



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:45 PM JST

PDB ID : 21VV / pdb_000021vv
EMDB ID : EMD-68040
Title : Cryo-EM structure of ncBAF bound to the nucleosome
Authors : Xu, W.; Cheng, J.; Chen, Y.
Deposited on : 2025-12-31
Resolution : 4.70 Å(reported)
Based on initial models : 7Y8R, .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

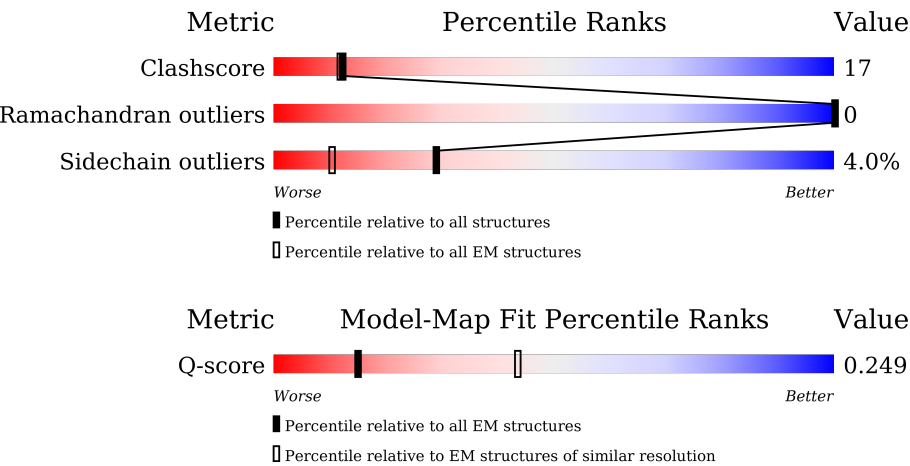
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.70 Å.

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



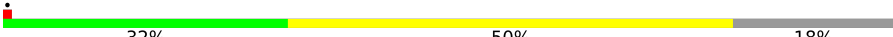
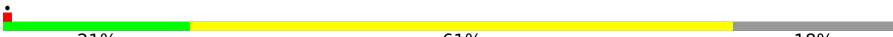
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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

Mol	Chain	Length	Quality of chain
1	A	135	43% 29% 27%
1	E	135	52% 19% 27%
2	B	102	43% 34% 21%
2	F	102	50% 31% 17%

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	125	
4	H	125	
5	N	216	
6	X	167	
7	Y	167	
8	I	1711	
9	J	381	
10	K	435	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23277 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			807	509	156	139	3		
1	E	98	Total	C	N	O	S	0	0
			807	509	156	139	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
2	F	85	Total	C	N	O	S	0	0
			682	430	136	115	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			825	519	163	143		
3	G	112	Total	C	N	O	0	0
			858	539	170	149		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			756	475	138	141	2		
4	H	94	Total	C	N	O	S	0	0
			735	463	132	138	2		

- Molecule 5 is a protein called B-cell CLL/lymphoma 7 protein family member A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	44	Total	C	N	O	0	0
			366	231	71	64		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	211	HIS	-	expression tag	UNP Q4VC05
N	212	HIS	-	expression tag	UNP Q4VC05
N	213	HIS	-	expression tag	UNP Q4VC05
N	214	HIS	-	expression tag	UNP Q4VC05
N	215	HIS	-	expression tag	UNP Q4VC05
N	216	HIS	-	expression tag	UNP Q4VC05

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	137	Total	C	N	O	P	0	0
			2791	1326	504	824	137		

- Molecule 7 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	137	Total	C	N	O	P	0	0
			2826	1337	532	820	137		

- Molecule 8 is a protein called SMARCA4 isoform 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	658	Total	C	N	O	S	0	0
			5409	3441	969	973	26		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-9	GLY	-	expression tag	UNP Q9HBD4
I	-8	PRO	-	expression tag	UNP Q9HBD4
I	-7	GLY	-	expression tag	UNP Q9HBD4
I	-6	GLY	-	expression tag	UNP Q9HBD4
I	-5	SER	-	expression tag	UNP Q9HBD4
I	-4	GLY	-	expression tag	UNP Q9HBD4
I	-3	GLY	-	expression tag	UNP Q9HBD4
I	-2	SER	-	expression tag	UNP Q9HBD4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q9HBD4
I	0	THR	-	expression tag	UNP Q9HBD4
I	1680	ASP	-	expression tag	UNP Q9HBD4
I	1681	TYR	-	expression tag	UNP Q9HBD4
I	1682	LYS	-	expression tag	UNP Q9HBD4
I	1683	ASP	-	expression tag	UNP Q9HBD4
I	1684	HIS	-	expression tag	UNP Q9HBD4
I	1685	ASP	-	expression tag	UNP Q9HBD4
I	1686	GLY	-	expression tag	UNP Q9HBD4
I	1687	ASP	-	expression tag	UNP Q9HBD4
I	1688	TYR	-	expression tag	UNP Q9HBD4
I	1689	LYS	-	expression tag	UNP Q9HBD4
I	1690	ASP	-	expression tag	UNP Q9HBD4
I	1691	HIS	-	expression tag	UNP Q9HBD4
I	1692	ASP	-	expression tag	UNP Q9HBD4
I	1693	ILE	-	expression tag	UNP Q9HBD4
I	1694	ASP	-	expression tag	UNP Q9HBD4
I	1695	TYR	-	expression tag	UNP Q9HBD4
I	1696	LYS	-	expression tag	UNP Q9HBD4
I	1697	ASP	-	expression tag	UNP Q9HBD4
I	1698	ASP	-	expression tag	UNP Q9HBD4
I	1699	ASP	-	expression tag	UNP Q9HBD4
I	1700	ASP	-	expression tag	UNP Q9HBD4
I	1701	LYS	-	expression tag	UNP Q9HBD4

- Molecule 9 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	329	Total	C	N	O	S	0	0
			2585	1647	428	490	20		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	376	HIS	-	expression tag	UNP P60709
J	377	HIS	-	expression tag	UNP P60709
J	378	HIS	-	expression tag	UNP P60709
J	379	HIS	-	expression tag	UNP P60709
J	380	HIS	-	expression tag	UNP P60709
J	381	HIS	-	expression tag	UNP P60709

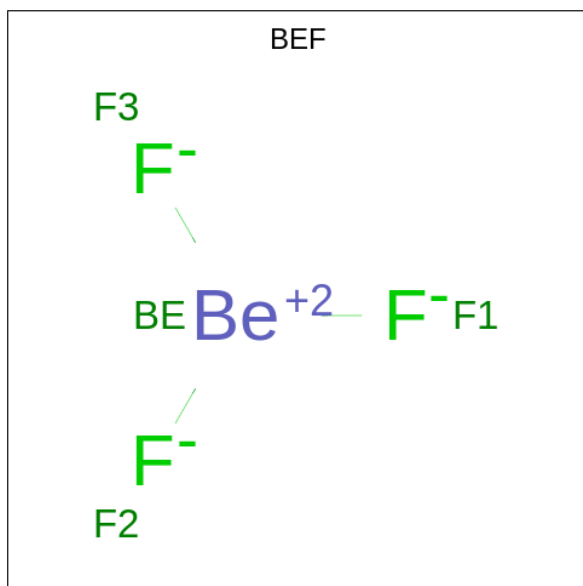
- Molecule 10 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	404	Total	C	N	O	S	0	0
			3152	1994	536	598	24		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	430	HIS	-	expression tag	UNP O96019
K	431	HIS	-	expression tag	UNP O96019
K	432	HIS	-	expression tag	UNP O96019
K	433	HIS	-	expression tag	UNP O96019
K	434	HIS	-	expression tag	UNP O96019
K	435	HIS	-	expression tag	UNP O96019

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).

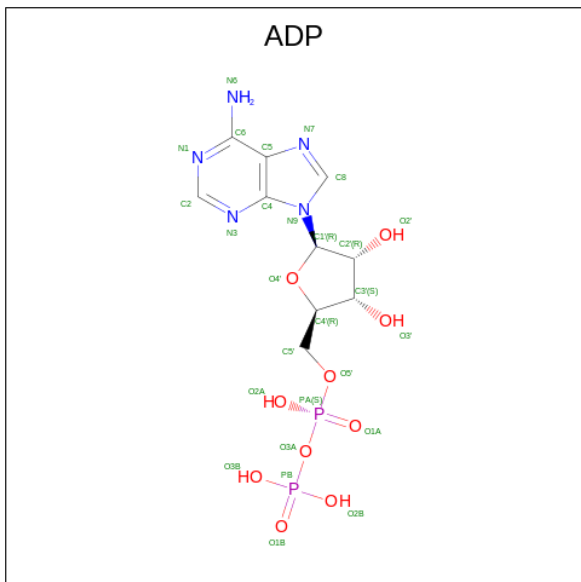


Mol	Chain	Residues	Atoms			AltConf
11	I	1	Total	Be	F	0
			4	1	3	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	I	1	Total	Mg	0
			1	1	

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

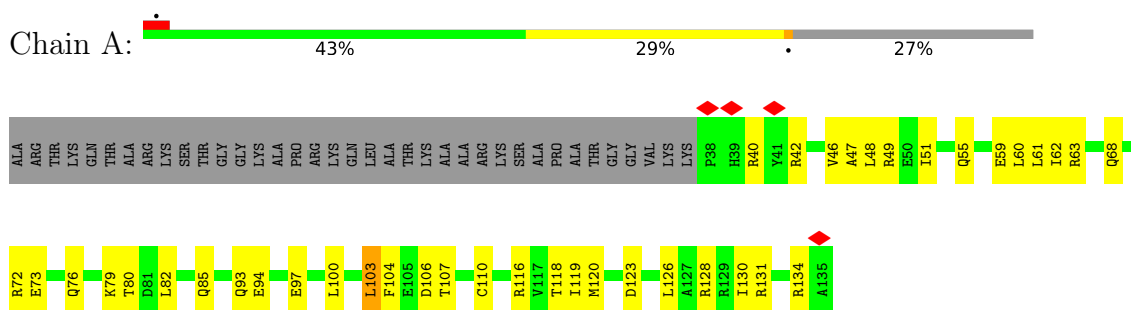


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	I	1	27	10	5	10	2	0

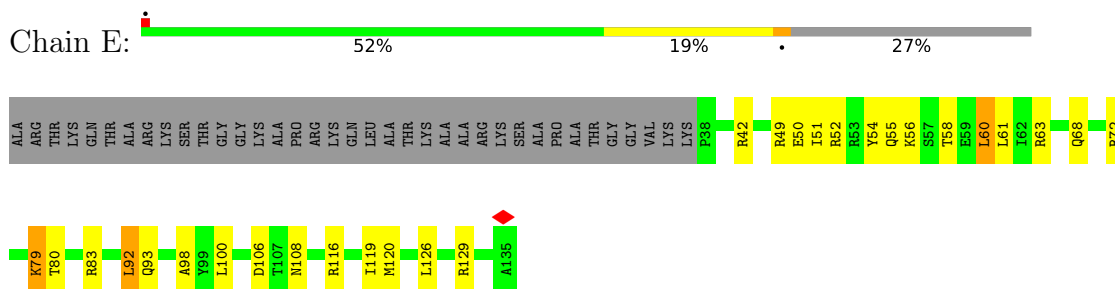
3 Residue-property plots [i](#)

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.

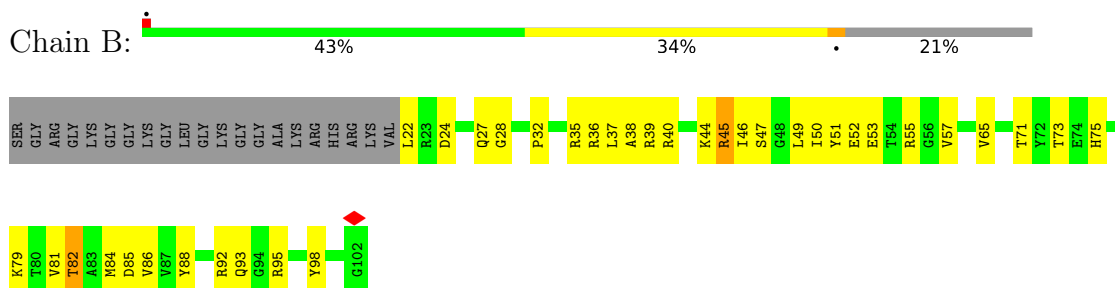
• Molecule 1: Histone H3



• Molecule 1: Histone H3



• Molecule 2: Histone H4



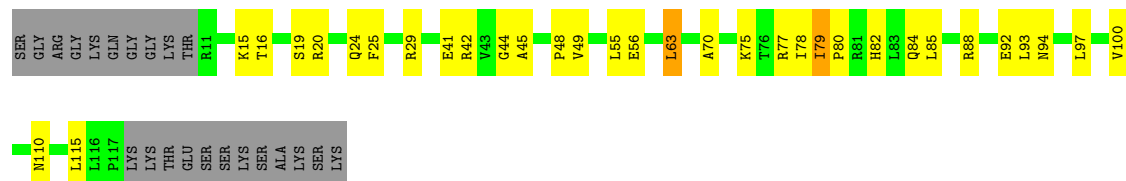
• Molecule 2: Histone H4





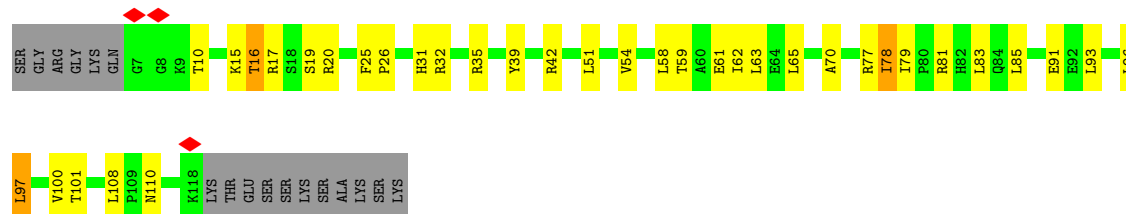
• Molecule 3: Histone H2A

Chain C: 57% 24% 17%



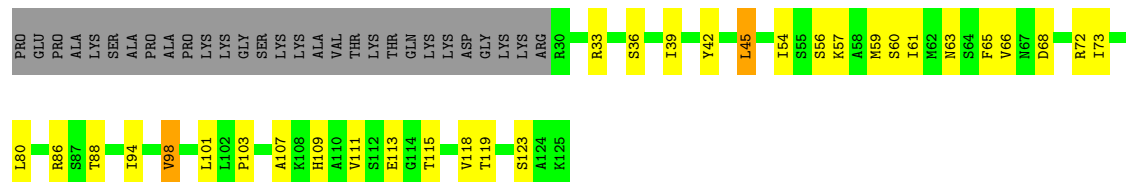
• Molecule 3: Histone H2A

Chain G: 59% 26% 13%



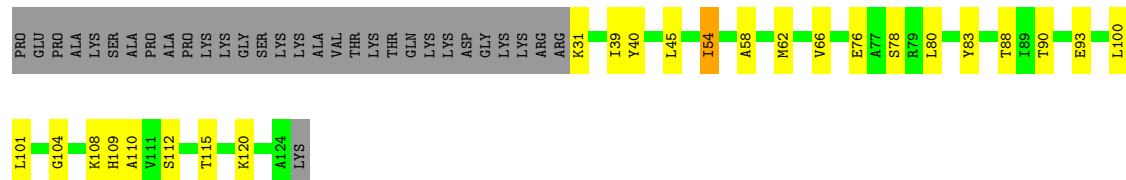
• Molecule 4: Histone H2B

Chain D: 51% 24% 23%

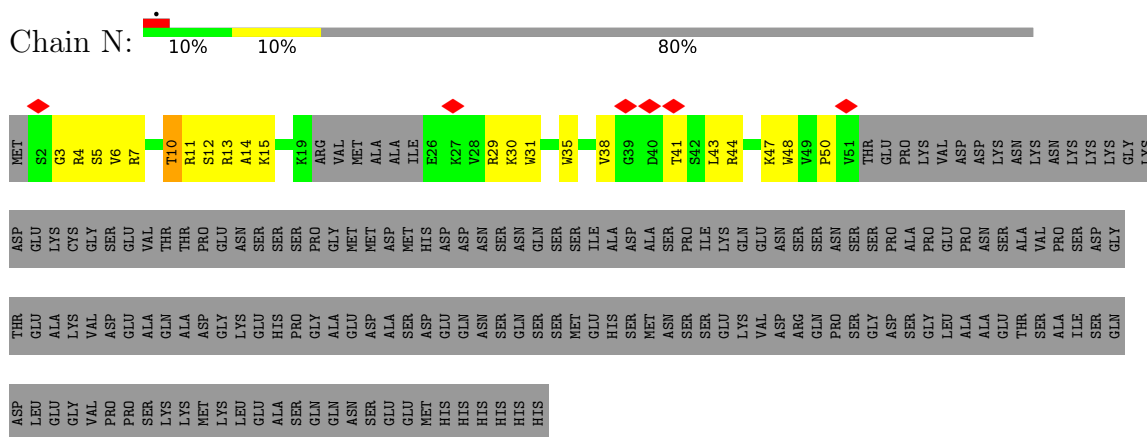


• Molecule 4: Histone H2B

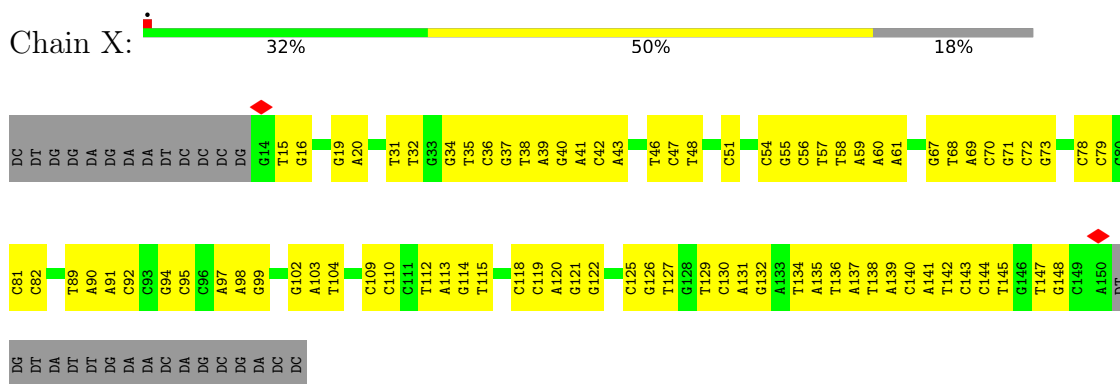
Chain H: 56% 18% 25%



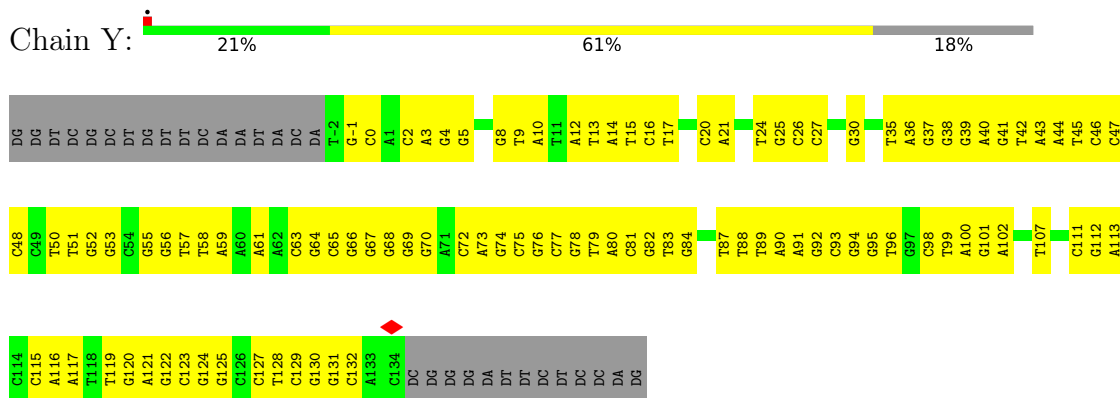
• Molecule 5: B-cell CLL/lymphoma 7 protein family member A



