HA2	1:A:1357:ARG:HH22	1.80	0.46
6:H:404:SER:HB3	5:I:73:ARG:HH12	1.81	0.46
12:Y:-16:DT:H2"	12:Y:-15:DA:H5'	1.98	0.46
2:B:242:LEU:O	2:B:245:ALA:HB3	2.16	0.46
6:J:162:THR:OG1	6:J:163:THR:N	2.48	0.46
10:W:69:ARG:NH2	12:Y:17:DA:OP1	2.49	0.46
12:Y:-30:DG:H1'	12:Y:-29:DC:C6	2.50	0.46
12:Y:-12:DC:H2"	12:Y:-11:DG:C8	2.50	0.46
1:A:1322:ARG:NE	13:Z:-18:DG:OP1	2.49	0.46
12:Y:-17:DT:H2"	12:Y:-16:DT:C6	2.51	0.46
2:B:596:LEU:HB2	2:B:609:PHE:CD1	2.51	0.46
3:C:189:LEU:HB2	3:C:349:MET:HG3	1.97	0.46
5:I:134:LYS:HB3	5:I:244:VAL:HG22	1.98	0.46
5:I:137:LYS:NZ	5:I:203:GLU:OE2	2.33	0.46
1:A:944:LYS:HD2	1:A:1352:GLN:NE2	2.31	0.46
5:I:413:ARG:HH12	6:J:350:ARG:HH21	1.64	0.46
6:J:147:ARG:HA	6:J:147:ARG:HD2	1.82	0.46
12:Y:-31:DA:H2"	12:Y:-30:DG:H2'	1.98	0.46
13:Z:53:DC:H6	13:Z:53:DC:OP2	1.99	0.46
4:D:195:ILE:O	4:D:199:LYS:HG2	2.16	0.45
7:K:441:LEU:HD22	7:K:445:GLN:HB3	1.98	0.45
8:Q:86:LEU:O	8:Q:90:ASN:ND2	2.33	0.45
10:U:103:LEU:HD22	11:V:57:VAL:HG11	1.99	0.45
1:A:718:ILE:HD12	1:A:850:LEU:O	2.17	0.45
12:Y:-95:DA:H2"	12:Y:-94:DT:C6	2.51	0.45
1:A:745:TRP:HB2	2:B:241:ARG:NH2	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:275:THR:HG23	6:J:276:LYS:HD2	1.98	0.45
2:B:696:PRO:HG3	7:K:96:LYS:HG3	1.98	0.45
2:B:771:TRP:HE3	7:K:589:TYR:HE2	1.63	0.45
4:D:126:VAL:HA	7:K:66:THR:HG21	1.98	0.45
12:Y:29:DA:H2'	12:Y:30:DT:H71	1.98	0.45
13:Z:-7:DG:H2"	13:Z:-6:DG:N7	2.31	0.45
4:D:255:SER:OG	4:D:260:GLY:HA2	2.17	0.45
5:E:26:ALA:O	14:E:901:ADP:O2'	2.33	0.45
6:F:135:LEU:HD22	6:F:233:LYS:HD3	1.97	0.45
5:G:280:ILE:HG23	5:G:284:LEU:HD23	1.99	0.45
5:G:441:GLU:OE2	6:H:52:ARG:NH1	2.47	0.45
2:B:598:ASP:OD1	2:B:599:PHE:N	2.50	0.45
2:B:788:ALA:O	2:B:791:VAL:HG13	2.17	0.45
3:C:36:LYS:HE2	3:C:36:LYS:HB2	1.79	0.45
6:H:22:ALA:O	6:H:371:ARG:NH1	2.50	0.45
5:I:429:SER:OG	5:I:431:ARG:NH1	2.49	0.45
8:S:43:ARG:NE	13:Z:39:DA:H5'	2.32	0.45
11:V:35:ARG:NH1	13:Z:8:DG:OP2	2.37	0.45
1:A:775:THR:HG22	1:A:800:ILE:HD11	1.98	0.45
2:B:696:PRO:HA	7:K:608:ARG:HH11	1.81	0.45
3:C:335:LEU:HD11	3:C:376:GLN:HG3	1.98	0.45
5:G:277:LYS:HD3	6:H:266:ARG:HH22	1.82	0.45
5:G:448:ASP:OD1	5:G:451:ARG:NE	2.32	0.45
5:I:51:GLN:HG2	5:I:375:TYR:HE1	1.82	0.45
10:W:50:GLU:OE1	11:X:39:ARG:NH2	2.49	0.45
12:Y:48:DG:H2"	12:Y:49:DC:C5	2.52	0.45
6:H:83:ALA:HB2	14:H:501:ADP:H5'2	1.98	0.45
11:X:29:ILE:O	11:X:29:ILE:HG13	2.17	0.45
11:X:38:ALA:HB1	11:X:43:VAL:HG21	1.99	0.45
2:B:269:ASN:ND2	12:Y:13:DT:OP1	2.43	0.44
1:A:721:ASP:H	1:A:727:LYS:CE	2.28	0.44
2:B:223:ARG:CZ	13:Z:65:DA:H5"	2.48	0.44
2:B:764:ASP:HA	2:B:768:ARG:NH2	2.32	0.44
3:C:136:PHE:HA	3:C:139:PHE:HD2	1.82	0.44
3:C:343:GLU:HA	3:C:346:ARG:NE	2.32	0.44
5:E:414:TYR:O	5:E:418:LEU:HD23	2.18	0.44
8:S:58:TYR:CD1	9:T:116:GLU:HG3	2.53	0.44
9:T:43:TYR:O	9:T:47:VAL:HG12	2.17	0.44
1:A:725:LEU:HD22	1:A:937:VAL:HG11	1.99	0.44
1:A:1225:HIS:CE1	5:E:263:GLN:HB3	2.53	0.44
3:C:336:GLU:O	3:C:340:MET:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:106:VAL:HB	5:G:109:GLU:HG3	1.99	0.44
6:H:397:ARG:NH2	14:H:501:ADP:O2A	2.48	0.44
7:K:83:PRO:HD3	7:K:590:ASN:HB3	1.99	0.44
13:Z:68:DC:C6	13:Z:69:DT:H72	2.53	0.44
1:A:922:HIS:O	1:A:926:ARG:HG3	2.17	0.44
2:B:791:VAL:HB	2:B:795:PHE:CG	2.53	0.44
7:K:179:ILE:HG23	7:K:182:LYS:HE3	2.00	0.44
8:Q:26:PHE:HB2	8:Q:53:THR:HG23	1.99	0.44
10:U:129:ARG:HE	10:W:109:LEU:HG	1.83	0.44
3:C:57:PHE:O	4:D:109:ASN:ND2	2.47	0.44
3:C:154:ASP:OD1	3:C:154:ASP:N	2.50	0.44
5:E:359:VAL:HG13	5:E:363:LEU:HD23	1.98	0.44
8:S:55:VAL:HG21	9:T:101:VAL:HG21	1.98	0.44
12:Y:67:DA:H2'	12:Y:68:DT:H71	1.99	0.44
13:Z:58:DC:H2"	13:Z:59:DA:C8	2.53	0.44
13:Z:76:DC:C4	13:Z:77:DG:C6	3.06	0.44
13:Z:99:DA:H2"	13:Z:100:DT:C7	2.44	0.44
3:C:55:ILE:HG23	3:C:57:PHE:HE1	1.81	0.44
5:E:23:ARG:NH1	6:F:290:PRO:HG3	2.33	0.44
6:J:98:PHE:CD2	6:J:292:VAL:HB	2.53	0.44
10:U:62:ILE:HD11	11:V:37:LEU:HD21	1.99	0.44
12:Y:-4:DC:H2"	12:Y:-3:DG:C8	2.53	0.44
2:B:638:HIS:H	5:I:156:LEU:HB3	1.82	0.44
5:E:264:ASP:OD1	5:E:265:VAL:N	2.50	0.44
5:I:274:LYS:NZ	6:J:110:GLU:OE2	2.47	0.44
13:Z:5:DT:H2"	13:Z:6:DA:C8	2.52	0.44
5:G:128:ALA:HB3	5:G:334:PRO:HG3	1.99	0.44
6:H:249:SER:OG	6:H:250:ARG:N	2.50	0.44
8:Q:43:ARG:HB3	9:R:91:THR:HG22	1.99	0.44
12:Y:-7:DG:H2"	12:Y:-6:DT:H71	2.00	0.44
13:Z:16:DA:H1'	13:Z:17:DA:C8	2.52	0.44
3:C:274:TYR:HA	3:C:287:VAL:HA	2.00	0.44
5:G:121:LEU:HD23	5:G:323:TYR:HD2	1.83	0.44
8:Q:80:ILE:HB	8:Q:81:PRO:HD2	2.00	0.44
12:Y:63:DA:H2'	12:Y:64:DT:H71	1.99	0.44
5:E:418:LEU:HD12	5:E:442:ALA:HB1	1.99	0.43
13:Z:-27:DC:H2"	13:Z:-26:DC:C5	2.52	0.43
1:A:830:LYS:HB2	1:A:862:GLU:HG2	1.99	0.43
1:A:950:TYR:HB3	1:A:1372:GLU:HG2	1.99	0.43
6:F:25:HIS:HE1	14:F:501:ADP:N3	2.16	0.43
6:F:124:SER:HB2	6:F:319:PRO:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:80:VAL:HA	7:K:589:TYR:HA	2.00	0.43
9:R:99:THR:O	9:R:103:LEU:HG	2.18	0.43
12:Y:52:DG:H2'	12:Y:53:DT:H71	2.00	0.43
13:Z:5:DT:H2"	13:Z:6:DA:C5	2.53	0.43
13:Z:65:DA:C8	13:Z:66:DT:H72	2.52	0.43
1:A:826:ALA:N	1:A:852:THR:HB	2.33	0.43
1:A:1074:GLU:HG3	6:H:206:PHE:CE1	2.53	0.43
1:A:1217:CYS:O	1:A:1220:VAL:HG12	2.18	0.43
4:D:104:GLU:O	4:D:107:THR:HG22	2.18	0.43
5:I:117:LYS:HB2	5:I:320:ILE:HD11	1.99	0.43
5:I:309:PHE:CD1	5:I:337:VAL:HG23	2.53	0.43
3:C:407:ASP:HA	3:C:410:ARG:HE	1.82	0.43
7:K:160:MET:HG2	7:K:551:LEU:HD22	2.00	0.43
7:K:619:ARG:O	7:K:623:HIS:ND1	2.51	0.43
12:Y:-54:DA:C8	12:Y:-54:DA:O5'	2.72	0.43
1:A:699:TYR:O	1:A:932:ARG:NH1	2.51	0.43
1:A:749:LEU:HB2	1:A:818:TRP:CE3	2.54	0.43
2:B:764:ASP:HA	2:B:768:ARG:CZ	2.48	0.43
5:E:174:LYS:HE3	5:E:235:GLY:HA2	1.99	0.43
6:F:83:ALA:HB2	14:F:501:ADP:H2'	2.00	0.43
6:F:331:LYS:HA	6:F:338:LYS:HA	2.00	0.43
5:G:79:GLY:HA3	5:G:372:THR:OG1	2.18	0.43
5:I:106:VAL:HG21	6:J:308:PHE:HD1	1.83	0.43
12:Y:29:DA:C2'	12:Y:30:DT:H71	2.48	0.43
3:C:228:LYS:NZ	3:C:242:THR:HG22	2.34	0.43
4:D:272:HIS:HA	4:D:276:ARG:HB3	2.01	0.43
5:G:126:ARG:HD3	5:G:285:ARG:HH11	1.83	0.43
1:A:1089:PHE:CD1	1:A:1105:LYS:HD2	2.52	0.43
1:A:1182:VAL:HG11	6:F:280:TRP:CZ2	2.53	0.43
1:A:1209:THR:OG1	5:I:263:GLN:OE1	2.26	0.43
3:C:343:GLU:HA	3:C:346:ARG:HE	1.84	0.43
6:H:158:LEU:HB3	6:H:171:LEU:HD21	1.99	0.43
6:J:79:THR:HG22	6:J:79:THR:O	2.19	0.43
11:X:56:GLY:HA2	11:X:59:LYS:HE2	2.00	0.43
12:Y:-39:DT:H2"	12:Y:-38:DC:C5	2.54	0.43
1:A:889:ALA:HB1	1:A:893:TRP:CZ2	2.53	0.43
2:B:209:LYS:HE2	8:S:73:ASP:OD1	2.19	0.43
2:B:728:TYR:CE1	2:B:734:TYR:HD2	2.37	0.43
3:C:83:PRO:HB3	3:C:90:ASP:HB2	1.99	0.43
3:C:199:TRP:CZ3	3:C:215:LYS:HB2	2.54	0.43
6:J:101:ILE:HD12	6:J:106:ILE:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:116:ARG:NH1	10:U:120:MET:SD	2.91	0.43
10:U:117:VAL:O	11:V:45:ARG:HB3	2.19	0.43
10:W:73:GLU:OE1	11:X:25:ASN:ND2	2.29	0.43
1:A:1142:ASP:O	1:A:1146:LYS:N	2.51	0.43
1:A:1225:HIS:HE1	5:E:263:GLN:HB3	1.84	0.43
5:G:77:LEU:N	5:G:338:LEU:O	2.46	0.43
5:I:359:VAL:HG13	5:I:363:LEU:HD23	2.00	0.43
7:K:470:LYS:HE2	7:K:470:LYS:HA	1.99	0.43
9:R:95:ARG:NH2	11:X:75:HIS:HA	2.34	0.43
12:Y:-18:DC:H2'	12:Y:-17:DT:H72	2.01	0.43
13:Z:-44:DG:C8	13:Z:-44:DG:H5'	2.53	0.43
13:Z:81:DG:C5	13:Z:82:DC:N4	2.87	0.43
5:E:150:GLU:OE2	5:E:180:ARG:NE	2.41	0.43
6:F:345:LEU:HA	6:F:348:LEU:HB2	2.00	0.43
5:G:241:LYS:HE3	5:G:241:LYS:HB2	1.86	0.43
5:G:314:ASN:HD22	5:G:342:ARG:CG	2.32	0.43
9:T:108:GLU:CG	9:T:112:HIS:HE1	2.32	0.43
12:Y:54:DG:H5'	12:Y:54:DG:C8	2.54	0.43
1:A:1054:LEU:HD12	1:A:1054:LEU:HA	1.91	0.42
5:G:314:ASN:HD22	5:G:342:ARG:HG3	1.83	0.42
8:S:79:ILE:HB	9:T:57:ILE:HD13	2.01	0.42
8:S:82:ARG:NH1	8:S:107:GLY:HA3	2.34	0.42
1:A:724:GLY:N	14:A:1601:ADP:O1B	2.37	0.42
1:A:1061:GLU:HG2	6:H:137:GLU:OE1	2.19	0.42
1:A:1253:ILE:HG13	1:A:1254:LEU:N	2.35	0.42
2:B:730:ASP:OD1	2:B:733:ALA:N	2.37	0.42
6:H:78:SER:N	14:H:501:ADP:O3B	2.44	0.42
8:S:101:VAL:HG11	11:X:98:TYR:CE2	2.54	0.42
1:A:811:HIS:O	1:A:814:LYS:HG2	2.19	0.42
2:B:700:VAL:HG13	2:B:720:PHE:HB2	2.02	0.42
5:I:25:ALA:HB1	6:J:314:GLU:O	2.19	0.42
6:J:454:VAL:HG13	6:J:456:ILE:HG13	2.01	0.42
7:K:619:ARG:HB3	7:K:623:HIS:CE1	2.54	0.42
12:Y:-70:DG:H2"	12:Y:-69:DA:C8	2.54	0.42
12:Y:4:DC:H2'	12:Y:4:DC:OP2	2.19	0.42
12:Y:22:DC:H2"	12:Y:23:DA:C5'	2.49	0.42
12:Y:27:DG:H1'	12:Y:28:DG:C8	2.54	0.42
2:B:199:VAL:HG12	8:S:66:LEU:HD21	2.00	0.42
2:B:745:SER:OG	2:B:766:GLN:OE1	2.25	0.42
3:C:123:TYR:HD2	3:C:125:PHE:HE2	1.66	0.42
6:F:71:VAL:O	6:F:322:MET:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:83:PRO:HD3	7:K:590:ASN:CB	2.50	0.42
10:U:56:LYS:HE2	10:U:56:LYS:HB2	1.76	0.42
10:U:78:PHE:CE1	11:V:67:ARG:HG2	2.55	0.42
10:W:67:PHE:O	10:W:71:VAL:HG22	2.20	0.42
3:C:97:HIS:O	3:C:125:PHE:HD1	2.03	0.42
5:E:96:LEU:HB3	5:E:100:VAL:HG21	2.00	0.42
6:H:58:LEU:HD11	6:H:62:GLN:HE21	1.85	0.42
12:Y:-38:DC:H6	12:Y:-38:DC:OP2	2.03	0.42
12:Y:-7:DG:H2"	12:Y:-6:DT:C7	2.50	0.42
13:Z:4:DG:H2"	13:Z:5:DT:C6	2.55	0.42
1:A:1271:MET:O	1:A:1274:VAL:HG22	2.20	0.42
5:E:56:GLU:CD	6:J:425:ARG:HH22	2.22	0.42
5:E:63:ASP:OD2	6:J:412:LYS:HD3	2.19	0.42
6:F:162:THR:HG22	6:F:163:THR:H	1.84	0.42
6:F:243:GLU:HA	6:F:257:LEU:HD21	2.01	0.42
6:H:57:ILE:O	6:H:61:VAL:HG23	2.20	0.42
12:Y:47:DG:H2"	12:Y:48:DG:N7	2.34	0.42
6:H:364:ILE:HG22	6:H:388:THR:HG23	2.02	0.42
8:S:19:SER:O	8:S:23:GLY:N	2.48	0.42
11:V:68:ASP:O	11:V:71:THR:HG22	2.20	0.42
10:W:79:LYS:NZ	11:X:74:GLU:OE2	2.26	0.42
1:A:1322:ARG:NH2	13:Z:-18:DG:H5'	2.35	0.42
2:B:270:ARG:HH21	5:E:220:THR:HB	1.84	0.42
3:C:25:PRO:HB3	3:C:397:TRP:CD2	2.54	0.42
3:C:335:LEU:HD12	4:D:237:VAL:HG21	2.02	0.42
6:H:269:VAL:O	6:H:273:ILE:HG12	2.19	0.42
6:H:391:GLY:HA2	6:H:395:SER:O	2.20	0.42
5:I:116:LYS:HG3	5:I:119:GLU:H	1.84	0.42
6:J:134:GLU:O	6:J:194:LYS:N	2.34	0.42
6:J:382:ASP:N	6:J:382:ASP:OD1	2.52	0.42
8:S:75:LYS:O	8:S:75:LYS:HD3	2.19	0.42
11:V:33:ALA:O	11:V:37:LEU:HD13	2.20	0.42
12:Y:45:DC:H2"	12:Y:46:DA:C8	2.54	0.42
1:A:796:PHE:CE1	1:A:799:CYS:HB2	2.55	0.42
1:A:829:ILE:HG22	1:A:837:TRP:HD1	1.84	0.42
3:C:342:PRO:HB2	3:C:345:VAL:HG12	2.02	0.42
6:F:345:LEU:HD13	6:J:454:VAL:HG12	2.01	0.42
6:H:158:LEU:HD21	6:H:160:ILE:HG13	2.00	0.42
5:I:36:ASP:N	5:I:40:VAL:O	2.45	0.42
9:T:108:GLU:HG2	9:T:112:HIS:HE1	1.85	0.42
1:A:1112:LEU:O	1:A:1115:THR:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:ASN:HB3	2:B:608:ASP:HB2	2.01	0.42
6:F:122:ARG:NE	6:F:245:ASP:OD2	2.45	0.42
8:Q:113:HIS:CE1	8:Q:115:ASN:HB2	2.54	0.42
10:W:79:LYS:HB3	10:W:82:LEU:HD11	2.02	0.42
4:D:170:GLU:OE1	4:D:173:ARG:NH1	2.53	0.41
4:D:212:LEU:O	4:D:222:LYS:NZ	2.38	0.41
6:H:440:VAL:HG23	6:H:447:TYR:CD2	2.55	0.41
12:Y:-98:DG:H2'	12:Y:-97:DT:H71	2.02	0.41
12:Y:38:DT:H2'	12:Y:39:DA:C8	2.55	0.41
13:Z:32:DT:H3'	13:Z:33:DG:C8	2.54	0.41
1:A:1252:ALA:HB2	1:A:1281:PHE:HZ	1.85	0.41
2:B:216:LYS:HE3	12:Y:-63:DC:H5"	2.02	0.41
2:B:720:PHE:HA	2:B:727:PRO:HA	2.02	0.41
5:E:322:THR:HG21	6:J:300:MET:HG3	2.01	0.41
6:J:57:ILE:O	6:J:61:VAL:HG23	2.20	0.41
10:W:110:CYS:SG	10:W:126:LEU:HD23	2.60	0.41
12:Y:26:DG:H5'	12:Y:26:DG:H8	1.82	0.41
13:Z:80:DC:C2	13:Z:81:DG:N7	2.88	0.41
1:A:831:ASN:ND2	12:Y:21:DC:OP2	2.36	0.41
1:A:1147:ASP:OD1	1:A:1147:ASP:N	2.53	0.41
1:A:1269:THR:HG21	1:A:1274:VAL:HG23	2.02	0.41
1:A:1270:GLN:H	1:A:1340:ASP:CG	2.24	0.41
1:A:1308:PHE:CE1	1:A:1317:PHE:HB2	2.54	0.41
6:F:306:PHE:CZ	6:F:343:LEU:HD22	2.55	0.41
7:K:157:ASP:OD1	7:K:158:CYS:N	2.53	0.41
8:Q:43:ARG:HH11	12:Y:40:DG:C5'	2.34	0.41
10:U:79:LYS:HB3	10:U:82:LEU:HD11	2.03	0.41
12:Y:-48:DC:H2"	12:Y:-47:DT:C7	2.51	0.41
1:A:920:LYS:O	1:A:924:VAL:HG23	2.20	0.41
2:B:203:THR:HA	2:B:206:VAL:HG12	2.02	0.41
3:C:99:LEU:O	3:C:128:LEU:HA	2.20	0.41
5:E:75:ILE:HG12	5:E:337:VAL:HG12	2.02	0.41
6:F:164:ASP:OD1	6:F:164:ASP:N	2.53	0.41
6:H:23:HIS:CG	6:H:86:MET:HG3	2.55	0.41
6:J:69:ARG:HD3	6:J:69:ARG:HA	1.89	0.41
9:R:102:ARG:HA	9:R:110:ALA:HB1	2.03	0.41
10:U:69:ARG:NH2	13:Z:17:DA:OP2	2.45	0.41
11:X:38:ALA:O	11:X:43:VAL:HG22	2.20	0.41
12:Y:-56:DC:H1'	12:Y:-55:DG:C8	2.54	0.41
1:A:1107:SER:O	1:A:1110:GLN:HG2	2.21	0.41
3:C:273:GLU:HG2	3:C:290:PRO:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:47:GLN:HB3	6:H:50:ALA:HB3	2.02	0.41
7:K:121:TYR:HB2	7:K:467:TYR:CE2	2.56	0.41
8:Q:44:ILE:O	12:Y:39:DA:H5"	2.19	0.41
12:Y:67:DA:H8	12:Y:67:DA:H5'	1.85	0.41
13:Z:36:DA:H2"	13:Z:37:DC:C5	2.56	0.41
1:A:760:TRP:O	1:A:763:GLU:HG3	2.21	0.41
8:S:72:ARG:NH2	9:T:54:ASP:OD1	2.53	0.41
10:U:68:GLN:HA	10:U:71:VAL:HG12	2.02	0.41
12:Y:-66:DA:C8	12:Y:-65:DT:H72	2.55	0.41
13:Z:74:DG:C6	13:Z:75:DG:C6	3.07	0.41
1:A:1245:CYS:SG	1:A:1247:LYS:HB2	2.60	0.41
1:A:1350:GLN:O	1:A:1354:ARG:HG2	2.21	0.41
3:C:148:ARG:HH12	3:C:367:GLN:NE2	2.17	0.41
3:C:351:GLY:O	3:C:384:HIS:HB2	2.21	0.41
5:E:73:ARG:NH1	6:J:404:SER:HB2	2.35	0.41
6:F:99:THR:HB	6:F:293:LEU:HD12	2.02	0.41
6:J:98:PHE:HD2	6:J:292:VAL:HB	1.85	0.41
7:K:498:LYS:O	7:K:501:THR:OG1	2.30	0.41
8:Q:80:ILE:HG12	8:Q:83:HIS:CE1	2.55	0.41
12:Y:67:DA:C4	13:Z:-66:DG:N2	2.88	0.41
1:A:1145:THR:HA	6:H:248:ASN:OD1	2.21	0.41
4:D:224:VAL:O	4:D:228:ASN:HB2	2.20	0.41
5:E:395:VAL:HG22	5:E:434:ILE:HD12	2.01	0.41
5:I:134:LYS:NZ	5:I:300:VAL:O	2.42	0.41
7:K:560:GLN:OE1	7:K:564:ASN:ND2	2.49	0.41
10:W:117:VAL:HG21	11:X:45:ARG:HH21	1.85	0.41
11:X:25:ASN:O	11:X:28:GLY:N	2.53	0.41
12:Y:-67:DA:H2"	12:Y:-66:DA:C8	2.55	0.41
12:Y:-27:DC:H2"	12:Y:-26:DT:C5	2.56	0.41
13:Z:45:DT:H2"	13:Z:46:DG:N7	2.35	0.41
5:E:72:GLY:O	5:E:328:LEU:HD22	2.20	0.41
5:G:136:THR:HB	5:G:242:GLU:HG2	2.02	0.41
6:H:45:VAL:HG11	6:H:366:THR:OG1	2.21	0.41
6:H:204:ARG:O	6:H:221:PHE:HA	2.21	0.41
6:H:240:SER:O	6:H:244:ILE:HG13	2.20	0.41
7:K:180:GLU:O	7:K:184:GLN:HG3	2.21	0.41
9:R:47:VAL:O	9:R:51:THR:HG23	2.21	0.41
12:Y:-26:DT:H2"	12:Y:-25:DA:N7	2.35	0.41
12:Y:-6:DT:H2"	12:Y:-5:DA:N7	2.35	0.41
13:Z:-21:DG:H4'	13:Z:-20:DC:OP1	2.21	0.41
1:A:1275:LEU:HD11	1:A:1320:SER:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ALA:HA	3:C:56:THR:O	2.21	0.41
6:H:280:TRP:CD1	6:H:285:LYS:HD3	2.56	0.41
5:I:140:TYR:HB2	5:I:202:ILE:HB	2.03	0.41
11:V:97:LEU:HD21	11:V:100:PHE:CE2	2.55	0.41
10:W:55:GLN:HA	11:X:40:ARG:HD3	2.03	0.41
11:X:24:ASP:OD1	11:X:26:ILE:HG22	2.21	0.41
1:A:1025:LEU:HD12	6:J:244:ILE:HG23	2.03	0.40
5:G:26:ALA:HA	5:G:387:ARG:HH22	1.86	0.40
6:H:399:SER:O	6:H:403:ILE:HG13	2.21	0.40
6:H:402:LEU:HD22	6:H:426:ALA:HB1	2.03	0.40
13:Z:52:DC:H2"	13:Z:53:DC:C5	2.55	0.40
13:Z:77:DG:C2	13:Z:78:DG:C6	3.09	0.40
1:A:815:ARG:HH12	13:Z:60:DC:H1'	1.85	0.40
1:A:1057:TYR:O	1:A:1060:GLU:HG2	2.20	0.40
3:C:361:ASN:OD1	3:C:362:LEU:N	2.55	0.40
6:J:386:LEU:O	6:J:389:LYS:HG2	2.20	0.40
12:Y:-88:DC:H2'	12:Y:-87:DT:H72	2.03	0.40
12:Y:11:DG:C8	12:Y:12:DT:H72	2.56	0.40
13:Z:11:DC:H2'	13:Z:12:DG:C8	2.57	0.40
13:Z:94:DA:H2"	13:Z:95:DT:C6	2.56	0.40
1:A:953:LEU:HD12	1:A:958:ARG:CZ	2.51	0.40
3:C:261:PHE:O	3:C:265:LYS:HG2	2.20	0.40
4:D:196:VAL:O	4:D:200:LYS:HG2	2.21	0.40
5:G:127:ARG:HE	5:G:250:HIS:CD2	2.39	0.40
6:H:216:GLY:O	6:H:219:THR:HG22	2.22	0.40
7:K:174:LEU:HB3	7:K:453:GLU:CB	2.48	0.40
8:Q:111:ASN:OD1	8:Q:111:ASN:N	2.54	0.40
1:A:1046:VAL:HA	5:I:256:ASN:OD1	2.22	0.40
3:C:140:THR:HA	3:C:143:TYR:CE1	2.57	0.40
6:F:146:ASP:N	6:F:155:GLN:O	2.39	0.40
5:I:79:GLY:O	5:I:341:ASN:HA	2.22	0.40
6:J:190:ILE:HD12	6:J:201:LYS:HA	2.03	0.40
8:S:80:ILE:HG12	8:S:83:HIS:CE1	2.56	0.40
12:Y:-87:DT:O2	13:Z:88:DG:N2	2.54	0.40
13:Z:78:DG:C5	13:Z:79:DC:C4	3.10	0.40
1:A:707:LEU:HB3	1:A:734:LEU:HD22	2.04	0.40
3:C:191:ILE:HD12	3:C:200:ILE:HD12	2.03	0.40
6:H:183:LYS:HE3	6:H:183:LYS:HB3	1.93	0.40
5:I:417:GLN:HE22	6:J:350:ARG:HA	1.87	0.40
6:J:135:LEU:HA	6:J:193:ASP:HA	2.04	0.40
10:U:75:ALA:HB1	10:U:82:LEU:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:67:DT:H2"	13:Z:68:DC:C5	2.56	0.40
13:Z:90:DG:H1'	13:Z:91:DT:O4'	2.21	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	716/1544 (46%)	698 (98%)	18 (2%)	0	100	100
2	B	293/795 (37%)	280 (96%)	13 (4%)	0	100	100
3	C	407/438 (93%)	392 (96%)	15 (4%)	0	100	100
4	D	198/280 (71%)	192 (97%)	6 (3%)	0	100	100
5	E	422/837 (50%)	411 (97%)	11 (3%)	0	100	100
5	G	432/837 (52%)	421 (98%)	11 (2%)	0	100	100
5	I	434/837 (52%)	425 (98%)	9 (2%)	0	100	100
6	F	441/471 (94%)	431 (98%)	10 (2%)	0	100	100
6	H	437/471 (93%)	427 (98%)	10 (2%)	0	100	100
6	J	420/471 (89%)	407 (97%)	13 (3%)	0	100	100
7	K	314/625 (50%)	303 (96%)	11 (4%)	0	100	100
8	Q	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
8	S	104/132 (79%)	101 (97%)	3 (3%)	0	100	100
9	R	89/131 (68%)	89 (100%)	0	0	100	100
9	T	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
10	U	105/136 (77%)	103 (98%)	2 (2%)	0	100	100
10	W	96/136 (71%)	93 (97%)	3 (3%)	0	100	100
11	V	79/103 (77%)	76 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	X	79/103 (77%)	76 (96%)	3 (4%)	0	100	100
All	All	5263/8610 (61%)	5118 (97%)	145 (3%)	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	659/1400 (47%)	657 (100%)	2 (0%)	91	92
2	B	280/732 (38%)	276 (99%)	4 (1%)	62	76
3	C	372/396 (94%)	371 (100%)	1 (0%)	91	92
4	D	197/261 (76%)	196 (100%)	1 (0%)	86	90
5	E	363/688 (53%)	363 (100%)	0	100	100
5	G	367/688 (53%)	367 (100%)	0	100	100
5	I	369/688 (54%)	368 (100%)	1 (0%)	91	92
6	F	377/403 (94%)	377 (100%)	0	100	100
6	H	375/403 (93%)	375 (100%)	0	100	100
6	J	366/403 (91%)	366 (100%)	0	100	100
7	K	298/570 (52%)	298 (100%)	0	100	100
8	Q	86/99 (87%)	86 (100%)	0	100	100
8	S	85/99 (86%)	85 (100%)	0	100	100
9	R	79/109 (72%)	79 (100%)	0	100	100
9	T	81/109 (74%)	81 (100%)	0	100	100
10	U	90/111 (81%)	90 (100%)	0	100	100
10	W	85/111 (77%)	84 (99%)	1 (1%)	67	79
11	V	66/79 (84%)	66 (100%)	0	100	100
11	X	66/79 (84%)	66 (100%)	0	100	100
All	All	4661/7428 (63%)	4651 (100%)	10 (0%)	91	94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1149	ARG
1	A	1193	ARG
2	B	195	LYS
2	B	205	LYS
2	B	209	LYS
2	B	215	LYS
3	C	410	ARG
4	D	220	MET
5	I	43	ARG
10	W	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
6	H	23	HIS
6	H	223	GLN
9	R	87	ASN
10	U	55	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 20 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
15	BEF	A	1602	14	0,3,3	-	-	-		
14	ADP	G	901	16	24,29,29	0.89	1 (4%)	29,45,45	1.26	2 (6%)
14	ADP	J	501	16	24,29,29	0.95	1 (4%)	29,45,45	1.15	2 (6%)
15	BEF	C	502	-	0,3,3	-	-	-		
14	ADP	E	901	16	24,29,29	0.88	0	29,45,45	1.18	2 (6%)
14	ADP	C	501	16	24,29,29	0.91	0	29,45,45	1.18	2 (6%)
14	ADP	I	901	16	24,29,29	0.91	1 (4%)	29,45,45	1.18	2 (6%)
14	ADP	F	501	16	24,29,29	0.91	1 (4%)	29,45,45	1.12	2 (6%)
14	ADP	H	501	16	24,29,29	0.90	1 (4%)	29,45,45	1.26	3 (10%)
14	ADP	A	1601	16,15	24,29,29	0.87	0	29,45,45	1.15	2 (6%)

