



Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 10:56 AM EDT

PDB ID : 9CA8 / pdb_00009ca8
EMDB ID : EMD-45382
Title : Cryo-EM structure of human SRCAP-nucleosome complex in the partially-engaged state (composite structure)
Authors : Louder, R.K.; Park, G.; Patel, A.B.
Deposited on : 2024-06-17
Resolution : 3.92 Å(reported)

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

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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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

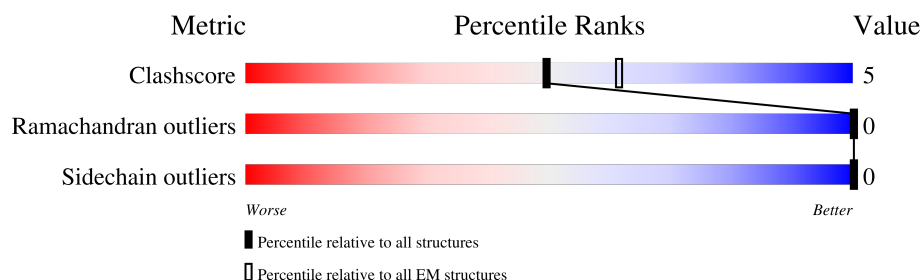
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.92 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.





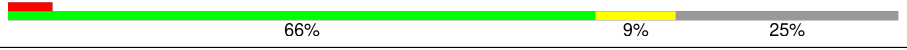



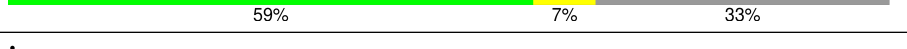
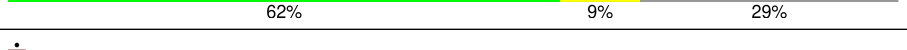
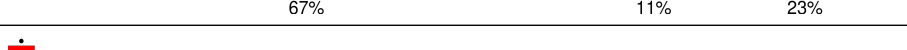
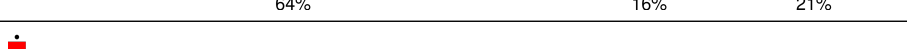
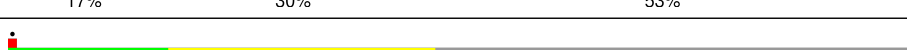
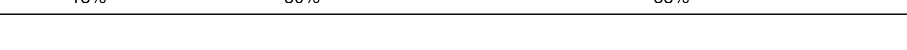
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	3230	
2	B	364	
3	C	396	
4	D	154	
5	E	456	
5	G	456	
5	I	456	
6	F	463	

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Mol	Chain	Length	Quality of chain
6	H	463	
6	J	463	
7	Q	128	
7	S	128	
8	R	125	
8	T	125	
9	U	135	
9	W	135	
10	V	102	
10	X	102	
11	Y	285	
12	Z	285	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 42947 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 SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	736	Total	C	N	O	S	0	0
			6036	3860	1095	1046	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	137	Total	C	N	O	S	0	0
			1125	715	205	201	4		

- Molecule 3 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3226	2064	528	616	18		

- Molecule 4 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	105	Total	C	N	O	S	0	0
			831	508	164	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	433	Total	C	N	O	S	0	0
			3344	2107	574	646	17		
5	G	445	Total	C	N	O	S	0	0
			3430	2159	588	665	18		
5	I	436	Total	C	N	O	S	0	0
			3365	2119	577	652	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	438	Total	C	N	O	S	0	0
			3395	2121	596	662	16		
6	H	432	Total	C	N	O	S	0	0
			3361	2101	590	654	16		
6	J	418	Total	C	N	O	S	0	0
			3254	2039	568	632	15		

- Molecule 7 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	96	Total	C	N	O	0	0
			742	465	147	130		
7	S	104	Total	C	N	O	0	0
			800	504	156	140		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	99	ARG	GLY	conflict	UNP P06897
Q	123	SER	-	expression tag	UNP P06897
Q	124	LYS	-	expression tag	UNP P06897
Q	125	SER	-	expression tag	UNP P06897
Q	126	LYS	-	expression tag	UNP P06897
Q	127	SER	-	expression tag	UNP P06897
Q	128	LYS	-	expression tag	UNP P06897
S	99	ARG	GLY	conflict	UNP P06897
S	123	SER	-	expression tag	UNP P06897
S	124	LYS	-	expression tag	UNP P06897
S	125	SER	-	expression tag	UNP P06897
S	126	LYS	-	expression tag	UNP P06897
S	127	SER	-	expression tag	UNP P06897
S	128	LYS	-	expression tag	UNP P06897

- Molecule 8 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
8	T	95	Total	C	N	O	S	0	0
			745	469	134	140	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	32	THR	SER	conflict	UNP P02281
T	32	THR	SER	conflict	UNP P02281

- Molecule 9 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	90	Total	C	N	O	S	0	0
			740	467	140	130	3		
9	W	96	Total	C	N	O	S	0	0
			795	501	154	137	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	102	ALA	GLY	variant	UNP P84233
W	102	ALA	GLY	variant	UNP P84233

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
10	X	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

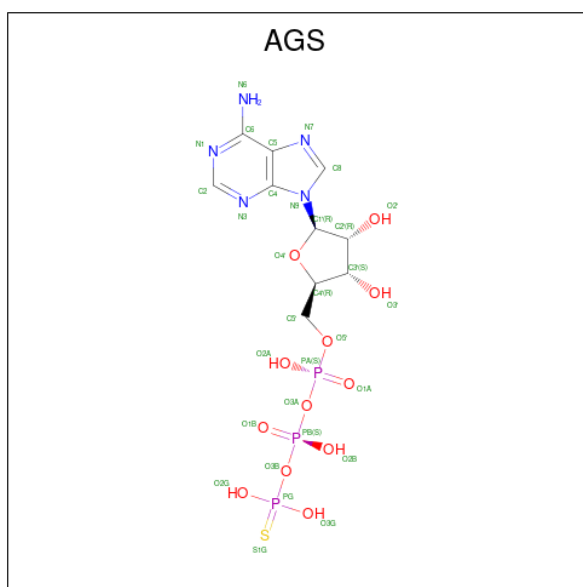
- Molecule 11 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	135	Total	C	N	O	P	0	0
			2753	1305	501	812	135		

- Molecule 12 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	135	Total	C	N	O	P	0	0
			2782	1314	525	808	135		

- Molecule 13 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms					AltConf	
13	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
13	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

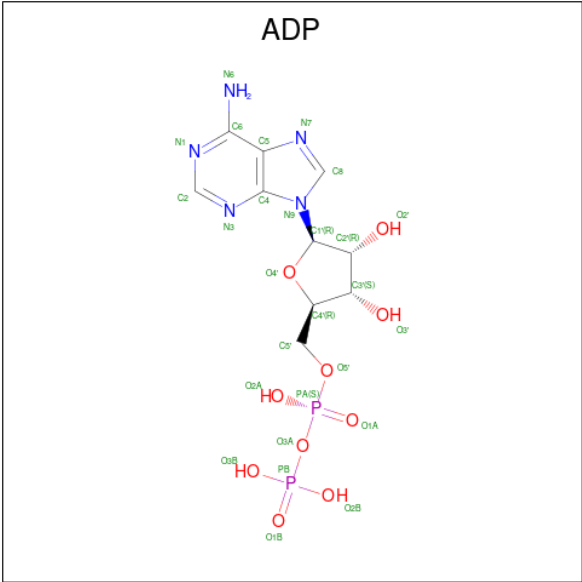
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	
14	C	1	Total	Mg	0
			1	1	
14	E	1	Total	Mg	0
			1	1	
14	F	1	Total	Mg	0
			1	1	
14	H	1	Total	Mg	0
			1	1	

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

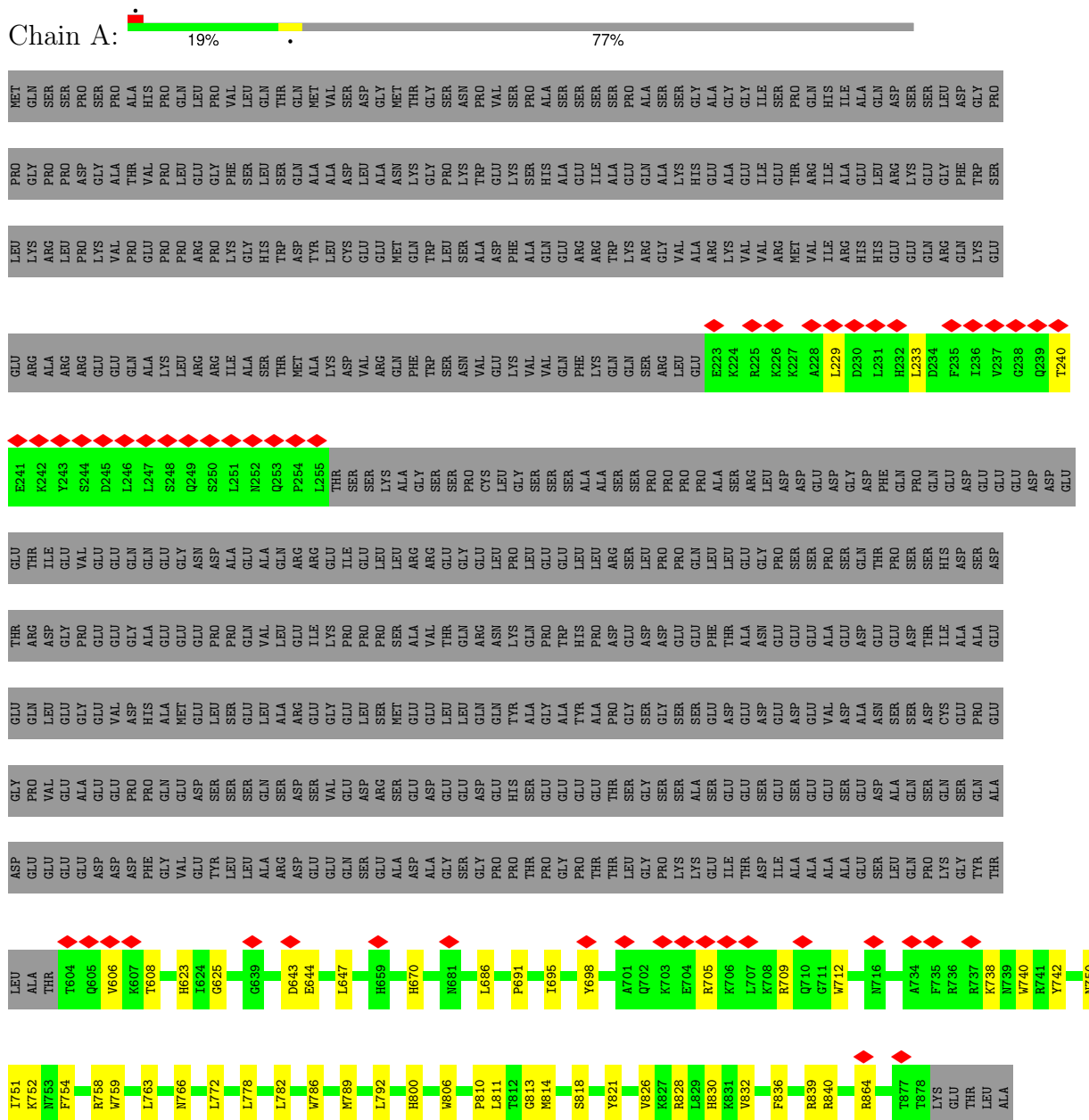


Mol	Chain	Residues	Atoms					AltConf
16	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

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

• Molecule 1: Helicase SRCAP

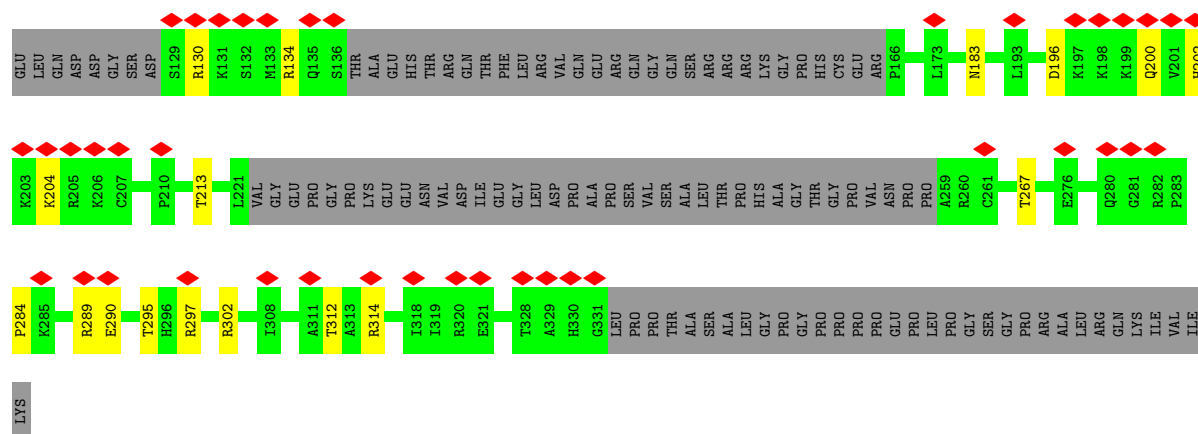




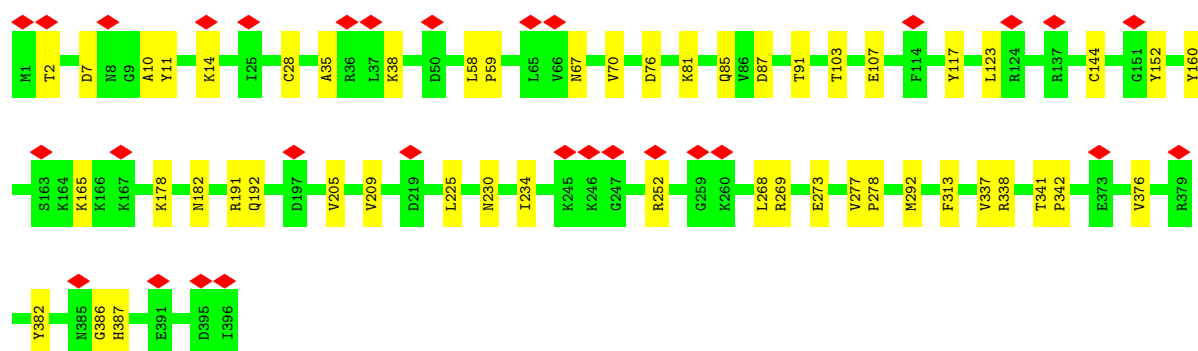
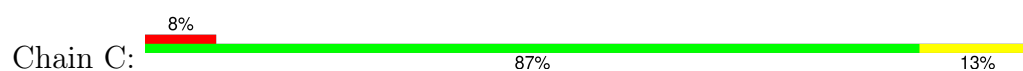
[illegible]

- Molecule 2: Vacuolar protein sorting-associated protein 72 homolog

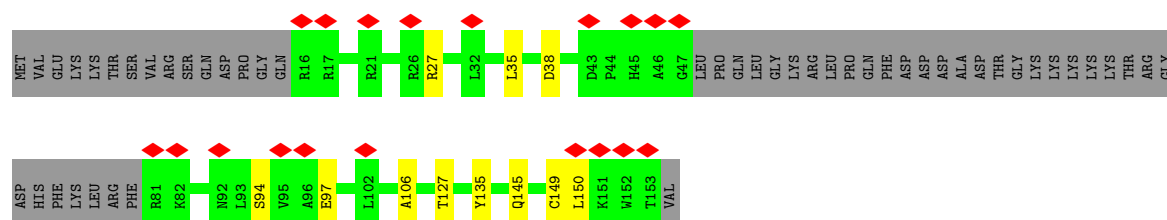
[illegible]



