



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:56 AM UTC

PDB ID : 9GCG / pdb_00009gcg
EMDB ID : EMD-51229
Title : CryoEM structure of the human INO80 core- H2A.Z nucleosome complex
Authors : Aggarwal, P.; Sharma, M.; Hopfner, K.P.
Deposited on : 2024-08-01
Resolution : 3.43 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

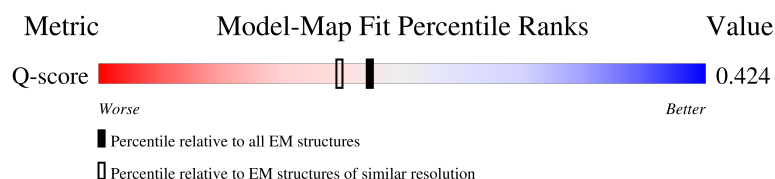
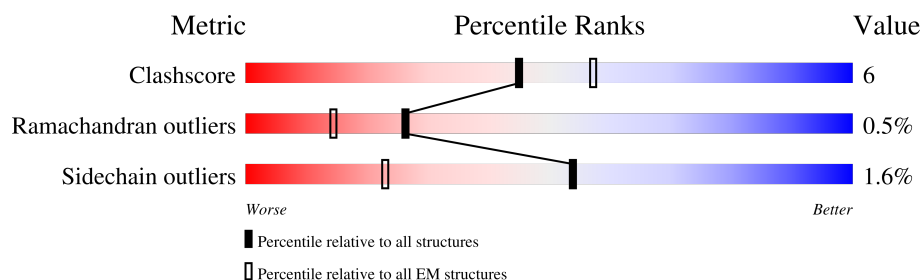
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.43 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.





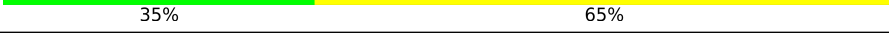
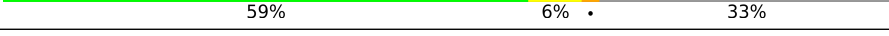
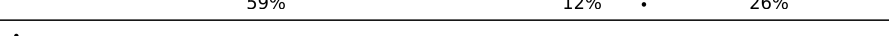
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13927 (2.93 - 3.93)

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	456	 89% 6% 5%
1	B	456	 91% 7% .
1	C	456	 93% . .
2	D	463	 81% 10% . 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	463	
2	F	463	
3	I	192	
4	G	1556	
5	H	356	
6	J	607	
7	K	152	
8	L	152	
9	M	136	
9	Q	136	
10	N	102	
10	R	102	
11	O	127	
12	P	125	
12	T	125	
13	S	127	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 43167 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	443	Total	C	N	O	S	0	0
			3412	2148	585	662	17		
1	A	434	Total	C	N	O	S	0	0
			3344	2107	575	646	16		
1	B	447	Total	C	N	O	S	0	0
			3453	2173	592	672	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	439	Total	C	N	O	S	0	0
			3403	2125	597	665	16		
2	D	426	Total	C	N	O	S	0	0
			3317	2074	583	645	15		
2	F	434	Total	C	N	O	S	0	0
			3376	2110	592	658	16		

- Molecule 3 is a protein called INO80 complex subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	107	Total	C	N	O	0	0
			850	545	150	155		

- Molecule 4 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	682	Total	C	N	O	S	0	0
			5608	3599	1004	975	30		

- Molecule 5 is a protein called INO80 complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	101	Total	C	N	O	S	0	0
			785	478	161	137	9		

- Molecule 6 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	412	Total	C	N	O	S	0	0
			3277	2088	572	596	21		

- Molecule 7 is a DNA chain called Nucleosomal DNA Strand 1 (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	152	Total	C	N	O	P	0	0
			3132	1483	590	907	152		

- Molecule 8 is a DNA chain called Nucleosomal DNA Strand 2 (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	152	Total	C	N	O	P	0	0
			3100	1474	557	917	152		

- Molecule 9 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	91	Total	C	N	O	S	0	0
			739	467	138	130	4		
9	Q	97	Total	C	N	O	S	0	0
			800	503	155	138	4		

- Molecule 10 is a protein called Histone H4.