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
14	ADP	G	901	16	-	4/12/32/32	0/3/3/3
14	ADP	J	501	16	-	1/12/32/32	0/3/3/3
14	ADP	E	901	16	-	4/12/32/32	0/3/3/3
14	ADP	C	501	16	-	3/12/32/32	0/3/3/3
14	ADP	I	901	16	-	5/12/32/32	0/3/3/3
14	ADP	F	501	16	-	3/12/32/32	0/3/3/3
14	ADP	H	501	16	-	3/12/32/32	0/3/3/3
14	ADP	A	1601	16,15	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	501	ADP	O4'-C1'	2.19	1.43	1.40
14	H	501	ADP	O4'-C1'	2.15	1.43	1.40
14	F	501	ADP	O4'-C1'	2.12	1.43	1.40
14	G	901	ADP	O4'-C1'	2.07	1.43	1.40
14	I	901	ADP	O4'-C1'	2.01	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	I	901	ADP	N3-C2-N1	-3.76	123.56	128.67
14	H	501	ADP	N3-C2-N1	-3.74	123.60	128.67
14	G	901	ADP	N3-C2-N1	-3.72	123.62	128.67
14	J	501	ADP	N3-C2-N1	-3.71	123.63	128.67
14	C	501	ADP	N3-C2-N1	-3.68	123.67	128.67
14	E	901	ADP	N3-C2-N1	-3.64	123.73	128.67
14	F	501	ADP	N3-C2-N1	-3.64	123.73	128.67
14	A	1601	ADP	N3-C2-N1	-3.58	123.81	128.67
14	J	501	ADP	C4-C5-N7	-2.66	106.53	109.34
14	E	901	ADP	C4-C5-N7	-2.64	106.55	109.34
14	A	1601	ADP	C4-C5-N7	-2.61	106.58	109.34
14	H	501	ADP	O4'-C1'-N9	2.59	112.18	108.75
14	F	501	ADP	C4-C5-N7	-2.58	106.61	109.34
14	C	501	ADP	C4-C5-N7	-2.58	106.62	109.34
14	I	901	ADP	C4-C5-N7	-2.56	106.64	109.34
14	H	501	ADP	C4-C5-N7	-2.54	106.65	109.34
14	G	901	ADP	C4-C5-N7	-2.48	106.72	109.34