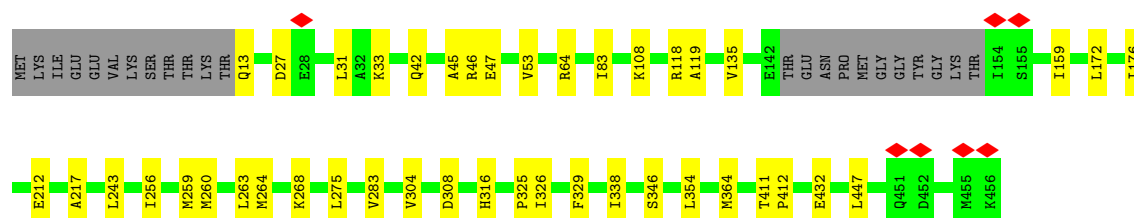
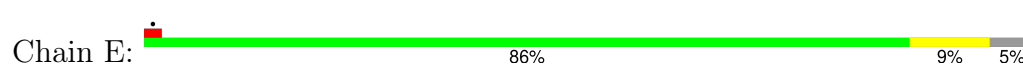
• Molecule 3: Actin-related protein 6



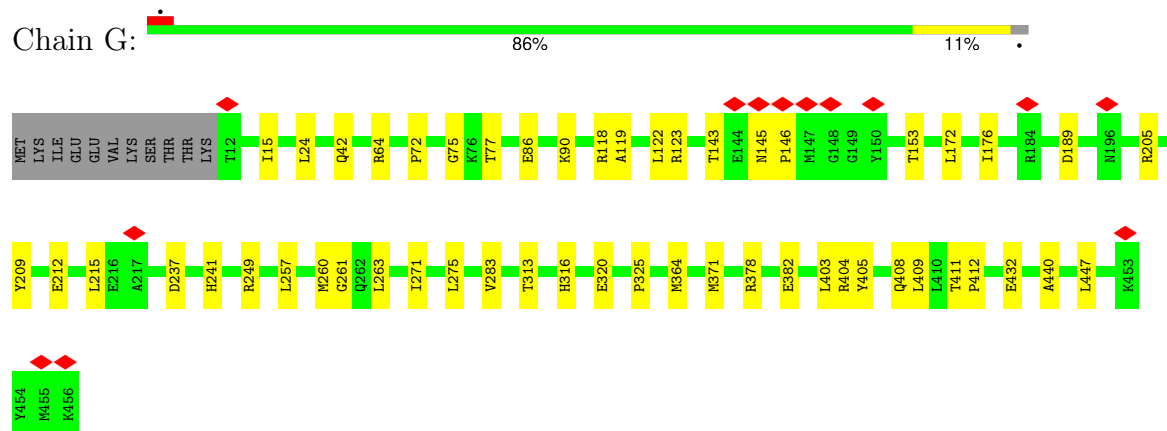
• Molecule 4: Zinc finger HIT domain-containing protein 1



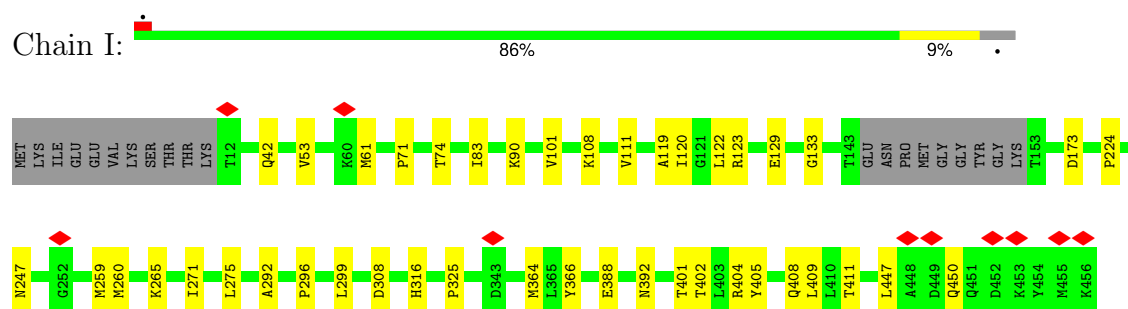
• Molecule 5: RuvB-like 1



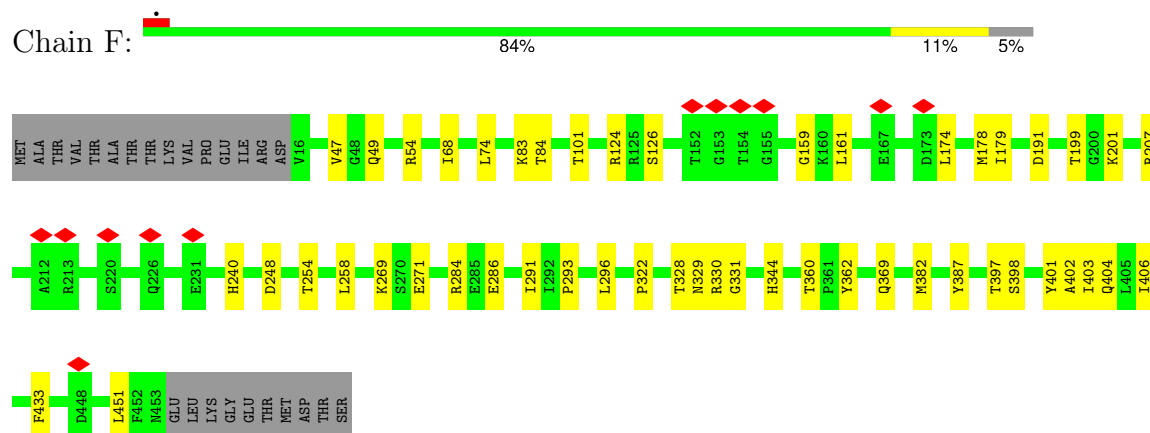
- Molecule 5: RuvB-like 1



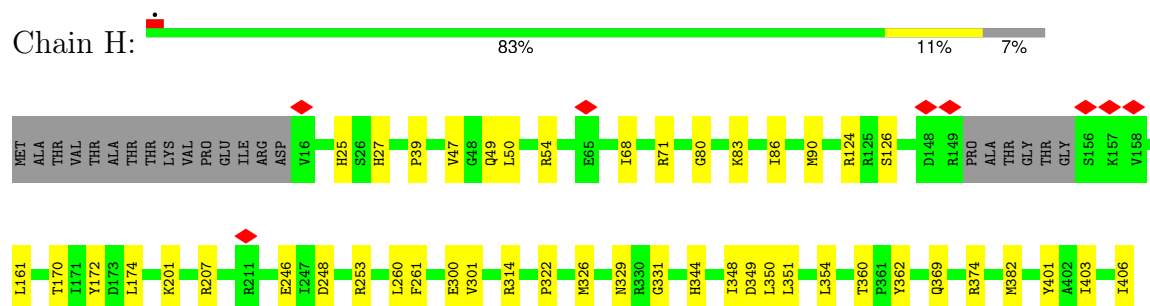
- Molecule 5: RuvB-like 1

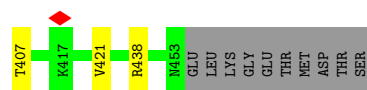


- Molecule 6: RuvB-like 2

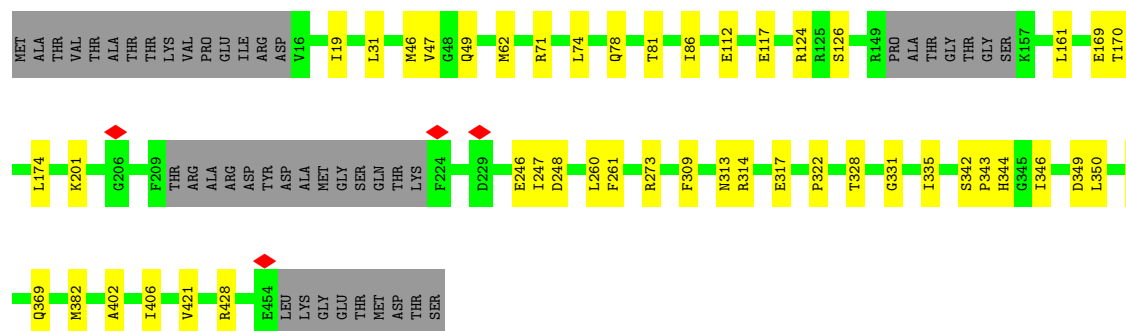
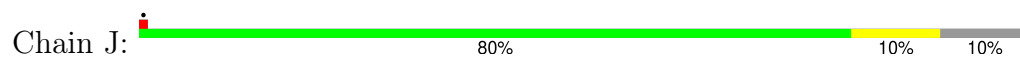


- Molecule 6: RuvB-like 2

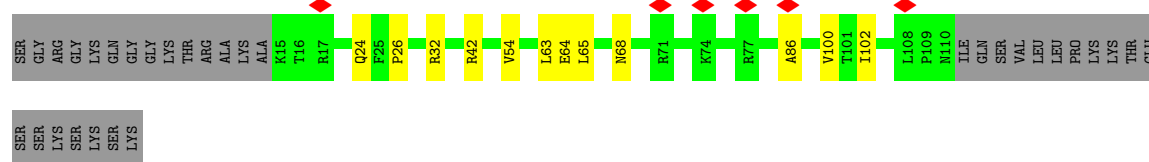




• Molecule 6: RuvB-like 2



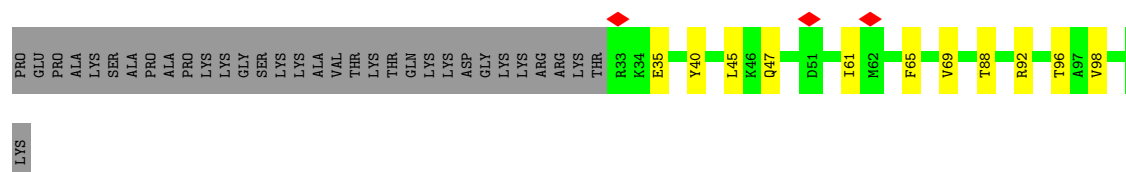
• Molecule 7: Histone H2A type 1



• Molecule 7: Histone H2A type 1



• Molecule 8: Histone H2B 1.1



• Molecule 8: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24701	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.078	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	393.59998, 393.59998, 393.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.025, 1.025, 1.025	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, AGS, ZN, 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	0.11	0/6186	0.29	0/8369
2	B	0.09	0/1151	0.23	0/1553
3	C	0.09	0/3300	0.25	0/4467
4	D	0.09	0/848	0.25	0/1147
5	E	0.11	0/3387	0.25	0/4561
5	G	0.11	0/3476	0.24	0/4683
5	I	0.11	0/3408	0.24	0/4591
6	F	0.11	0/3435	0.24	0/4625
6	H	0.12	0/3399	0.24	0/4573
6	J	0.12	0/3290	0.23	0/4426
7	Q	0.09	0/751	0.21	0/1013
7	S	0.10	0/810	0.22	0/1095
8	R	0.09	0/730	0.20	0/983
8	T	0.10	0/756	0.21	0/1015
9	U	0.10	0/748	0.22	0/1003
9	W	0.10	0/806	0.22	0/1081
10	V	0.12	0/634	0.22	0/848
10	X	0.12	0/653	0.23	0/873
11	Y	0.20	0/3084	0.43	0/4754
12	Z	0.20	0/3124	0.40	0/4823
All	All	0.13	0/43976	0.28	0/60483

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	6036	0	6121	70	0
2	B	1125	0	1148	14	0
3	C	3226	0	3147	31	0
4	D	831	0	798	9	0
5	E	3344	0	3449	34	0
5	G	3430	0	3530	44	0
5	I	3365	0	3470	34	0
6	F	3395	0	3468	37	0
6	H	3361	0	3434	37	0
6	J	3254	0	3330	34	0
7	Q	742	0	784	10	0
7	S	800	0	851	8	0
8	R	719	0	740	10	0
8	T	745	0	773	5	0
9	U	740	0	781	9	0
9	W	795	0	833	11	0
10	V	627	0	663	9	0
10	X	646	0	687	13	0
11	Y	2753	0	1514	81	0
12	Z	2782	0	1512	68	0
13	A	31	0	12	0	0
13	C	31	0	12	1	0
14	A	1	0	0	0	0
14	C	1	0	0	0	0
14	E	1	0	0	0	0
14	F	1	0	0	0	0
14	H	1	0	0	0	0
15	D	2	0	0	0	0
16	E	27	0	12	0	0
16	F	27	0	12	3	0
16	G	27	0	12	2	0
16	H	27	0	12	3	0
16	I	27	0	12	1	0
16	J	27	0	12	1	0
All	All	42947	0	41129	460	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 5.