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

- Molecule 11 is a protein called Histone H2A.Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	106	Total	C	N	O	0	0
			803	504	157	142		

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 12 | P | 94 | Total
735 | C
462 | N
132 | O
139 | S
2 | 0 | 0 |
| 12 | T | 92 | Total
720 | C
453 | N
129 | O
136 | S
2 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 13 | S | 108 | Total
819 | C
514 | N
160 | O
145 | 0 | 0 |

Chain	Residue	Modelled	Actual	Comment	Reference
S	108	LEU	ILE	conflict	UNP P0C0S5

- # ADP

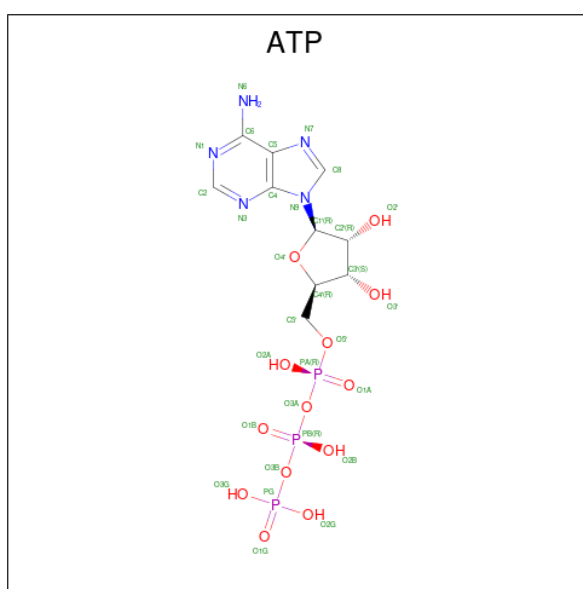
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total 27	C 10	N 5	O 10	P 2	0
14	E	1	Total 27	C 10	N 5	O 10	P 2	0
14	B	1	Total 27	C 10	N 5	O 10	P 2	0



Continued from previous page...

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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	H	1	Total	Zn	0
			1	1	

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.