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	501	ADP	C5'-O5'-PA-O2A
14	E	901	ADP	PA-O3A-PB-O2B
14	F	501	ADP	C5'-O5'-PA-O1A
14	G	901	ADP	C5'-O5'-PA-O2A
14	G	901	ADP	C5'-O5'-PA-O3A
14	H	501	ADP	PA-O3A-PB-O2B
14	I	901	ADP	PA-O3A-PB-O3B
14	I	901	ADP	O4'-C4'-C5'-O5'
14	I	901	ADP	C3'-C4'-C5'-O5'
14	A	1601	ADP	O4'-C4'-C5'-O5'
14	E	901	ADP	O4'-C4'-C5'-O5'
14	E	901	ADP	C3'-C4'-C5'-O5'
14	J	501	ADP	PA-O3A-PB-O1B
14	C	501	ADP	C5'-O5'-PA-O1A
14	C	501	ADP	C5'-O5'-PA-O3A
14	F	501	ADP	C5'-O5'-PA-O2A
14	F	501	ADP	C5'-O5'-PA-O3A
14	H	501	ADP	C5'-O5'-PA-O1A
14	E	901	ADP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	901	ADP	C3'-C4'-C5'-O5'
14	G	901	ADP	PB-O3A-PA-O2A
14	I	901	ADP	C4'-C5'-O5'-PA
14	H	501	ADP	PA-O3A-PB-O1B
14	I	901	ADP	PA-O3A-PB-O2B
14	A	1601	ADP	PB-O3A-PA-O1A
14	A	1601	ADP	PB-O3A-PA-O2A
14	A	1601	ADP	C3'-C4'-C5'-O5'