All (460) 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)
11:Y:39:DA:H2'	11:Y:40:DG:C8	2.18	0.79
5:E:411:THR:HG21	6:F:68:ILE:HG13	1.67	0.76
1:A:2119:ARG:HH22	11:Y:22:DC:H5''	1.51	0.75
12:Z:49:DC:H2'	12:Z:50:DG:C8	2.24	0.73
12:Z:-25:DC:H2'	12:Z:-24:DT:H71	1.71	0.72
5:G:411:THR:HG21	6:H:68:ILE:HG13	1.71	0.70
12:Z:39:DA:H2''	12:Z:40:DC:H5''	1.74	0.70
3:C:182:ASN:ND2	4:D:35:LEU:O	2.24	0.70
5:G:189:ASP:OD1	5:G:205:ARG:NH1	2.26	0.68
1:A:2141:ASN:ND2	11:Y:22:DC:OP1	2.27	0.68
8:R:92:ARG:NH2	10:X:75:HIS:O	2.26	0.67
12:Z:21:DG:H2'	12:Z:22:DT:H71	1.77	0.66
6:F:191:ASP:OD1	6:F:207:ARG:NH1	2.28	0.66
6:H:401:TYR:OH	6:H:438:ARG:NH2	2.29	0.66
11:Y:-57:DC:H2''	11:Y:-56:DG:C8	2.30	0.65
12:Z:-14:DA:H2''	12:Z:-13:DA:H5''	1.77	0.65
6:F:159:GLY:HA3	6:F:179:ILE:HD11	1.79	0.65
10:X:30:THR:HG22	10:X:32:PRO:HD2	1.80	0.64
7:Q:54:VAL:HG21	8:R:98:VAL:HG21	1.78	0.64
12:Z:15:DT:H2''	12:Z:16:DA:C8	2.33	0.64
1:A:2183:LYS:NZ	11:Y:23:DA:OP1	2.31	0.64
11:Y:27:DG:H2'	11:Y:28:DG:C8	2.32	0.64
11:Y:-44:DA:H2'	11:Y:-43:DT:H71	1.79	0.64
1:A:1971:GLU:OE1	6:F:240:HIS:NE2	2.26	0.63
5:G:313:THR:HA	5:G:316:HIS:CD2	2.33	0.63
6:F:258:LEU:HD12	5:G:257:LEU:HD13	1.81	0.63
1:A:922:CYS:SG	6:J:201:LYS:NZ	2.69	0.63
1:A:1924:ASP:OD2	6:H:201:LYS:NZ	2.31	0.63
11:Y:-27:DC:H2''	11:Y:-26:DT:H71	1.81	0.63
1:A:2179:LYS:NZ	11:Y:24:DA:OP1	2.32	0.62
12:Z:37:DC:H2''	12:Z:38:DG:C8	2.34	0.62
5:G:172:LEU:HB3	5:G:176:ILE:HD12	1.81	0.62
6:H:382:MET:HG2	6:H:421:VAL:HB	1.80	0.62
11:Y:29:DA:H2'	11:Y:30:DT:H71	1.79	0.62
2:B:289:ARG:NH2	5:G:212:GLU:OE2	2.32	0.62
2:B:213:THR:HB	2:B:267:THR:HB	1.82	0.62
12:Z:43:DA:H2''	12:Z:44:DT:H5''	1.81	0.61
5:G:119:ALA:HB3	5:G:325:PRO:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:LYS:N	16:F:501:ADP:O1B	2.30	0.60
12:Z:0:DG:H2'	12:Z:1:DC:C6	2.36	0.60
9:U:72:ARG:NH1	11:Y:-23:DC:OP1	2.34	0.60
12:Z:2:DG:H2''	12:Z:3:DC:H5''	1.82	0.60
1:A:2134:VAL:HG22	1:A:2164:TYR:HB2	1.82	0.60
10:X:52:GLU:OE2	10:X:55:ARG:NH1	2.34	0.60
5:G:447:LEU:HD22	6:H:331:GLY:HA2	1.83	0.60
6:J:49:GLN:NE2	6:J:81:THR:O	2.25	0.60
11:Y:25:DG:H2''	11:Y:26:DG:C8	2.37	0.60
11:Y:-20:DC:H2'	11:Y:-19:DG:C8	2.36	0.60
1:A:2036:ARG:NH2	6:F:286:GLU:O	2.30	0.60
11:Y:-22:DA:H2''	11:Y:-21:DC:H5''	1.84	0.59
11:Y:30:DT:H2'	11:Y:31:DT:C6	2.37	0.59
12:Z:50:DG:H2''	12:Z:51:DG:C8	2.37	0.59
1:A:229:LEU:HB3	1:A:806:TRP:HE1	1.67	0.59
6:F:49:GLN:NE2	6:F:360:THR:O	2.35	0.59
7:S:29:ARG:NH2	12:Z:49:DC:OP1	2.27	0.59
11:Y:-47:DT:H2''	11:Y:-46:DC:C5	2.37	0.59
11:Y:28:DG:H1'	11:Y:29:DA:N7	2.16	0.59
2:B:290:GLU:OE2	2:B:302:ARG:NH1	2.35	0.59
3:C:123:LEU:HB2	3:C:376:VAL:HG12	1.85	0.59
9:W:83:ARG:NH2	12:Z:-24:DT:OP1	2.34	0.59
12:Z:35:DT:H2''	12:Z:36:DA:C8	2.38	0.59
1:A:2089:LEU:HB3	1:A:2116:LEU:HD23	1.85	0.59
1:A:772:LEU:HG	1:A:792:LEU:HD21	1.84	0.58
6:F:124:ARG:NE	6:F:248:ASP:OD2	2.36	0.58
6:J:46:MET:HE1	6:J:86:ILE:HA	1.83	0.58
3:C:192:GLN:NE2	3:C:269:ARG:O	2.37	0.58
5:I:450:GLN:OE1	6:J:78:GLN:NE2	2.36	0.58
11:Y:8:DC:H2''	11:Y:9:DG:C8	2.38	0.58
5:G:408:GLN:O	6:H:71:ARG:NH2	2.37	0.57
6:F:199:THR:HG23	6:F:201:LYS:H	1.69	0.57
6:J:124:ARG:NE	6:J:248:ASP:OD2	2.38	0.57
9:W:62:ILE:O	9:W:93:GLN:NE2	2.38	0.57
11:Y:45:DC:H2''	11:Y:46:DA:C8	2.39	0.57
5:I:42:GLN:NE2	5:I:364:MET:O	2.38	0.57
1:A:778:LEU:HD23	1:A:2187:GLY:HA2	1.87	0.56
8:T:71:GLU:OE1	10:X:91:LYS:NZ	2.38	0.56
9:W:51:ILE:HG13	10:X:39:ARG:HD2	1.87	0.56
1:A:782:LEU:HD11	1:A:811:LEU:HD12	1.87	0.56
1:A:826:VAL:HG12	1:A:830:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:THR:HG23	1:A:2098:ARG:HG2	1.87	0.56
7:Q:64:GLU:OE2	7:Q:68:ASN:ND2	2.37	0.56
11:Y:26:DG:H2''	11:Y:27:DG:H8	1.70	0.56
12:Z:42:DA:H2''	12:Z:43:DA:H5''	1.86	0.56
4:D:27:ARG:NH2	4:D:150:LEU:O	2.32	0.56
5:I:402:THR:HG22	5:I:404:ARG:H	1.69	0.56
11:Y:26:DG:H2''	11:Y:27:DG:C8	2.41	0.56
11:Y:56:DC:H2''	11:Y:57:DA:C8	2.41	0.55
12:Z:74:DC:H2''	12:Z:75:DA:C8	2.40	0.55
1:A:233:LEU:HG	1:A:828:ARG:HH21	1.71	0.55
1:A:240:THR:HG21	1:A:832:VAL:HA	1.87	0.55
9:W:96:SER:HB2	10:X:58:LEU:HD11	1.88	0.55
1:A:1973:ILE:HG23	1:A:1977:ILE:HD12	1.87	0.55
5:I:265:LYS:NZ	6:J:112:GLU:OE2	2.40	0.55
12:Z:20:DG:H2'	12:Z:21:DG:H8	1.71	0.55
3:C:11:TYR:HB2	3:C:152:TYR:CG	2.42	0.55
5:I:447:LEU:HD11	6:J:344:HIS:CE1	2.41	0.55
7:Q:102:ILE:HG23	8:R:61:ILE:HD12	1.88	0.55
11:Y:47:DG:H2''	11:Y:48:DG:N7	2.22	0.55
12:Z:20:DG:H2'	12:Z:21:DG:C8	2.41	0.55
6:F:74:LEU:HD11	6:F:328:THR:HG22	1.89	0.55
5:E:432:GLU:OE2	6:F:54:ARG:NH1	2.36	0.54
12:Z:54:DT:H2''	12:Z:55:DG:N7	2.22	0.54
12:Z:-37:DG:H2''	12:Z:-36:DG:N7	2.22	0.54
1:A:750:ASN:HB3	1:A:758:ARG:HH11	1.72	0.54
6:H:124:ARG:NE	6:H:248:ASP:OD2	2.40	0.54
3:C:107:GLU:OE2	3:C:387:HIS:NE2	2.41	0.54
12:Z:53:DC:H2''	12:Z:54:DT:C6	2.43	0.54
5:E:304:VAL:HG21	5:E:329:PHE:HB3	1.89	0.54
9:U:106:ASP:OD2	9:U:131:ARG:NH2	2.30	0.54
9:W:119:ILE:HD11	10:X:46:ILE:HG23	1.89	0.54
11:Y:-62:DC:H2'	11:Y:-61:DG:C8	2.42	0.54
5:G:263:LEU:HD22	5:I:260:MET:HE2	1.89	0.53
4:D:135:TYR:OH	6:J:169:GLU:O	2.23	0.53
6:F:404:GLN:HA	5:G:64:ARG:HH21	1.72	0.53
6:H:246:GLU:HA	6:H:260:LEU:HD21	1.91	0.53
11:Y:-21:DC:H2'	11:Y:-20:DC:C6	2.44	0.53
12:Z:58:DC:H2''	12:Z:59:DA:C8	2.44	0.53
1:A:644:GLU:OE2	1:A:839:ARG:NH2	2.31	0.53
6:F:451:LEU:HD21	5:G:72:PRO:HG3	1.89	0.53
1:A:712:TRP:NE1	12:Z:62:DG:OP1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-5:DG:H2''	12:Z:-4:DG:C8	2.44	0.53
5:G:313:THR:HA	5:G:316:HIS:HD2	1.73	0.53
5:I:119:ALA:HB3	5:I:325:PRO:HG3	1.90	0.53
3:C:338:ARG:NH2	3:C:342:PRO:O	2.41	0.53
5:E:42:GLN:HE22	5:E:364:MET:H	1.56	0.53
5:E:260:MET:HE1	5:I:260:MET:HE3	1.91	0.53
3:C:59:PRO:HA	3:C:67:ASN:HB3	1.92	0.52
6:F:404:GLN:HA	5:G:64:ARG:NH2	2.24	0.52
1:A:670:HIS:ND1	1:A:742:TYR:HB2	2.24	0.52
1:A:751:ILE:HG22	1:A:759:TRP:HD1	1.73	0.52
12:Z:-20:DC:H2'	12:Z:-19:DG:C8	2.45	0.52
5:E:275:LEU:HD13	6:J:261:PHE:HB3	1.90	0.52
6:F:161:LEU:HB2	6:F:174:LEU:HD11	1.91	0.52
11:Y:-57:DC:H2''	11:Y:-56:DG:N7	2.24	0.52
1:A:686:LEU:HD13	1:A:695:ILE:HD12	1.91	0.52
11:Y:-54:DA:H2''	11:Y:-53:DG:C8	2.45	0.52
1:A:2120:SER:HB3	12:Z:-19:DG:H5''	1.91	0.52
5:G:15:ILE:HD13	5:G:382:GLU:HA	1.91	0.52
10:X:26:ILE:HD13	10:X:59:LYS:HD3	1.90	0.52
11:Y:-72:DT:H2''	11:Y:-71:DG:C8	2.44	0.52
11:Y:-66:DA:H2''	11:Y:-65:DT:H5''	1.91	0.52
5:E:283:VAL:HB	6:J:19:ILE:HD11	1.90	0.52
3:C:28:CYS:HB3	3:C:58:LEU:HD13	1.92	0.52
5:I:122:LEU:HD11	5:I:292:ALA:HB1	1.92	0.52
11:Y:52:DC:H2'	11:Y:53:DT:C6	2.45	0.52
1:A:813:GLY:O	1:A:818:SER:N	2.43	0.51
6:F:401:TYR:OH	6:F:433:PHE:O	2.28	0.51
11:Y:33:DC:H2'	11:Y:34:DT:C6	2.46	0.51
12:Z:19:DC:H2''	12:Z:20:DG:H8	1.75	0.51
7:S:63:LEU:HD13	8:T:45:LEU:HB2	1.91	0.51
1:A:2105:PHE:CE2	1:A:2114:PHE:HB2	2.45	0.51
5:G:123:ARG:NH2	5:G:237:ASP:OD2	2.44	0.51
10:X:29:ILE:HD13	10:X:58:LEU:HD23	1.93	0.51
11:Y:-71:DG:H2''	11:Y:-70:DG:C8	2.45	0.51
11:Y:-26:DT:H2''	11:Y:-25:DA:C8	2.45	0.51
11:Y:29:DA:H2''	11:Y:30:DT:H5''	1.91	0.51
11:Y:38:DT:H2''	11:Y:39:DA:N7	2.24	0.51
11:Y:-7:DC:H2''	11:Y:-6:DT:C6	2.46	0.51
5:G:447:LEU:HD11	6:H:344:HIS:CE1	2.44	0.51
7:Q:32:ARG:NH2	8:R:35:GLU:OE1	2.36	0.51
1:A:766:ASN:HD21	11:Y:-58:DG:H5''	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:-28:DT:H2''	11:Y:-27:DC:C6	2.46	0.51
5:I:90:LYS:HB2	5:I:123:ARG:HH22	1.75	0.51
11:Y:-55:DC:H2''	11:Y:-54:DA:N7	2.26	0.51
12:Z:66:DT:H2'	12:Z:67:DT:H71	1.93	0.51
5:I:71:PRO:HD2	5:I:74:THR:HG21	1.92	0.50
6:J:342:SER:OG	6:J:346:ILE:O	2.26	0.50
3:C:191:ARG:NH1	3:C:273:GLU:OE2	2.43	0.50
5:E:108:LYS:NZ	5:E:308:ASP:OD2	2.36	0.50
10:V:24:ASP:OD1	10:V:24:ASP:N	2.44	0.50
5:G:77:THR:OG1	6:H:314:ARG:NH1	2.44	0.50
6:J:31:LEU:HD23	6:J:46:MET:HE3	1.92	0.50
6:J:47:VAL:HG11	6:J:369:GLN:HB3	1.92	0.50
12:Z:-2:DC:H2''	12:Z:-1:DA:H8	1.77	0.50
3:C:2:THR:HG23	3:C:91:THR:HG23	1.93	0.50
11:Y:-40:DG:H2'	11:Y:-39:DT:C6	2.46	0.50
1:A:643:ASP:HB3	1:A:647:LEU:HD12	1.94	0.50
6:H:47:VAL:HG11	6:H:369:GLN:HB3	1.93	0.50
11:Y:25:DG:H2''	11:Y:26:DG:H8	1.77	0.50
12:Z:1:DC:H2''	12:Z:2:DG:C8	2.46	0.50
6:J:335:ILE:HD11	6:J:342:SER:HB2	1.93	0.50
12:Z:-48:DC:H2''	12:Z:-47:DC:C6	2.47	0.50
1:A:2103:GLU:OE1	2:B:202:HIS:NE2	2.45	0.49
2:B:295:THR:HG23	2:B:297:ARG:H	1.77	0.49
5:E:411:THR:OG1	5:E:412:PRO:HD3	2.12	0.49
11:Y:46:DA:H2''	11:Y:47:DG:C8	2.47	0.49
1:A:1936:ILE:HD11	1:A:1959:VAL:HB	1.95	0.49
4:D:127:THR:H	6:J:170:THR:HG23	1.75	0.49
6:F:328:THR:HG21	6:F:344:HIS:HB3	1.94	0.49
1:A:1903:ARG:HE	5:I:129:GLU:CD	2.21	0.49
3:C:292:MET:HG2	4:D:106:ALA:HB1	1.95	0.49
5:E:119:ALA:HB3	5:E:325:PRO:HG3	1.95	0.49
9:U:103:LEU:O	9:U:107:THR:HG23	2.13	0.49
1:A:814:MET:SD	1:A:821:TYR:HA	2.53	0.48
11:Y:-14:DA:H2''	11:Y:-13:DA:C8	2.48	0.48
6:F:126:SER:HB2	6:F:322:PRO:HG3	1.94	0.48
6:H:27:HIS:HD2	6:H:374:ARG:HH11	1.59	0.48
12:Z:5:DT:H2''	12:Z:6:DA:N7	2.28	0.48
1:A:766:ASN:ND2	11:Y:-58:DG:H5''	2.28	0.48
3:C:7:ASP:HB3	3:C:14:LYS:HB2	1.95	0.48
1:A:752:LYS:NZ	11:Y:22:DC:OP2	2.45	0.48
6:F:329:ASN:OD1	6:F:330:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:22:DC:H2'	11:Y:23:DA:C8	2.49	0.48
1:A:2009:GLN:HB3	5:I:259:MET:HE1	1.96	0.48
10:V:31:LYS:HG3	10:V:51:TYR:CE1	2.48	0.48
3:C:178:LYS:NZ	4:D:38:ASP:OD1	2.37	0.48
10:V:79:LYS:N	12:Z:28:DA:OP1	2.45	0.48
12:Z:-33:DG:H2'	12:Z:-32:DT:H71	1.96	0.48
1:A:691:PRO:O	2:B:183:ASN:ND2	2.33	0.47
1:A:810:PRO:O	1:A:814:MET:HG3	2.14	0.47
11:Y:24:DA:H2''	11:Y:25:DG:H5''	1.95	0.47
6:J:313:ASN:HD21	6:J:350:LEU:HB2	1.79	0.47
11:Y:-2:DC:H2''	11:Y:-1:DG:C8	2.49	0.47
11:Y:15:DT:H2''	11:Y:16:DA:N7	2.28	0.47
5:E:259:MET:HE1	6:F:254:THR:HG21	1.96	0.47
6:H:351:LEU:HD23	6:H:354:LEU:HD11	1.97	0.47
12:Z:8:DC:H2'	12:Z:9:DT:H71	1.96	0.47
5:E:13:GLN:OE1	6:F:284:ARG:NH2	2.47	0.47
6:J:126:SER:HB2	6:J:322:PRO:HG3	1.97	0.47
11:Y:-69:DA:H2''	11:Y:-68:DG:C8	2.49	0.47
12:Z:-46:DT:H2''	12:Z:-45:DG:C8	2.49	0.47
1:A:892:ASN:O	1:A:896:GLN:HG2	2.14	0.47
9:U:117:VAL:HG13	10:V:44:LYS:HE3	1.96	0.47
2:B:134:ARG:NH1	7:S:92:GLU:OE1	2.43	0.47
5:E:47:GLU:OE1	6:J:428:ARG:NH2	2.40	0.47
6:F:291:ILE:HG22	6:F:293:PRO:HD3	1.97	0.47
6:H:49:GLN:NE2	6:H:360:THR:O	2.45	0.47
6:J:402:ALA:O	6:J:406:ILE:HG13	2.14	0.47
11:Y:30:DT:H4'	11:Y:31:DT:OP1	2.15	0.47
1:A:926:ALA:HB3	1:A:929:VAL:HG23	1.97	0.47
2:B:312:THR:HG22	2:B:314:ARG:H	1.79	0.47
5:G:42:GLN:HE22	5:G:364:MET:N	2.13	0.47
1:A:606:VAL:HG11	1:A:623:HIS:HD1	1.79	0.47
3:C:182:ASN:HD22	4:D:35:LEU:C	2.19	0.47
5:I:133:GLY:HA2	5:I:224:PRO:HG2	1.97	0.47
6:H:126:SER:HB2	6:H:322:PRO:HG3	1.96	0.47
1:A:789:MET:HE1	1:A:836:PHE:HB2	1.97	0.46
5:G:411:THR:OG1	5:G:412:PRO:HD3	2.15	0.46
7:S:88:ARG:HB2	7:S:108:LEU:HD21	1.98	0.46
9:U:72:ARG:NH2	11:Y:-23:DC:OP2	2.48	0.46
11:Y:39:DA:H2''	11:Y:40:DG:O5'	2.15	0.46
12:Z:-53:DA:H2''	12:Z:-52:DG:C8	2.50	0.46
5:G:24:LEU:HD12	5:G:86:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:382:TYR:CD1	3:C:386:GLY:HA3	2.49	0.46
7:Q:26:PRO:HD3	8:R:40:TYR:CD1	2.51	0.46
1:A:2073:ASP:OD1	1:A:2088:ARG:NH1	2.47	0.46
16:J:501:ADP:H5'1	16:J:501:ADP:H8	1.79	0.46
6:F:403:ILE:HA	6:F:406:ILE:HD12	1.98	0.46
5:G:432:GLU:OE2	6:H:54:ARG:NH2	2.43	0.46
12:Z:9:DT:H2''	12:Z:10:DG:H8	1.81	0.46
5:E:33:LYS:O	5:E:46:ARG:NH2	2.49	0.46
6:J:74:LEU:HD11	6:J:328:THR:HG22	1.98	0.46
11:Y:14:DT:H5'	11:Y:14:DT:C6	2.51	0.46
7:S:115:LEU:HB3	10:X:44:LYS:HD2	1.98	0.46
11:Y:-63:DC:H2''	11:Y:-62:DC:C6	2.50	0.46
6:H:301:VAL:HG21	6:H:326:MET:HB3	1.98	0.46
11:Y:-18:DC:H2''	11:Y:-17:DT:H5'	1.98	0.46
7:Q:65:LEU:HB3	7:Q:86:ALA:HB1	1.98	0.46
11:Y:28:DG:H1'	11:Y:29:DA:C8	2.51	0.46
1:A:969:LEU:HD13	1:A:974:LEU:HD13	1.99	0.45
3:C:35:ALA:HB1	3:C:38:LYS:HB3	1.98	0.45
5:E:217:ALA:HB2	6:F:178:MET:HE2	1.98	0.45
11:Y:36:DC:H2''	11:Y:37:DC:C5	2.51	0.45
12:Z:51:DG:H1'	12:Z:52:DC:H5'	1.98	0.45
5:G:249:ARG:NH2	5:G:261:GLY:O	2.49	0.45
1:A:1983:VAL:HG11	5:E:243:LEU:HD23	1.97	0.45
6:H:161:LEU:HB3	6:H:174:LEU:HD21	1.99	0.45
6:J:49:GLN:NE2	6:J:359:THR:HB	2.32	0.45
11:Y:-32:DC:H2''	11:Y:-31:DA:C8	2.51	0.45
12:Z:-54:DC:H2''	12:Z:-53:DA:H8	1.81	0.45
1:A:608:THR:O	1:A:623:HIS:HE1	2.00	0.45
3:C:205:VAL:O	3:C:209:VAL:HG22	2.17	0.45
8:R:96:THR:HG21	10:X:75:HIS:HB2	1.99	0.45
7:S:54:VAL:HG21	8:T:98:VAL:HG21	1.99	0.45
6:H:86:ILE:HG22	6:H:90:MET:HE2	1.98	0.45
5:I:411:THR:HG21	6:J:62:MET:HE3	1.99	0.45
2:B:284:PRO:HG2	5:G:209:TYR:CZ	2.51	0.45
3:C:144:CYS:HB3	3:C:313:PHE:CE1	2.52	0.45
3:C:225:LEU:O	3:C:230:ASN:ND2	2.50	0.45
5:E:42:GLN:NE2	5:E:364:MET:O	2.50	0.45
5:G:263:LEU:HD22	5:I:260:MET:HB3	1.99	0.45
6:J:117:GLU:OE2	6:J:273:ARG:NH2	2.33	0.45
9:W:69:ARG:NH1	11:Y:17:DA:OP2	2.43	0.45
11:Y:17:DA:H2''	11:Y:18:DC:H2'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:64:DG:H1'	12:Z:65:DA:H5'	1.99	0.45
5:G:447:LEU:HD11	6:H:344:HIS:NE2	2.32	0.45
6:H:83:LYS:HE3	6:H:329:ASN:HB3	1.99	0.45
8:R:65:PHE:O	8:R:69:VAL:HG12	2.17	0.45
1:A:902:ASN:ND2	1:A:2068:MET:SD	2.90	0.44
1:A:910:ARG:NH1	1:A:2041:ASP:OD2	2.47	0.44
6:H:407:THR:HG21	5:I:61:MET:HG3	1.98	0.44
1:A:1882:SER:HB3	1:A:1885:TYR:HB2	2.00	0.44
6:H:27:HIS:CD2	6:H:374:ARG:HH11	2.35	0.44
6:J:382:MET:HE2	6:J:421:VAL:HG11	1.98	0.44
6:H:261:PHE:HD2	5:I:275:LEU:HD13	1.81	0.44
4:D:94:SER:HB2	4:D:97:GLU:HG3	1.98	0.44
5:E:53:VAL:HG22	5:E:83:ILE:HG23	1.99	0.44
6:H:80:GLY:N	16:H:501:ADP:O1B	2.30	0.44
1:A:786:TRP:CH2	1:A:800:HIS:HB3	2.52	0.44
6:F:47:VAL:HG11	6:F:369:GLN:HB3	1.99	0.44
6:H:300:GLU:OE2	5:I:316:HIS:ND1	2.41	0.44
6:J:62:MET:HE1	6:J:71:ARG:CZ	2.47	0.44
9:U:107:THR:HG21	9:U:124:ILE:HG12	2.00	0.44
12:Z:-50:DT:H2''	12:Z:-49:DG:C8	2.52	0.44
5:E:172:LEU:HD13	5:E:176:ILE:HG21	1.99	0.44
5:G:143:THR:HG22	5:G:145:ASN:H	1.82	0.44
5:I:447:LEU:HD22	6:J:331:GLY:HA2	1.99	0.44
6:J:309:PHE:O	6:J:313:ASN:ND2	2.41	0.44
5:G:271:ILE:HG23	5:G:275:LEU:HD23	2.00	0.44
6:H:39:PRO:HG3	6:H:50:LEU:O	2.18	0.44
10:V:32:PRO:O	10:V:36:ARG:HG3	2.18	0.44
11:Y:-75:DT:H2''	11:Y:-74:DG:C8	2.53	0.44
12:Z:-54:DC:H2''	12:Z:-53:DA:C8	2.53	0.44
1:A:2065:PHE:HB3	1:A:2118:THR:HG23	2.00	0.43
5:I:119:ALA:HB2	5:I:299:LEU:HB2	1.99	0.43
12:Z:-40:DC:H1'	12:Z:-39:DT:H5'	2.00	0.43
12:Z:19:DC:H2''	12:Z:20:DG:C8	2.52	0.43
3:C:87:ASP:O	3:C:91:THR:OG1	2.32	0.43
5:E:42:GLN:HB3	5:E:45:ALA:HB3	2.00	0.43
11:Y:29:DA:H5''	11:Y:29:DA:H8	1.83	0.43
1:A:606:VAL:HG11	1:A:623:HIS:ND1	2.34	0.43
3:C:7:ASP:HB3	3:C:14:LYS:HE2	1.99	0.43
5:E:118:ARG:NH1	6:F:271:GLU:OE2	2.49	0.43
5:E:338:ILE:HD11	5:E:346:SER:OG	2.19	0.43
11:Y:-29:DC:H2'	11:Y:-28:DT:H71	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-53:DA:H2''	12:Z:-52:DG:N7	2.34	0.43
1:A:698:TYR:CE2	1:A:705:ARG:HD2	2.53	0.43
6:H:207:ARG:NH1	5:I:173:ASP:OD1	2.51	0.43
11:Y:-62:DC:H2'	11:Y:-61:DG:H8	1.82	0.43
6:H:362:TYR:OH	16:H:501:ADP:N7	2.46	0.43
5:I:366:TYR:OH	16:I:501:ADP:N6	2.46	0.43
7:Q:42:ARG:NH1	8:R:88:THR:OG1	2.40	0.43
9:W:82:LEU:HD23	9:W:82:LEU:HA	1.88	0.43
1:A:754:PHE:HA	1:A:759:TRP:CG	2.53	0.43
1:A:2126:ASN:OD1	1:A:2154:ARG:HD2	2.19	0.43
5:E:42:GLN:HE22	5:E:364:MET:N	2.17	0.43
9:U:54:TYR:O	10:V:40:ARG:NE	2.51	0.43
9:W:118:THR:HG22	10:X:45:ARG:HE	1.84	0.43
1:A:864:ARG:NH2	1:A:908:ASP:O	2.50	0.43
2:B:196:ASP:O	2:B:200:GLN:HG2	2.18	0.43
5:I:401:THR:O	5:I:402:THR:OG1	2.32	0.43
5:I:447:LEU:HD13	6:J:343:PRO:O	2.19	0.43
6:J:314:ARG:HA	6:J:314:ARG:HD3	1.82	0.43
3:C:59:PRO:HB3	3:C:70:VAL:HG13	2.00	0.43
6:F:84:THR:HG21	5:G:320:GLU:OE1	2.18	0.43
6:F:382:MET:HB3	6:F:387:TYR:CE2	2.54	0.43
5:I:101:VAL:HA	5:I:111:VAL:HG11	2.00	0.43
7:Q:24:GLN:NE2	8:R:47:GLN:OE1	2.51	0.43
1:A:759:TRP:CH2	1:A:763:LEU:HD22	2.54	0.43
1:A:1996:PRO:HB3	1:A:1998:TRP:CZ2	2.54	0.43
1:A:2061:ARG:HB2	1:A:2130:ALA:HA	2.00	0.43
3:C:76:ASP:OD1	3:C:117:TYR:OH	2.28	0.43
5:E:260:MET:HB3	5:E:264:MET:HE2	2.01	0.43
6:F:397:THR:OG1	6:F:398:SER:N	2.52	0.43
5:G:405:TYR:O	5:G:409:LEU:HG	2.19	0.43
5:I:53:VAL:HG22	5:I:83:ILE:HG23	2.01	0.43
9:U:62:ILE:HD11	10:V:37:LEU:HD11	2.00	0.43
12:Z:-41:DA:H2''	12:Z:-40:DC:H5''	2.00	0.43
1:A:948:LEU:N	5:I:247:ASN:OD1	2.37	0.42
12:Z:-44:DG:H2''	12:Z:-43:DA:H8	1.84	0.42
3:C:192:GLN:OE1	3:C:268:LEU:HD12	2.18	0.42
5:G:263:LEU:O	6:H:253:ARG:NH2	2.52	0.42
6:J:246:GLU:HA	6:J:260:LEU:HD21	2.01	0.42
10:X:73:THR:HG21	10:X:81:VAL:HA	2.00	0.42
12:Z:-29:DT:H6	12:Z:-29:DT:H2'	1.69	0.42
12:Z:5:DT:H2''	12:Z:6:DA:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:65:LEU:HB3	11:Y:17:DA:H5'	2.01	0.42
12:Z:38:DG:H2''	12:Z:39:DA:C8	2.54	0.42
5:E:27:ASP:OD1	5:E:31:LEU:N	2.53	0.42
5:I:271:ILE:HG23	5:I:275:LEU:HD23	2.01	0.42
12:Z:38:DG:H2''	12:Z:39:DA:H8	1.84	0.42
5:E:316:HIS:HD2	5:E:354:LEU:HD13	1.84	0.42
6:H:25:HIS:NE2	16:H:501:ADP:O1A	2.41	0.42
12:Z:-56:DG:H2''	12:Z:-55:DA:H8	1.84	0.42
12:Z:-18:DG:H2''	12:Z:-17:DT:H5'	2.01	0.42
1:A:2119:ARG:HH22	11:Y:22:DC:C5'	2.26	0.42
5:G:440:ALA:HB1	6:H:348:ILE:HD11	2.02	0.42
9:U:108:ASN:HB2	10:V:43:VAL:HG22	2.00	0.42
11:Y:39:DA:H8	11:Y:39:DA:H5''	1.84	0.42
12:Z:-23:DT:H2''	12:Z:-22:DG:C8	2.54	0.42
12:Z:-19:DG:H2''	12:Z:-18:DG:C8	2.54	0.42
12:Z:22:DT:H4'	12:Z:23:DG:OP1	2.20	0.42
6:J:314:ARG:NH1	6:J:317:GLU:OE2	2.52	0.42
7:S:51:LEU:HB2	8:T:94:ILE:HD13	2.01	0.42
11:Y:3:DT:H2'	11:Y:4:DC:C5	2.55	0.42
3:C:81:LYS:HA	3:C:85:GLN:HG2	2.02	0.42
5:E:64:ARG:HB2	5:E:326:ILE:HD12	2.02	0.42
5:E:256:ILE:O	5:E:260:MET:HG2	2.19	0.42
5:G:411:THR:OG1	6:H:71:ARG:NH1	2.52	0.42
5:I:388:GLU:O	5:I:392:ASN:ND2	2.43	0.42
7:Q:63:LEU:HD13	8:R:45:LEU:HB2	2.01	0.42
11:Y:6:DC:H2''	11:Y:7:DC:C5	2.55	0.42
2:B:284:PRO:HG3	5:G:205:ARG:NH2	2.35	0.42
3:C:103:THR:O	3:C:107:GLU:HG3	2.19	0.42
5:E:263:LEU:HB2	5:G:260:MET:HE3	2.01	0.42
5:G:146:PRO:HA	5:G:153:THR:HG22	2.01	0.42
7:Q:100:VAL:HG11	10:V:98:TYR:CE2	2.54	0.42
5:I:120:ILE:HD13	5:I:296:PRO:O	2.20	0.42
11:Y:-7:DC:H2''	11:Y:-6:DT:C5	2.55	0.42
12:Z:45:DT:H2''	12:Z:46:DG:N7	2.35	0.42
1:A:929:VAL:HG13	6:J:247:ILE:HG12	2.01	0.41
6:H:403:ILE:HA	6:H:406:ILE:HD12	2.02	0.41
5:I:405:TYR:O	5:I:409:LEU:HG	2.20	0.41
12:Z:-32:DT:H2''	12:Z:-31:DA:H8	1.85	0.41
12:Z:51:DG:C8	12:Z:51:DG:H5'	2.55	0.41
12:Z:62:DG:H2''	12:Z:63:DG:C8	2.55	0.41
1:A:2062:VAL:O	1:A:2113:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:THR:O	6:F:296:LEU:HD12	2.19	0.41
6:H:349:ASP:OD1	6:H:350:LEU:N	2.53	0.41
12:Z:-31:DA:H2''	12:Z:-30:DA:H5'	2.02	0.41
5:G:404:ARG:NH2	16:G:501:ADP:O3A	2.49	0.41
11:Y:-42:DT:H2''	11:Y:-41:DG:H8	1.85	0.41
11:Y:3:DT:H2'	11:Y:4:DC:C6	2.55	0.41
11:Y:53:DT:H2''	11:Y:54:DG:C8	2.54	0.41
2:B:130:ARG:HB3	8:T:48:VAL:HA	2.03	0.41
5:I:408:GLN:HE21	5:I:408:GLN:HB2	1.63	0.41
1:A:698:TYR:OH	1:A:709:ARG:NH1	2.53	0.41
3:C:277:VAL:HB	3:C:278:PRO:HD3	2.03	0.41
3:C:337:VAL:O	3:C:341:THR:OG1	2.30	0.41
5:G:90:LYS:HE3	5:G:123:ARG:HD2	2.02	0.41
5:G:122:LEU:HD22	5:G:283:VAL:HG22	2.02	0.41
6:J:161:LEU:HB2	6:J:174:LEU:HD11	2.02	0.41
3:C:234:ILE:HG22	3:C:252:ARG:HH21	1.84	0.41
2:B:204:LYS:NZ	5:E:212:GLU:OE1	2.33	0.41
5:E:135:VAL:HG22	5:E:159:ILE:HD11	2.01	0.41
5:G:378:ARG:HA	5:G:378:ARG:HD2	1.87	0.41
5:I:108:LYS:NZ	5:I:308:ASP:OD2	2.40	0.41
12:Z:47:DA:H2''	12:Z:48:DG:C8	2.55	0.41
1:A:738:LYS:HD3	1:A:740:TRP:CH2	2.56	0.41
1:A:2098:ARG:O	1:A:2102:MET:HG2	2.21	0.41
6:F:362:TYR:OH	16:F:501:ADP:N7	2.40	0.41
5:G:75:GLY:N	16:G:501:ADP:O1A	2.47	0.41
5:G:118:ARG:HE	5:G:241:HIS:CE1	2.38	0.41
11:Y:-42:DT:H2''	11:Y:-41:DG:C8	2.56	0.41
11:Y:14:DT:H5'	11:Y:14:DT:H6	1.85	0.41
6:F:402:ALA:O	6:F:406:ILE:HG13	2.21	0.41
5:G:215:LEU:HD13	6:H:172:TYR:CD1	2.56	0.41
6:J:349:ASP:OD1	6:J:350:LEU:N	2.54	0.41
7:S:106:GLY:HA3	9:W:58:THR:HG22	2.03	0.41
9:W:116:ARG:HD3	12:Z:-3:DA:H3'	2.02	0.41
11:Y:-59:DT:H2''	11:Y:-58:DG:C8	2.56	0.41
1:A:625:GLY:CA	1:A:840:ARG:HH22	2.34	0.41
3:C:160:TYR:CE2	3:C:165:LYS:HD3	2.56	0.41
1:A:903:HIS:ND1	1:A:905:ASN:HB2	2.36	0.40
3:C:10:ALA:N	13:C:401:AGS:S1G	2.86	0.40
11:Y:4:DC:H2''	11:Y:5:DC:C5	2.56	0.40
4:D:145:GLN:HA	4:D:149:CYS:HB2	2.04	0.40
11:Y:50:DA:C2	12:Z:-49:DG:N2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-45:DG:H2''	12:Z:-44:DG:C8	2.57	0.40
5:E:447:LEU:HD11	6:F:344:HIS:CE1	2.56	0.40
5:G:371:MET:HG2	5:G:403:LEU:HD13	2.04	0.40
11:Y:26:DG:OP2	11:Y:26:DG:H2'	2.21	0.40
12:Z:42:DA:H2''	12:Z:43:DA:C8	2.57	0.40
5:E:268:LYS:HG2	6:F:269:LYS:HE2	2.02	0.40
6:F:47:VAL:O	16:F:501:ADP:N6	2.54	0.40
12:Z:50:DG:H2''	12:Z:51:DG:H8	1.80	0.40
1:A:2063:LEU:HD22	1:A:2114:PHE:HB3	2.03	0.40
2:B:302:ARG:N	6:H:170:THR:OG1	2.43	0.40
5:E:447:LEU:HD22	6:F:331:GLY:HA2	2.02	0.40
11:Y:-14:DA:H2''	11:Y:-13:DA:H8	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	728/3230 (22%)	714 (98%)	14 (2%)	0	100	100
2	B	131/364 (36%)	128 (98%)	3 (2%)	0	100	100
3	C	394/396 (100%)	382 (97%)	12 (3%)	0	100	100
4	D	101/154 (66%)	99 (98%)	2 (2%)	0	100	100
5	E	429/456 (94%)	424 (99%)	5 (1%)	0	100	100
5	G	443/456 (97%)	440 (99%)	3 (1%)	0	100	100
5	I	432/456 (95%)	425 (98%)	7 (2%)	0	100	100
6	F	436/463 (94%)	429 (98%)	7 (2%)	0	100	100
6	H	428/463 (92%)	418 (98%)	10 (2%)	0	100	100
6	J	412/463 (89%)	405 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Q	94/128 (73%)	91 (97%)	3 (3%)	0	100	100
7	S	102/128 (80%)	101 (99%)	1 (1%)	0	100	100
8	R	90/125 (72%)	88 (98%)	2 (2%)	0	100	100
8	T	93/125 (74%)	91 (98%)	2 (2%)	0	100	100
9	U	88/135 (65%)	87 (99%)	1 (1%)	0	100	100
9	W	94/135 (70%)	92 (98%)	2 (2%)	0	100	100
10	V	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
10	X	79/102 (78%)	78 (99%)	1 (1%)	0	100	100
All	All	4651/7881 (59%)	4568 (98%)	83 (2%)	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	664/2721 (24%)	664 (100%)	0	100	100
2	B	124/312 (40%)	124 (100%)	0	100	100
3	C	361/361 (100%)	361 (100%)	0	100	100
4	D	89/133 (67%)	89 (100%)	0	100	100
5	E	367/387 (95%)	367 (100%)	0	100	100
5	G	376/387 (97%)	376 (100%)	0	100	100
5	I	370/387 (96%)	370 (100%)	0	100	100
6	F	368/390 (94%)	368 (100%)	0	100	100
6	H	365/390 (94%)	365 (100%)	0	100	100
6	J	354/390 (91%)	354 (100%)	0	100	100
7	Q	75/101 (74%)	75 (100%)	0	100	100
7	S	82/101 (81%)	82 (100%)	0	100	100
8	R	78/105 (74%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	T	81/105 (77%)	81 (100%)	0	100	100
9	U	79/110 (72%)	79 (100%)	0	100	100
9	W	84/110 (76%)	84 (100%)	0	100	100
10	V	64/78 (82%)	64 (100%)	0	100	100
10	X	66/78 (85%)	66 (100%)	0	100	100
All	All	4047/6646 (61%)	4047 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	659	HIS
1	A	766	ASN
1	A	768	GLN
1	A	780	ASN
1	A	1963	GLN
1	A	1991	HIS
1	A	2157	GLN
2	B	200	GLN
2	B	215	HIS
2	B	296	HIS
3	C	126	ASN
3	C	203	ASN
3	C	316	ASN
6	F	221	GLN
6	F	275	GLN
5	G	316	HIS
6	H	146	GLN
6	H	245	HIS
6	H	453	ASN
5	I	115	ASN
5	I	169	GLN
5	I	241	HIS
5	I	393	HIS
6	J	404	GLN
8	R	67	ASN
9	U	85	GLN
10	X	27	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 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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$
16	ADP	G	501	-	24,29,29	0.86	0	29,45,45	1.20	2 (6%)
13	AGS	A	3301	14	28,33,33	0.84	1 (3%)	31,52,52	1.69	4 (12%)
13	AGS	C	401	14	28,33,33	0.81	0	31,52,52	0.95	2 (6%)
16	ADP	E	501	-	24,29,29	0.87	0	29,45,45	1.20	2 (6%)
16	ADP	H	501	14	24,29,29	0.90	0	29,45,45	1.23	2 (6%)
16	ADP	J	501	14	24,29,29	0.89	0	29,45,45	1.20	2 (6%)
16	ADP	F	501	14	24,29,29	0.83	0	29,45,45	1.19	2 (6%)
16	ADP	I	501	-	24,29,29	0.83	0	29,45,45	1.20	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
16	ADP	G	501	-	-	5/12/32/32	0/3/3/3
13	AGS	A	3301	14	-	4/17/38/38	0/3/3/3
13	AGS	C	401	14	-	0/17/38/38	0/3/3/3
16	ADP	E	501	-	-	3/12/32/32	0/3/3/3
16	ADP	H	501	14	-	4/12/32/32	0/3/3/3
16	ADP	J	501	14	-	5/12/32/32	0/3/3/3
16	ADP	F	501	14	-	3/12/32/32	0/3/3/3
16	ADP	I	501	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3301	AGS	PG-S1G	2.08	1.95	1.90