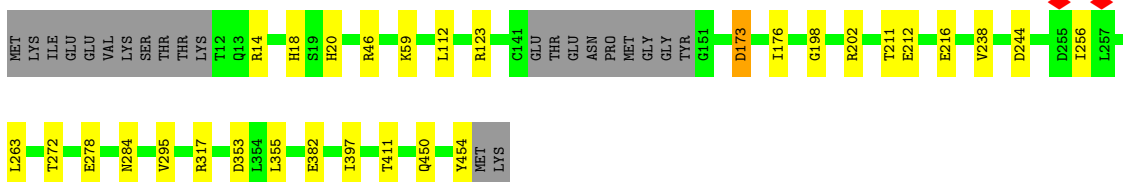
- Molecule 1: RuvB-like 1

Chain C:  93%



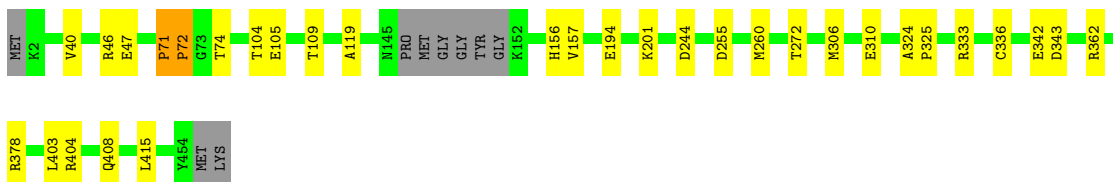
- Molecule 1: RuvB-like 1

Chain A:  89% 6% 5%



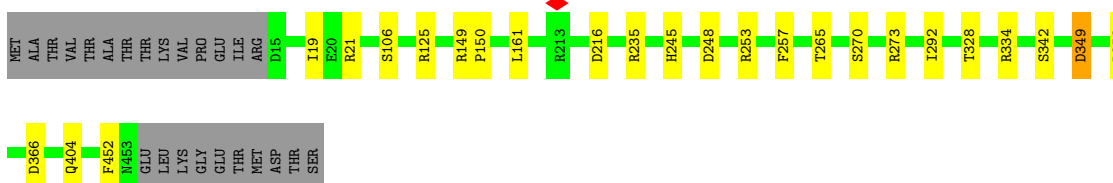
- Molecule 1: RuvB-like 1

Chain B:  91% 7%

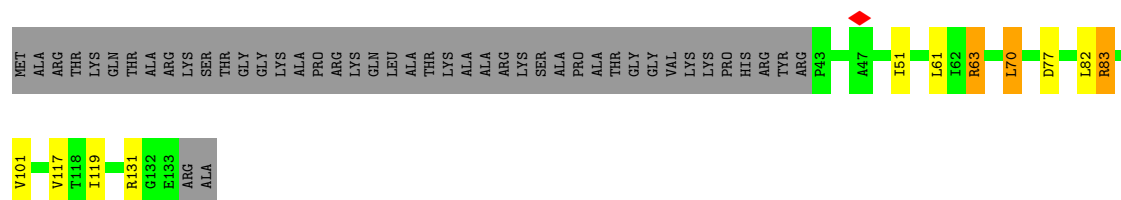


- Molecule 2: RuvB-like 2

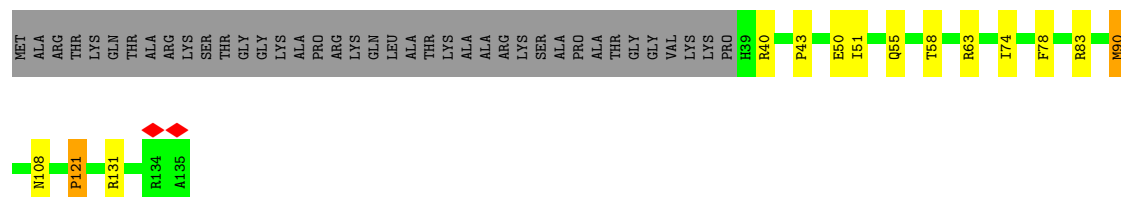
Chain E:  89% 5% 5%



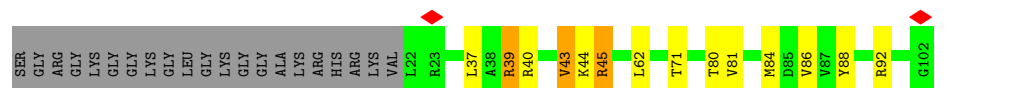




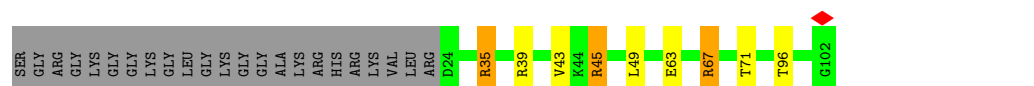
• Molecule 9: Histone H3.1



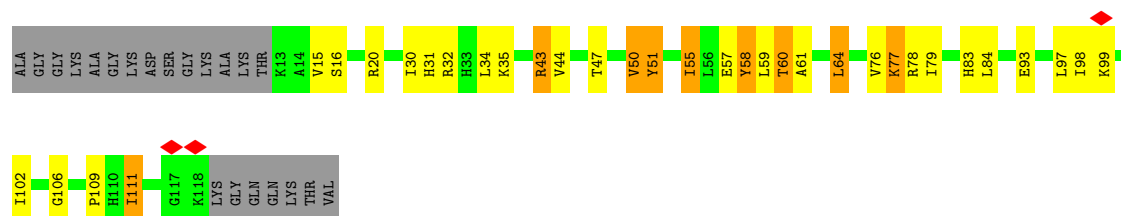
• Molecule 10: Histone H4



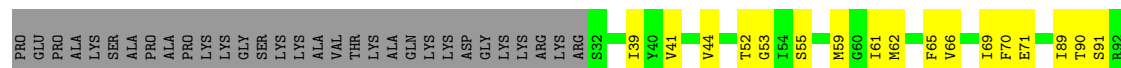
• Molecule 10: Histone H4

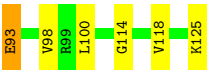


• Molecule 11: Histone H2A.Z

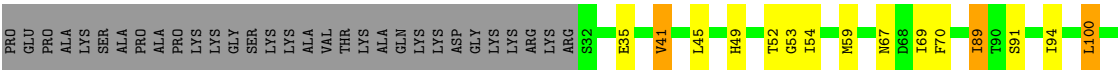


• Molecule 12: Histone H2B type 2-E

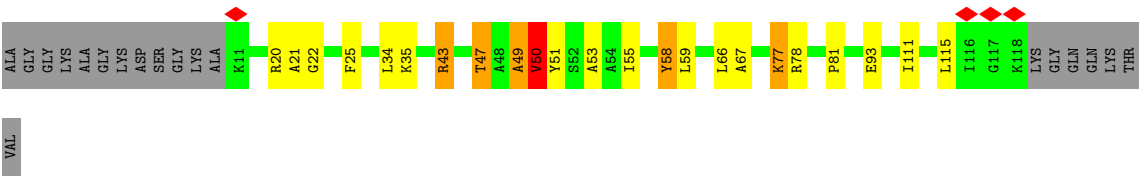




- Molecule 12: Histone H2B type 2-E



- Molecule 13: Histone H2A.Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94892	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.592	Depositor