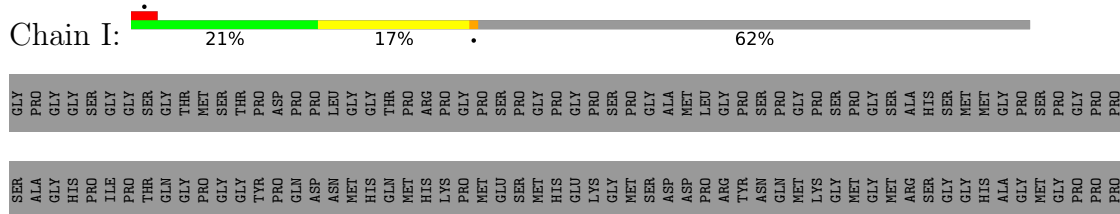
- Molecule 6: DNA (167-MER)



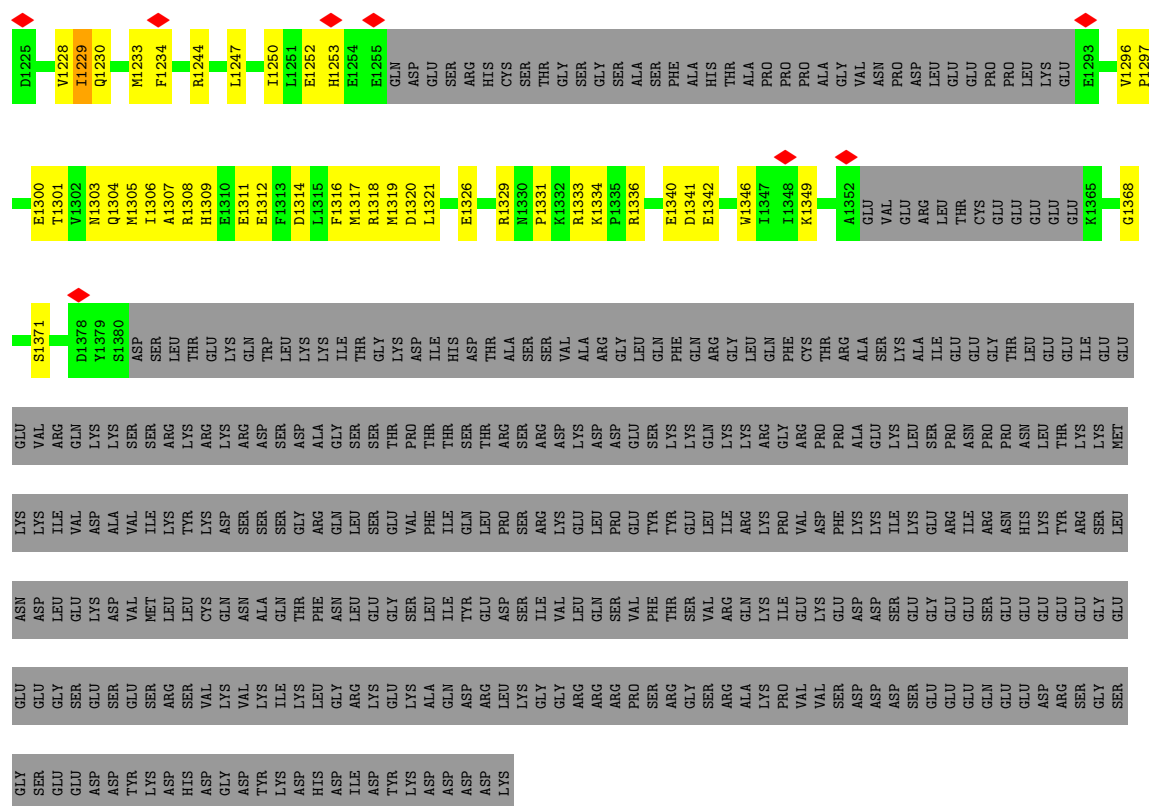
- Molecule 7: DNA (167-MER)



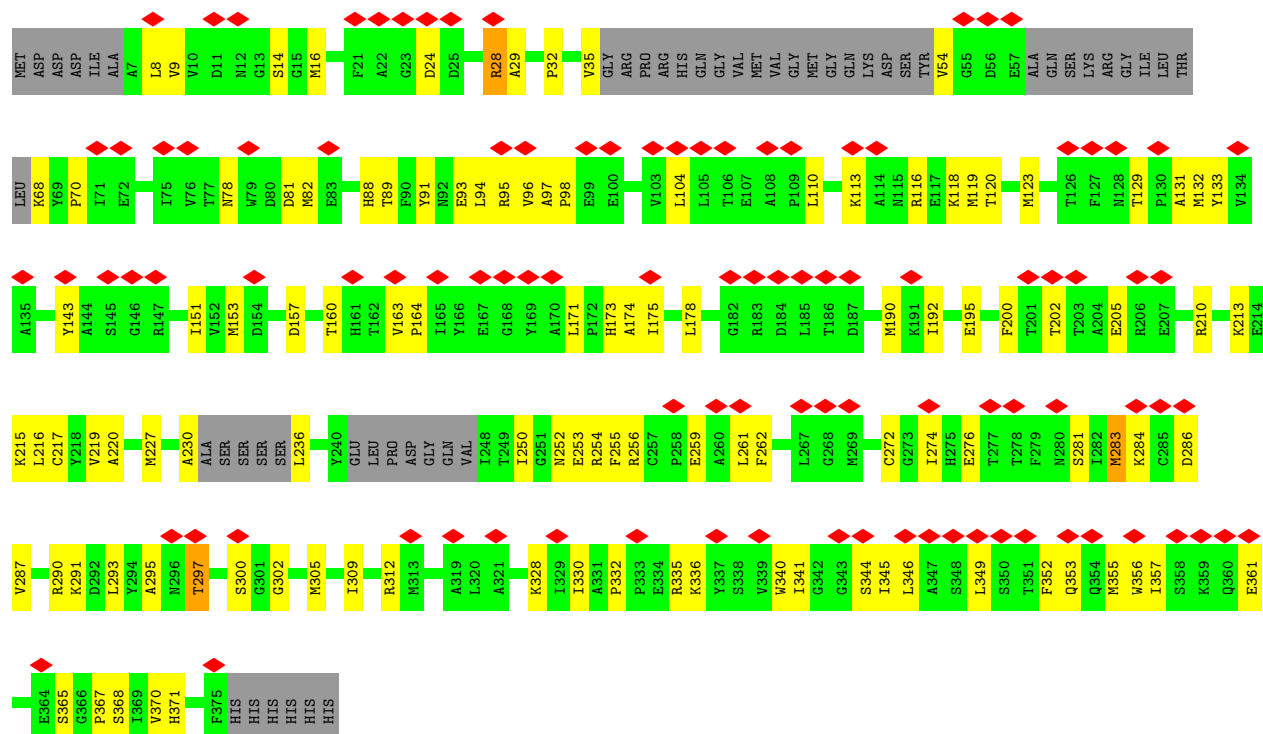
- Molecule 8: SMARCA4 isoform 2



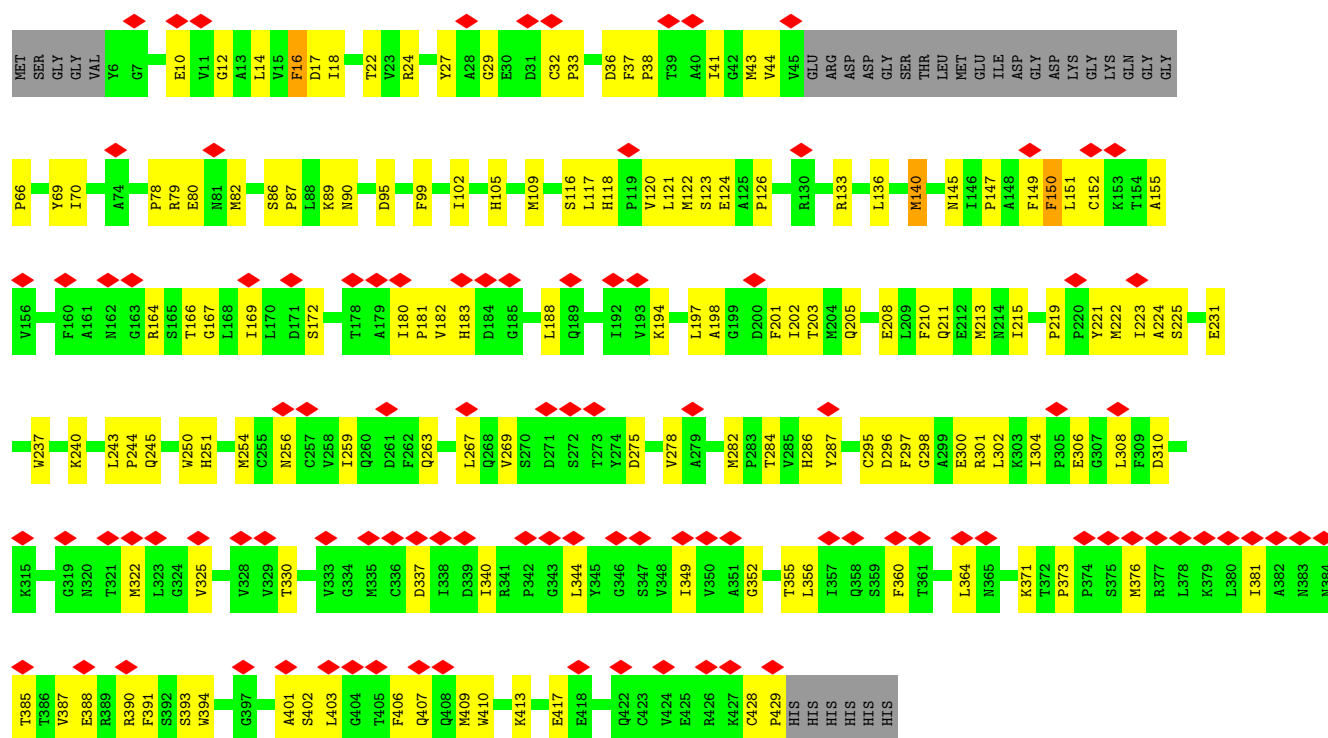




• Molecule 9: Actin, cytoplasmic 1



• Molecule 10: Actin-like protein 6A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/819	0.36	0/1099
1	E	0.18	0/819	0.34	0/1099
2	B	0.21	0/653	0.37	0/873
2	F	0.19	0/690	0.34	0/923
3	C	0.17	0/835	0.33	0/1127
3	G	0.20	0/868	0.39	0/1169
4	D	0.17	0/767	0.34	0/1029
4	H	0.19	0/746	0.35	0/1004
5	N	0.11	0/372	0.28	0/498
6	X	0.22	0/3126	0.39	0/4818
7	Y	0.22	0/3174	0.38	0/4901
8	I	0.14	0/5510	0.33	0/7409
9	J	0.10	0/2640	0.26	0/3573
10	K	0.11	0/3224	0.27	0/4372
All	All	0.17	0/24243	0.34	0/33894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	807	0	846	29	0
1	E	807	0	846	32	0
2	B	646	0	687	29	0
2	F	682	0	729	30	0
3	C	825	0	882	35	0
3	G	858	0	921	27	0
4	D	756	0	786	23	0
4	H	735	0	760	20	0
5	N	366	0	376	23	0
6	X	2791	0	1539	90	0
7	Y	2826	0	1537	101	0
8	I	5409	0	5490	236	0
9	J	2585	0	2552	84	0
10	K	3152	0	3093	96	0
11	I	4	0	0	1	0
12	I	1	0	0	0	0
13	I	27	0	12	4	0
All	All	23277	0	21056	747	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 17.