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3301	AGS	C4'-O4'-C1'	-6.47	104.00	109.92
13	A	3301	AGS	PB-O3B-PG	-4.22	117.74	133.17
16	I	501	ADP	N3-C2-N1	-3.62	123.76	128.67
16	F	501	ADP	N3-C2-N1	-3.60	123.79	128.67
16	H	501	ADP	N3-C2-N1	-3.59	123.81	128.67
16	G	501	ADP	N3-C2-N1	-3.54	123.87	128.67
16	E	501	ADP	N3-C2-N1	-3.50	123.92	128.67
16	J	501	ADP	N3-C2-N1	-3.48	123.95	128.67
16	H	501	ADP	C4-C5-N7	-2.61	106.58	109.34
16	J	501	ADP	C4-C5-N7	-2.55	106.64	109.34
13	C	401	AGS	PB-O3B-PG	-2.54	123.89	133.17
16	I	501	ADP	C4-C5-N7	-2.53	106.67	109.34
16	E	501	ADP	C4-C5-N7	-2.40	106.80	109.34
13	C	401	AGS	C5-C6-N6	2.36	123.91	120.31
16	F	501	ADP	C4-C5-N7	-2.35	106.85	109.34
16	G	501	ADP	C4-C5-N7	-2.33	106.87	109.34
13	A	3301	AGS	C5-C6-N6	2.30	123.81	120.31
13	A	3301	AGS	O2G-PG-O3B	2.11	111.70	104.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3301	AGS	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	3301	AGS	C5'-O5'-PA-O2A
13	A	3301	AGS	C5'-O5'-PA-O3A
16	E	501	ADP	PA-O3A-PB-O2B
16	F	501	ADP	C5'-O5'-PA-O2A
16	F	501	ADP	C5'-O5'-PA-O3A
16	G	501	ADP	C5'-O5'-PA-O1A
16	G	501	ADP	C5'-O5'-PA-O2A
16	G	501	ADP	C5'-O5'-PA-O3A
16	H	501	ADP	PA-O3A-PB-O3B
16	I	501	ADP	C5'-O5'-PA-O1A
16	I	501	ADP	C5'-O5'-PA-O2A
16	I	501	ADP	C5'-O5'-PA-O3A
16	J	501	ADP	C5'-O5'-PA-O1A
16	J	501	ADP	C5'-O5'-PA-O2A
16	J	501	ADP	C5'-O5'-PA-O3A
16	G	501	ADP	O4'-C4'-C5'-O5'
16	J	501	ADP	O4'-C4'-C5'-O5'
16	G	501	ADP	C3'-C4'-C5'-O5'
16	J	501	ADP	C3'-C4'-C5'-O5'
16	F	501	ADP	C5'-O5'-PA-O1A
13	A	3301	AGS	PA-O3A-PB-O2B
16	E	501	ADP	C3'-C4'-C5'-O5'
16	H	501	ADP	PA-O3A-PB-O1B
16	H	501	ADP	PA-O3A-PB-O2B
16	H	501	ADP	C4'-C5'-O5'-PA
16	E	501	ADP	O4'-C4'-C5'-O5'