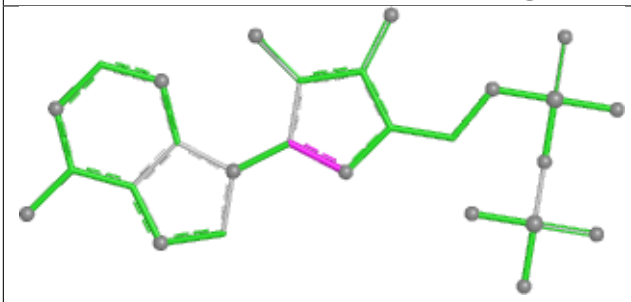
There are no ring outliers.

9 monomers are involved in 16 short contacts:

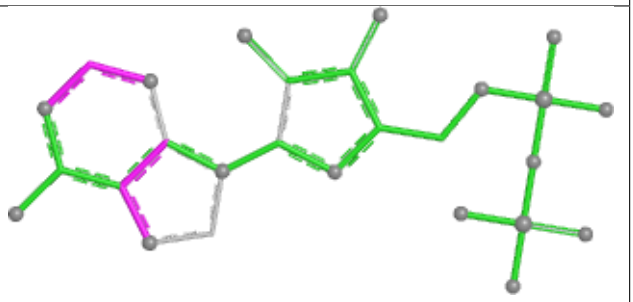
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1602	BEF	1	0
14	J	501	ADP	1	0
15	C	502	BEF	1	0
14	E	901	ADP	1	0
14	C	501	ADP	1	0
14	I	901	ADP	2	0
14	F	501	ADP	4	0
14	H	501	ADP	4	0
14	A	1601	ADP	3	0

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.