All (747) 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:X:143:DC:O2	7:Y:5:DG:N2	1.98	0.97
6:X:95:DC:O2	7:Y:53:DG:N2	2.03	0.91
6:X:148:DG:N2	7:Y:0:DC:O2	2.04	0.90
8:I:970:LYS:HA	8:I:973:ARG:HG3	1.57	0.87
6:X:143:DC:N3	7:Y:5:DG:N1	2.24	0.84
6:X:70:DC:H42	7:Y:78:DG:H1	1.27	0.82
3:C:42:ARG:HG2	7:Y:113:DA:H5'	1.63	0.81
10:K:407:GLN:HA	10:K:410:TRP:HD1	1.45	0.81
9:J:35:VAL:HG21	9:J:81:ASP:HB3	1.63	0.81
10:K:403:LEU:HB3	10:K:406:PHE:HB2	1.65	0.77
8:I:1078:ALA:HA	8:I:1336:ARG:HH12	1.50	0.76
2:B:73:THR:HG21	2:B:81:VAL:HG12	1.67	0.76
4:D:36:SER:HB2	4:D:63:ASN:HD21	1.50	0.76
8:I:1164:ASN:HA	8:I:1192:ARG:HH12	1.48	0.76
6:X:95:DC:N3	7:Y:53:DG:N1	2.31	0.75
8:I:925:LEU:HB2	8:I:934:LYS:HE3	1.70	0.72
9:J:151:ILE:O	9:J:297:THR:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:1000:MET:SD	8:I:1000:MET:N	2.62	0.71
9:J:349:LEU:HB2	9:J:352:PHE:HB2	1.71	0.70
8:I:778:ALA:HB3	8:I:976:LEU:HD11	1.73	0.70
8:I:1166:GLN:O	8:I:1195:GLN:NE2	2.25	0.70
10:K:231:GLU:HG3	10:K:295:CYS:HA	1.74	0.69
5:N:10:THR:HG22	5:N:13:ARG:HH21	1.57	0.69
10:K:205:GLN:HB3	10:K:304:ILE:HD12	1.74	0.69
9:J:353:GLN:HA	9:J:356:TRP:HD1	1.58	0.68
6:X:81:DC:H42	7:Y:67:DG:H1	1.41	0.68
9:J:28:ARG:NH2	9:J:93:GLU:O	2.26	0.68
10:K:251:HIS:HA	10:K:254:MET:HE2	1.76	0.68
3:C:75:LYS:HE2	3:C:77:ARG:HB3	1.75	0.68
10:K:150:PHE:HZ	10:K:409:MET:HG2	1.58	0.68
6:X:148:DG:N1	7:Y:0:DC:N3	2.29	0.67
8:I:1124:LEU:HD11	8:I:1149:TYR:HB3	1.75	0.67
2:B:49:LEU:H	2:B:49:LEU:HD12	1.60	0.67
1:E:61:LEU:O	2:F:36:ARG:NH2	2.27	0.67
9:J:300:SER:HA	9:J:335:ARG:HB2	1.76	0.67
2:B:92:ARG:NH2	4:H:76:GLU:OE1	2.26	0.67
9:J:283:MET:O	9:J:290:ARG:NH2	2.28	0.67
8:I:480:LEU:O	8:I:484:LYS:NZ	2.24	0.66
10:K:286:HIS:ND1	10:K:296:ASP:OD1	2.25	0.66
2:B:45:ARG:HH12	2:B:47:SER:HB2	1.60	0.66
5:N:35:TRP:HE3	5:N:44:ARG:HB2	1.60	0.66
3:G:77:ARG:NH2	6:X:132:DG:O4'	2.29	0.66
8:I:1342:GLU:HA	8:I:1346:TRP:HB3	1.77	0.66
8:I:991:LYS:HA	8:I:1199:VAL:HB	1.77	0.66
1:E:83:ARG:HH22	7:Y:100:DA:H4'	1.59	0.65
8:I:1300:GLU:OE1	8:I:1303:ASN:ND2	2.29	0.65
9:J:287:VAL:O	9:J:291:LYS:NZ	2.29	0.65
9:J:131:ALA:HB1	9:J:356:TRP:HB3	1.79	0.65
8:I:875:TRP:NE1	8:I:902:VAL:O	2.28	0.65
8:I:1164:ASN:OD1	8:I:1192:ARG:NH2	2.26	0.65
8:I:1103:CYS:SG	8:I:1104:GLN:N	2.70	0.64
8:I:1301:THR:HB	8:I:1304:GLN:HE21	1.63	0.64
10:K:181:PRO:HG2	10:K:188:LEU:HB2	1.79	0.64
3:C:41:GLU:HG2	3:C:42:ARG:HG3	1.78	0.64
7:Y:130:DG:H2''	7:Y:131:DG:C8	2.32	0.64
9:J:24:ASP:HB2	9:J:340:TRP:HH2	1.62	0.64
8:I:784:GLY:HA2	13:I:1803:ADP:H5'2	1.78	0.64
8:I:1000:MET:O	8:I:1005:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:263:GLN:HA	10:K:267:LEU:HD13	1.80	0.64
2:F:29:ILE:O	2:F:55:ARG:NH1	2.30	0.64
3:G:78:ILE:HG22	4:H:54:ILE:HA	1.80	0.64
8:I:874:ARG:NH2	8:I:902:VAL:O	2.31	0.64
8:I:922:TRP:HH2	8:I:937:SER:HA	1.62	0.64
10:K:167:GLY:HA2	10:K:344:LEU:HA	1.79	0.64
5:N:6:VAL:O	5:N:10:THR:OG1	2.16	0.64
8:I:784:GLY:O	8:I:788:GLN:NE2	2.31	0.63
2:B:93:GLN:OE1	2:B:95:ARG:NH2	2.25	0.63
2:B:27:GLN:OE1	2:B:55:ARG:NH1	2.31	0.63
2:F:93:GLN:OE1	2:F:95:ARG:NH2	2.32	0.63
9:J:353:GLN:HA	9:J:356:TRP:CD1	2.34	0.63
8:I:1006:VAL:HG23	8:I:1007:LEU:HD22	1.80	0.63
10:K:12:GLY:O	10:K:118:HIS:ND1	2.32	0.63
8:I:497:ILE:HD12	8:I:500:LEU:HD21	1.80	0.62
10:K:197:LEU:HG	10:K:322:MET:HE2	1.82	0.62
8:I:753:VAL:H	13:I:1803:ADP:HN62	1.48	0.62
8:I:926:ASN:OD1	8:I:934:LYS:NZ	2.23	0.62
8:I:781:MET:SD	8:I:781:MET:N	2.72	0.62
8:I:486:PHE:HZ	10:K:29:GLY:HA2	1.65	0.61
8:I:1320:ASP:OD1	8:I:1321:LEU:N	2.32	0.61
8:I:1126:LEU:HD11	8:I:1135:ARG:HG2	1.82	0.61
10:K:70:ILE:HD13	10:K:102:ILE:HA	1.83	0.61
3:C:29:ARG:NH2	7:Y:123:DC:OP1	2.31	0.61
10:K:41:ILE:HD11	10:K:70:ILE:HG12	1.81	0.61
10:K:164:ARG:HH21	10:K:349:ILE:HD13	1.65	0.61
1:E:49:ARG:HA	1:E:52:ARG:HG2	1.81	0.61
10:K:116:SER:HA	10:K:147:PRO:HD3	1.83	0.61
8:I:767:SER:O	8:I:771:ASN:ND2	2.33	0.61
2:B:39:ARG:NH2	2:B:44:LYS:O	2.34	0.60
1:E:42:ARG:H	6:X:144:DC:H5'	1.66	0.60
8:I:891:CYS:O	8:I:894:THR:OG1	2.20	0.60
9:J:163:VAL:HG13	9:J:175:ILE:HG12	1.83	0.60
6:X:136:DT:H2'	6:X:137:DA:C8	2.37	0.60
1:E:100:LEU:HB3	2:F:37:LEU:HD21	1.83	0.60
1:A:40:ARG:O	1:A:42:ARG:NH2	2.33	0.60
3:C:78:ILE:HB	4:D:54:ILE:HA	1.83	0.60
10:K:17:ASP:OD2	10:K:24:ARG:NH2	2.34	0.60
2:F:23:ARG:HD2	2:F:27:GLN:HG3	1.83	0.59
8:I:969:HIS:CE1	8:I:973:ARG:HG2	2.36	0.59
10:K:126:PRO:HG2	10:K:180:ILE:HD13	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.85	0.59
8:I:1326:GLU:OE1	8:I:1329:ARG:NH2	2.35	0.59
3:G:42:ARG:HB2	4:H:88:THR:HG22	1.84	0.59
7:Y:4:DG:H2''	7:Y:5:DG:H5'	1.84	0.59
8:I:833:SER:HA	8:I:857:LEU:HB2	1.84	0.59
3:G:63:LEU:HD21	4:H:45:LEU:HD12	1.84	0.58
8:I:1105:MET:HG2	8:I:1108:LEU:HG	1.84	0.58
8:I:1174:PHE:HA	8:I:1204:LEU:HD12	1.85	0.58
10:K:22:THR:HG22	10:K:38:PRO:HA	1.84	0.58
7:Y:45:DT:H2''	7:Y:46:DC:C5	2.38	0.58
8:I:1165:LEU:HD12	8:I:1189:ARG:HB3	1.84	0.58
3:G:42:ARG:HH12	6:X:112:DT:H4'	1.68	0.58
6:X:31:DT:H1'	6:X:32:DT:H5'	1.84	0.58
1:A:73:GLU:O	1:A:76:GLN:NE2	2.27	0.58
9:J:9:VAL:HG21	9:J:344:SER:HA	1.85	0.58
8:I:1084:LEU:HA	8:I:1087:ARG:HB2	1.86	0.58
1:E:83:ARG:HB2	2:F:80:THR:HG22	1.86	0.57
5:N:41:THR:HG22	5:N:43:LEU:H	1.70	0.57
6:X:36:DC:H2''	6:X:37:DG:C8	2.39	0.57
6:X:120:DA:H2''	6:X:121:DG:N7	2.20	0.57
8:I:926:ASN:HA	8:I:930:PRO:HA	1.84	0.57
10:K:275:ASP:HB3	10:K:278:VAL:HG22	1.86	0.57
7:Y:4:DG:H2''	7:Y:5:DG:H2'	1.87	0.57
2:F:51:TYR:O	2:F:54:THR:OG1	2.17	0.57
8:I:916:ASN:HB2	8:I:1221:LYS:HB2	1.87	0.57
9:J:16:MET:SD	9:J:210:ARG:NH2	2.78	0.57
8:I:754:LEU:HD23	8:I:754:LEU:H	1.69	0.57
8:I:1062:HIS:NE2	8:I:1340:GLU:OE1	2.38	0.57
10:K:208:GLU:O	10:K:211:GLN:NE2	2.36	0.57
2:B:82:THR:N	2:B:85:ASP:OD1	2.27	0.57
4:D:33:ARG:HD2	7:Y:123:DC:H4'	1.87	0.57
10:K:16:PHE:HE2	10:K:120:VAL:HG13	1.69	0.57
9:J:153:MET:HE1	9:J:160:THR:HG23	1.87	0.56
6:X:104:DT:H3	7:Y:44:DA:H2	1.51	0.56
8:I:482:HIS:NE2	10:K:402:SER:O	2.38	0.56
8:I:877:TYR:CZ	8:I:907:LEU:HD23	2.41	0.56
10:K:243:LEU:HD12	10:K:244:PRO:HD2	1.86	0.56
4:D:57:LYS:O	4:D:60:SER:OG	2.21	0.56
5:N:31:TRP:HB3	5:N:48:TRP:HB3	1.88	0.56
6:X:89:DT:H2''	6:X:90:DA:C8	2.41	0.56
9:J:132:MET:SD	9:J:132:MET:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:305:MET:HA	9:J:335:ARG:HH21	1.68	0.56
8:I:1074:ASP:N	8:I:1074:ASP:OD1	2.36	0.56
8:I:1180:PRO:HG3	8:I:1222:LEU:HB2	1.86	0.56
8:I:1200:ARG:HH11	8:I:1308:ARG:HG2	1.70	0.56
8:I:1018:LEU:HA	8:I:1032:THR:HG22	1.88	0.56
8:I:833:SER:OG	8:I:835:LYS:NZ	2.38	0.56
3:C:15:LYS:NZ	6:X:31:DT:O3'	2.33	0.56
8:I:836:GLY:O	8:I:841:ARG:NH1	2.37	0.56
8:I:922:TRP:CH2	8:I:937:SER:HA	2.41	0.56
8:I:1173:ILE:O	8:I:1203:ARG:NH1	2.39	0.56
9:J:160:THR:HB	9:J:178:LEU:O	2.06	0.56
6:X:135:DA:H2'	6:X:136:DT:C6	2.41	0.55
8:I:994:TYR:HB3	8:I:1305:MET:HE3	1.86	0.55
4:D:86:ARG:HH12	6:X:40:DG:H3'	1.70	0.55
1:A:59:GLU:OE1	1:A:59:GLU:N	2.33	0.55
2:B:24:ASP:O	2:B:28:GLY:N	2.39	0.55
6:X:55:DG:OP1	8:I:1155:SER:OG	2.24	0.55
8:I:1010:HIS:HE1	8:I:1016:VAL:HG23	1.71	0.55
10:K:43:MET:O	10:K:82:MET:HA	2.06	0.55
10:K:124:GLU:HB3	10:K:151:LEU:HD11	1.88	0.55
7:Y:40:DA:H2''	7:Y:41:DG:H8	1.71	0.55
2:B:49:LEU:O	2:B:53:GLU:HG2	2.07	0.55
7:Y:101:DG:H2''	7:Y:102:DA:H8	1.72	0.55
8:I:1130:THR:O	8:I:1135:ARG:NH2	2.38	0.55
6:X:68:DT:H2''	6:X:69:DA:N7	2.21	0.55
8:I:796:LEU:HD12	8:I:800:LYS:HB2	1.87	0.55
8:I:1009:ARG:HA	8:I:1012:GLN:HE21	1.72	0.55
9:J:35:VAL:HA	9:J:54:VAL:HG13	1.89	0.55
9:J:104:LEU:HD13	9:J:133:TYR:HB3	1.88	0.55
5:N:29:ARG:HH22	9:J:367:PRO:HD3	1.71	0.54
8:I:961:THR:HA	8:I:964:ILE:HG12	1.88	0.54
8:I:1119:ARG:HB3	8:I:1121:PHE:CD2	2.42	0.54
9:J:215:LYS:HG3	9:J:216:LEU:HG	1.88	0.54
9:J:361:GLU:O	9:J:365:SER:OG	2.25	0.54
4:D:57:LYS:O	4:D:61:ILE:HG12	2.08	0.54
6:X:31:DT:H3	7:Y:117:DA:H2	1.55	0.54
6:X:99:DG:N2	7:Y:50:DT:O2	2.41	0.54
8:I:972:LEU:HB2	8:I:975:PHE:HB2	1.89	0.54
8:I:995:VAL:HG12	8:I:1203:ARG:HB2	1.89	0.54
8:I:1244:ARG:HA	8:I:1247:LEU:HG	1.89	0.54
9:J:200:PHE:HD1	9:J:205:GLU:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:ASP:OD2	4:D:72:ARG:NH2	2.41	0.54
3:G:39:TYR:HB3	4:H:78:SER:HB3	1.90	0.54
6:X:144:DC:H2'	6:X:145:DT:C6	2.42	0.54
8:I:1125:ARG:HA	8:I:1153:LEU:HG	1.87	0.54
9:J:151:ILE:HA	9:J:164:PRO:HA	1.89	0.54
7:Y:90:DA:H2''	7:Y:91:DA:N7	2.23	0.54
1:E:56:LYS:O	3:G:81:ARG:NH2	2.41	0.54
1:E:108:ASN:ND2	2:F:42:GLY:O	2.40	0.54
6:X:54:DC:N3	7:Y:95:DG:N2	2.56	0.54
9:J:259:GLU:HA	9:J:262:PHE:HD2	1.73	0.54
1:E:60:LEU:HD12	1:E:93:GLN:HE22	1.72	0.53
8:I:881:ASP:OD1	8:I:882:GLU:N	2.41	0.53
8:I:1126:LEU:HD22	8:I:1138:LEU:HD11	1.89	0.53
2:B:84:MET:HG3	4:H:83:TYR:OH	2.08	0.53
1:E:116:ARG:HH12	6:X:71:DG:H3'	1.72	0.53
1:A:106:ASP:OD2	1:A:131:ARG:NH2	2.41	0.53
3:C:24:GLN:N	3:C:56:GLU:OE1	2.41	0.53
7:Y:20:DC:H2''	7:Y:21:DA:C8	2.42	0.53
7:Y:77:DC:H2''	7:Y:78:DG:N7	2.23	0.53
8:I:1250:ILE:HA	8:I:1253:HIS:CD2	2.43	0.53
7:Y:55:DG:H2''	7:Y:56:DG:C5	2.43	0.53
3:C:44:GLY:HA2	7:Y:112:DG:H5''	1.90	0.53
1:E:42:ARG:HG2	6:X:144:DC:H5''	1.91	0.53
8:I:569:ARG:HH22	8:I:572:LYS:HZ1	1.56	0.53
8:I:868:HIS:CD2	8:I:869:ILE:HG23	2.43	0.53
8:I:871:ALA:HA	8:I:875:TRP:HH2	1.74	0.53
8:I:1127:ASP:O	8:I:1130:THR:OG1	2.20	0.53
7:Y:68:DG:H2''	7:Y:69:DG:C8	2.44	0.53
8:I:487:LYS:O	8:I:491:ARG:HG2	2.09	0.53
10:K:78:PRO:HB2	10:K:244:PRO:HG2	1.89	0.53
10:K:219:PRO:HB2	10:K:221:TYR:HD2	1.74	0.53
7:Y:9:DT:H2''	7:Y:10:DA:C8	2.44	0.53
8:I:547:ASP:HB3	8:I:550:LEU:HB3	1.89	0.53
1:E:50:GLU:HB3	2:F:39:ARG:HG2	1.91	0.53
2:F:48:GLY:N	7:Y:81:DC:OP1	2.40	0.53
8:I:922:TRP:HD1	8:I:926:ASN:HD21	1.55	0.53
8:I:998:CYS:N	8:I:1205:CYS:O	2.41	0.53
8:I:1098:LYS:O	8:I:1170:THR:OG1	2.24	0.53
8:I:962:ILE:HG23	8:I:1247:LEU:HD11	1.90	0.53
3:G:16:THR:O	3:G:19:SER:OG	2.24	0.53
1:E:129:ARG:O	1:E:129:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:111:DC:H2"	7:Y:112:DG:C8	2.44	0.52
9:J:120:THR:HB	9:J:367:PRO:HB3	1.90	0.52
3:C:16:THR:HG22	3:C:19:SER:H	1.74	0.52
4:H:39:ILE:HG13	4:H:40:TYR:HD2	1.73	0.52
8:I:879:ILE:HG23	8:I:907:LEU:HD11	1.90	0.52
8:I:996:ILE:HD11	8:I:1202:LEU:HD12	1.91	0.52
8:I:741:ARG:NH1	8:I:763:GLU:OE2	2.42	0.52
9:J:14:SER:HB2	9:J:157:ASP:HB3	1.90	0.52
9:J:202:THR:HG23	9:J:205:GLU:H	1.74	0.52
2:B:82:THR:HG23	2:B:84:MET:H	1.74	0.52
1:E:98:ALA:HB1	3:G:101:THR:HG21	1.90	0.52
1:E:119:ILE:O	2:F:47:SER:OG	2.27	0.52
8:I:831:LYS:HA	8:I:855:VAL:HB	1.91	0.52
2:F:27:GLN:NE2	2:F:52:GLU:OE2	2.43	0.52
8:I:1213:LYS:H	8:I:1213:LYS:HD2	1.73	0.52
7:Y:121:DA:H2"	7:Y:122:DG:C8	2.45	0.52
10:K:373:PRO:HD2	10:K:376:MET:HE2	1.91	0.52
1:A:119:ILE:HD11	2:B:46:ILE:HG22	1.92	0.52
8:I:1206:THR:O	8:I:1209:SER:OG	2.27	0.52
9:J:192:ILE:O	9:J:195:GLU:HG2	2.10	0.52
10:K:17:ASP:OD2	10:K:393:SER:OG	2.28	0.52
5:N:38:VAL:HB	10:K:407:GLN:CD	2.34	0.52
6:X:89:DT:H2"	6:X:90:DA:N7	2.25	0.52
6:X:112:DT:H2"	6:X:113:DA:C8	2.45	0.52
8:I:1124:LEU:HD22	8:I:1142:PHE:HB2	1.93	0.51
10:K:356:LEU:HD11	10:K:390:ARG:HD2	1.91	0.51
1:A:104:PHE:HD2	2:B:38:ALA:HA	1.76	0.51
10:K:352:GLY:O	10:K:355:THR:OG1	2.23	0.51
1:A:47:ALA:O	1:A:51:ILE:HG12	2.10	0.51
7:Y:24:DT:H2"	7:Y:25:DG:C8	2.44	0.51
7:Y:36:DA:H2"	7:Y:37:DG:C8	2.45	0.51
8:I:922:TRP:CD1	8:I:926:ASN:HD21	2.27	0.51
8:I:755:LYS:HB2	8:I:758:GLN:HG3	1.92	0.51
8:I:756:GLN:O	8:I:760:LYS:HG2	2.11	0.51
8:I:1076:TYR:CE1	8:I:1083:GLU:HA	2.46	0.51
8:I:1314:ASP:HB2	8:I:1318:ARG:NH2	2.26	0.51
8:I:1331:PRO:O	8:I:1333:ARG:NH1	2.43	0.51
3:C:25:PHE:HE2	3:C:55:LEU:HB3	1.76	0.51
7:Y:-1:DG:H2"	7:Y:0:DC:C5	2.45	0.51
8:I:861:GLU:OE1	8:I:861:GLU:N	2.43	0.51
3:C:75:LYS:HG3	3:C:77:ARG:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:566:GLU:OE2	8:I:570:GLN:NE2	2.43	0.51
8:I:1163:LEU:O	8:I:1192:ARG:NH1	2.44	0.51
8:I:1169:ASP:OD2	8:I:1308:ARG:NH2	2.43	0.51
1:A:94:GLU:O	1:A:97:GLU:HG3	2.10	0.51
3:C:55:LEU:HD12	4:D:66:VAL:HG23	1.92	0.51
3:C:79:ILE:HD12	3:C:80:PRO:HD2	1.92	0.51
6:X:81:DC:N4	7:Y:67:DG:H1	2.07	0.51
8:I:1076:TYR:CE1	8:I:1086:ASP:HB3	2.46	0.51
4:H:109:HIS:HE1	5:N:5:SER:HA	1.75	0.51
10:K:155:ALA:HB1	10:K:169:ILE:HD13	1.93	0.51
7:Y:99:DT:H2''	7:Y:100:DA:C8	2.46	0.51
8:I:781:MET:O	8:I:1192:ARG:HD2	2.11	0.51
9:J:330:ILE:HG22	9:J:332:PRO:HD3	1.93	0.51
1:A:134:ARG:NE	1:A:134:ARG:O	2.41	0.50
7:Y:101:DG:H2''	7:Y:102:DA:C8	2.45	0.50
8:I:915:GLN:HG3	8:I:916:ASN:H	1.75	0.50
8:I:507:TYR:HA	8:I:510:ASN:HD21	1.76	0.50
8:I:1076:TYR:HE2	8:I:1334:LYS:HG3	1.74	0.50
8:I:776:ILE:HD12	8:I:908:LEU:HD23	1.94	0.50
8:I:997:LYS:HZ2	8:I:1297:PRO:HA	1.77	0.50
1:A:110:CYS:HA	1:E:126:LEU:HD11	1.92	0.50
10:K:145:ASN:O	10:K:413:LYS:NZ	2.45	0.50
2:F:39:ARG:NH1	2:F:44:LYS:O	2.45	0.50
4:D:107:ALA:O	4:D:111:VAL:HG12	2.11	0.50
3:G:10:THR:HA	4:H:120:LYS:HE3	1.94	0.50
8:I:783:LEU:HD23	8:I:783:LEU:H	1.77	0.50
9:J:190:MET:HG2	9:J:200:PHE:HB2	1.94	0.50
9:J:250:ILE:HG21	9:J:254:ARG:HE	1.77	0.50
6:X:94:DG:H2'	6:X:95:DC:C6	2.46	0.50
9:J:163:VAL:HG22	9:J:175:ILE:HG23	1.94	0.50
10:K:80:GLU:OE2	10:K:245:GLN:N	2.43	0.50
4:D:39:ILE:HD11	7:Y:123:DC:OP2	2.12	0.50
4:D:72:ARG:HD2	4:D:101:LEU:HD21	1.94	0.50
7:Y:35:DT:H2''	7:Y:36:DA:C8	2.47	0.50
7:Y:46:DC:H2''	7:Y:47:DC:C6	2.47	0.50
1:A:120:MET:N	1:A:123:ASP:OD2	2.42	0.49
6:X:58:DT:H2''	6:X:59:DA:N7	2.27	0.49
8:I:466:ARG:HH21	8:I:469:ARG:HG3	1.76	0.49
8:I:922:TRP:HD1	8:I:926:ASN:ND2	2.11	0.49
1:A:62:ILE:HB	1:A:93:GLN:HE22	1.76	0.49
3:C:63:LEU:HD12	4:D:45:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:31:HIS:CE1	3:G:35:ARG:HH22	2.31	0.49
7:Y:75:DC:H2''	7:Y:76:DG:C8	2.47	0.49
8:I:1166:GLN:NE2	13:I:1803:ADP:O3'	2.45	0.49
8:I:1177:ASP:HB2	8:I:1182:GLN:NE2	2.27	0.49
10:K:223:ILE:HA	10:K:237:TRP:CZ3	2.47	0.49
6:X:70:DC:H2''	6:X:71:DG:C8	2.48	0.49
6:X:138:DT:H2''	6:X:139:DA:N7	2.28	0.49
6:X:140:DC:H2''	6:X:141:DA:N7	2.27	0.49
8:I:1184:LEU:HA	8:I:1187:GLN:HE21	1.77	0.49
10:K:87:PRO:HB3	10:K:95:ASP:HB3	1.94	0.49
10:K:269:VAL:HG21	10:K:360:PHE:HD1	1.78	0.49
7:Y:69:DG:H2''	7:Y:70:DG:C8	2.46	0.49
8:I:1001:SER:N	8:I:1004:GLN:OE1	2.45	0.49
7:Y:93:DC:H2''	7:Y:94:DG:H8	1.78	0.49
8:I:1077:ARG:HG2	8:I:1336:ARG:HB2	1.95	0.49
8:I:1099:VAL:HA	8:I:1170:THR:O	2.12	0.49
2:F:91:LYS:NZ	2:F:96:THR:HB	2.28	0.49
5:N:29:ARG:H	5:N:29:ARG:HD3	1.77	0.49
6:X:38:DT:H2''	6:X:39:DA:N7	2.27	0.49
7:Y:12:DA:H2'	7:Y:13:DT:H71	1.95	0.49
9:J:174:ALA:HA	9:J:284:LYS:HD2	1.94	0.49
1:E:51:ILE:O	1:E:55:GLN:HB2	2.13	0.49
10:K:16:PHE:HB2	10:K:122:MET:SD	2.53	0.49
1:E:54:TYR:OH	2:F:36:ARG:HD2	2.13	0.49
7:Y:81:DC:H2''	7:Y:82:DG:C8	2.48	0.49
8:I:929:LEU:HD12	8:I:930:PRO:HD2	1.95	0.49
2:B:51:TYR:HB3	2:B:55:ARG:HH21	1.78	0.48
8:I:736:HIS:O	8:I:736:HIS:ND1	2.46	0.48
11:I:1801:BEF:F3	13:I:1803:ADP:O1B	2.21	0.48
9:J:290:ARG:O	9:J:293:LEU:HB2	2.12	0.48
1:A:61:LEU:HD21	2:B:40:ARG:CZ	2.43	0.48
4:D:86:ARG:NH2	6:X:41:DA:OP2	2.36	0.48
6:X:98:DA:H5'	6:X:98:DA:C8	2.49	0.48
7:Y:47:DC:H4'	7:Y:48:DC:H5'	1.95	0.48
8:I:871:ALA:HA	8:I:875:TRP:CH2	2.48	0.48
9:J:217:CYS:SG	9:J:254:ARG:NH1	2.86	0.48
2:B:44:LYS:HB2	3:C:115:LEU:HD11	1.95	0.48
3:C:15:LYS:NZ	6:X:32:DT:H5''	2.28	0.48
6:X:121:DG:H2''	6:X:122:DG:C8	2.48	0.48
7:Y:92:DG:C8	7:Y:92:DG:H5'	2.48	0.48
3:C:70:ALA:HA	3:C:82:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:20:DA:H8	6:X:20:DA:H5''	1.79	0.48
10:K:330:THR:HG21	10:K:371:LYS:HD3	1.94	0.48
1:A:68:GLN:OE1	1:A:72:ARG:NH2	2.47	0.48
4:H:109:HIS:O	4:H:112:SER:OG	2.28	0.48
10:K:413:LYS:O	10:K:417:GLU:HG2	2.13	0.48
7:Y:124:DG:H2''	7:Y:125:DG:H8	1.77	0.48
8:I:959:GLU:HG3	8:I:961:THR:HG22	1.96	0.48
8:I:1048:HIS:HE1	8:I:1050:TYR:CG	2.32	0.48
10:K:105:HIS:O	10:K:109:MET:HG3	2.13	0.48
10:K:267:LEU:HA	10:K:301:ARG:HB2	1.95	0.48
3:C:42:ARG:HB2	4:D:88:THR:HG22	1.95	0.48
7:Y:116:DA:H2''	7:Y:117:DA:C8	2.49	0.48
3:C:88:ARG:HD3	3:C:94:ASN:ND2	2.28	0.48
6:X:46:DT:H2''	6:X:47:DC:C6	2.49	0.48
8:I:891:CYS:SG	8:I:893:LEU:HB3	2.53	0.48
6:X:135:DA:H2'	6:X:136:DT:H6	1.79	0.48
8:I:1109:MET:HE3	8:I:1125:ARG:HH21	1.79	0.48
8:I:1229:ILE:HG13	8:I:1230:GLN:H	1.79	0.48
10:K:69:TYR:CE2	10:K:79:ARG:HD2	2.49	0.48
8:I:778:ALA:HA	8:I:910:THR:O	2.14	0.47
8:I:994:TYR:HE2	8:I:1200:ARG:HH21	1.62	0.47
3:C:92:GLU:HB2	4:D:103:PRO:HG3	1.95	0.47
7:Y:51:DT:H2'	7:Y:52:DG:H8	1.79	0.47
8:I:1101:LEU:HB2	8:I:1151:ILE:HD11	1.96	0.47
7:Y:26:DC:H2''	7:Y:27:DC:C5	2.48	0.47
8:I:486:PHE:CZ	10:K:29:GLY:HA2	2.48	0.47
8:I:1008:TYR:HD1	8:I:1045:ILE:HD11	1.79	0.47
4:D:94:ILE:O	4:D:98:VAL:HG22	2.14	0.47
7:Y:65:DC:H2''	7:Y:66:DG:C8	2.49	0.47
8:I:991:LYS:HZ3	8:I:1188:ASP:HA	1.79	0.47
4:D:56:SER:HA	4:D:59:MET:HG2	1.97	0.47
8:I:1052:PHE:HB3	8:I:1054:HIS:CE1	2.49	0.47
9:J:295:ALA:HB1	9:J:328:LYS:HD2	1.95	0.47
10:K:282:MET:SD	10:K:301:ARG:NH2	2.85	0.47
3:C:97:LEU:HD21	4:D:65:PHE:HE1	1.78	0.47
6:X:72:DC:H2''	6:X:73:DG:C8	2.50	0.47
8:I:1048:HIS:HE1	8:I:1050:TYR:CD2	2.32	0.47
10:K:213:MET:HG2	10:K:215:ILE:HG13	1.96	0.47
8:I:498:GLN:O	8:I:502:LYS:HG2	2.14	0.47
8:I:550:LEU:HD23	8:I:554:LEU:HD23	1.96	0.47
8:I:749:MET:HE3	8:I:749:MET:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:98:PRO:HB2	9:J:129:THR:HG22	1.96	0.47