Minimum map value	-0.268	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	414.92, 414.92, 414.92	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.943, 0.943, 0.943	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.76	2/3387 (0.1%)	1.23	6/4564 (0.1%)
1	B	0.71	0/3496	1.17	15/4710 (0.3%)
1	C	0.71	0/3458	1.16	2/4662 (0.0%)
2	D	0.75	2/3353 (0.1%)	1.25	12/4510 (0.3%)
2	E	0.69	0/3443	1.21	12/4636 (0.3%)
2	F	0.74	1/3415 (0.0%)	1.28	22/4596 (0.5%)
3	I	0.67	0/873	1.15	2/1183 (0.2%)
4	G	0.63	0/5744	1.11	15/7759 (0.2%)
5	H	0.66	0/802	1.06	0/1080
6	J	0.69	0/3362	1.13	5/4558 (0.1%)
7	K	0.58	0/3518	0.95	2/5431 (0.0%)
8	L	0.59	0/3472	0.96	0/5353
9	M	0.75	0/748	1.31	3/1003 (0.3%)
9	Q	0.74	0/811	1.30	0/1086
10	N	0.76	0/653	1.28	0/873
10	R	0.76	0/634	1.36	2/848 (0.2%)
11	O	0.90	1/814 (0.1%)	1.68	12/1095 (1.1%)
12	P	0.74	0/746	1.28	2/1001 (0.2%)
12	T	0.72	0/731	1.23	0/983
13	S	0.88	0/830	1.49	8/1116 (0.7%)
All	All	0.70	6/44290 (0.0%)	1.17	120/61047 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
2	D	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	2
2	F	0	4
3	I	0	1
4	G	0	5
5	H	0	1
6	J	0	2
9	M	0	2
9	Q	0	3
10	N	0	3
10	R	0	1
11	O	0	3
12	P	0	1
13	S	0	1
All	All	0	37