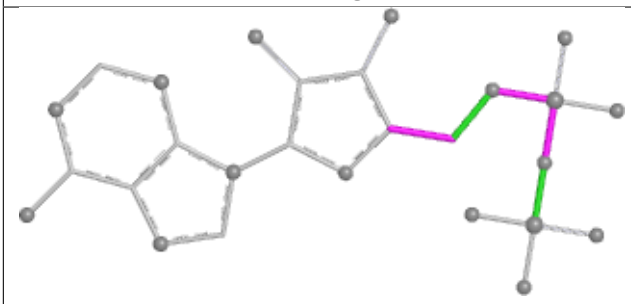
Ligand ADP G 901



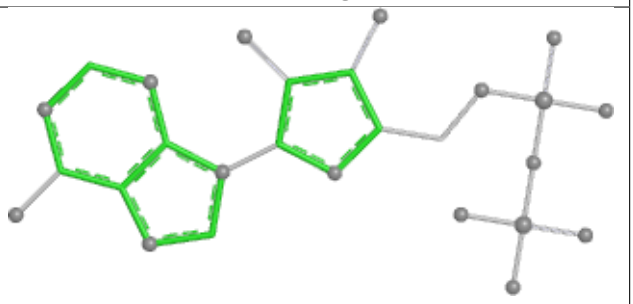
Bond lengths



Bond angles

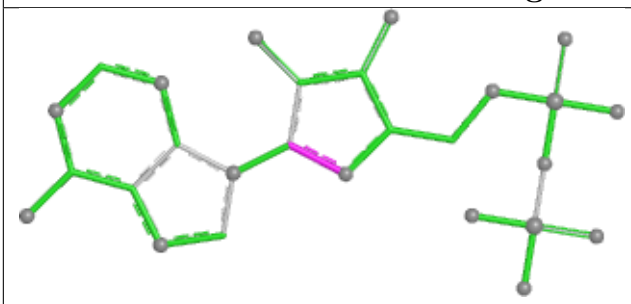


Torsions

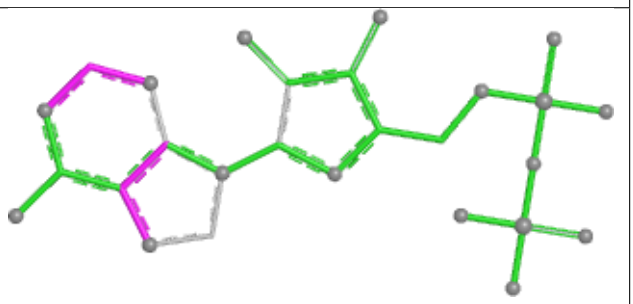


Rings

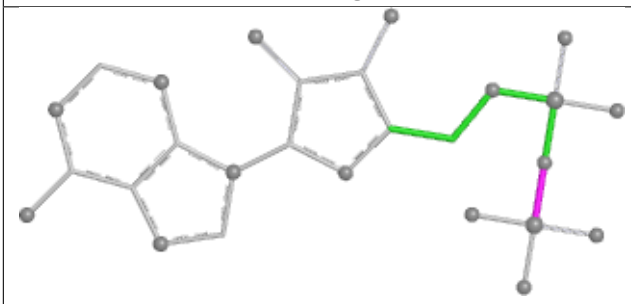
Ligand ADP J 501



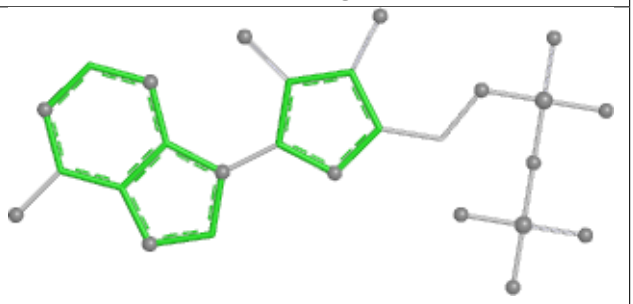
Bond lengths



Bond angles

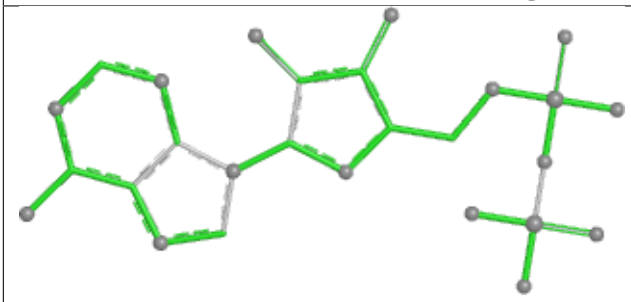


Torsions

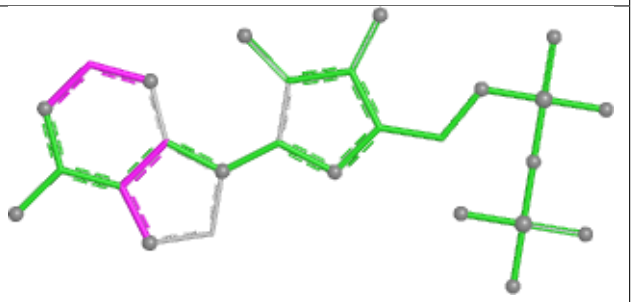


Rings

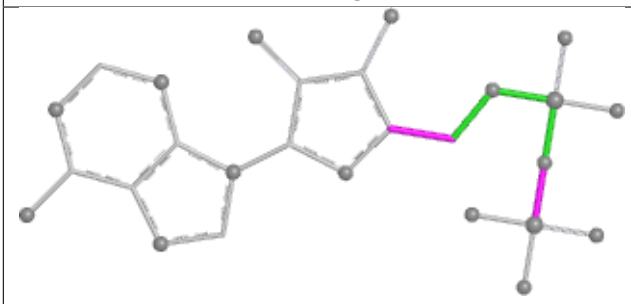
Ligand ADP E 901



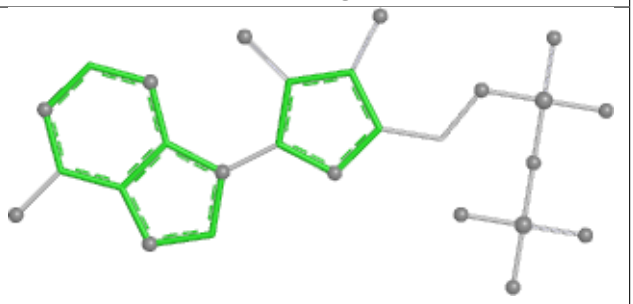
Bond lengths



Bond angles

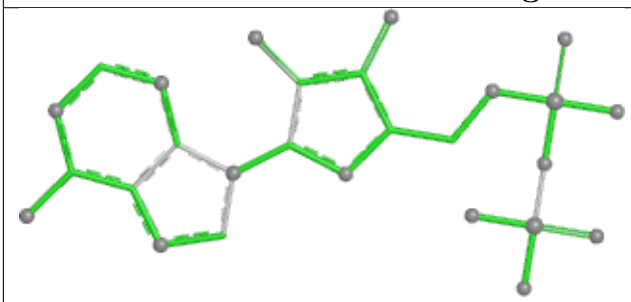


Torsions

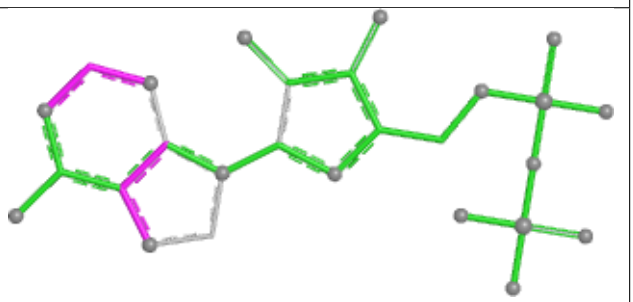


Rings

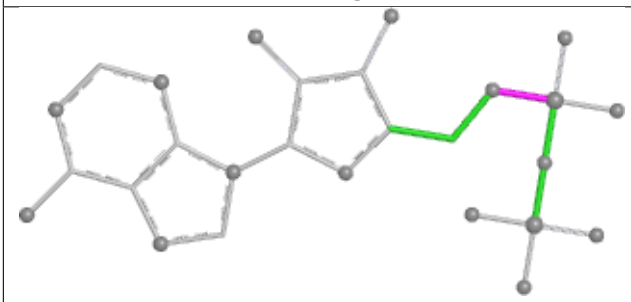
Ligand ADP C 501



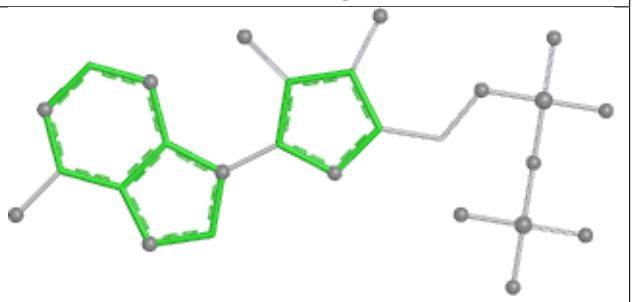
Bond lengths



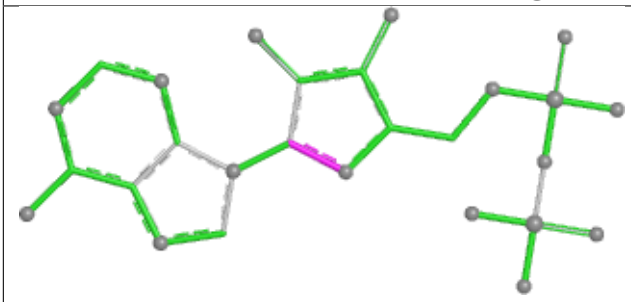
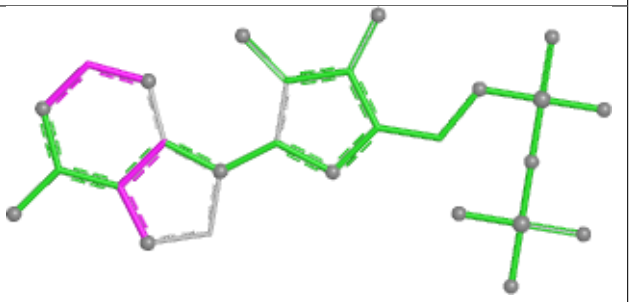
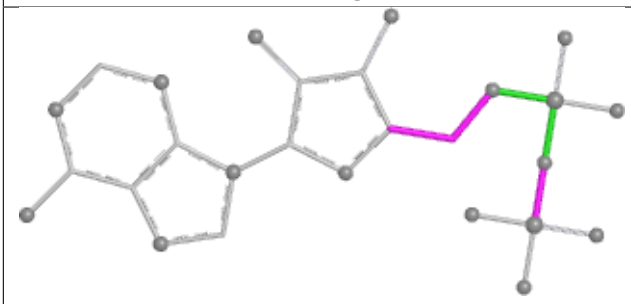
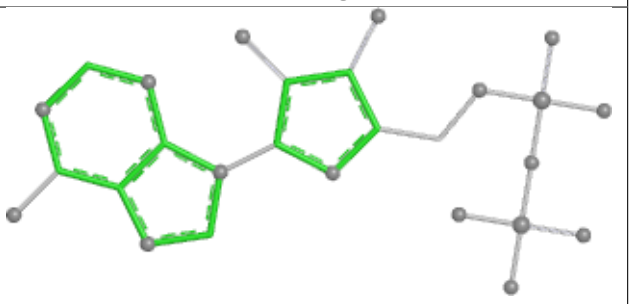
Bond angles

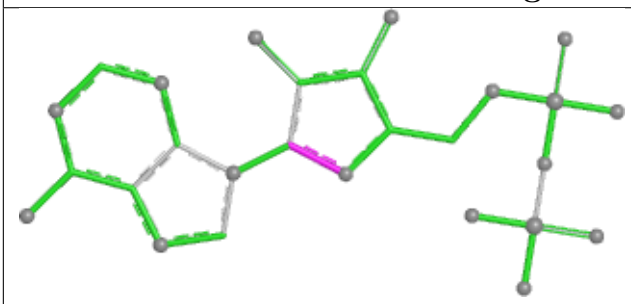
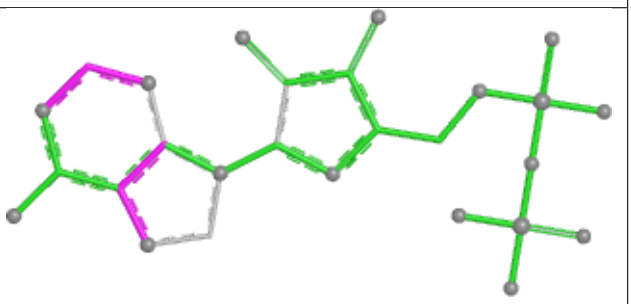
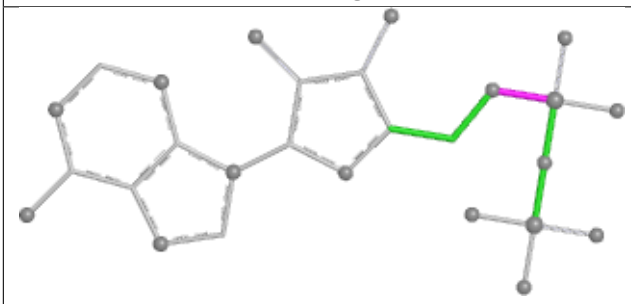
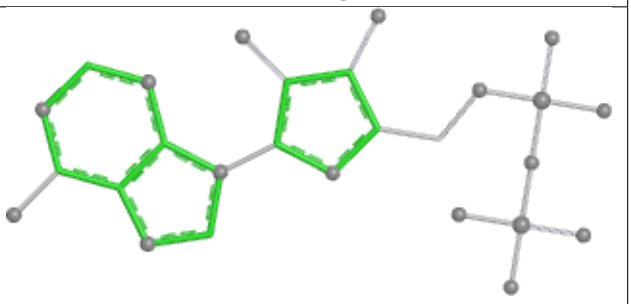


Torsions

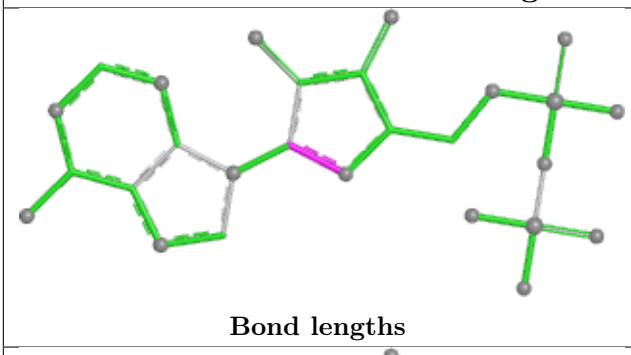


Rings

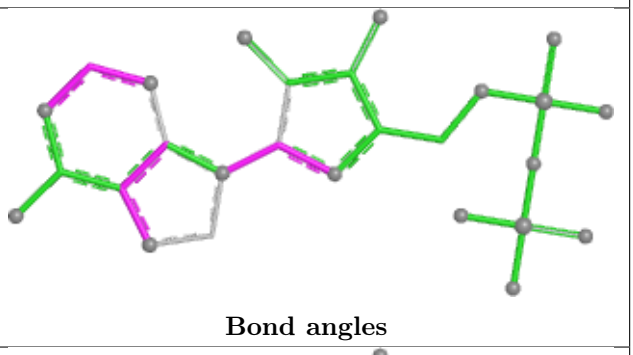
Ligand ADP I 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