9:J:113:LYS:HD3	9:J:116:ARG:HH21	1.79	0.47
10:K:225:SER:O	10:K:237:TRP:HB2	2.15	0.47
4:D:109:HIS:O	4:D:113:GLU:HG2	2.13	0.47
6:X:57:DT:O3'	8:I:865:LYS:NZ	2.34	0.47
8:I:480:LEU:O	8:I:484:LYS:HG2	2.15	0.47
8:I:877:TYR:HB2	8:I:905:ARG:HH21	1.80	0.47
8:I:929:LEU:HG	8:I:932:ILE:HB	1.96	0.47
8:I:1173:ILE:HB	8:I:1203:ARG:HH11	1.79	0.47
6:X:19:DG:H2''	6:X:20:DA:N7	2.30	0.47
7:Y:51:DT:H2'	7:Y:52:DG:C8	2.50	0.46
8:I:758:GLN:O	8:I:762:LEU:HG	2.15	0.46
8:I:891:CYS:O	8:I:895:GLN:HG3	2.15	0.46
5:N:43:LEU:HD23	10:K:407:GLN:HG2	1.96	0.46
8:I:918:LEU:N	8:I:919:PRO:HD2	2.30	0.46
1:A:130:ILE:HD11	1:E:106:ASP:HB3	1.98	0.46
2:B:36:ARG:NH2	7:Y:61:DA:OP1	2.49	0.46
5:N:13:ARG:NH2	5:N:14:ALA:HB2	2.30	0.46
10:K:222:MET:HE1	10:K:251:HIS:HE1	1.81	0.46
3:G:15:LYS:HA	3:G:20:ARG:HH21	1.81	0.46
3:G:96:LEU:HG	3:G:97:LEU:HD22	1.98	0.46
8:I:978:ARG:NH2	8:I:979:ARG:O	2.34	0.46
8:I:1009:ARG:HH22	8:I:1349:LYS:HE2	1.81	0.46
8:I:1038:THR:O	8:I:1042:LEU:HG	2.16	0.46
10:K:123:SER:HA	10:K:152:CYS:O	2.15	0.46
8:I:1009:ARG:NH1	8:I:1010:HIS:HB2	2.29	0.46
9:J:220:ALA:O	9:J:312:ARG:NH1	2.49	0.46
5:N:43:LEU:HB3	10:K:407:GLN:HE21	1.80	0.46
9:J:210:ARG:O	9:J:213:LYS:HG3	2.15	0.46
2:F:70:VAL:HA	2:F:73:THR:HG22	1.97	0.46
3:G:97:LEU:HD13	3:G:97:LEU:HA	1.65	0.46
3:G:25:PHE:HZ	3:G:59:THR:HG21	1.80	0.46
5:N:29:ARG:HG3	5:N:50:PRO:HG3	1.98	0.46
7:Y:79:DT:H2''	7:Y:80:DA:N7	2.30	0.46
8:I:960:GLU:O	8:I:964:ILE:HG23	2.15	0.46
8:I:1307:ALA:HB2	8:I:1316:PHE:HE2	1.80	0.46
7:Y:87:DT:H2''	7:Y:88:DT:C6	2.51	0.46
8:I:1228:VAL:HG23	8:I:1229:ILE:HG23	1.98	0.46
10:K:14:LEU:HD13	10:K:27:TYR:HA	1.98	0.46
4:D:115:THR:HA	4:D:118:VAL:HG12	1.98	0.45
1:E:55:GLN:NE2	3:G:110:ASN:H	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:LYS:C	3:G:81:ARG:HH22	2.24	0.45
2:F:91:LYS:HB2	2:F:91:LYS:HE2	1.78	0.45
5:N:47:LYS:HD3	10:K:10:GLU:HA	1.98	0.45
6:X:119:DC:H2''	6:X:120:DA:N7	2.30	0.45
8:I:1342:GLU:CD	8:I:1342:GLU:H	2.23	0.45
8:I:929:LEU:O	8:I:933:PHE:HB2	2.16	0.45
3:C:63:LEU:HD13	3:C:63:LEU:HA	1.82	0.45
9:J:286:ASP:O	9:J:290:ARG:HG3	2.16	0.45
6:X:81:DC:H1'	6:X:82:DC:H5'	1.98	0.45
7:Y:43:DA:H2''	7:Y:44:DA:C8	2.52	0.45
7:Y:119:DT:H2''	7:Y:120:DG:N7	2.31	0.45
8:I:1009:ARG:NH2	8:I:1349:LYS:HE2	2.31	0.45
10:K:43:MET:SD	10:K:66:PRO:HB2	2.56	0.45
1:E:68:GLN:NE2	1:E:72:ARG:HH21	2.15	0.45
6:X:126:DG:C8	6:X:127:DT:H72	2.51	0.45
8:I:1041:GLN:HA	8:I:1044:LYS:HD3	1.99	0.45
8:I:1137:MET:HE3	8:I:1137:MET:HB3	1.89	0.45
10:K:86:SER:O	10:K:89:LYS:NZ	2.39	0.45
10:K:224:ALA:HB2	10:K:240:LYS:HE3	1.99	0.45
1:A:60:LEU:H	1:A:60:LEU:HD23	1.81	0.45
1:E:68:GLN:HE22	1:E:72:ARG:HH21	1.63	0.45
8:I:552:TYR:O	8:I:556:GLN:NE2	2.49	0.45
8:I:882:GLU:N	8:I:909:LEU:O	2.49	0.45
2:B:35:ARG:HG2	2:B:46:ILE:HD11	1.98	0.45
1:E:92:LEU:HD22	2:F:86:VAL:HG21	1.98	0.45
6:X:143:DC:N4	7:Y:5:DG:O6	2.42	0.45
8:I:1076:TYR:HE1	8:I:1086:ASP:HB3	1.81	0.45
8:I:1177:ASP:OD1	8:I:1178:TRP:N	2.50	0.45
3:C:75:LYS:HE3	7:Y:132:DC:O5'	2.16	0.45
7:Y:123:DC:H2''	7:Y:124:DG:C8	2.52	0.45
8:I:1090:PRO:HB3	8:I:1093:ARG:HH21	1.82	0.45
1:E:42:ARG:HH22	6:X:69:DA:P	2.40	0.45
10:K:250:TRP:CH2	10:K:254:MET:HE1	2.51	0.45
2:B:49:LEU:O	2:B:52:GLU:HG2	2.17	0.44
5:N:3:GLY:O	5:N:7:ARG:HG2	2.17	0.44
5:N:7:ARG:O	5:N:11:ARG:HG2	2.18	0.44
6:X:92:DC:H5'	6:X:92:DC:C6	2.52	0.44
7:Y:2:DC:H2''	7:Y:3:DA:H5'	1.99	0.44
8:I:494:THR:HA	8:I:497:ILE:HG22	1.99	0.44
8:I:570:GLN:NE2	8:I:735:ALA:O	2.41	0.44
8:I:1122:LYS:HB3	8:I:1149:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:24:ARG:HG3	10:K:36:ASP:HB2	1.98	0.44
1:A:85:GLN:OE1	7:Y:50:DT:H5''	2.17	0.44
1:E:72:ARG:HH22	6:X:51:DC:P	2.40	0.44
1:E:63:ARG:HD3	7:Y:91:DA:H4'	1.99	0.44
5:N:35:TRP:HZ2	10:K:117:LEU:HA	1.82	0.44
6:X:120:DA:H2''	6:X:121:DG:C8	2.52	0.44
7:Y:40:DA:H2''	7:Y:41:DG:C8	2.51	0.44
8:I:964:ILE:O	8:I:968:LEU:HG	2.17	0.44
8:I:1014:LYS:HB3	8:I:1016:VAL:HG22	1.98	0.44
8:I:1098:LYS:HB2	8:I:1168:ALA:HA	2.00	0.44
9:J:116:ARG:HA	9:J:119:MET:SD	2.57	0.44
9:J:143:TYR:CE2	9:J:346:LEU:HG	2.52	0.44
9:J:253:GLU:HA	9:J:256:ARG:HB2	1.98	0.44
9:J:302:GLY:HA2	9:J:336:LYS:HD3	1.98	0.44
1:A:76:GLN:HA	1:A:79:LYS:O	2.18	0.44
2:F:76:ALA:O	2:F:78:ARG:HG3	2.18	0.44
7:Y:15:DT:H4'	7:Y:16:DC:OP1	2.17	0.44
7:Y:127:DC:H2''	7:Y:128:DT:H5'	1.98	0.44
10:K:133:ARG:HA	10:K:136:LEU:HD12	1.99	0.44
10:K:325:VAL:HG13	10:K:364:LEU:HD21	2.00	0.44
1:A:103:LEU:HD13	1:A:103:LEU:HA	1.85	0.44
6:X:42:DC:H2''	6:X:43:DA:C8	2.52	0.44
8:I:1173:ILE:HB	8:I:1203:ARG:HD2	1.99	0.44
2:F:23:ARG:HH11	2:F:27:GLN:HB3	1.83	0.44
7:Y:91:DA:C4	7:Y:92:DG:C6	3.06	0.44
8:I:1100:LEU:HB2	8:I:1171:VAL:HG23	2.00	0.44
8:I:1126:LEU:HD13	8:I:1138:LEU:HD21	1.98	0.44
8:I:1200:ARG:HD2	8:I:1308:ARG:HG2	1.99	0.44
8:I:1211:GLU:OE2	8:I:1212:GLU:HG2	2.18	0.44
10:K:203:THR:HG21	10:K:256:ASN:HB3	1.98	0.44
2:F:98:TYR:CE1	3:G:100:VAL:HG21	2.52	0.44
6:X:55:DG:C5	6:X:56:DC:C4	3.05	0.44
8:I:997:LYS:HD2	8:I:1296:VAL:O	2.18	0.44
10:K:172:SER:HB3	10:K:355:THR:HG23	2.00	0.44
1:E:79:LYS:HG3	1:E:80:THR:O	2.18	0.44
8:I:844:PHE:O	8:I:848:LEU:HG	2.17	0.44
8:I:1038:THR:HA	8:I:1041:GLN:HE21	1.82	0.44
9:J:91:TYR:HE1	9:J:97:ALA:HA	1.82	0.44
10:K:140:MET:N	10:K:140:MET:SD	2.91	0.44
10:K:337:ASP:HB3	10:K:340:ILE:HG12	1.99	0.44
1:E:42:ARG:N	6:X:144:DC:OP1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:130:DC:H2"	6:X:131:DA:N7	2.33	0.44
7:Y:44:DA:C4	7:Y:45:DT:C4	3.06	0.44
8:I:789:THR:O	8:I:793:ILE:HG12	2.18	0.44
8:I:1309:HIS:HD1	8:I:1311:GLU:HB3	1.82	0.44
9:J:195:GLU:OE2	9:J:256:ARG:NH2	2.51	0.44
10:K:202:ILE:HD11	10:K:308:LEU:HD23	2.00	0.44
3:C:88:ARG:HD3	3:C:94:ASN:HD21	1.82	0.43
6:X:54:DC:H2"	6:X:55:DG:C8	2.52	0.43
7:Y:83:DT:H2"	7:Y:84:DG:H8	1.83	0.43
8:I:929:LEU:HB3	8:I:933:PHE:CG	2.53	0.43
8:I:993:GLU:N	8:I:993:GLU:OE2	2.51	0.43
8:I:1077:ARG:HE	8:I:1336:ARG:HA	1.83	0.43
8:I:1119:ARG:HA	8:I:1119:ARG:HD3	1.81	0.43
9:J:157:ASP:OD1	9:J:210:ARG:NH2	2.51	0.43
2:B:79:LYS:N	6:X:102:DG:OP1	2.39	0.43
8:I:746:SER:HA	8:I:754:LEU:HD11	1.99	0.43
8:I:1223:ASN:OD1	8:I:1224:VAL:N	2.52	0.43
8:I:1247:LEU:HA	8:I:1250:ILE:HG12	2.00	0.43
9:J:35:VAL:O	9:J:68:LYS:N	2.51	0.43
7:Y:50:DT:H6	7:Y:50:DT:H2'	1.64	0.43
8:I:805:PRO:HG3	8:I:875:TRP:HA	2.00	0.43
8:I:847:GLN:O	8:I:850:SER:OG	2.27	0.43
8:I:967:ARG:HA	8:I:970:LYS:HG2	2.00	0.43
9:J:261:LEU:HB3	9:J:274:ILE:HD13	2.00	0.43
3:C:77:ARG:HH11	4:D:54:ILE:N	2.16	0.43
3:G:79:ILE:HG13	3:G:81:ARG:H	1.83	0.43
7:Y:98:DC:H5"	8:I:1178:TRP:CZ3	2.52	0.43
7:Y:107:DT:H6	7:Y:107:DT:H2'	1.65	0.43
8:I:878:MET:HE3	8:I:906:ARG:HE	1.82	0.43
9:J:94:LEU:HB3	9:J:96:VAL:HG12	1.99	0.43
1:A:46:VAL:O	1:A:49:ARG:HG2	2.18	0.43
1:E:49:ARG:NH1	7:Y:8:DG:O5'	2.51	0.43
3:G:42:ARG:NH1	6:X:112:DT:H4'	2.33	0.43
5:N:35:TRP:CE3	5:N:44:ARG:HB2	2.48	0.43
6:X:109:DC:H2"	6:X:110:DC:C6	2.53	0.43
7:Y:78:DG:H2"	7:Y:79:DT:C5	2.54	0.43
8:I:992:VAL:N	8:I:1199:VAL:O	2.51	0.43
9:J:16:MET:HA	9:J:32:PRO:HA	2.00	0.43
9:J:272:CYS:HB3	9:J:276:GLU:HB2	1.99	0.43
9:J:367:PRO:O	9:J:370:VAL:HG12	2.19	0.43
1:A:63:ARG:HD3	6:X:91:DA:H5"	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:39:ILE:HG13	4:H:40:TYR:CD2	2.52	0.43
8:I:554:LEU:O	8:I:557:THR:OG1	2.37	0.43
9:J:89:THR:HA	9:J:93:GLU:HB2	1.99	0.43
9:J:173:HIS:CE1	10:K:32:CYS:HB2	2.54	0.43
10:K:219:PRO:HB2	10:K:221:TYR:CD2	2.52	0.43
6:X:56:DC:H2"	6:X:57:DT:C7	2.48	0.43
8:I:755:LYS:HG2	8:I:758:GLN:NE2	2.33	0.43
9:J:116:ARG:CZ	9:J:371:HIS:HB3	2.49	0.43
9:J:230:ALA:HB2	9:J:236:LEU:HD12	1.99	0.43
3:C:16:THR:O	3:C:20:ARG:N	2.45	0.43
1:E:50:GLU:OE1	2:F:39:ARG:NE	2.51	0.43
2:F:51:TYR:O	2:F:55:ARG:HG3	2.18	0.43
7:Y:115:DC:H2"	7:Y:116:DA:C8	2.54	0.43
8:I:922:TRP:CZ3	8:I:939:PHE:HB3	2.54	0.43
8:I:1007:LEU:HD13	8:I:1007:LEU:HA	1.88	0.43
9:J:78:ASN:ND2	9:J:81:ASP:OD2	2.51	0.43
10:K:213:MET:N	10:K:213:MET:SD	2.92	0.43
10:K:385:THR:HG23	10:K:388:GLU:HB3	2.01	0.43
3:G:70:ALA:HB2	3:G:78:ILE:HD12	2.01	0.43
7:Y:13:DT:H2"	7:Y:14:DA:C8	2.54	0.43
8:I:877:TYR:CE1	8:I:905:ARG:HG2	2.53	0.43
9:J:164:PRO:HD3	9:J:281:SER:OG	2.19	0.43
6:X:34:DG:H2"	6:X:35:DT:H5"	2.01	0.43
6:X:102:DG:H2"	6:X:103:DA:H8	1.84	0.43
6:X:129:DT:H2"	6:X:130:DC:C5	2.54	0.43
6:X:134:DT:H2"	6:X:135:DA:H8	1.84	0.43
9:J:171:LEU:O	9:J:175:ILE:HG13	2.18	0.43
10:K:387:VAL:HG13	10:K:391:PHE:HD2	1.84	0.43
1:A:55:GLN:CD	3:C:110:ASN:H	2.27	0.42
1:A:63:ARG:HH22	7:Y:61:DA:P	2.41	0.42
3:C:45:ALA:O	3:C:48:PRO:HD2	2.19	0.42
8:I:507:TYR:HA	8:I:510:ASN:ND2	2.33	0.42
8:I:1162:GLY:HA2	8:I:1189:ARG:CZ	2.49	0.42
3:G:17:ARG:HA	3:G:20:ARG:HG2	2.01	0.42
4:H:62:MET:O	4:H:66:VAL:HG23	2.19	0.42
6:X:142:DT:H2"	6:X:143:DC:C5	2.55	0.42
8:I:874:ARG:NH2	8:I:875:TRP:O	2.43	0.42
8:I:1252:GLU:N	8:I:1252:GLU:OE1	2.52	0.42
8:I:1306:ILE:HG13	8:I:1316:PHE:CZ	2.54	0.42
10:K:259:ILE:O	10:K:263:GLN:HG3	2.18	0.42
6:X:114:DG:H2'	6:X:115:DT:H71	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:56:DG:H1'	7:Y:57:DT:C2	2.54	0.42
8:I:496:LYS:O	8:I:499:LYS:HG2	2.19	0.42
8:I:548:LYS:NZ	8:I:960:GLU:OE1	2.53	0.42
8:I:737:ALA:N	8:I:771:ASN:OD1	2.52	0.42
8:I:780:GLU:N	8:I:978:ARG:HH22	2.18	0.42
8:I:1039:ILE:O	8:I:1043:ARG:HG3	2.19	0.42
10:K:287:TYR:HB3	10:K:297:PHE:CE2	2.55	0.42
2:B:98:TYR:CZ	3:C:100:VAL:HG11	2.54	0.42
5:N:12:SER:HA	5:N:15:LYS:HG2	2.02	0.42
8:I:465:GLU:O	8:I:469:ARG:HG2	2.19	0.42
8:I:1050:TYR:HB2	8:I:1111:ILE:CD1	2.49	0.42
9:J:132:MET:SD	9:J:357:ILE:HB	2.59	0.42
9:J:219:VAL:HG11	9:J:309:ILE:HA	2.01	0.42
6:X:39:DA:C5	6:X:40:DG:C6	3.07	0.42
6:X:51:DC:H5''	8:I:1036:MET:HE2	2.01	0.42
7:Y:128:DT:H2''	7:Y:129:DC:C5	2.55	0.42
8:I:755:LYS:H	8:I:758:GLN:CD	2.26	0.42
8:I:881:ASP:HA	8:I:909:LEU:HB2	2.01	0.42
10:K:90:ASN:HB3	10:K:194:LYS:HZ3	1.85	0.42
10:K:301:ARG:HG3	10:K:302:LEU:HD12	2.02	0.42
1:A:73:GLU:O	1:A:76:GLN:HG3	2.20	0.42
3:C:84:GLN:OE1	3:C:88:ARG:NH2	2.52	0.42
8:I:1122:LYS:HB2	8:I:1150:PHE:H	1.84	0.42
9:J:341:ILE:O	9:J:345:ILE:HG13	2.20	0.42
2:B:75:HIS:CD2	4:H:80:LEU:HD21	2.55	0.42
4:H:112:SER:O	4:H:115:THR:HG22	2.20	0.42
5:N:43:LEU:O	10:K:407:GLN:NE2	2.52	0.42
7:Y:16:DC:H4'	7:Y:17:DT:H5'	2.01	0.42
7:Y:39:DG:H2''	7:Y:40:DA:H8	1.85	0.42
8:I:1050:TYR:HB2	8:I:1111:ILE:HD11	2.01	0.42
10:K:210:PHE:HE2	10:K:259:ILE:HG12	1.85	0.42
2:B:32:PRO:O	2:B:35:ARG:HB2	2.19	0.42
4:D:119:THR:O	4:D:123:SER:OG	2.23	0.42
2:F:33:ALA:HA	2:F:36:ARG:CZ	2.50	0.42
4:H:90:THR:HG22	4:H:93:GLU:HG2	2.00	0.42
6:X:15:DT:H2''	6:X:16:DG:N7	2.35	0.42
8:I:1319:MET:HE3	8:I:1319:MET:HB3	1.91	0.42
10:K:198:ALA:H	10:K:201:PHE:HB3	1.84	0.42
6:X:57:DT:H3	7:Y:92:DG:H22	1.67	0.42
6:X:67:DG:H2''	6:X:68:DT:H72	2.02	0.42
6:X:99:DG:H22	7:Y:50:DT:H3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:118:DC:H2''	6:X:119:DC:C5	2.54	0.42
7:Y:96:DT:H6	7:Y:96:DT:H2'	1.58	0.42
10:K:298:GLY:N	10:K:300:GLU:OE1	2.53	0.42
2:B:53:GLU:O	2:B:57:VAL:HG23	2.20	0.41
7:Y:124:DG:H2''	7:Y:125:DG:C8	2.55	0.41
8:I:553:LEU:O	8:I:557:THR:HG23	2.20	0.41
8:I:1307:ALA:HA	8:I:1312:GLU:HG2	2.01	0.41
9:J:116:ARG:HH12	9:J:368:SER:HA	1.85	0.41
10:K:349:ILE:HG13	10:K:381:ILE:HB	2.02	0.41
4:H:104:GLY:O	4:H:108:LYS:HG2	2.20	0.41
7:Y:127:DC:H2'	7:Y:128:DT:H72	2.03	0.41
8:I:1124:LEU:O	8:I:1152:PHE:HD1	2.03	0.41
9:J:216:LEU:HB2	9:J:254:ARG:NH1	2.35	0.41
2:B:82:THR:HG23	2:B:84:MET:N	2.35	0.41
7:Y:45:DT:H2''	7:Y:46:DC:C4	2.54	0.41
7:Y:58:DT:H2''	7:Y:59:DA:C8	2.55	0.41
7:Y:94:DG:H4'	7:Y:95:DG:OP1	2.20	0.41
8:I:784:GLY:O	8:I:787:ILE:HG22	2.20	0.41
8:I:1075:LEU:HD12	8:I:1075:LEU:H	1.84	0.41
8:I:1341:ASP:OD1	8:I:1341:ASP:N	2.53	0.41
9:J:88:HIS:O	9:J:93:GLU:N	2.52	0.41
9:J:287:VAL:HA	9:J:290:ARG:HD2	2.02	0.41
10:K:121:LEU:HD12	10:K:401:ALA:HB2	2.02	0.41
2:B:24:ASP:CG	2:B:27:GLN:HB3	2.44	0.41
2:F:32:PRO:O	2:F:36:ARG:HG3	2.19	0.41
8:I:808:ILE:HB	8:I:857:LEU:HD13	2.02	0.41
10:K:33:PRO:HB3	10:K:394:TRP:CE2	2.55	0.41
10:K:90:ASN:HB3	10:K:194:LYS:NZ	2.35	0.41
2:B:98:TYR:CE2	3:C:100:VAL:HG11	2.55	0.41
3:C:88:ARG:HD3	3:C:88:ARG:HA	1.89	0.41
3:G:26:PRO:HD3	4:H:40:TYR:CD1	2.56	0.41
3:G:61:GLU:HG3	5:N:4:ARG:NH2	2.35	0.41
6:X:20:DA:H5''	6:X:20:DA:C8	2.56	0.41
6:X:47:DC:H2''	6:X:48:DT:H71	2.02	0.41
7:Y:38:DG:H2''	7:Y:39:DG:N7	2.36	0.41
7:Y:63:DC:H2''	7:Y:64:DG:H8	1.86	0.41
7:Y:73:DA:H2''	7:Y:74:DG:H8	1.85	0.41
8:I:469:ARG:NH1	8:I:469:ARG:HA	2.35	0.41
8:I:475:TYR:OH	10:K:406:PHE:HA	2.19	0.41
8:I:922:TRP:CE3	8:I:939:PHE:HB3	2.56	0.41
8:I:1326:GLU:HA	8:I:1329:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:118:LYS:HD2	9:J:118:LYS:HA	1.82	0.41
10:K:166:THR:HA	10:K:182:VAL:O	2.21	0.41
1:A:128:ARG:NH1	2:B:57:VAL:HG22	2.35	0.41
3:C:55:LEU:HD13	3:C:55:LEU:HA	1.92	0.41
2:F:73:THR:HG21	2:F:81:VAL:HG22	2.02	0.41
7:Y:93:DC:H2''	7:Y:94:DG:C8	2.54	0.41
8:I:834:TYR:CE1	8:I:841:ARG:HB3	2.56	0.41
8:I:1368:GLY:HA3	8:I:1371:SER:HB3	2.03	0.41
9:J:93:GLU:O	9:J:95:ARG:NE	2.54	0.41
10:K:306:GLU:HG3	10:K:310:ASP:HB3	2.02	0.41
2:F:31:LYS:O	2:F:34:ILE:HG22	2.20	0.41
3:G:54:VAL:HG22	4:H:110:ALA:HB1	2.02	0.41
9:J:123:MET:HE1	9:J:132:MET:HE2	2.02	0.41
1:E:120:MET:SD	2:F:47:SER:OG	2.79	0.41
3:G:32:ARG:HD3	7:Y:30:DG:OP2	2.20	0.41
3:G:51:LEU:HD12	3:G:51:LEU:HA	1.88	0.41
6:X:147:DT:H6	6:X:147:DT:H2'	1.72	0.41
8:I:780:GLU:HG2	8:I:978:ARG:NH2	2.35	0.41
9:J:227:MET:HE2	9:J:227:MET:HB2	1.94	0.41
4:H:31:LYS:NZ	6:X:125:DC:OP1	2.33	0.41
5:N:31:TRP:HB3	5:N:48:TRP:HE3	1.85	0.41
6:X:97:DA:N6	7:Y:52:DG:O6	2.54	0.41
6:X:103:DA:H2'	6:X:104:DT:H71	2.02	0.41
6:X:109:DC:H2''	6:X:110:DC:C5	2.55	0.41
8:I:768:LEU:HB2	8:I:773:LEU:HB3	2.03	0.41
8:I:1014:LYS:HE2	8:I:1014:LYS:HB2	1.87	0.41
8:I:1044:LYS:HE3	8:I:1051:MET:HE1	2.02	0.41
8:I:1062:HIS:CD2	8:I:1340:GLU:HB3	2.56	0.41
8:I:1077:ARG:HG3	8:I:1334:LYS:O	2.21	0.41
8:I:1317:MET:HA	8:I:1320:ASP:CG	2.45	0.41
9:J:8:LEU:HD12	9:J:94:LEU:HD13	2.02	0.41
9:J:70:PRO:HB3	9:J:81:ASP:HB2	2.03	0.41
9:J:252:ASN:HA	9:J:255:PHE:CE2	2.56	0.41
9:J:259:GLU:CD	9:J:312:ARG:HH22	2.29	0.41
9:J:355:MET:HE2	9:J:355:MET:HB2	1.91	0.41
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.74	0.41
3:C:92:GLU:HG2	3:C:93:LEU:HD22	2.02	0.41
7:Y:42:DT:C2	7:Y:43:DA:N7	2.89	0.41
8:I:747:ALA:H	8:I:754:LEU:HD22	1.86	0.41
9:J:28:ARG:HH21	9:J:29:ALA:HB2	1.85	0.41
9:J:116:ARG:HA	9:J:119:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:123:MET:HE2	9:J:123:MET:HB2	1.80	0.41
10:K:284:THR:HA	10:K:301:ARG:NH2	2.36	0.41
4:D:80:LEU:HD11	2:F:75:HIS:CD2	2.56	0.40
4:H:58:ALA:O	4:H:62:MET:HG2	2.21	0.40
6:X:40:DG:H2''	6:X:41:DA:C8	2.56	0.40
7:Y:72:DC:H2''	7:Y:73:DA:C8	2.56	0.40
7:Y:88:DT:H2''	7:Y:89:DT:C6	2.56	0.40
8:I:960:GLU:H	8:I:960:GLU:CD	2.29	0.40
8:I:973:ARG:HA	8:I:1234:PHE:HD2	1.86	0.40
8:I:997:LYS:HZ3	8:I:999:ASP:HB3	1.85	0.40
10:K:428:CYS:HA	10:K:429:PRO:HD2	1.90	0.40
1:A:116:ARG:HD2	1:A:118:THR:O	2.21	0.40
5:N:4:ARG:O	5:N:4:ARG:NH1	2.54	0.40
6:X:60:DA:H2''	6:X:61:DA:C8	2.56	0.40
8:I:1114:ASP:OD1	8:I:1114:ASP:N	2.51	0.40
1:A:104:PHE:HA	1:A:107:THR:HG22	2.03	0.40
6:X:34:DG:H2'	6:X:35:DT:H71	2.03	0.40
6:X:78:DC:H2''	6:X:79:DC:C5	2.56	0.40
7:Y:13:DT:H2''	7:Y:14:DA:H8	1.86	0.40
8:I:464:GLN:HG2	8:I:467:LYS:HD2	2.03	0.40
8:I:502:LYS:HA	8:I:502:LYS:HD3	1.82	0.40
9:J:82:MET:HE2	9:J:82:MET:HB2	1.69	0.40
10:K:166:THR:HG23	10:K:183:HIS:HA	2.04	0.40
8:I:837:SER:O	8:I:841:ARG:HG3	2.20	0.40
8:I:1000:MET:HB3	8:I:1004:GLN:HB2	2.03	0.40
10:K:44:VAL:HG23	10:K:82:MET:HG2	2.03	0.40
10:K:284:THR:HA	10:K:301:ARG:HH21	1.86	0.40
3:C:77:ARG:NH1	6:X:20:DA:H4'	2.37	0.40
2:F:31:LYS:HB3	2:F:32:PRO:HD3	2.03	0.40
8:I:796:LEU:HA	8:I:800:LYS:HG2	2.04	0.40
9:J:259:GLU:OE2	9:J:312:ARG:NH2	2.46	0.40
10:K:149:PHE:CZ	10:K:151:LEU:HB2	2.56	0.40
10:K:164:ARG:HH22	10:K:169:ILE:HG13	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
1	E	96/135 (71%)	96 (100%)	0	0	100	100
2	B	79/102 (78%)	79 (100%)	0	0	100	100
2	F	83/102 (81%)	75 (90%)	8 (10%)	0	100	100
3	C	105/129 (81%)	101 (96%)	4 (4%)	0	100	100
3	G	110/129 (85%)	103 (94%)	7 (6%)	0	100	100
4	D	94/125 (75%)	87 (93%)	7 (7%)	0	100	100
4	H	92/125 (74%)	91 (99%)	1 (1%)	0	100	100
5	N	40/216 (18%)	40 (100%)	0	0	100	100
8	I	644/1711 (38%)	600 (93%)	44 (7%)	0	100	100
9	J	319/381 (84%)	310 (97%)	9 (3%)	0	100	100
10	K	400/435 (92%)	394 (98%)	6 (2%)	0	100	100
All	All	2158/3725 (58%)	2068 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/110 (77%)	81 (95%)	4 (5%)	23	45
1	E	85/110 (77%)	81 (95%)	4 (5%)	23	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	66/78 (85%)	57 (86%)	9 (14%)	3	15
2	F	70/78 (90%)	65 (93%)	5 (7%)	13	36
3	C	84/101 (83%)	80 (95%)	4 (5%)	23	45
3	G	87/101 (86%)	76 (87%)	11 (13%)	4	17
4	D	82/105 (78%)	78 (95%)	4 (5%)	22	44
4	H	80/105 (76%)	77 (96%)	3 (4%)	29	51
5	N	39/188 (21%)	37 (95%)	2 (5%)	21	43
8	I	586/1473 (40%)	566 (97%)	20 (3%)	32	55
9	J	281/324 (87%)	277 (99%)	4 (1%)	59	72
10	K	346/370 (94%)	340 (98%)	6 (2%)	53	68
All	All	1891/3143 (60%)	1815 (96%)	76 (4%)	29	49