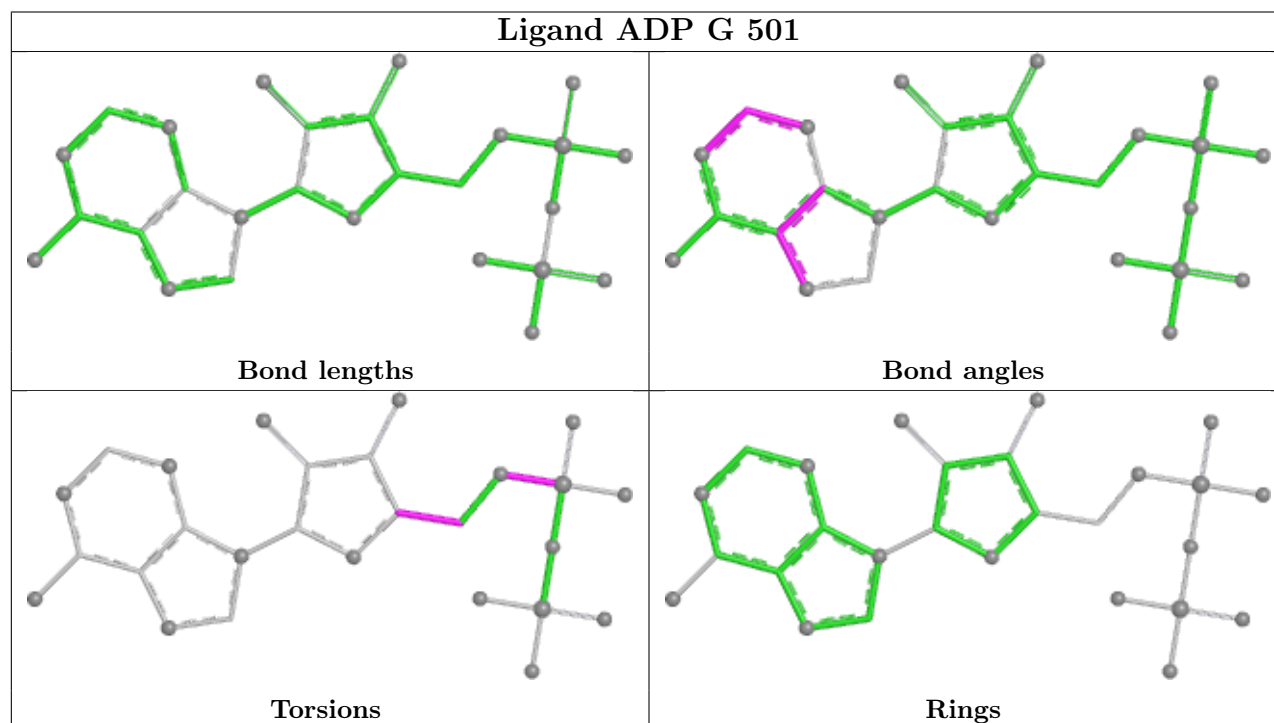
There are no ring outliers.