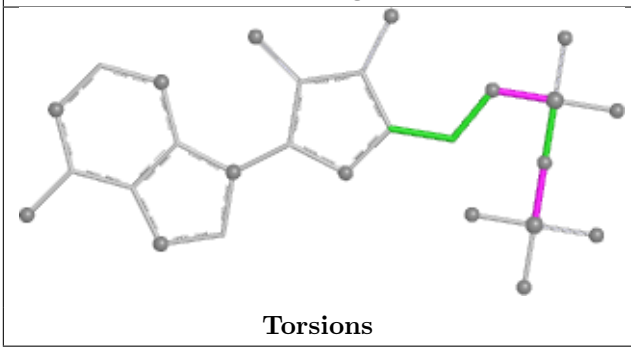
Ligand ADP H 501



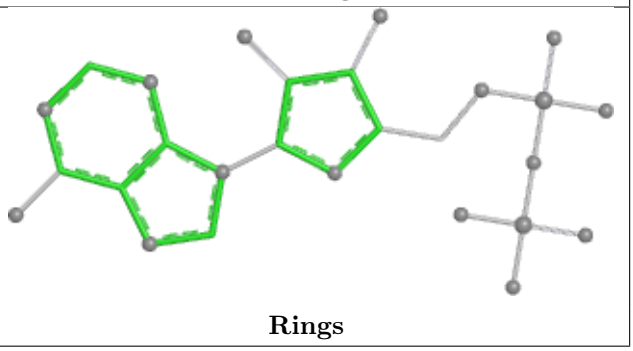
Bond lengths



Bond angles

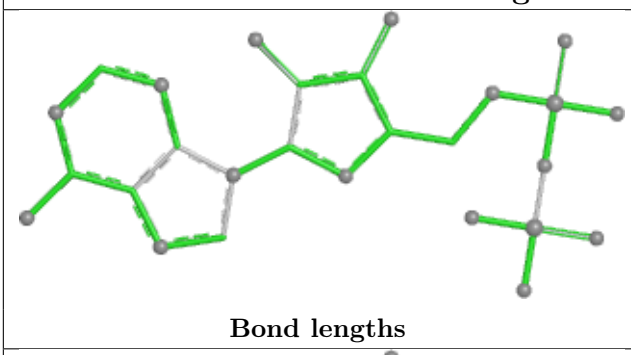


Torsions

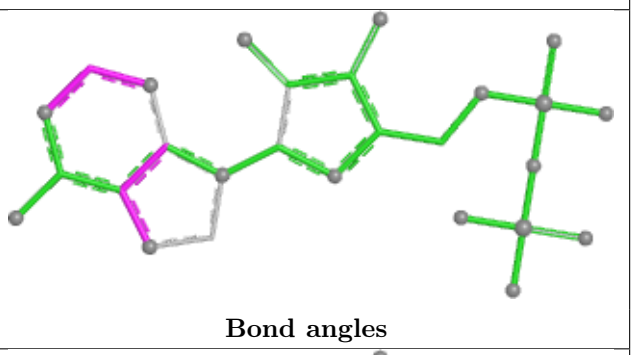


Rings

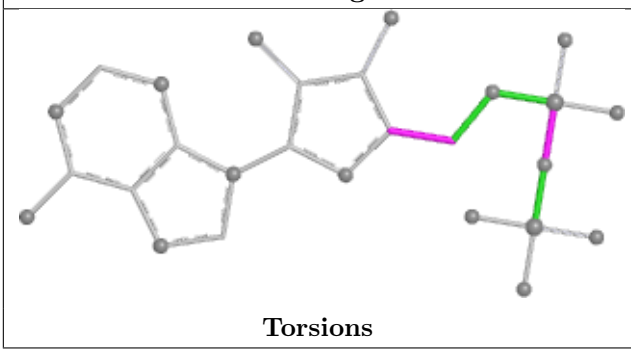
Ligand ADP A 1601



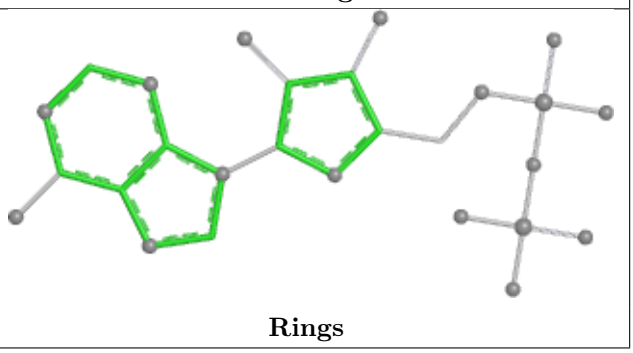
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

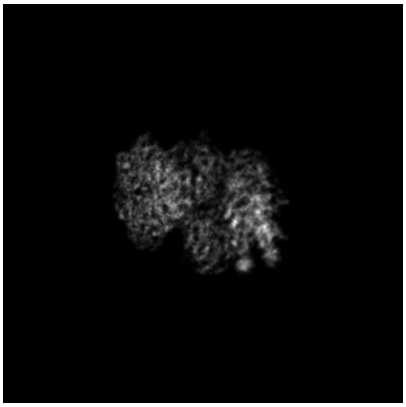
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44075. These allow visual inspection of the internal detail of the map and identification of artifacts.

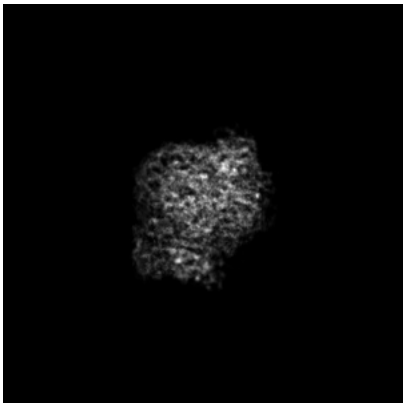
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



Y

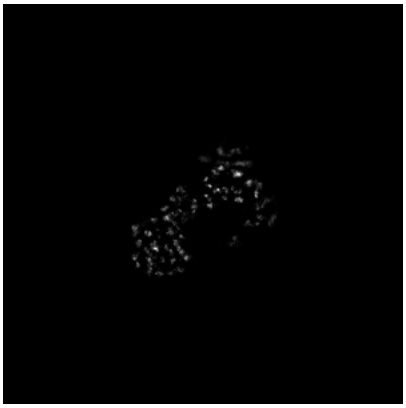
Z

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

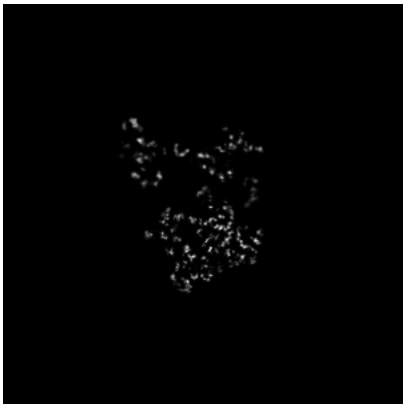
6.2 Central slices

6.2.1 Primary map

X Index: 192



Y Index: 192

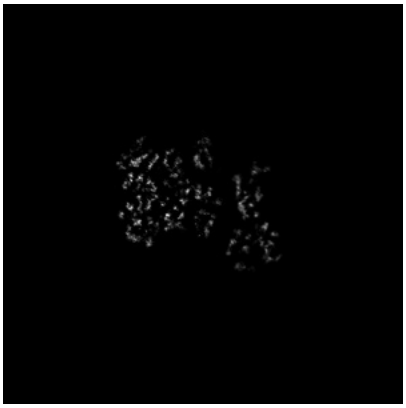


Z Index: 192

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

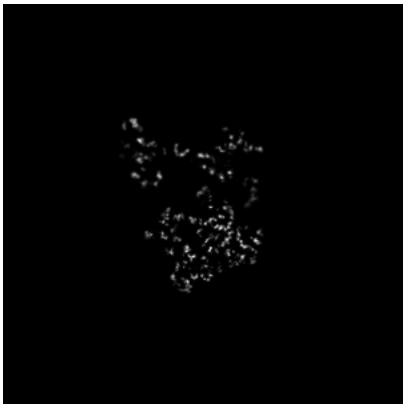
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 193

Y Index: 245

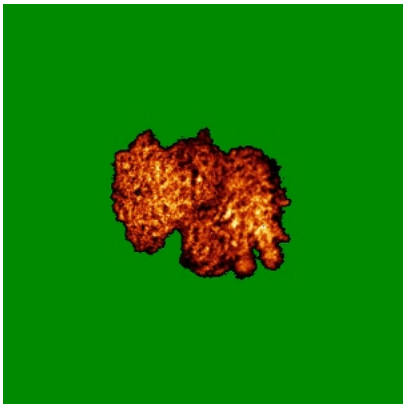


Z Index: 192

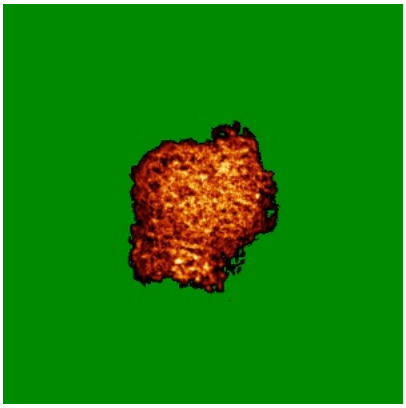
The images above show the largest variance slices of the map in three orthogonal directions.