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	80	THR
1	A	103	LEU
1	A	126	LEU
2	B	22	LEU
2	B	37	LEU
2	B	45	ARG
2	B	50	ILE
2	B	65	VAL
2	B	71	THR
2	B	82	THR
2	B	86	VAL
2	B	88	TYR
3	C	49	VAL
3	C	63	LEU
3	C	79	ILE
3	C	85	LEU
4	D	42	TYR
4	D	45	LEU
4	D	73	ILE
4	D	98	VAL
1	E	58	THR
1	E	60	LEU

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Mol	Chain	Res	Type
1	E	79	LYS
1	E	92	LEU
2	F	63	GLU
2	F	86	VAL
2	F	87	VAL
2	F	90	LEU
2	F	96	THR
3	G	16	THR
3	G	58	LEU
3	G	62	ILE
3	G	65	LEU
3	G	78	ILE
3	G	83	LEU
3	G	85	LEU
3	G	91	GLU
3	G	93	LEU
3	G	97	LEU
3	G	108	LEU
4	H	54	ILE
4	H	100	LEU
4	H	101	LEU
5	N	10	THR
5	N	30	LYS
8	I	498	GLN
8	I	567	LEU
8	I	748	LEU
8	I	749	MET
8	I	792	LEU
8	I	796	LEU
8	I	830	VAL
8	I	912	THR
8	I	972	LEU
8	I	1007	LEU
8	I	1038	THR
8	I	1039	ILE
8	I	1089	LEU
8	I	1092	LEU
8	I	1113	GLU
8	I	1153	LEU
8	I	1209	SER
8	I	1211	GLU
8	I	1229	ILE