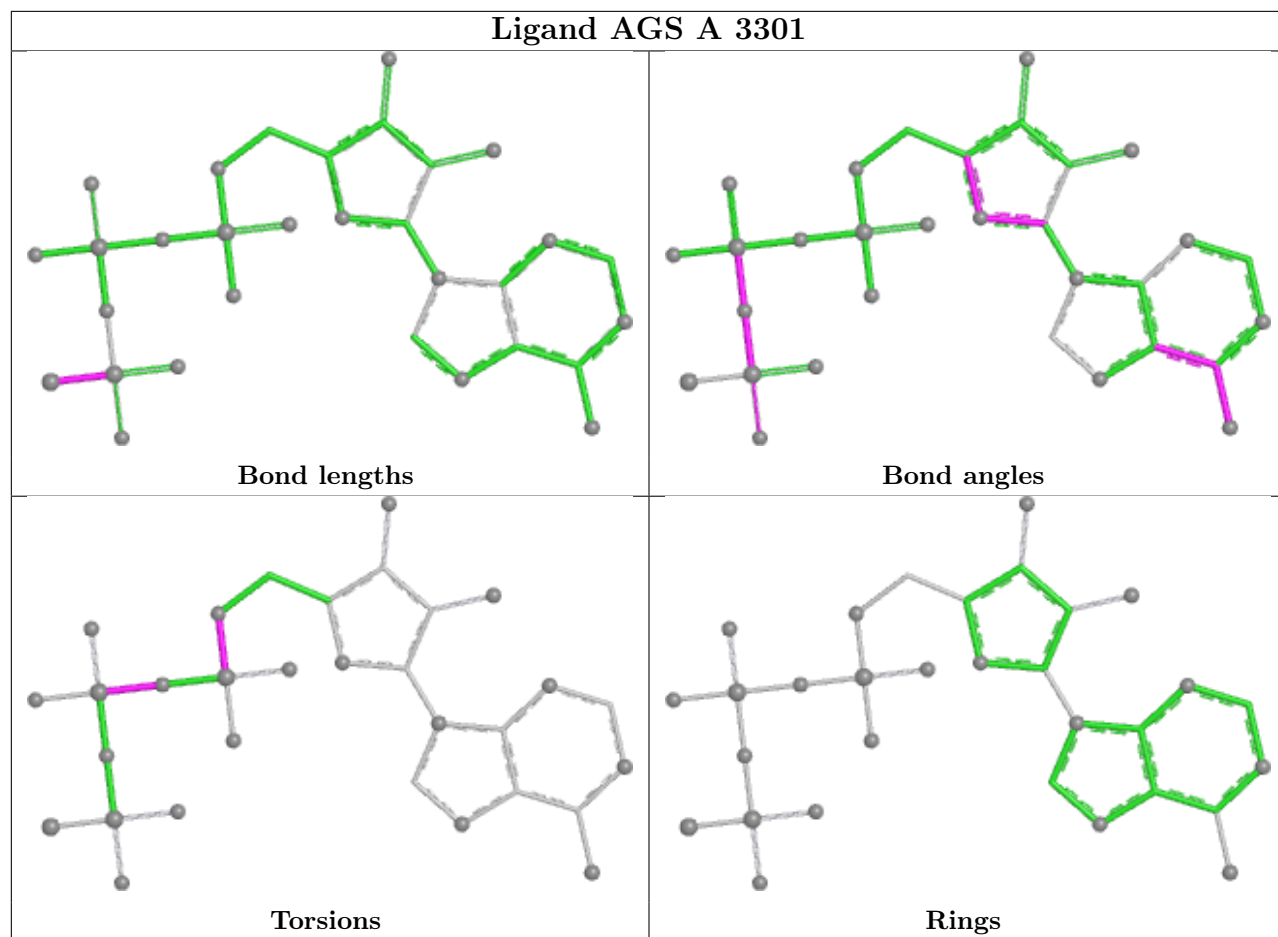
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	501	ADP	2	0
13	C	401	AGS	1	0
16	H	501	ADP	3	0
16	J	501	ADP	1	0
16	F	501	ADP	3	0
16	I	501	ADP	1	0

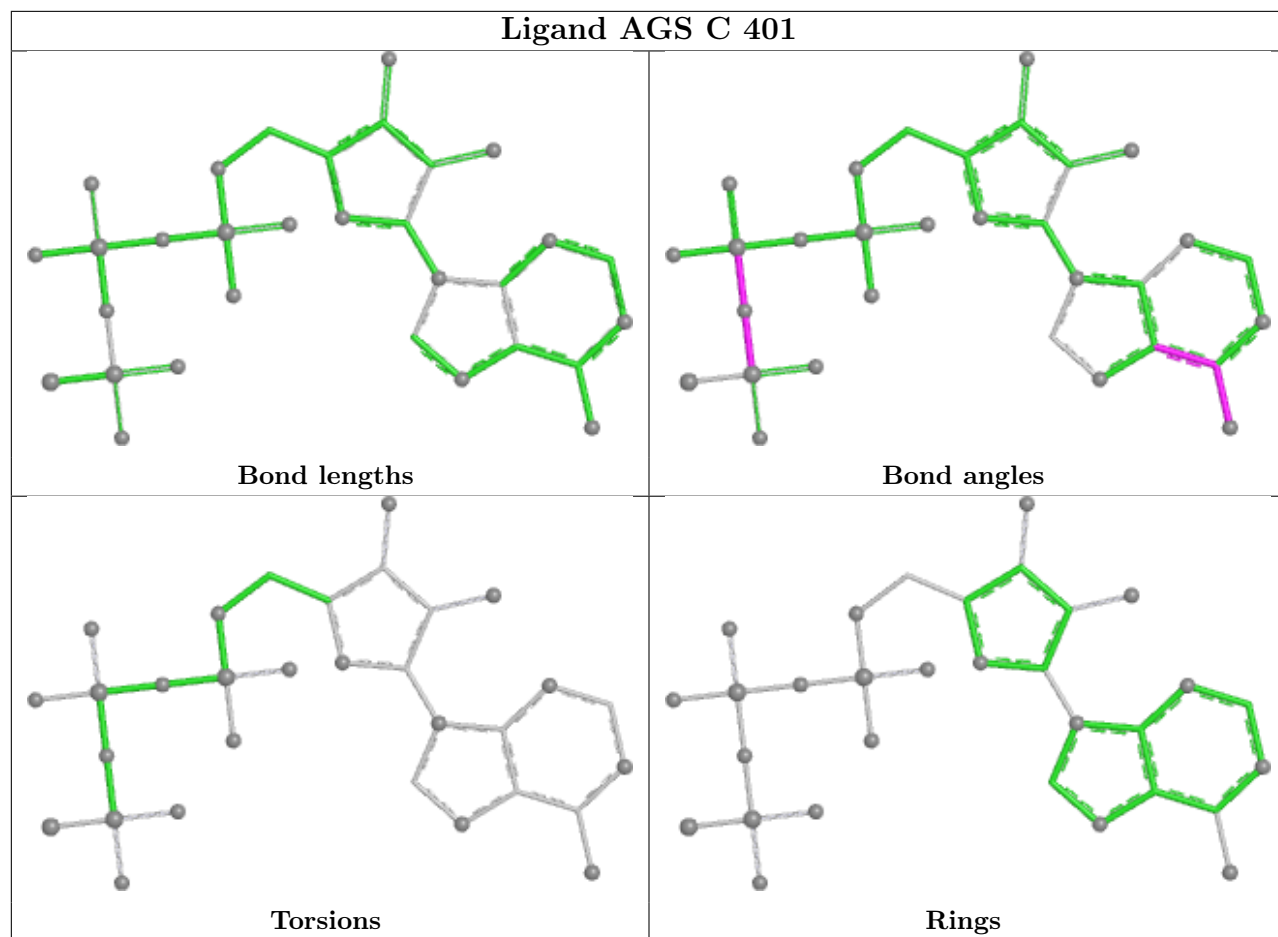
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

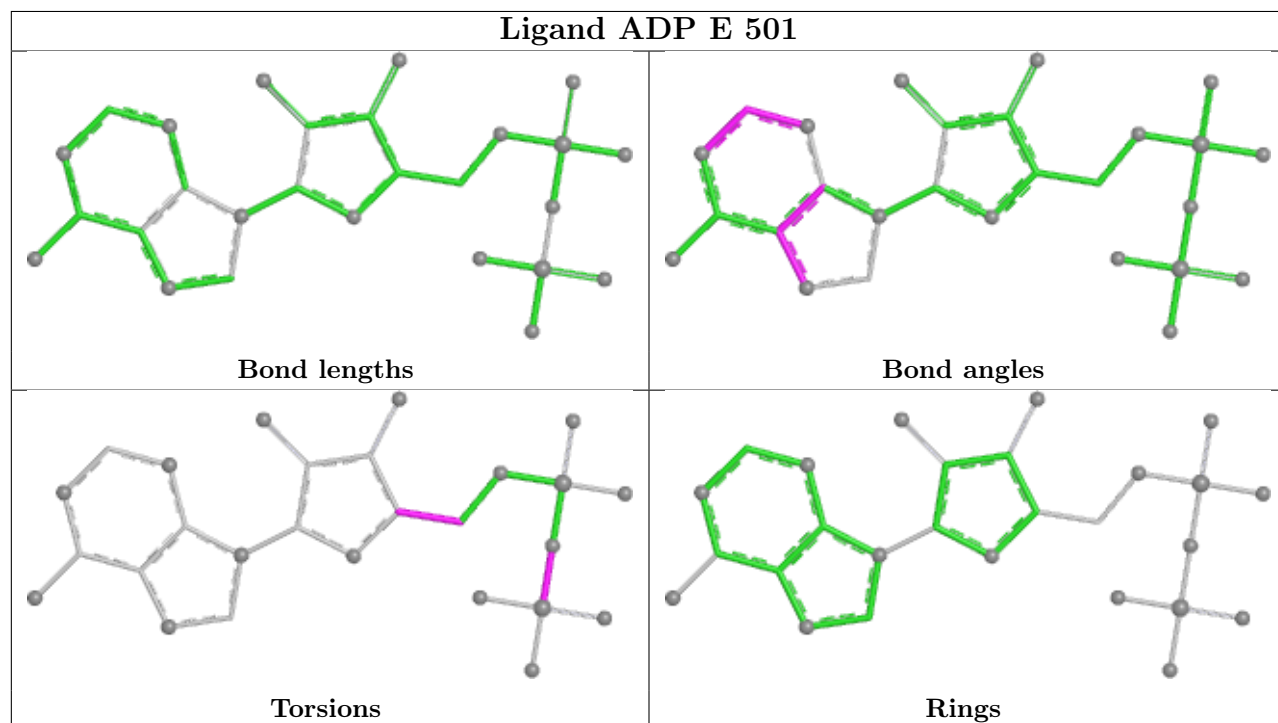


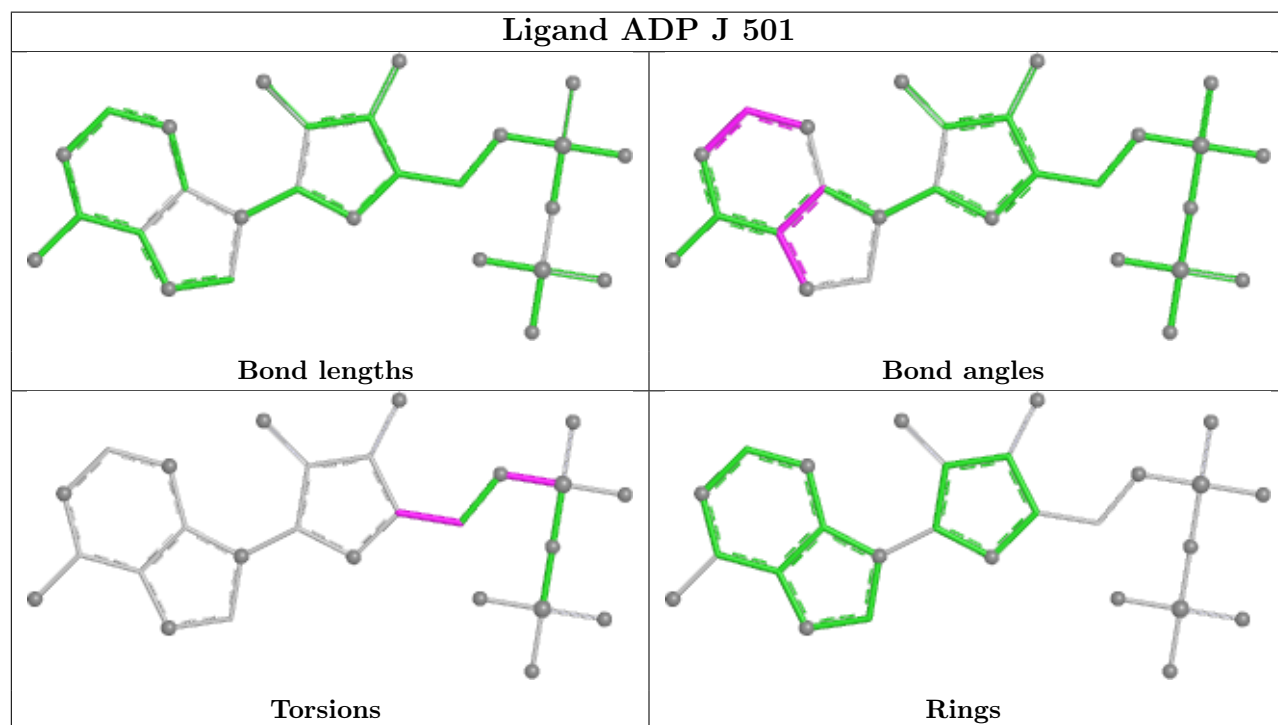
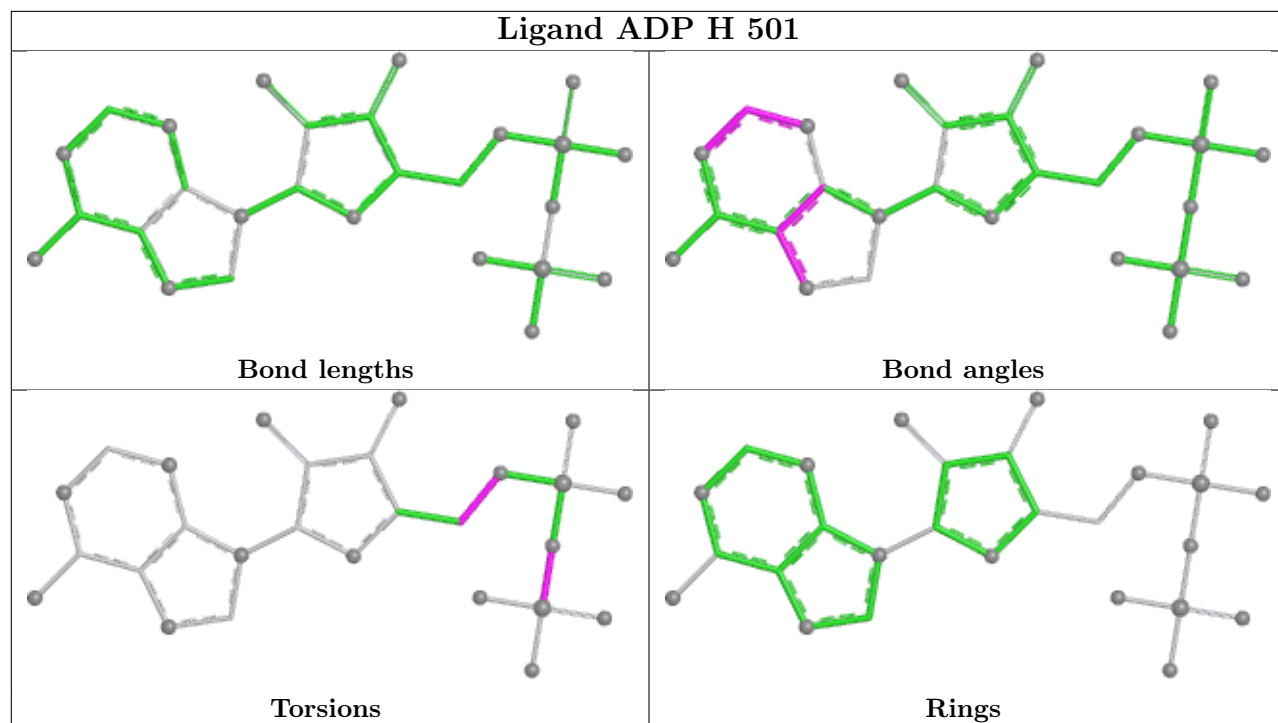