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	83	HIS	CG-CD2	-6.70	1.28	1.35
2	D	86	ILE	CB-CG1	-6.16	1.41	1.53
1	A	454	TYR	CA-C	5.65	1.64	1.52
2	D	335	ILE	CB-CG1	-5.27	1.43	1.53
1	A	46	ARG	NE-CZ	-5.09	1.27	1.33
2	F	370	ILE	CB-CG1	-5.09	1.43	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	64	LEU	N-CA-CB	8.80	125.37	110.49
10	R	45	ARG	NE-CZ-NH2	8.61	126.95	119.20
2	D	273	ARG	NE-CZ-NH1	-8.54	112.96	121.50
2	F	214	ASP	CA-CB-CG	7.81	120.41	112.60
11	O	50	VAL	N-CA-CB	7.39	123.42	111.23
13	S	50	VAL	CA-CB-CG1	7.25	122.72	110.40
11	O	50	VAL	CA-CB-CG2	7.19	122.62	110.40
12	P	93	GLU	CB-CA-C	7.12	122.16	110.90
1	B	403	LEU	N-CA-CB	7.09	121.26	110.28
11	O	58	TYR	N-CA-CB	7.01	120.51	110.13
11	O	57	GLU	N-CA-CB	6.92	122.18	110.49
13	S	50	VAL	N-CA-CB	6.91	122.63	111.23
2	E	248	ASP	CA-CB-CG	6.84	119.44	112.60
6	J	255	ASP	CA-CB-CG	6.83	119.43	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ASP	CA-CB-CG	6.71	119.31	112.60
13	S	35	LYS	N-CA-C	-6.69	100.37	110.28
13	S	81	PRO	N-CA-CB	6.68	110.16	103.48
6	J	477	ASP	CA-CB-CG	6.62	119.22	112.60
2	F	196	ASP	CA-CB-CG	6.57	119.17	112.60
2	E	245	HIS	CA-CB-CG	-6.54	107.26	113.80
2	D	273	ARG	NE-CZ-NH2	6.49	125.04	119.20
2	F	264	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	71	PRO	N-CA-C	6.45	118.57	110.70
2	E	216	ASP	CA-CB-CG	6.41	119.01	112.60
11	O	51	TYR	CA-CB-CG	-6.34	102.48	113.90
9	M	77	ASP	CA-CB-CG	6.28	118.88	112.60
2	D	319	ASP	CA-CB-CG	6.26	118.86	112.60
4	G	853	PHE	CA-CB-CG	6.26	120.06	113.80
2	D	264	ASP	CA-CB-CG	6.23	118.83	112.60
2	F	320	MET	CG-SD-CE	6.21	114.57	100.90
4	G	1028	ASP	CA-CB-CG	6.20	118.80	112.60
2	F	27	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	A	173	ASP	CA-CB-CG	6.12	118.72	112.60
10	R	67	ARG	NE-CZ-NH1	-6.09	115.41	121.50
11	O	51	TYR	N-CA-C	-6.05	101.65	111.04
2	E	265	THR	OG1-CB-CG2	6.02	121.35	109.30
1	B	46	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	B	324	ALA	N-CA-C	5.97	116.47	109.60
2	F	305	ASP	CA-CB-CG	5.96	118.56	112.60
7	K	-14	DG	O3'-P-O5'	-5.96	95.06	104.00
1	B	46	ARG	NE-CZ-NH1	-5.88	115.62	121.50
4	G	857	ARG	NE-CZ-NH2	5.86	124.47	119.20
2	F	273	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	B	156	HIS	CA-CB-CG	5.83	119.63	113.80
4	G	930	ARG	NE-CZ-NH2	5.83	124.44	119.20
4	G	1001	CYS	CB-CA-C	-5.81	102.66	109.80
3	I	167	ASP	CA-CB-CG	5.80	118.40	112.60
4	G	857	ARG	NE-CZ-NH1	-5.80	115.70	121.50
2	F	314	ARG	NE-CZ-NH2	5.77	124.39	119.20
13	S	58	TYR	N-CA-CB	5.77	118.37	110.01
2	E	273	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	F	453	ASN	CB-CA-C	5.71	120.96	110.10
13	S	49	ALA	CA-C-O	-5.70	114.83	120.70
2	F	248	ASP	CA-CB-CG	5.67	118.27	112.60
2	F	273	ARG	NE-CZ-NH2	5.66	124.29	119.20
4	G	1148	ASP	CA-CB-CG	5.65	118.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	ASP	CA-CB-CG	5.64	118.24	112.60