Continued on next page...

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Mol	Chain	Res	Type
8	I	1233	MET
9	J	28	ARG
9	J	110	LEU
9	J	283	MET
9	J	297	THR
10	K	16	PHE
10	K	18	ILE
10	K	37	PHE
10	K	99	PHE
10	K	140	MET
10	K	150	PHE

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

Mol	Chain	Res	Type
1	A	93	GLN
1	A	125	GLN
2	B	25	ASN
3	C	82	HIS
3	C	89	ASN
3	C	94	ASN
3	C	112	GLN
4	D	63	ASN
1	E	55	GLN
1	E	93	GLN
2	F	25	ASN
2	F	75	HIS
3	G	110	ASN
4	H	49	HIS
4	H	109	HIS
8	I	889	HIS
8	I	916	ASN
8	I	941	GLN
8	I	1012	GLN
8	I	1041	GLN
8	I	1047	ASN
8	I	1182	GLN
8	I	1185	GLN
8	I	1187	GLN
8	I	1303	ASN
8	I	1304	GLN
9	J	115	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	K	100	GLN
10	K	143	HIS
10	K	251	HIS
10	K	263	GLN
10	K	277	GLN
10	K	313	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	BEF	I	1801	13	0,3,3	-	-	-		
13	ADP	I	1803	11	27,29,29	1.35	4 (14%)	42,45,45	1.97	11 (26%)

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
13	ADP	I	1803	11	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	1803	ADP	C5-C4	4.52	1.47	1.39
13	I	1803	ADP	C5-C6	2.68	1.48	1.41
13	I	1803	ADP	C8-N7	2.42	1.36	1.31
13	I	1803	ADP	C5-N7	-2.10	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	1803	ADP	C5-C4-N3	-6.07	118.83	126.75
13	I	1803	ADP	N3-C4-N9	4.75	134.91	127.08
13	I	1803	ADP	C2-N3-C4	3.83	120.79	111.75
13	I	1803	ADP	PA-O3A-PB	-3.49	120.83	132.83
13	I	1803	ADP	C4-C5-N7	-3.27	106.64	110.62
13	I	1803	ADP	N3-C2-N1	-3.14	123.70	128.60
13	I	1803	ADP	C5-N7-C8	2.74	107.40	103.51
13	I	1803	ADP	C4-N9-C8	2.66	108.61	105.73
13	I	1803	ADP	C3'-C2'-C1'	2.32	105.83	101.43
13	I	1803	ADP	C6-C5-N7	2.22	136.15	132.02
13	I	1803	ADP	N9-C8-N7	-2.06	111.10	113.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	I	1803	ADP	O4'-C4'-C5'-O5'
13	I	1803	ADP	C3'-C4'-C5'-O5'

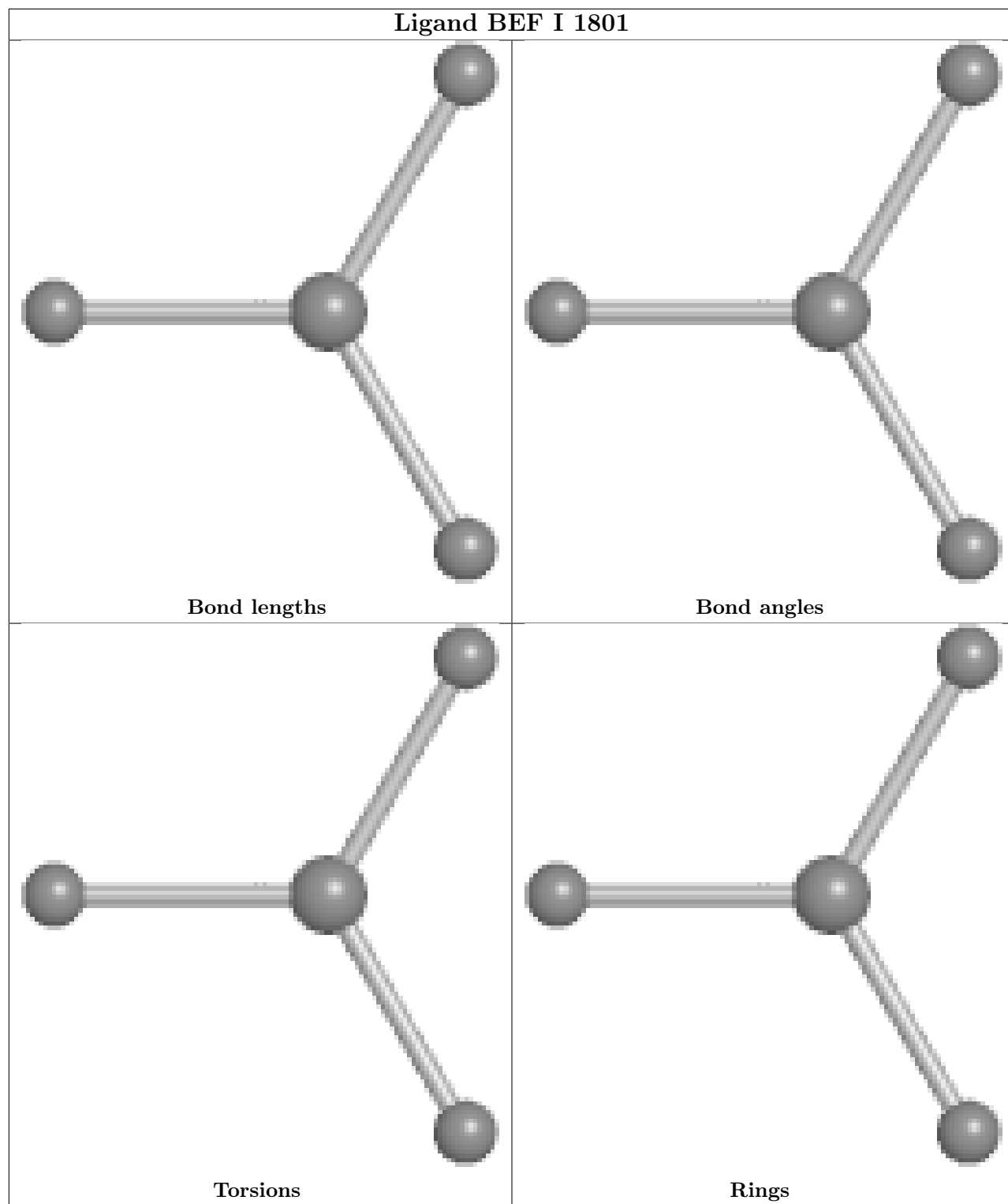
There are no ring outliers.

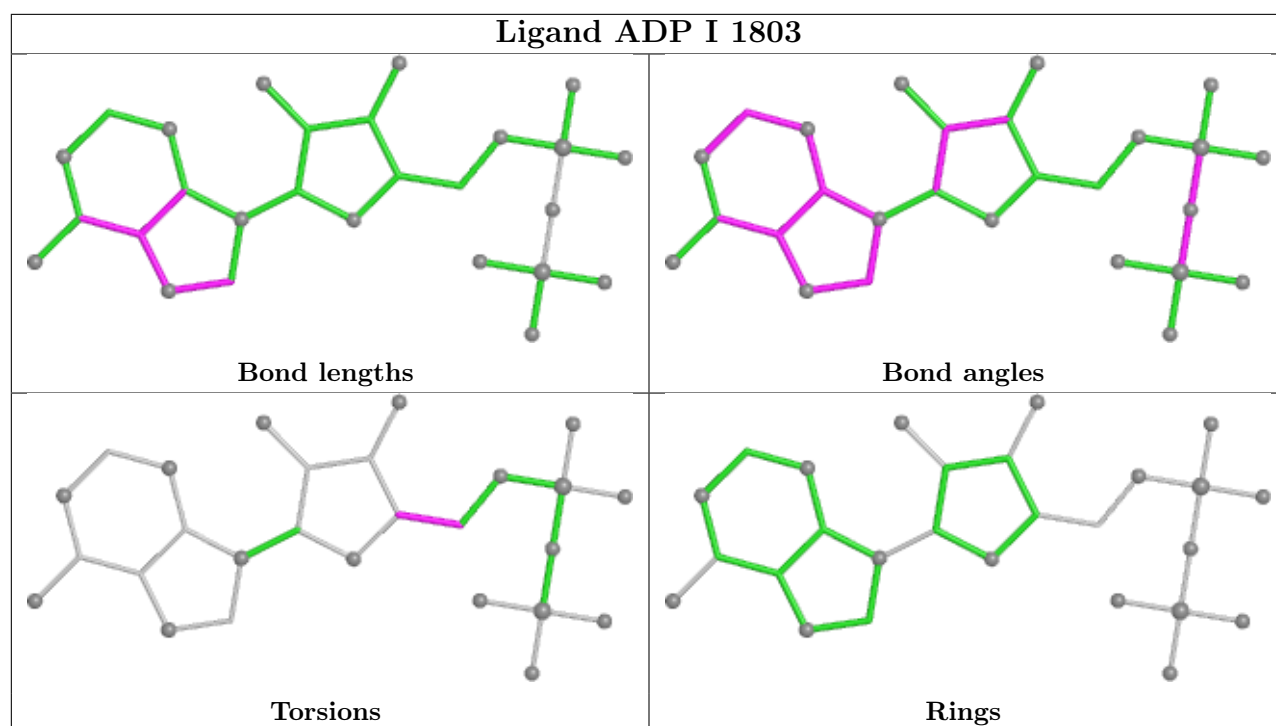
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	1801	BEF	1	0
13	I	1803	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

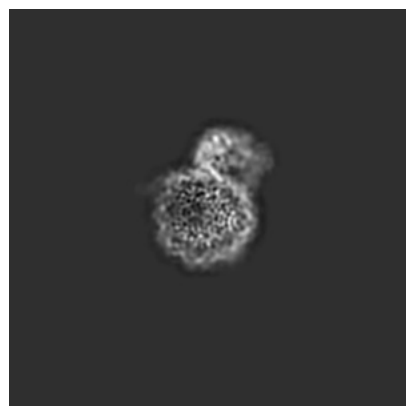
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68040. These allow visual inspection of the internal detail of the map and identification of artifacts.