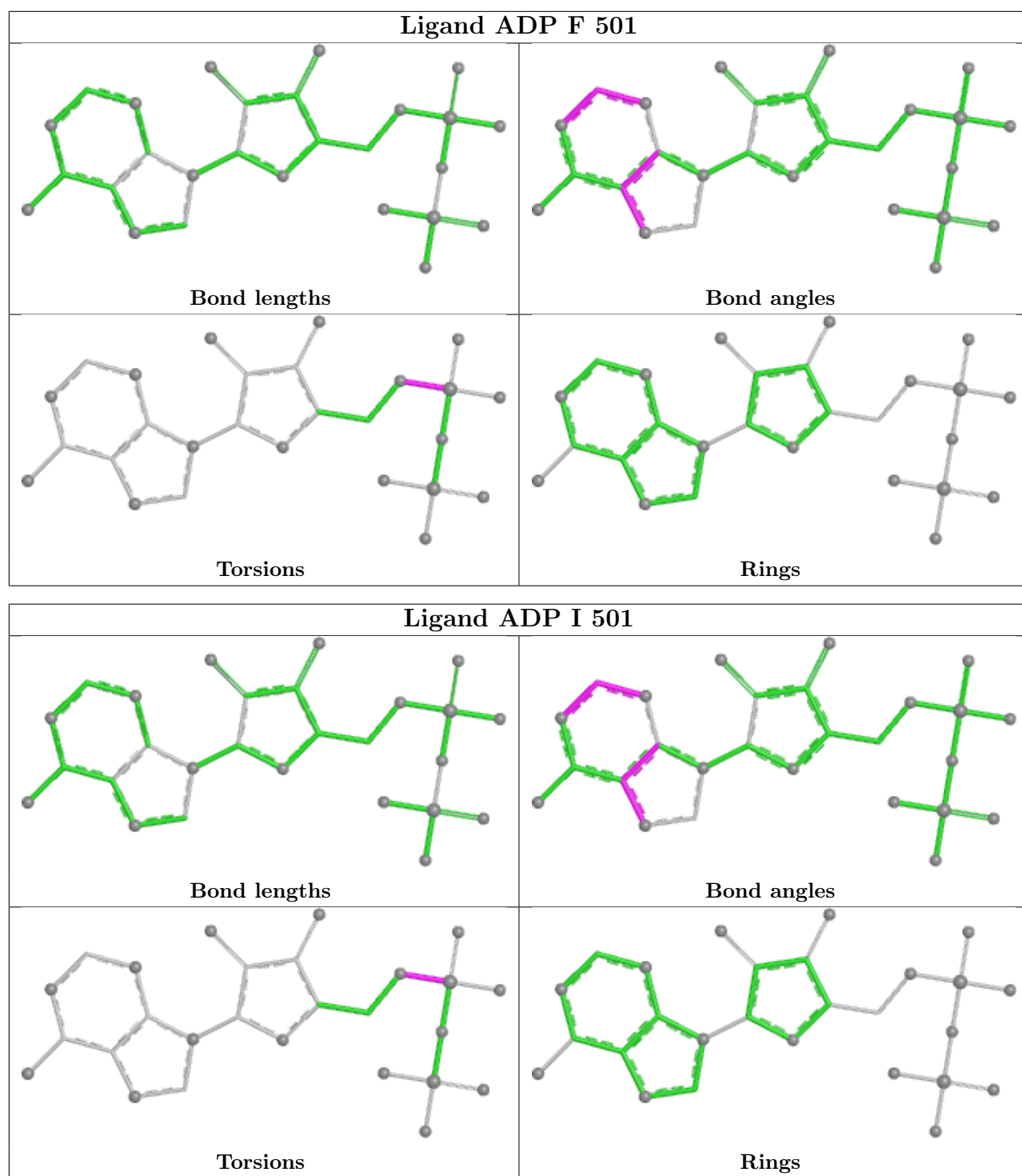
Ligand AGS C 401



Ligand ADP E 501







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

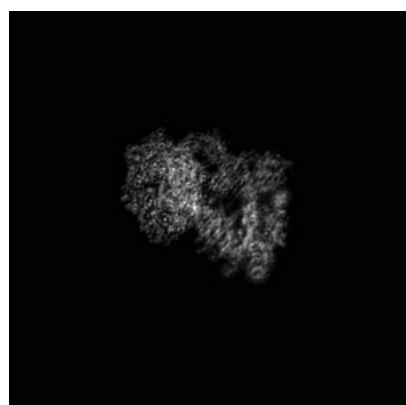
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45382. These allow visual inspection of the internal detail of the map and identification of artifacts.

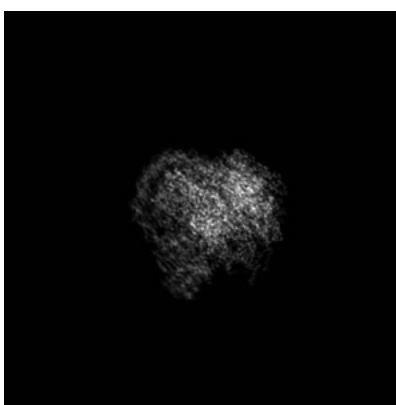
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

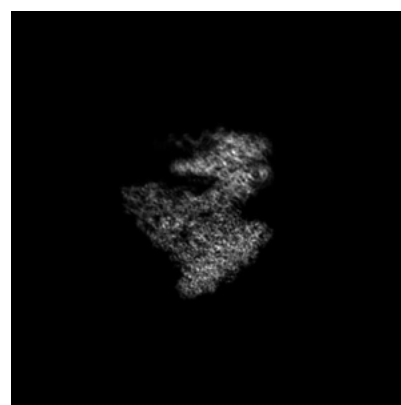
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 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: 204



Y Index: 168

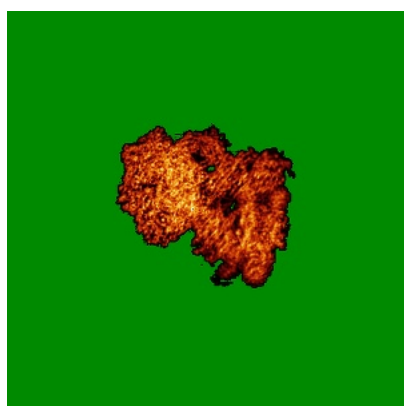


Z Index: 226

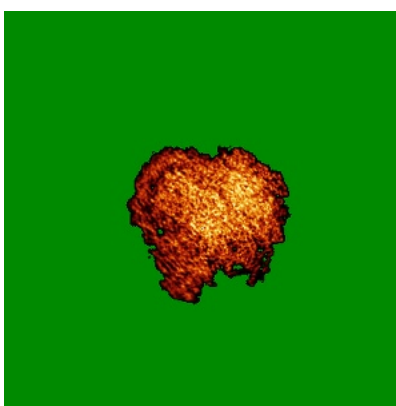
The images above show the largest variance slices of the map in three orthogonal directions.

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

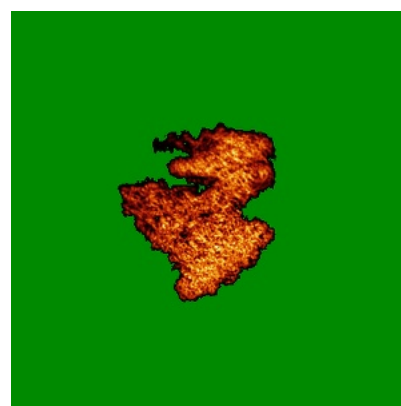
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

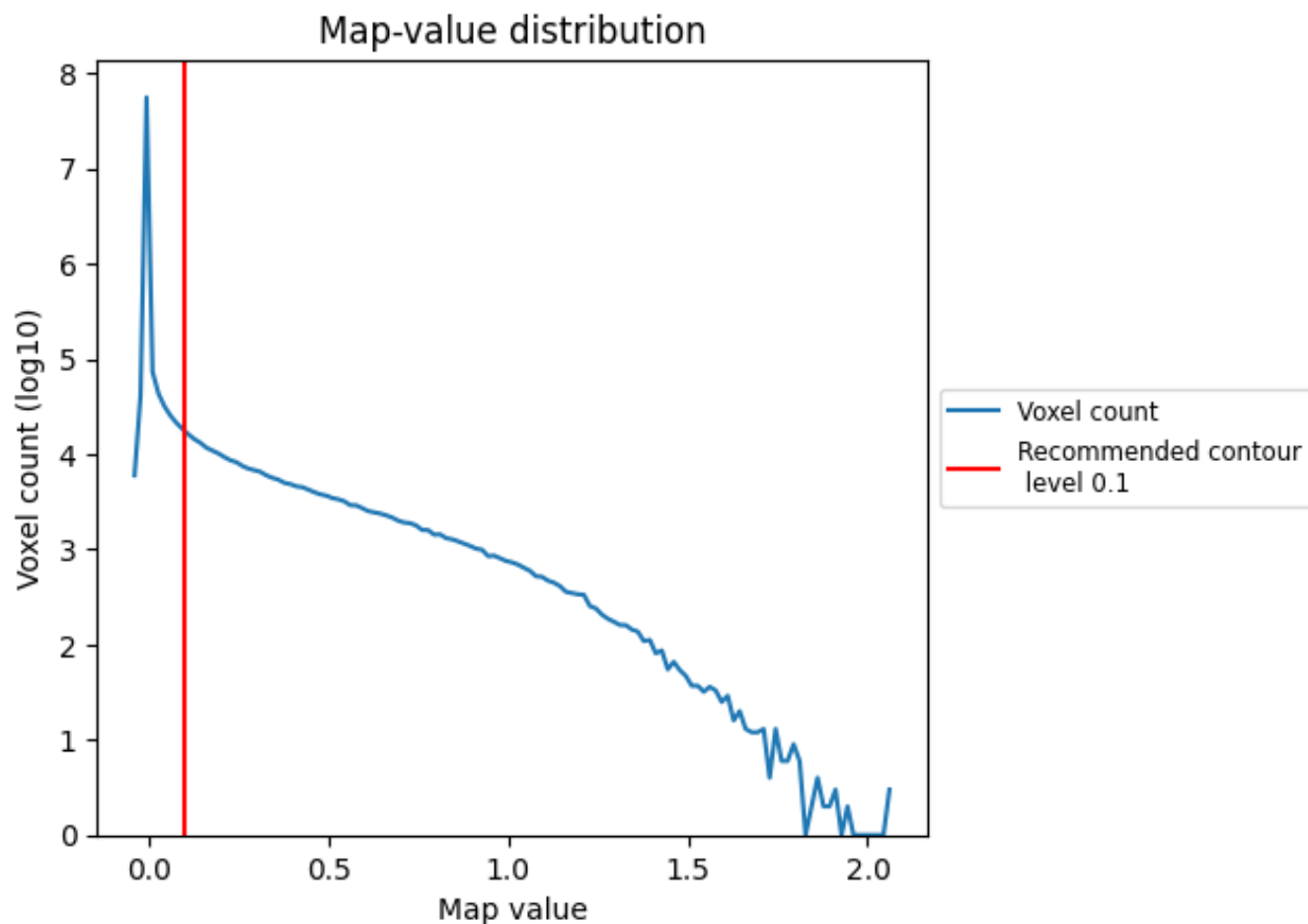
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

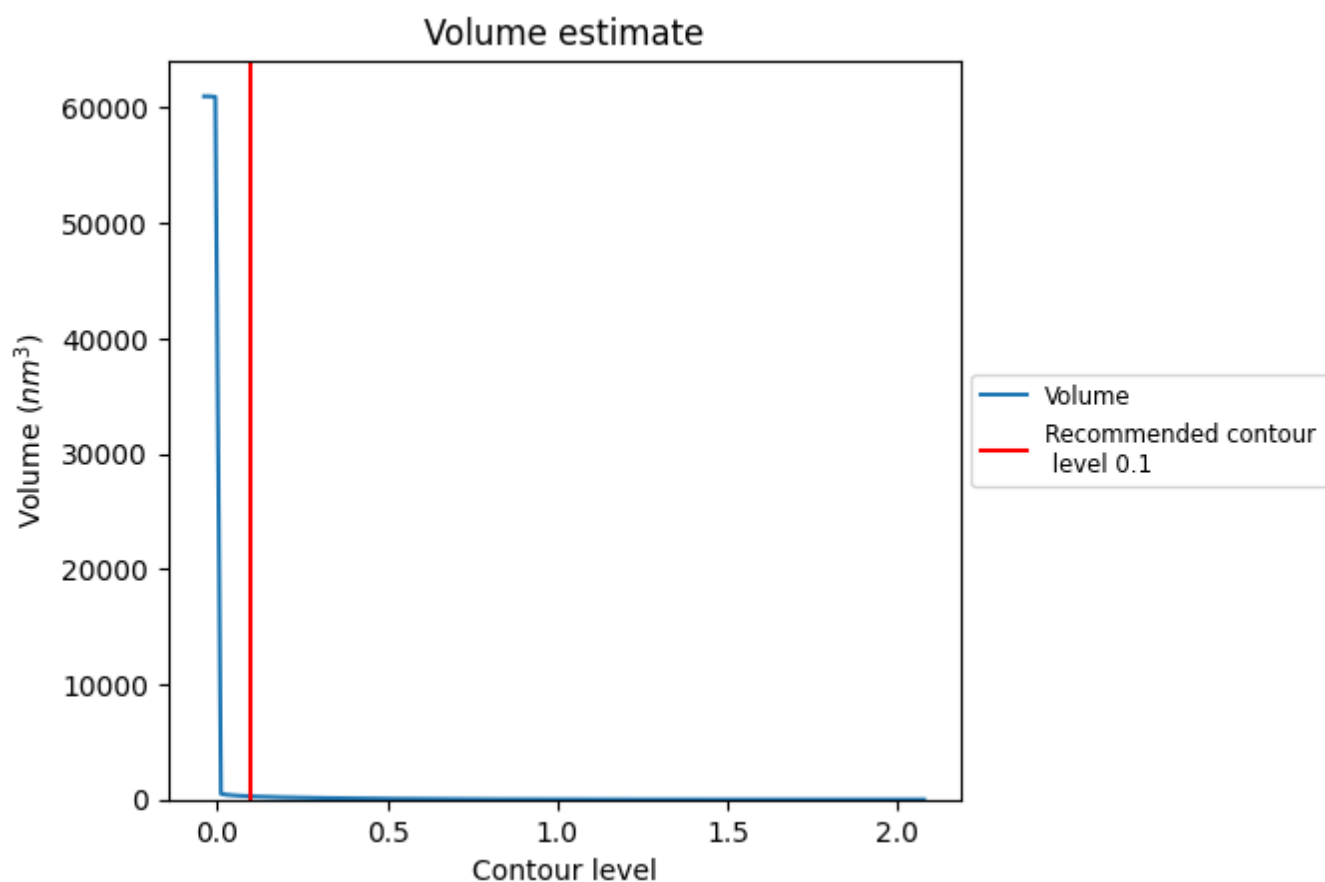
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