9	M	70	LEU	CD1-CG-CD2	5.64	123.20	110.80
2	D	349	ASP	CA-CB-CG	5.61	118.21	112.60
4	G	849	GLN	N-CA-CB	5.58	118.61	109.95
6	J	546	ASP	CA-CB-CG	5.58	118.18	112.60
4	G	898	PRO	N-CA-CB	5.57	109.61	103.26
1	B	104	THR	OG1-CB-CG2	-5.57	98.17	109.30
1	C	244	ASP	CA-CB-CG	5.56	118.16	112.60
2	D	148	ASP	CA-CB-CG	5.56	118.16	112.60
2	E	21	ARG	N-CA-CB	-5.54	101.12	110.49
2	E	334	ARG	N-CA-CB	5.54	118.53	109.95
11	O	51	TYR	N-CA-CB	5.53	117.95	110.10
1	A	244	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	355	LEU	N-CA-CB	-5.49	101.47	110.52
2	D	196	ASP	CA-CB-CG	5.48	118.08	112.60
7	K	-13	DG	O3'-P-O5'	-5.48	95.78	104.00
2	F	130	ARG	N-CA-CB	5.48	119.17	110.57
4	G	1168	ASP	CA-CB-CG	5.45	118.05	112.60
11	O	78	ARG	CA-CB-CG	-5.44	103.22	114.10
2	E	349	ASP	CB-CA-C	-5.42	101.46	110.68
1	A	212	GLU	N-CA-CB	-5.42	101.93	110.06
2	D	303	MET	CB-CG-SD	-5.42	96.45	112.70
2	F	303	MET	CB-CG-SD	-5.41	96.47	112.70
1	B	244	ASP	CA-CB-CG	5.41	118.01	112.60
4	G	893	PHE	CA-CB-CG	-5.39	108.41	113.80
2	F	31	LEU	N-CA-CB	-5.38	102.01	110.79
2	E	257	PHE	CA-CB-CG	-5.38	108.42	113.80
2	F	27	HIS	CB-CG-ND1	5.37	130.75	122.70
13	S	77	LYS	CG-CD-CE	5.36	123.63	111.30
4	G	842	LYS	N-CA-CB	5.36	117.99	110.12
1	B	310	GLU	CB-CA-C	-5.35	101.90	110.79
1	B	72	PRO	N-CA-CB	-5.34	98.38	103.19
2	D	400	ARG	NE-CZ-NH2	5.33	124.00	119.20
13	S	93	GLU	CG-CD-OE1	-5.33	106.14	118.40
1	C	353	ASP	CA-CB-CG	5.33	117.92	112.60
12	P	59	MET	CG-SD-CE	-5.33	89.19	100.90
2	F	83	LYS	N-CA-C	-5.32	105.40	111.14
4	G	897	SER	CA-C-N	5.30	125.36	119.32
4	G	897	SER	C-N-CA	5.30	125.36	119.32
1	B	378	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	B	194	GLU	CB-CA-C	5.25	118.79	110.19
2	F	448	ASP	CA-CB-CG	5.24	117.83	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	164	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	202	ARG	NE-CZ-NH1	-5.22	116.28	121.50
2	F	130	ARG	NE-CZ-NH2	5.22	123.90	119.20
11	O	77	LYS	CG-CD-CE	5.22	123.31	111.30
2	F	216	ASP	CA-CB-CG	5.21	117.81	112.60
2	F	349	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	124	ARG	NE-CZ-NH1	-5.21	116.30	121.50
1	B	343	ASP	CA-CB-CG	5.19	117.79	112.60
2	F	321	ALA	O-C-N	-5.18	118.39	121.71
6	J	515	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	E	366	ASP	CA-CB-CG	5.15	117.75	112.60
4	G	901	MET	CG-SD-CE	-5.13	89.61	100.90
2	D	303	MET	CG-SD-CE	5.12	112.17	100.90
2	E	342	SER	CA-C-N	5.09	125.01	119.76
2	E	342	SER	C-N-CA	5.09	125.01	119.76
9	M	63	ARG	CD-NE-CZ	5.09	131.53	124.40
2	F	355	LEU	N-CA-CB	-5.05	102.26	110.59
6	J	506	ARG	CB-CA-C	-5.04	102.42	110.79
1	B	306	MET	CB-CG-SD	-5.04	97.59	112.70
11	O	61	ALA	N-CA-C	-5.02	106.50	113.18
1	A	454	TYR	N-CA-CB	-5.01	101.98	110.50
11	O	43	ARG	CB-CA-C	-5.01	102.43	110.14