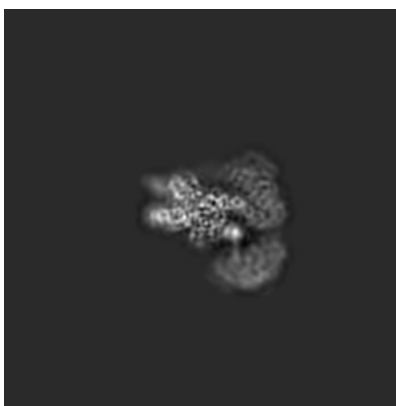
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

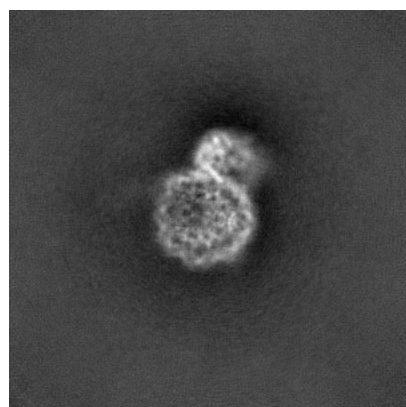


Y

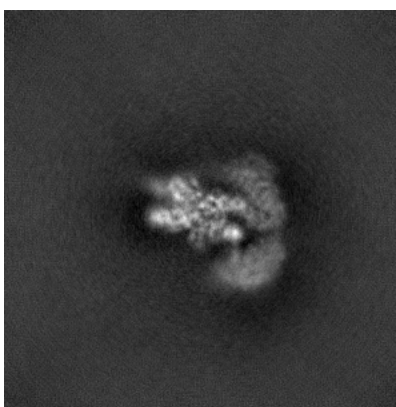


Z

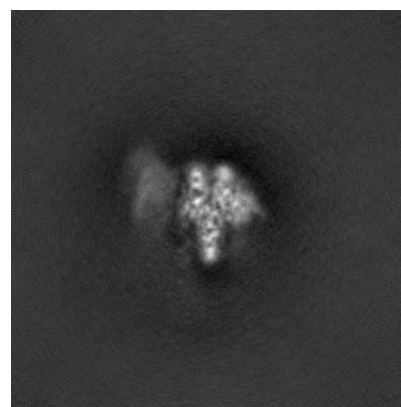
6.1.2 Raw map



X



Y

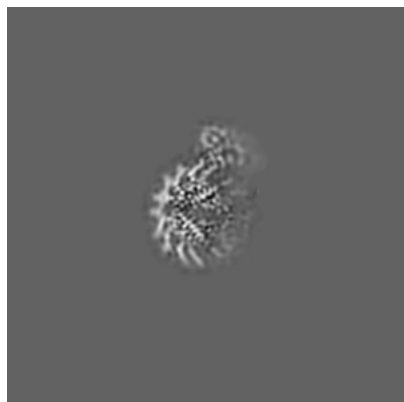


Z

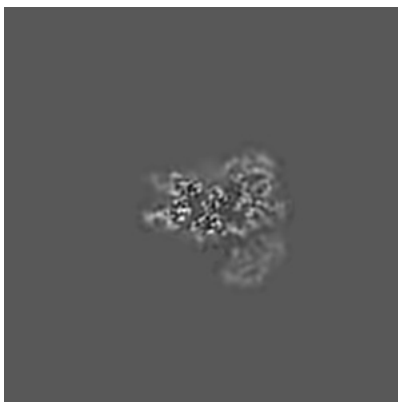
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

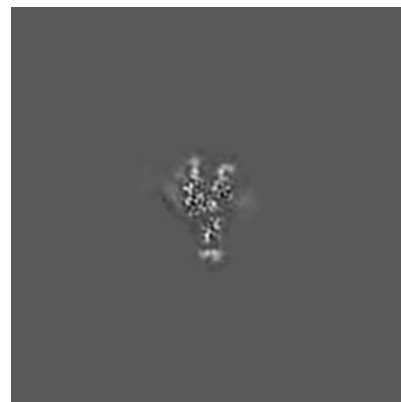
6.2.1 Primary map



X Index: 180

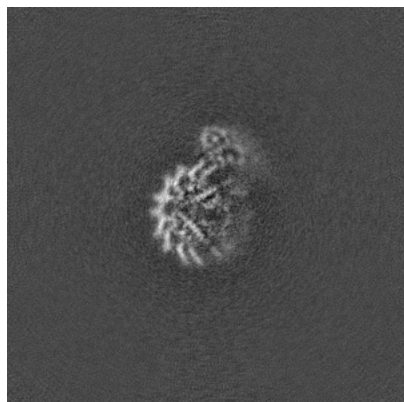


Y Index: 180

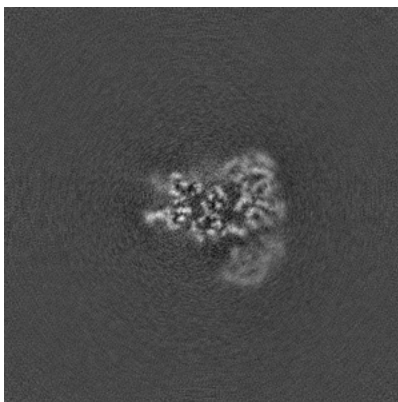


Z Index: 180

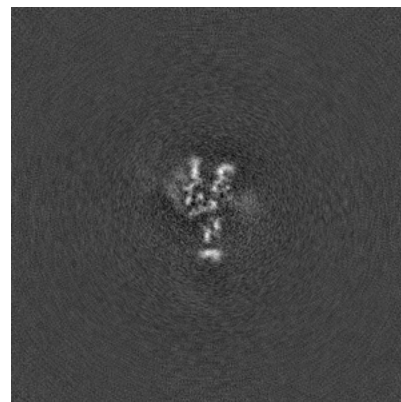
6.2.2 Raw map



X Index: 180



Y Index: 180

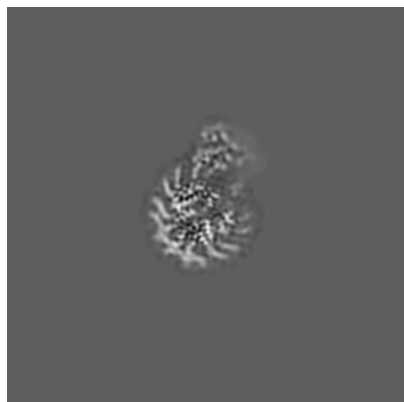


Z Index: 180

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

6.3 Largest variance slices [i](#)

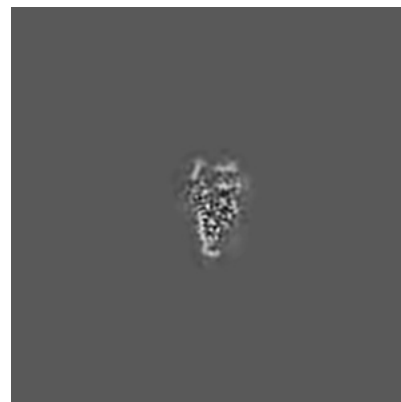
6.3.1 Primary map



X Index: 176

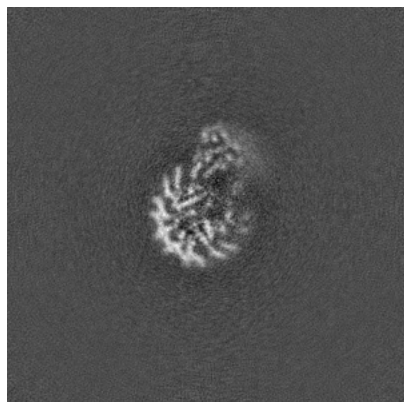


Y Index: 188

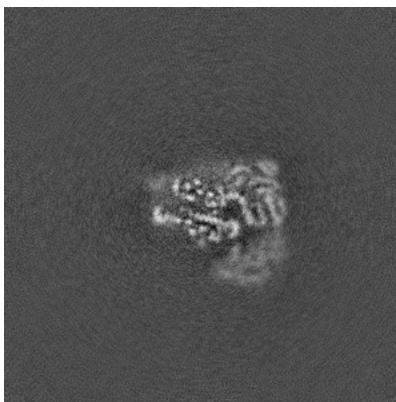


Z Index: 162

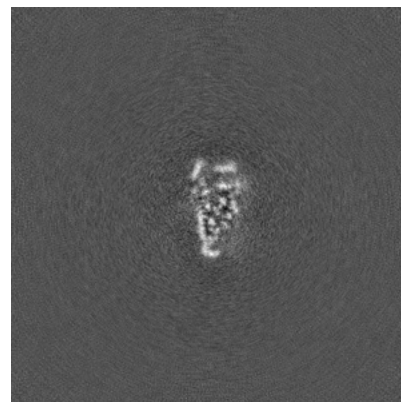
6.3.2 Raw map



X Index: 177



Y Index: 188

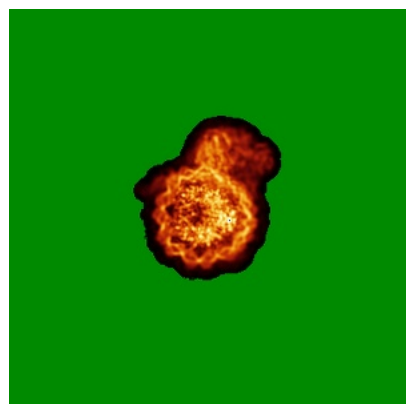


Z Index: 162

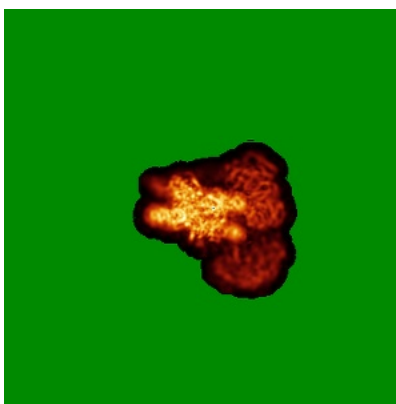
The images above show the largest variance slices of the map in three orthogonal directions.

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

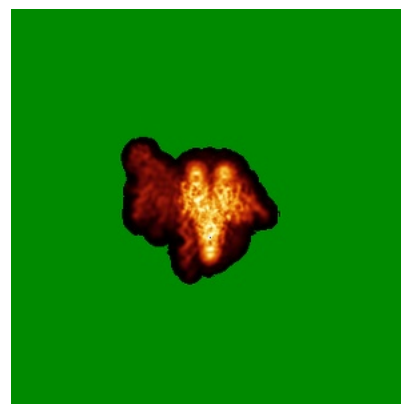
6.4.1 Primary map



X

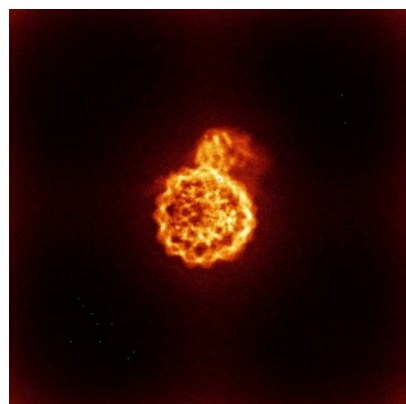


Y

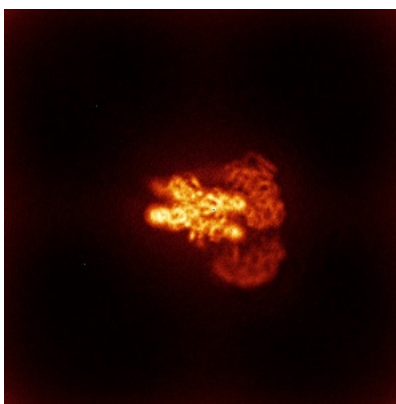


Z

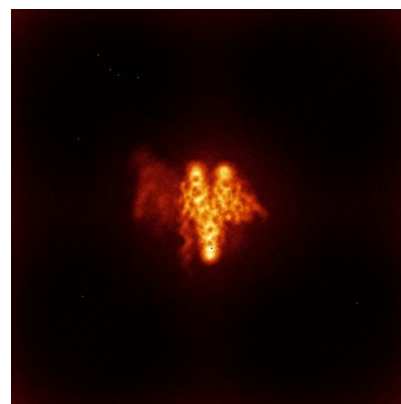
6.4.2 Raw map



X



Y



Z

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

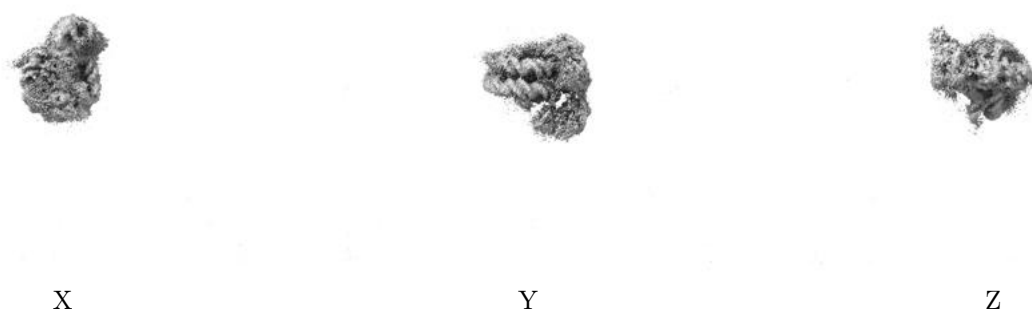
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

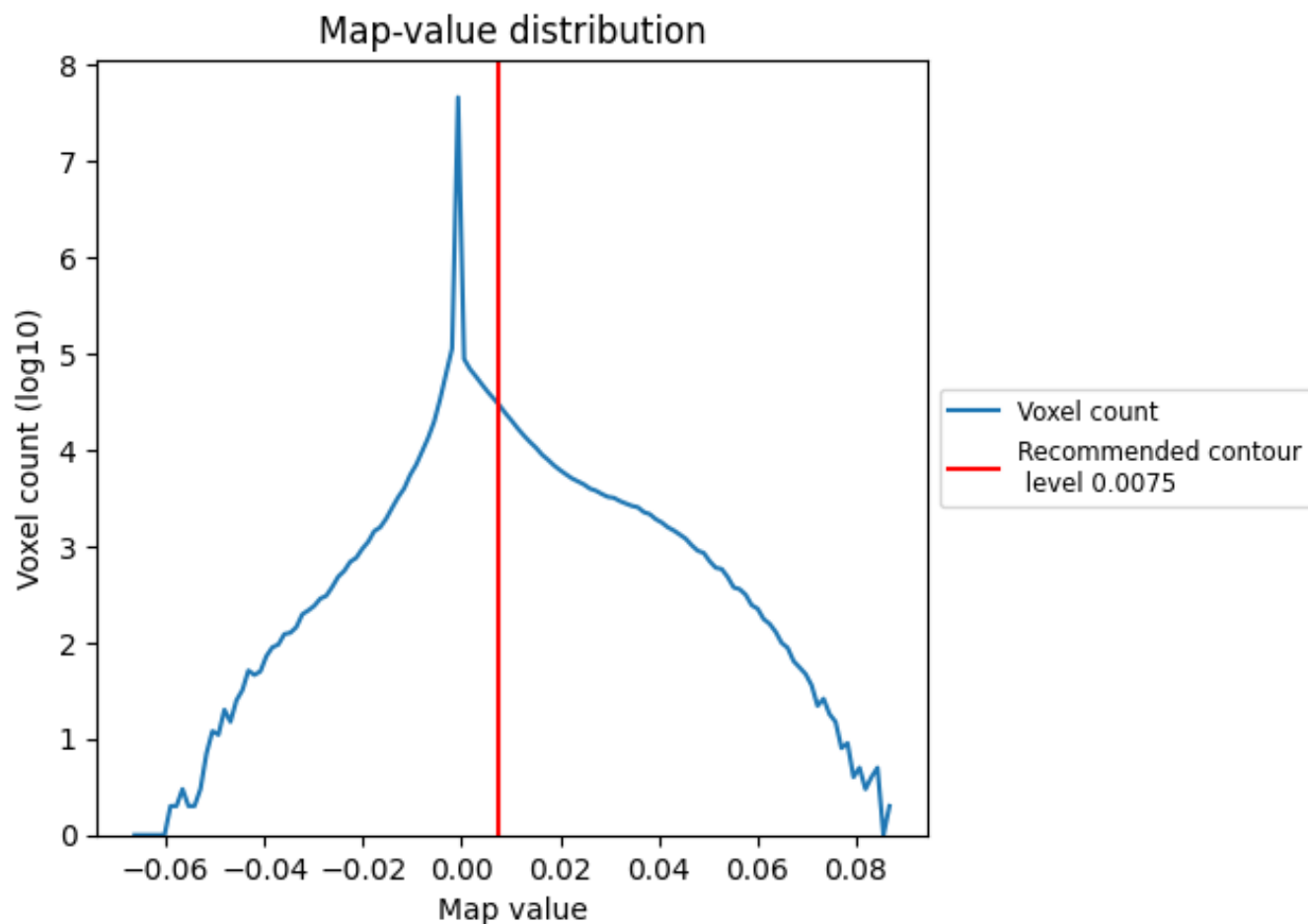
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

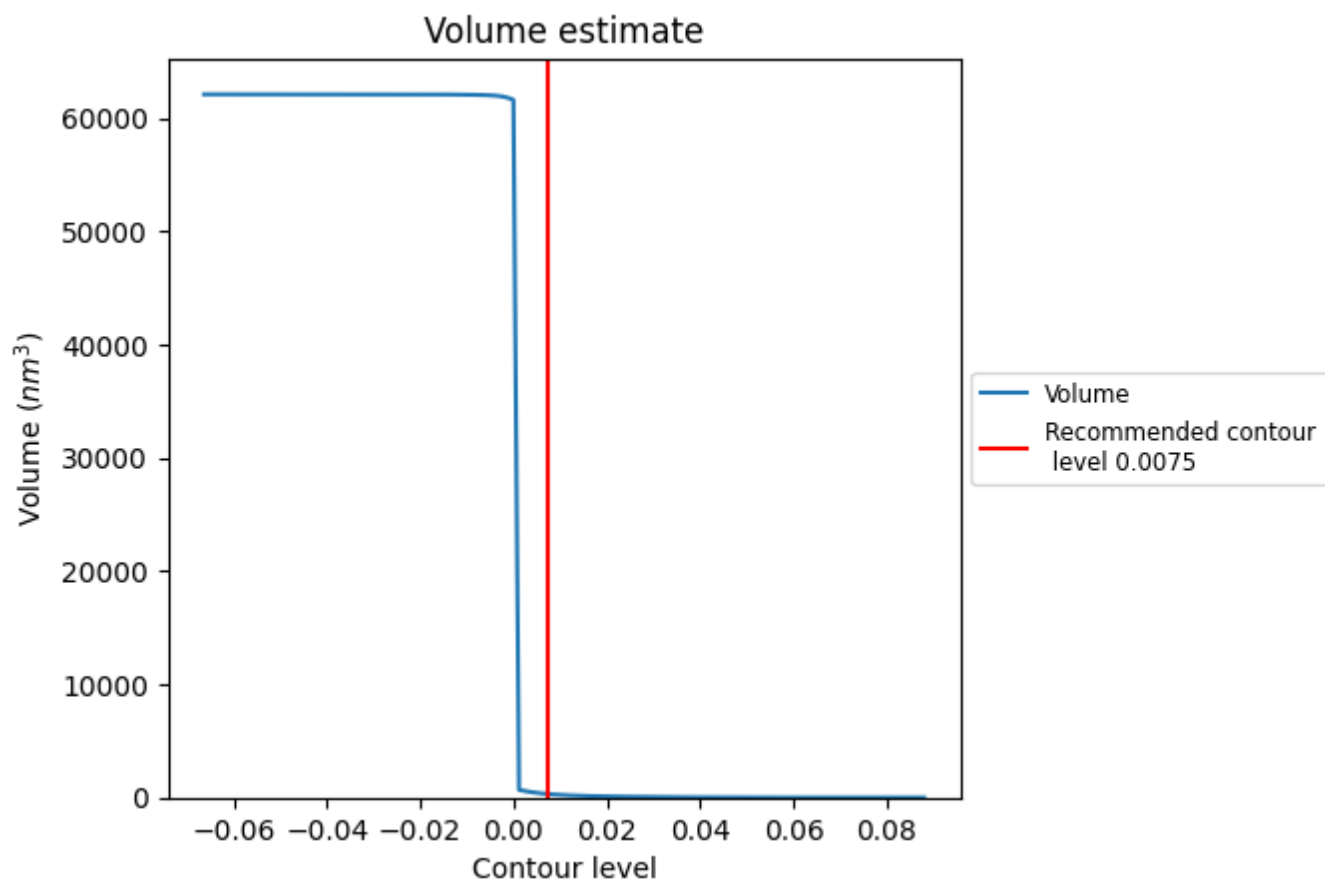
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