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

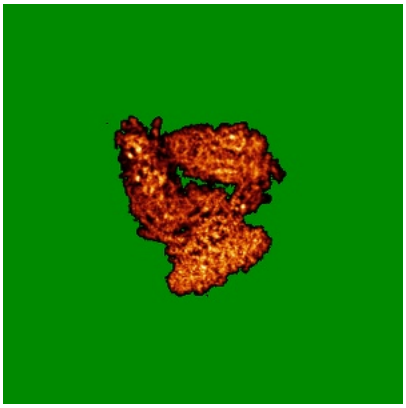
6.4.1 Primary map



X



Y

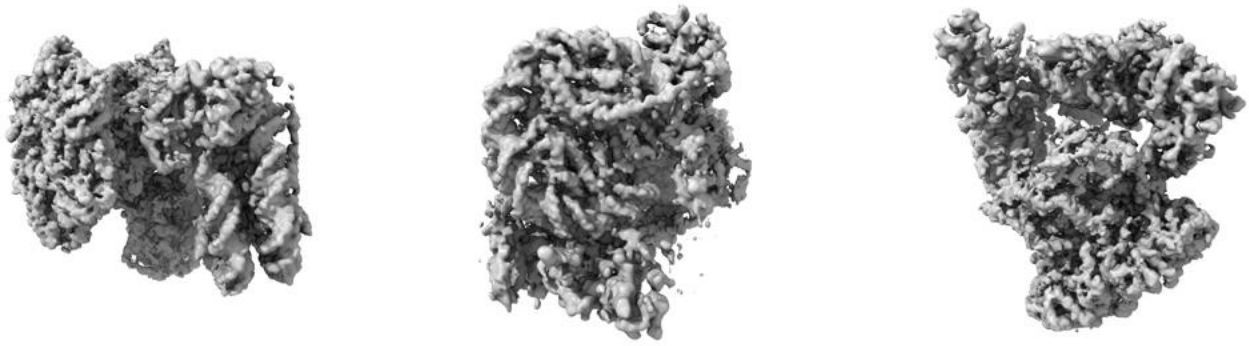


Z

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

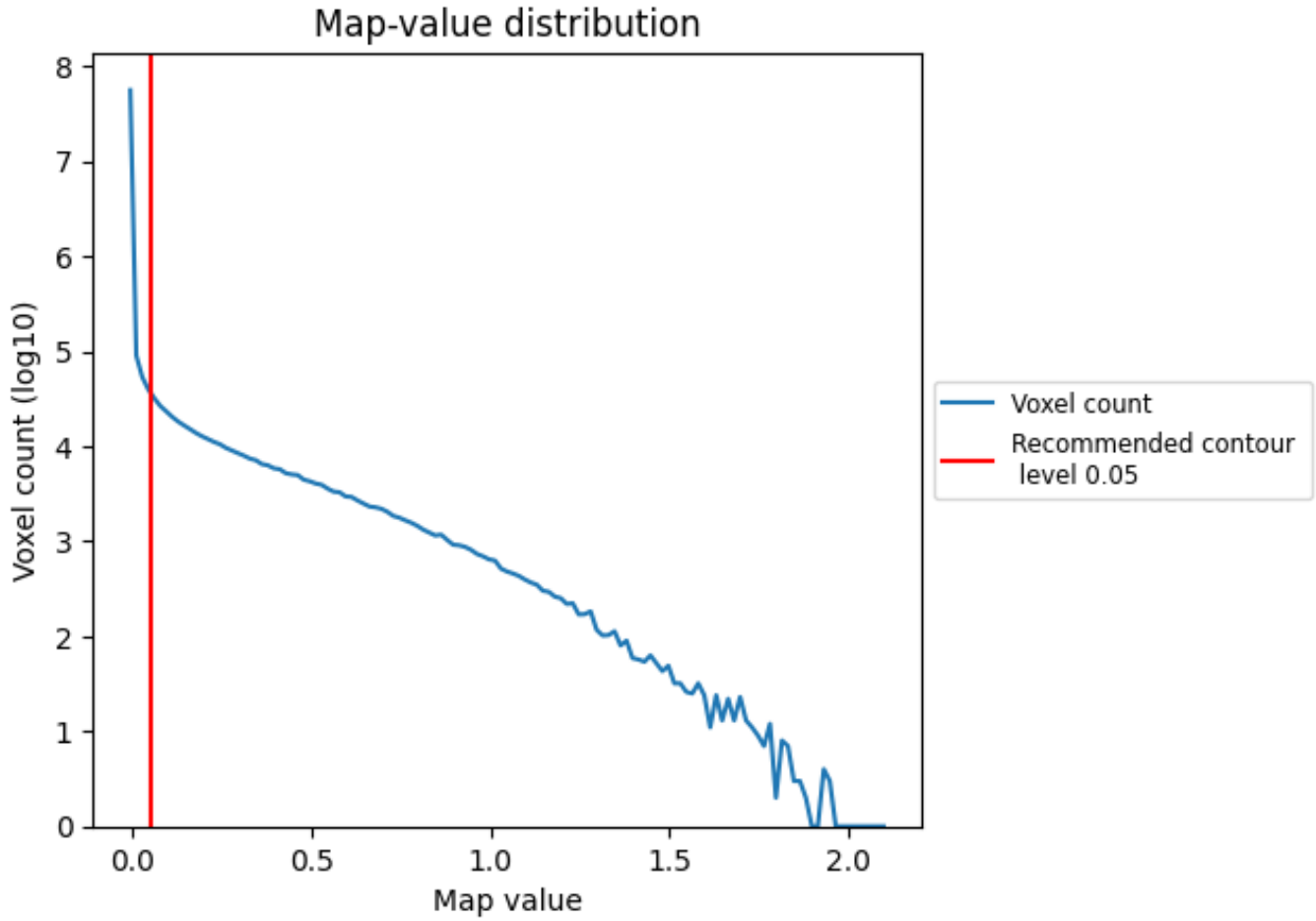
6.6 Mask visualisation (i)

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

7 Map analysis

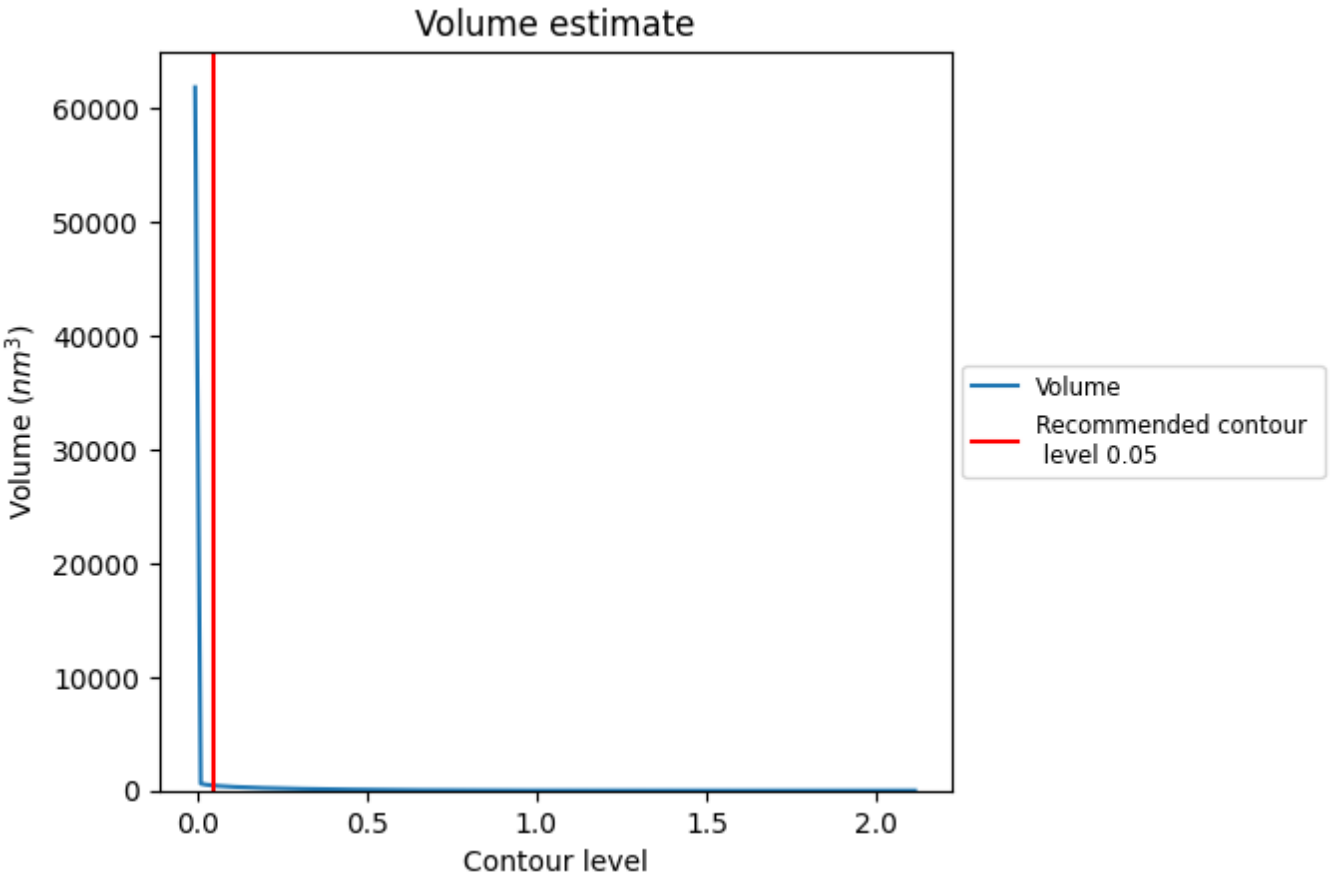
This section contains the results of statistical analysis of the map.

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.

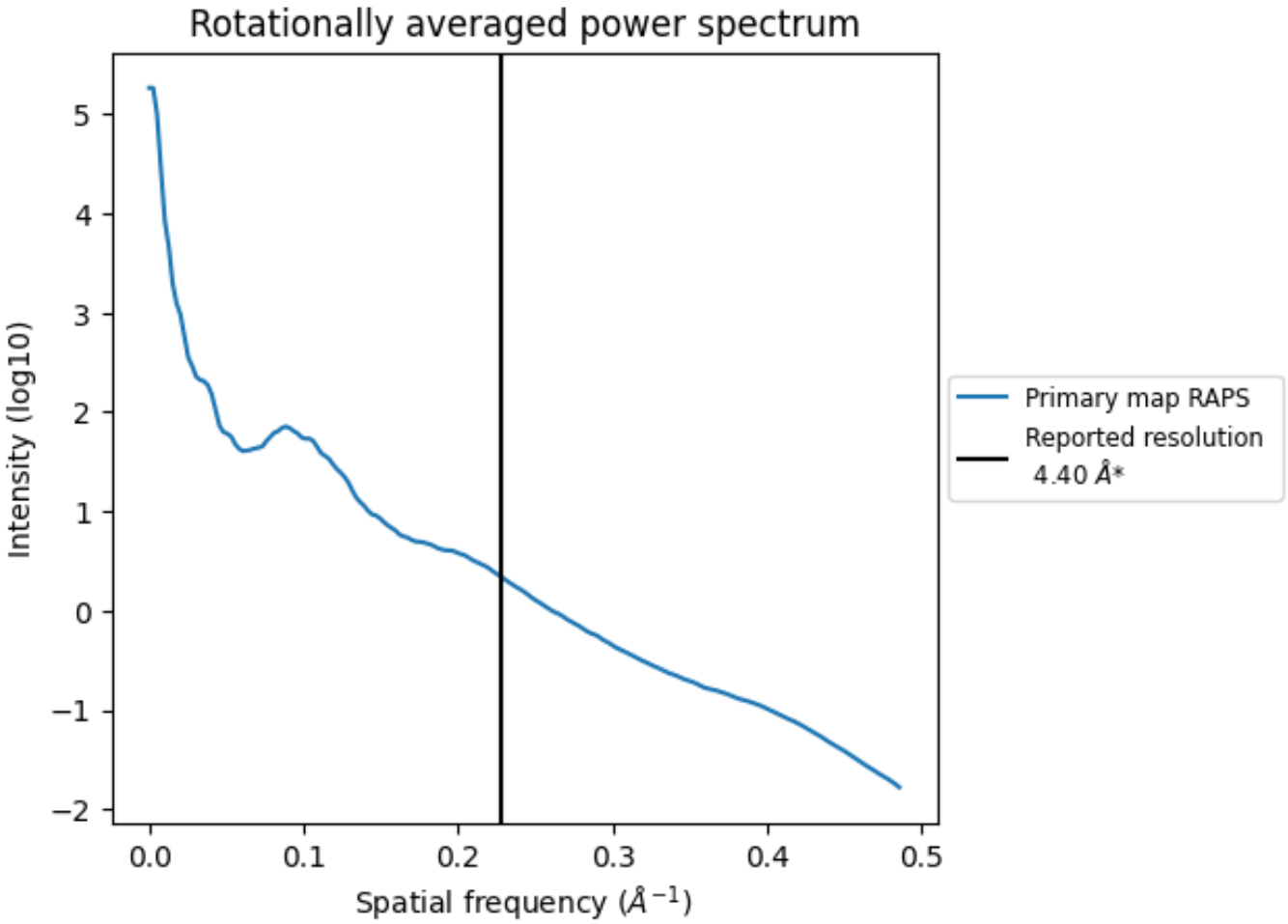
7.2 Volume estimate



The volume at the recommended contour level is 440 nm^3; this corresponds to an approximate mass of 398 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 0.227 Å^{-1}