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	A	317	ARG	Sidechain
1	C	64	ARG	Sidechain
2	D	124	ARG	Sidechain
2	D	314	ARG	Sidechain
2	D	400	ARG	Sidechain
2	D	416	ARG	Sidechain
2	D	64	ARG	Sidechain
2	E	125	ARG	Sidechain
2	E	253	ARG	Sidechain
2	F	21	ARG	Sidechain
2	F	438	ARG	Sidechain
2	F	53	ARG	Sidechain
2	F	54	ARG	Sidechain
4	G	1182	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	G	1212	ARG	Sidechain
4	G	664	ARG	Sidechain
4	G	824	ARG	Sidechain
4	G	930	ARG	Sidechain
5	H	319	ARG	Sidechain
3	I	138	ASN	Peptide
6	J	210	ARG	Sidechain
6	J	448	ARG	Sidechain
9	M	131	ARG	Sidechain
9	M	83	ARG	Sidechain
10	N	39	ARG	Sidechain
10	N	45	ARG	Sidechain
10	N	92	ARG	Sidechain
11	O	32	ARG	Sidechain
11	O	55	ILE	Peptide
11	O	60	THR	Peptide
12	P	98	VAL	Peptide
9	Q	131	ARG	Sidechain
9	Q	63	ARG	Sidechain
9	Q	83	ARG	Sidechain
10	R	35	ARG	Sidechain
13	S	43	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3451	17	0
1	B	3453	0	3563	17	0
1	C	3412	0	3508	16	0
2	D	3317	0	3395	29	0
2	E	3403	0	3472	9	0
2	F	3376	0	3446	20	0
3	I	850	0	852	31	0
4	G	5608	0	5651	50	0
5	H	785	0	794	19	0
6	J	3277	0	3215	31	0
7	K	3132	0	1705	119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	3100	0	1710	137	0
9	M	739	0	777	11	0
9	Q	800	0	836	20	0
10	N	646	0	687	16	0
10	R	627	0	663	18	0
11	O	803	0	853	46	0
12	P	735	0	755	31	0
12	T	720	0	740	17	0
13	S	819	0	873	31	0
14	B	27	0	12	0	0
14	C	27	0	12	0	0
14	D	27	0	12	0	0
14	E	27	0	12	0	0
14	F	27	0	12	1	0
14	G	27	0	12	0	0
14	J	27	0	12	0	0
15	A	31	0	12	3	0
16	H	1	0	0	0	0
All	All	43167	0	41042	458	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 6.