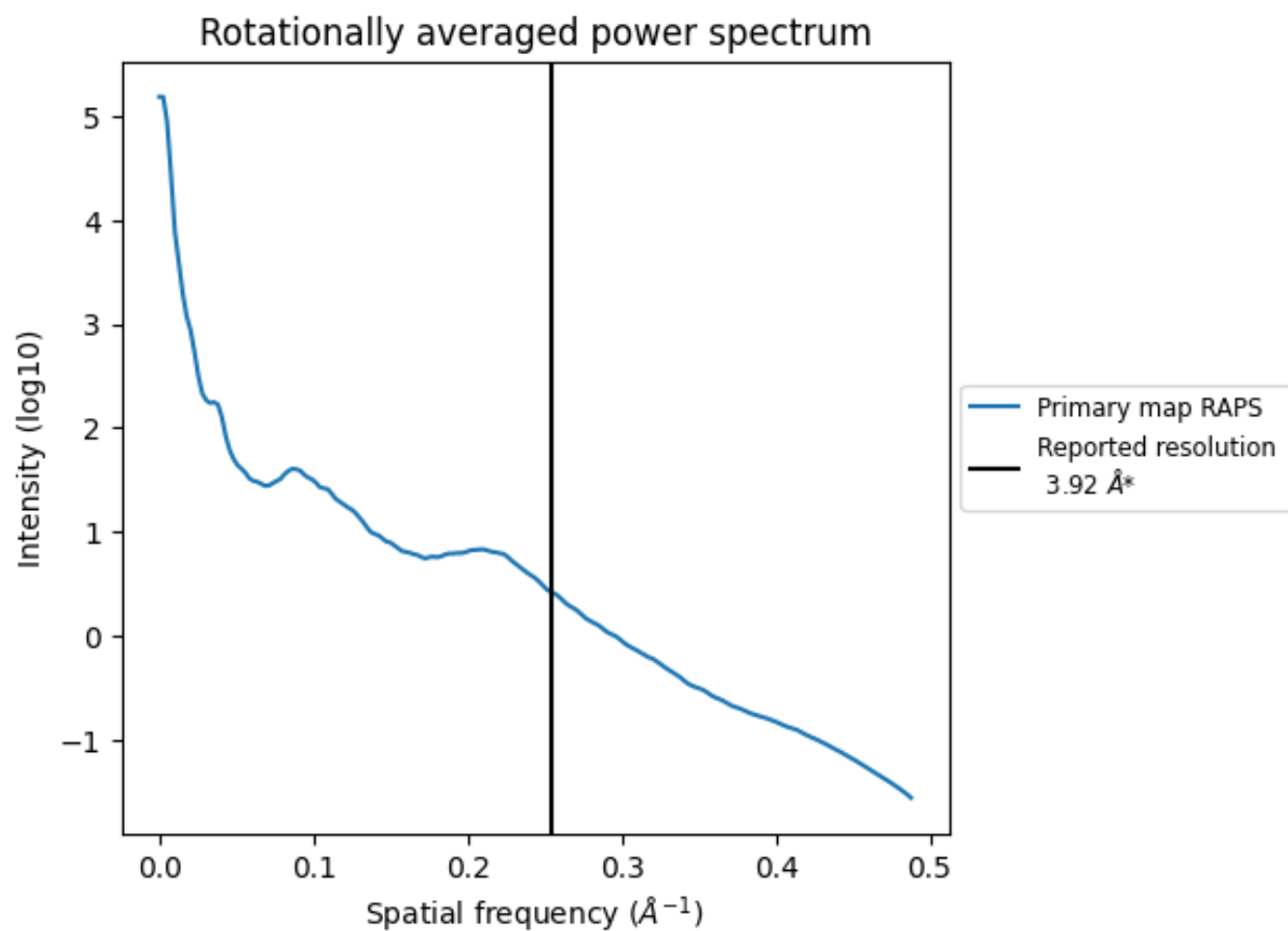
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 0.255 Å⁻¹

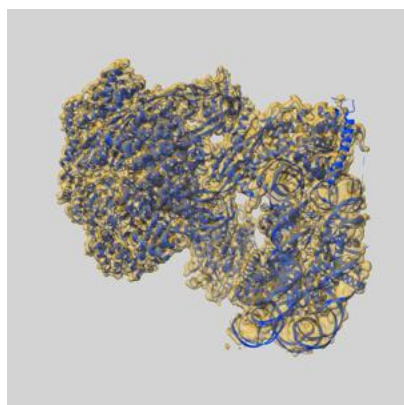
8 Fourier-Shell correlation ⓘ

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

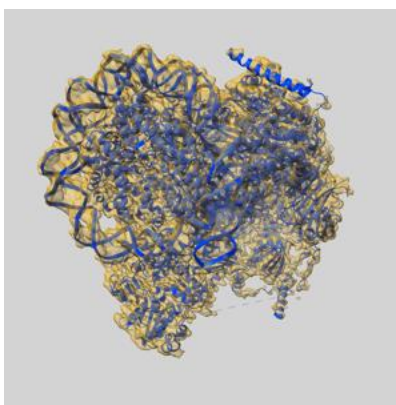
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45382 and PDB model 9CA8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

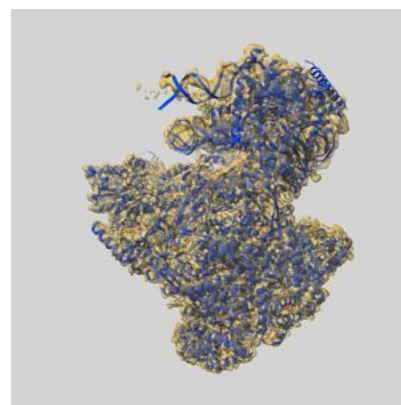
9.1 Map-model overlay [i](#)



X



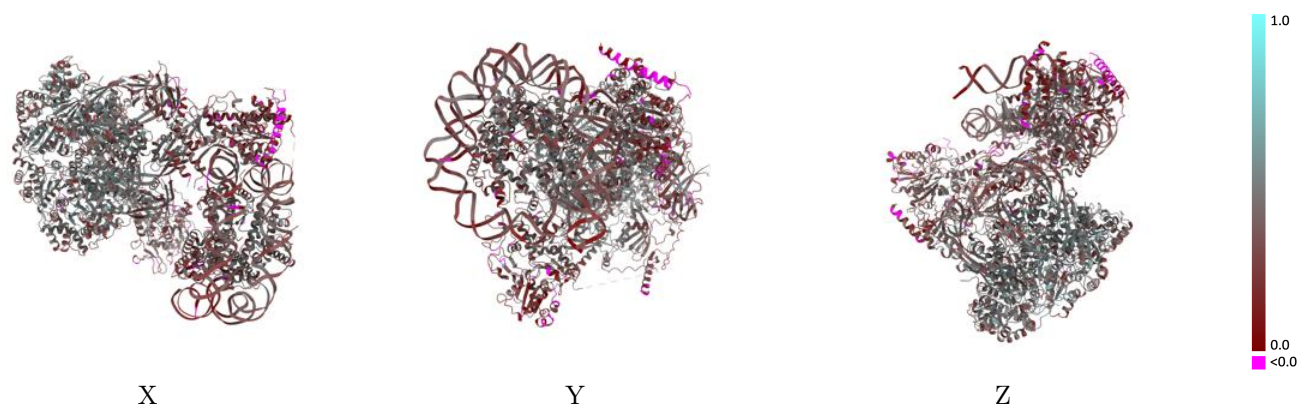
Y



Z

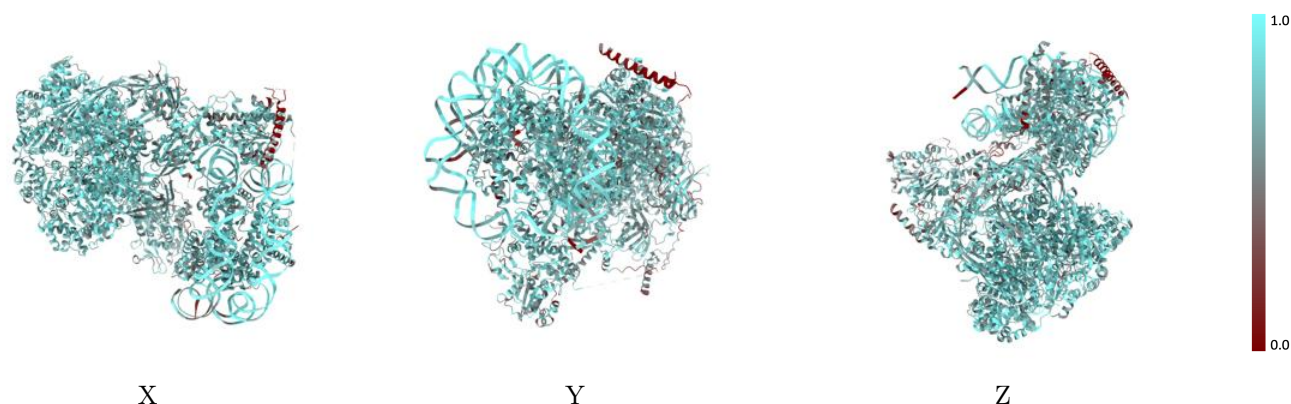
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



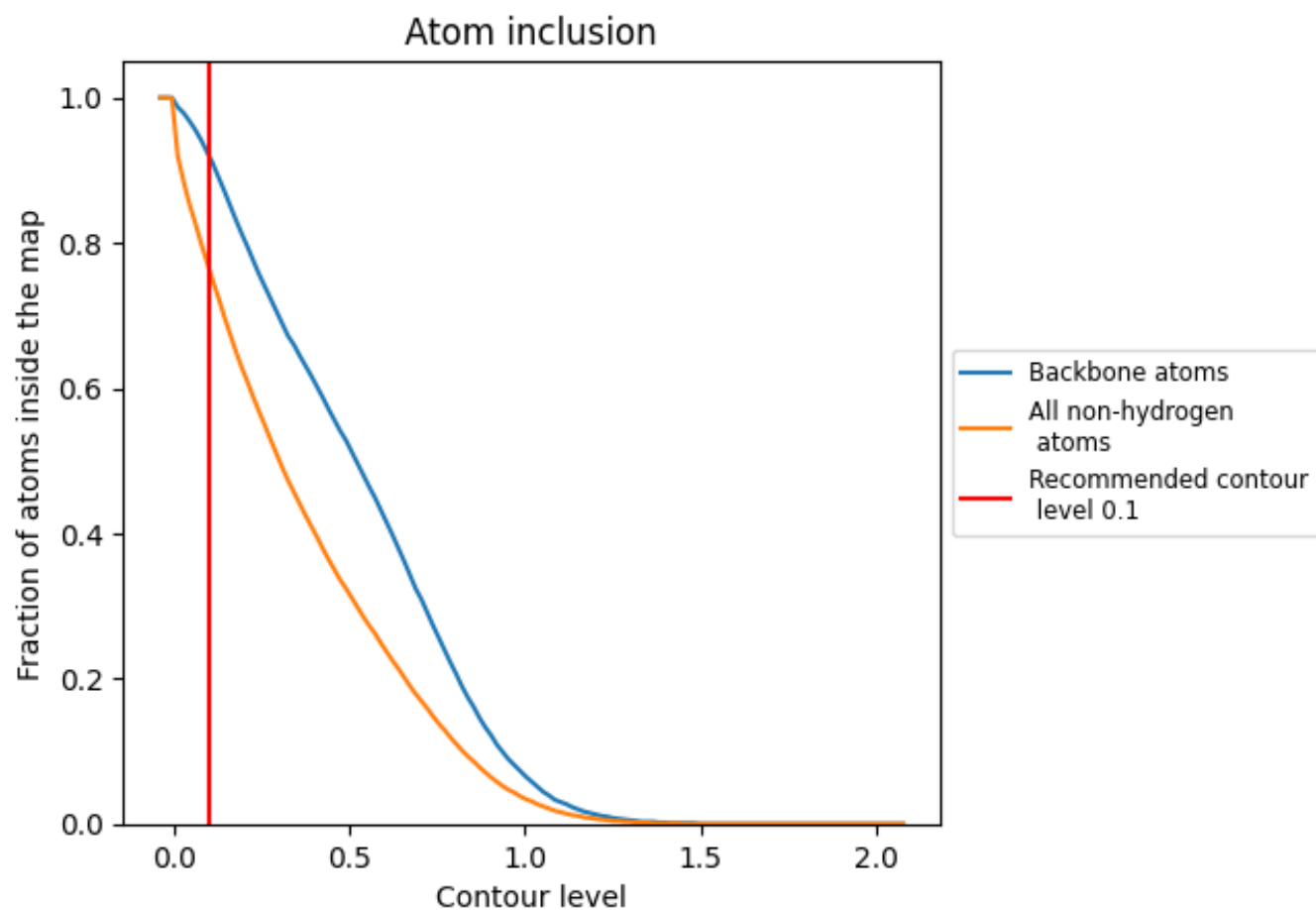
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.3680
A	 0.7120	 0.3230
B	 0.5190	 0.2040
C	 0.7220	 0.2900
D	 0.6720	 0.3010
E	 0.7990	 0.4380
F	 0.7780	 0.4140
G	 0.7660	 0.4130
H	 0.7890	 0.4220
I	 0.7940	 0.4300
J	 0.7940	 0.4360
Q	 0.7270	 0.3020
R	 0.7820	 0.3410
S	 0.8030	 0.4080
T	 0.8010	 0.3970
U	 0.6860	 0.3040
V	 0.8030	 0.3840
W	 0.7750	 0.3780
X	 0.8180	 0.4070
Y	 0.8210	 0.2970
Z	 0.8140	 0.2970