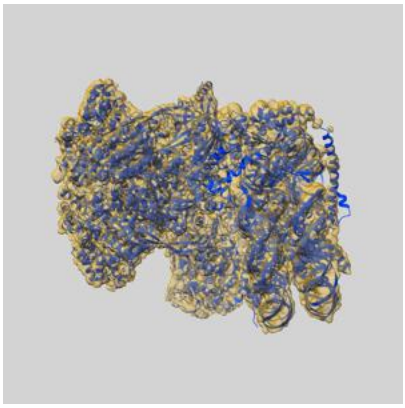
8 Fourier-Shell correlation (i)

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

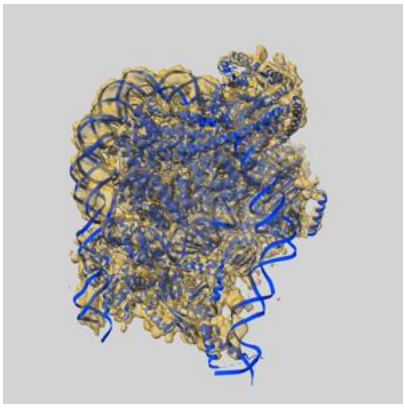
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44075 and PDB model 9B1E. Per-residue inclusion information can be found in section 3 on page 9.

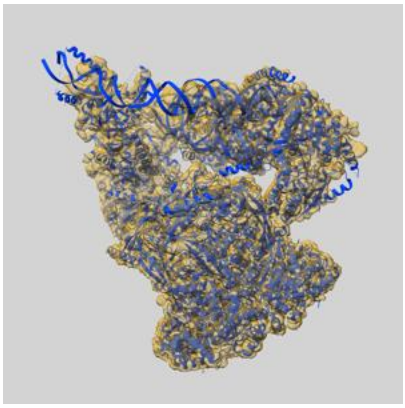
9.1 Map-model overlay



X



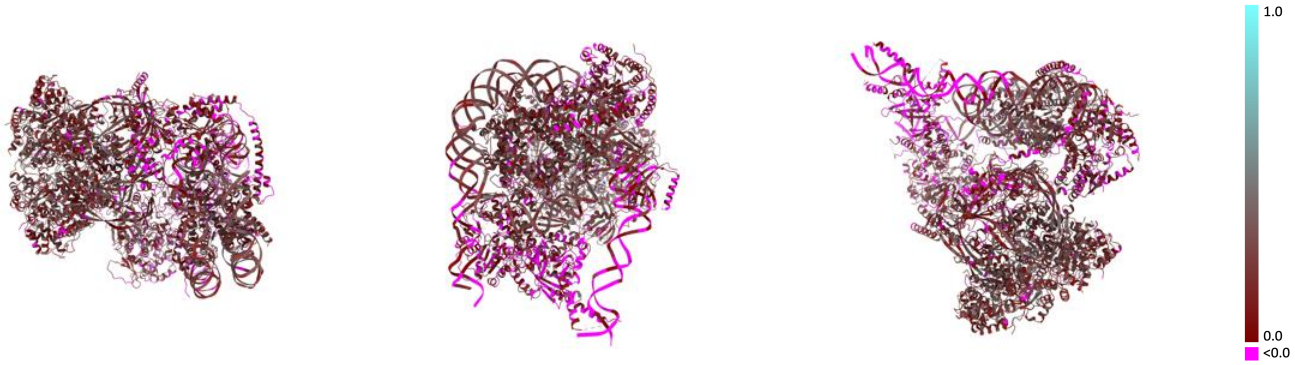
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

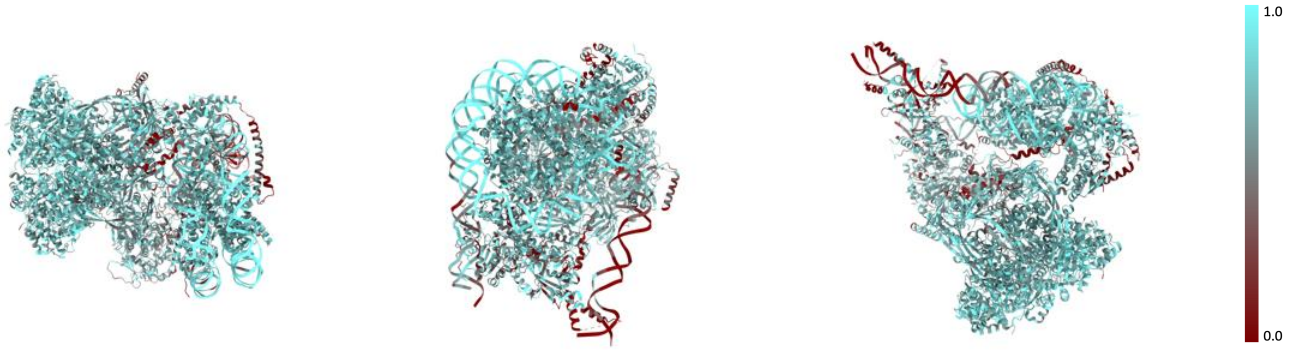
9.2 Q-score mapped to coordinate model (i)



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.

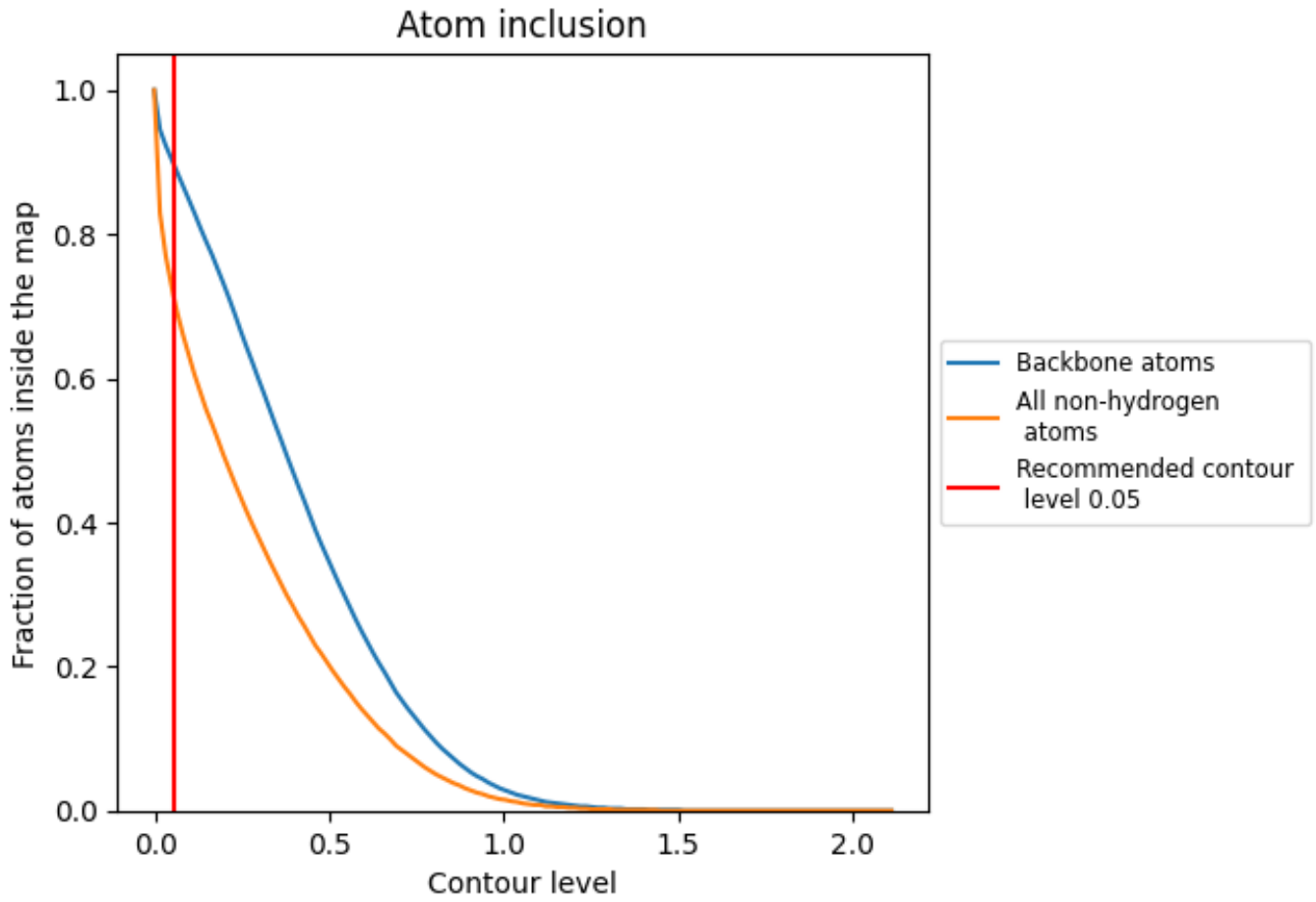
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.1910
A	0.6760	0.1640
B	0.5070	0.0720
C	0.6910	0.1560
D	0.5820	0.1300
E	0.7770	0.2490
F	0.7610	0.2370
G	0.7410	0.2120
H	0.7580	0.2410
I	0.7550	0.2340
J	0.7420	0.2280
K	0.5800	0.0380
Q	0.7520	0.2250
R	0.7920	0.2290
S	0.7890	0.2520
T	0.7830	0.2370
U	0.7280	0.2130
V	0.7810	0.2410
W	0.7580	0.2130
X	0.8060	0.2570
Y	0.7520	0.1870
Z	0.7350	0.1840