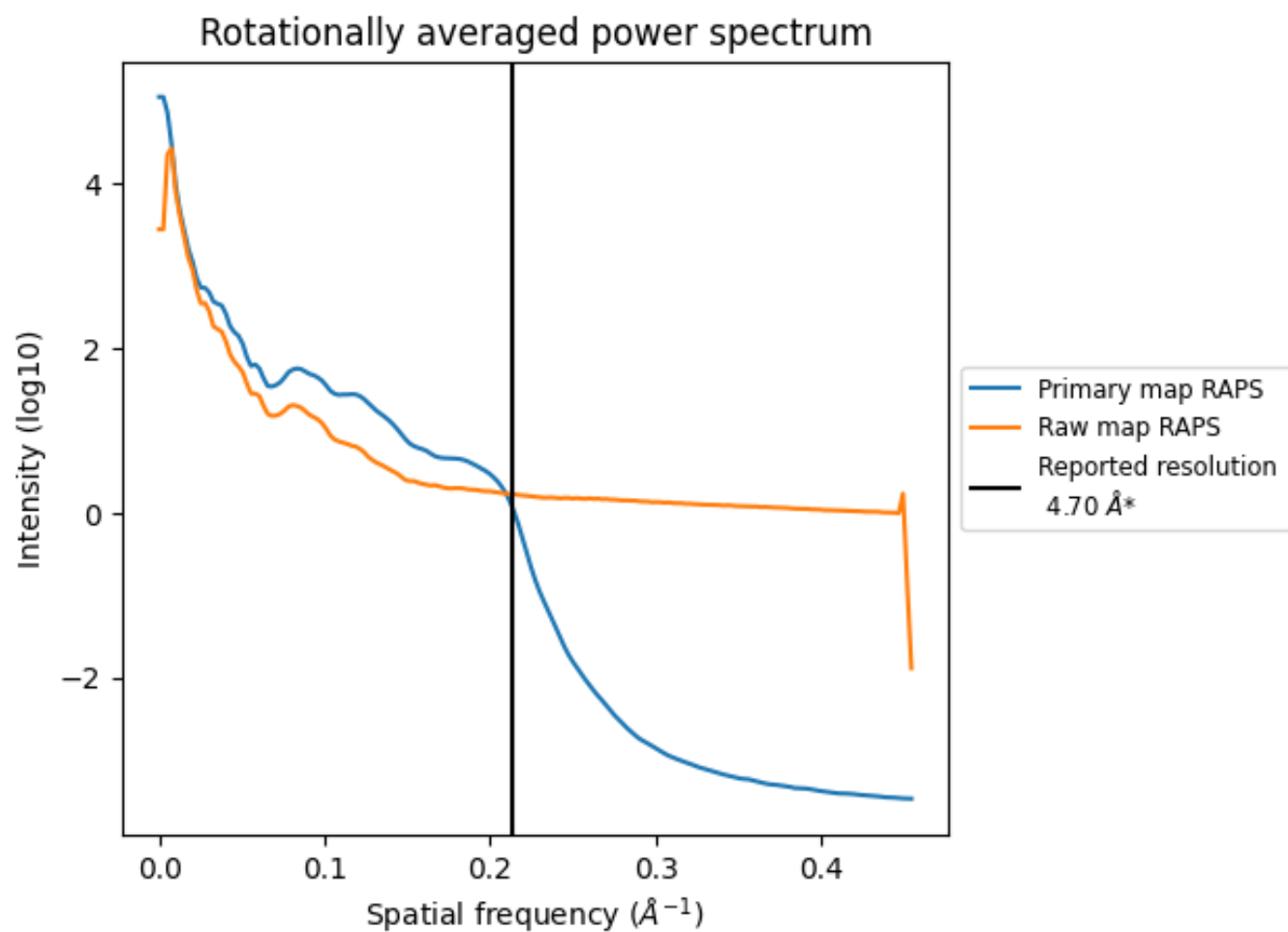
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 310 nm³; this corresponds to an approximate mass of 280 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

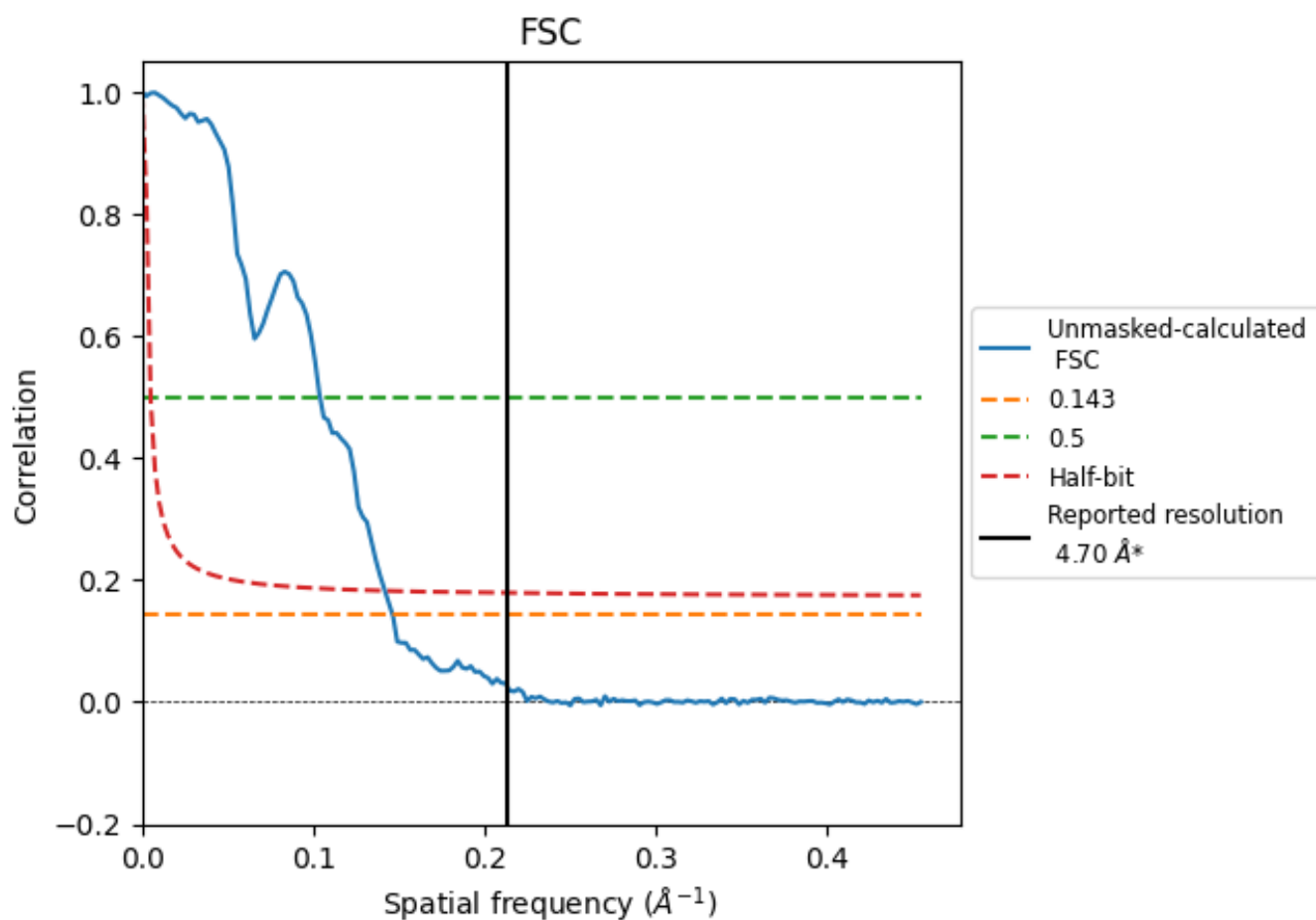


*Reported resolution corresponds to spatial frequency of $0.213 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

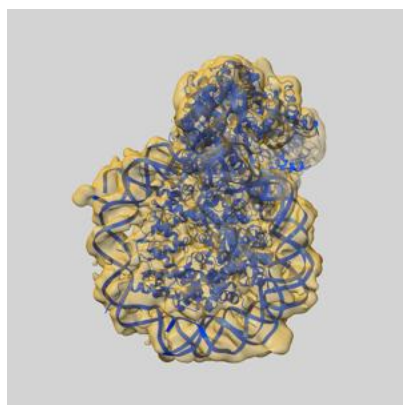
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.84	9.62	7.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 4.7 by more than 10 %

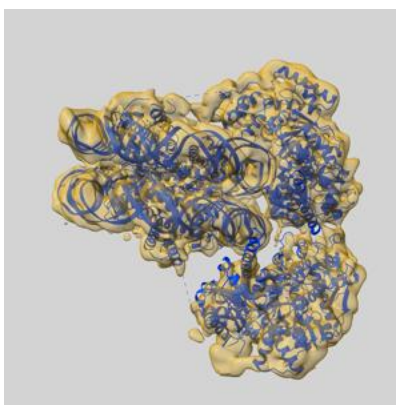
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68040 and PDB model 21VV. Per-residue inclusion information can be found in section [3](#) on page [9](#).

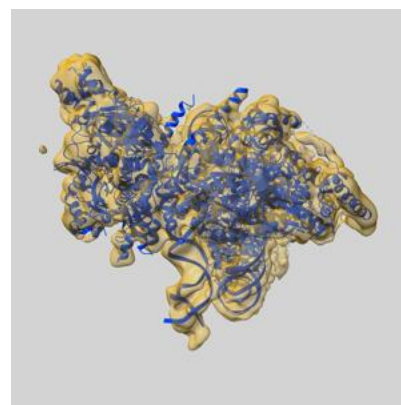
9.1 Map-model overlay [i](#)



X



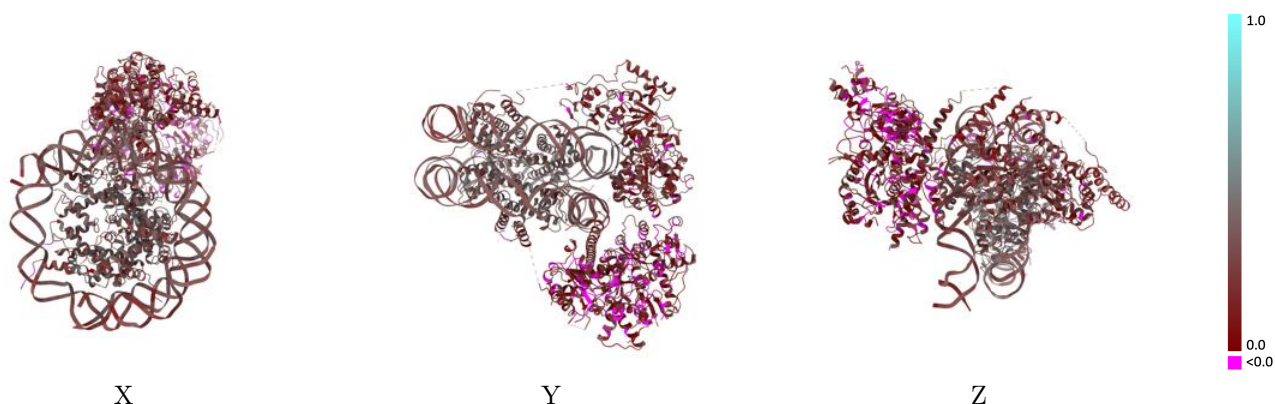
Y



Z

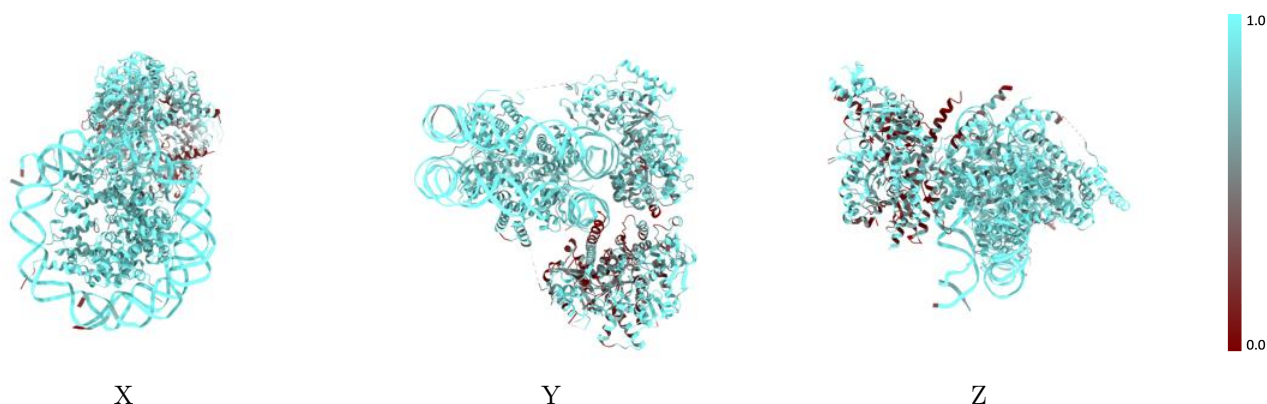
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



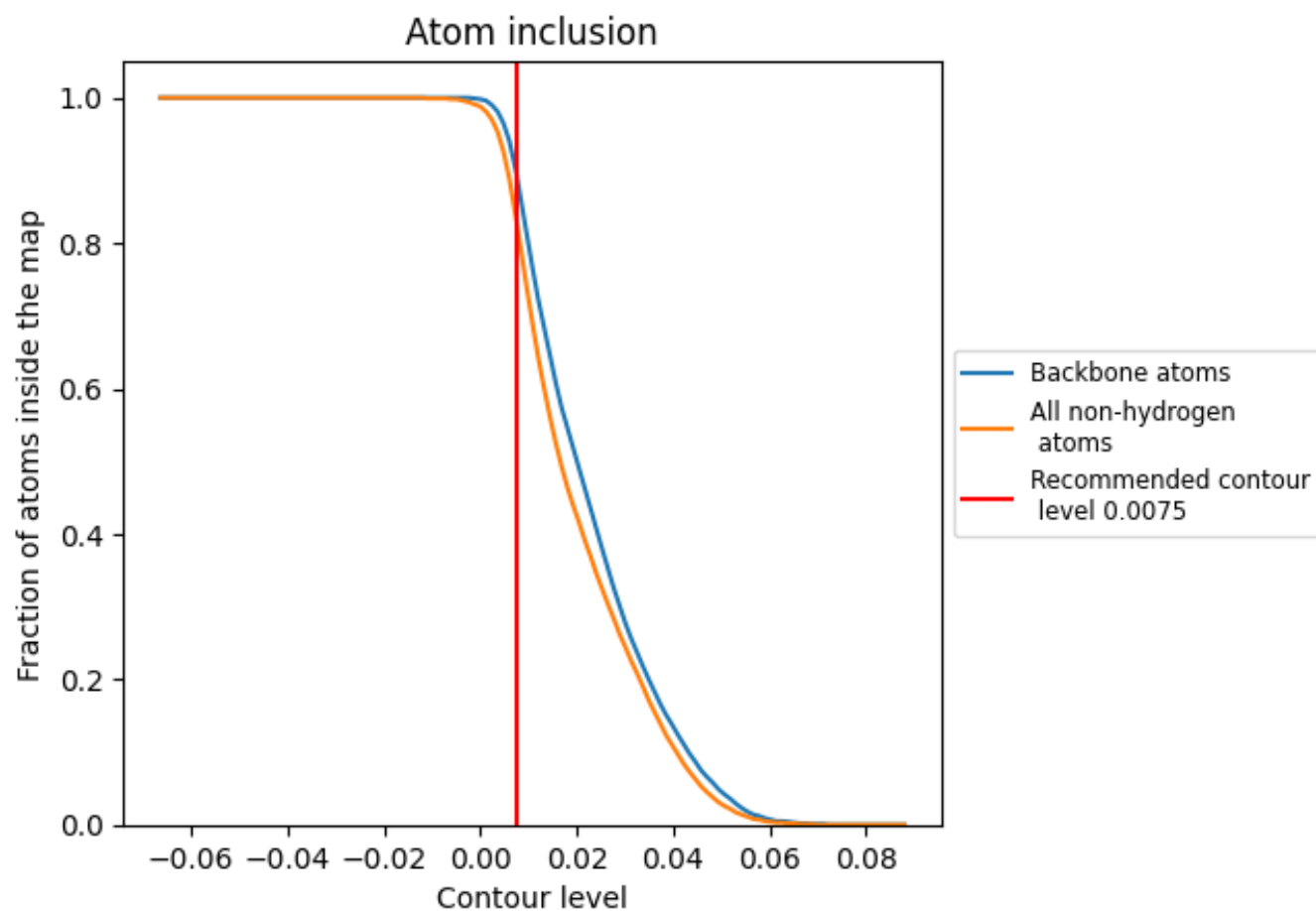
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.2490
A	0.8990	0.3330
B	0.9270	0.3580
C	0.9440	0.3520
D	0.9280	0.3360
E	0.9170	0.3800
F	0.8880	0.3750
G	0.9160	0.3620
H	0.9250	0.3590
I	0.7970	0.2140
J	0.6140	0.0960
K	0.6520	0.1260
N	0.8110	0.1620
X	0.9750	0.3070
Y	0.9660	0.3150

1.0

0.0

<0.0