All (458) 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)
4:G:1157:ARG:HH22	5:H:234:HIS:CE1	1.46	1.33
8:L:39:DA:OP1	11:O:35:LYS:HE2	1.40	1.17
5:H:216:ARG:NH1	8:L:14:DC:OP2	1.92	1.01
4:G:1157:ARG:NH2	5:H:234:HIS:CE1	2.29	1.00
6:J:69:ARG:HE	8:L:-30:DC:H1'	1.29	0.97
11:O:43:ARG:CZ	12:P:89:ILE:HG13	1.93	0.97
11:O:50:VAL:HG23	12:P:114:GLY:HA3	1.48	0.96
2:D:161:LEU:HD13	2:D:163:LEU:CD1	1.95	0.96
13:S:51:TYR:OH	12:T:70:PHE:CG	2.24	0.91
11:O:43:ARG:NH2	12:P:89:ILE:HG21	1.90	0.86
8:L:39:DA:OP1	11:O:35:LYS:CE	2.22	0.85
13:S:51:TYR:OH	12:T:70:PHE:CD2	2.28	0.85
9:Q:50:GLU:OE1	10:R:39:ARG:NH2	2.12	0.82
9:Q:78:PHE:HB2	10:R:67:ARG:CZ	2.10	0.81
8:L:35:DA:H1'	8:L:36:DG:C4	2.15	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:51:TYR:CZ	12:P:70:PHE:HD1	2.00	0.80
2:D:161:LEU:CD1	2:D:163:LEU:CD1	2.59	0.79
8:L:29:DC:H2'	8:L:30:DG:H8	1.48	0.79
11:O:47:THR:HG22	12:P:90:THR:C	2.09	0.78
7:K:48:DA:H61	8:L:-49:DC:H42	1.31	0.78
8:L:29:DC:H2'	8:L:30:DG:C8	2.19	0.77
1:B:272:THR:HG22	2:D:261:PHE:O	1.85	0.77
9:Q:78:PHE:HB2	10:R:67:ARG:NH1	2.00	0.77
6:J:184:LEU:HD13	6:J:472:LEU:CD1	2.16	0.76
9:Q:108:ASN:CG	10:R:43:VAL:HG12	2.11	0.76
13:S:50:VAL:HG22	13:S:50:VAL:O	1.85	0.75
6:J:69:ARG:NH2	8:L:-29:DG:N7	2.34	0.75
8:L:57:DT:H2''	8:L:58:DA:C8	2.23	0.74
9:M:51:ILE:HG21	13:S:111:ILE:CD1	2.18	0.74
7:K:3:DG:H1	8:L:-3:DC:H42	1.35	0.74
1:B:201:LYS:HB2	4:G:1088:ILE:HD11	1.70	0.73
7:K:24:DG:H4'	7:K:25:DC:H5'	1.69	0.73
6:J:461:ILE:HG22	6:J:462:GLY:H	1.52	0.73
1:B:71:PRO:HG2	1:B:74:THR:HG21	1.70	0.72
7:K:-8:DA:H1'	7:K:-7:DT:H5'	1.72	0.72
8:L:5:DG:H2''	8:L:6:DG:C8	2.25	0.71
4:G:664:ARG:HH11	7:K:72:DG:H4'	1.54	0.71
2:D:161:LEU:CD1	2:D:163:LEU:HD13	2.20	0.70
8:L:55:DT:H2''	8:L:56:DG:C8	2.27	0.70
6:J:184:LEU:CD1	6:J:472:LEU:HD11	2.23	0.69
7:K:-37:DT:H2''	7:K:-36:DC:C6	2.26	0.69
8:L:-32:DC:H2''	8:L:-31:DA:N7	2.07	0.69
2:D:161:LEU:HD13	2:D:163:LEU:HD12	1.74	0.69
1:C:256:ILE:HD13	4:G:1075:GLY:C	2.18	0.68
10:N:44:LYS:HG3	13:S:115:LEU:HD23	1.75	0.68
2:E:353:ARG:C	1:B:408:GLN:HE22	2.00	0.68
13:S:20:ARG:NH1	12:T:123:SER:O	2.26	0.68
8:L:-29:DG:H1'	8:L:-28:DT:H5'	1.76	0.68
8:L:51:DT:H2'	8:L:52:DG:H8	1.59	0.68
7:K:47:DT:H2''	7:K:48:DA:C8	2.29	0.67
7:K:-4:DC:H42	8:L:4:DG:H1	1.43	0.67
9:Q:78:PHE:CB	10:R:67:ARG:NH1	2.58	0.66
3:I:138:ASN:HD21	7:K:35:DT:P	2.19	0.66
8:L:-9:DT:H2''	8:L:-8:DT:H71	1.77	0.66
9:Q:78:PHE:CD1	10:R:67:ARG:NE	2.63	0.66
1:A:14:ARG:NH1	2:D:69:ALA:HA	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:11:DC:H2'	7:K:12:DG:C8	2.30	0.66
3:I:138:ASN:ND2	7:K:35:DT:P	2.69	0.65
9:Q:78:PHE:CG	10:R:67:ARG:NE	2.65	0.65
1:B:362:ARG:CZ	2:D:442:TYR:HB3	2.27	0.65
8:L:-56:DG:H2''	8:L:-55:DA:C8	2.32	0.65
8:L:38:DT:OP1	11:O:44:VAL:HG22	1.96	0.65
11:O:111:ILE:CG1	9:Q:51:ILE:HG21	2.27	0.65
3:I:136:LYS:NZ	8:L:-36:DA:C4	2.65	0.64
7:K:74:DC:H2'	7:K:75:DC:C6	2.31	0.64
8:L:51:DT:H2'	8:L:52:DG:C8	2.32	0.64
1:B:201:LYS:CB	4:G:1088:ILE:HD11	2.26	0.64
4:G:583:HIS:CB	5:H:234:HIS:CE1	2.80	0.64
6:J:184:LEU:HD13	6:J:472:LEU:HD11	1.79	0.64
13:S:50:VAL:HG23	12:T:114:GLY:HA3	1.78	0.64
3:I:138:ASN:ND2	7:K:34:DG:O3'	2.31	0.64
3:I:136:LYS:HD2	8:L:-36:DA:C5	2.33	0.64
8:L:-2:DG:H2'	8:L:-1:DC:C6	2.33	0.64
11:O:43:ARG:HH22	12:P:89:ILE:HG21	1.58	0.64
1:A:272:THR:HG21	2:F:260:LEU:O	1.97	0.64
8:L:32:DG:H1'	8:L:33:DT:H5''	1.79	0.64
1:C:153:THR:HG22	5:H:285:SER:CB	2.29	0.63
11:O:59:LEU:HD12	11:O:59:LEU:N	2.14	0.63
7:K:58:DA:H1'	7:K:59:DC:H5'	1.81	0.63
8:L:-45:DC:H2''	8:L:-44:DA:C8	2.34	0.63
1:A:238:VAL:HG21	4:G:861:LEU:HD11	1.81	0.63
8:L:5:DG:H2''	8:L:6:DG:N7	2.13	0.62
4:G:821:LEU:HD11	4:G:1129:MET:HE2	1.81	0.62
7:K:-7:DT:H2''	7:K:-6:DC:C5	2.35	0.62
7:K:55:DT:H2''	7:K:56:DC:C6	2.35	0.61
11:O:58:TYR:CE2	12:P:69:ILE:HG21	2.35	0.61
11:O:47:THR:CG2	12:P:90:THR:C	2.73	0.61
3:I:144:LEU:HD12	6:J:102:VAL:CG1	2.30	0.61
11:O:55:ILE:HD11	12:P:66:VAL:HG13	1.81	0.61
11:O:111:ILE:HG12	9:Q:51:ILE:HG21	1.83	0.61
4:G:632:GLN:HG2	8:L:-69:DT:H4'	1.82	0.61
4:G:818:HIS:HB2	4:G:1129:MET:HE1	1.82	0.60
8:L:11:DC:H2'	8:L:12:DT:H72	1.83	0.60
11:O:99:LYS:O	10:R:96:THR:HB	2.01	0.60
8:L:-48:DT:H4'	8:L:-47:DA:O5'	2.01	0.60
2:F:161:LEU:CD2	2:F:163:LEU:CD2	2.80	0.60
9:M:83:ARG:O	10:N:80:THR:HA	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:-59:DG:H2''	8:L:-58:DT:H72	1.83	0.60
8:L:-38:DT:H2'	8:L:-37:DA:C8	2.37	0.60
9:M:51:ILE:HG21	13:S:111:ILE:HD13	1.83	0.60
7:K:20:DC:H2''	7:K:21:DA:C8	2.37	0.59
9:M:51:ILE:CG2	13:S:111:ILE:CD1	2.80	0.59
2:E:349:ASP:OD2	1:B:333:ARG:NH1	2.35	0.59
2:F:174:LEU:CD1	2:F:179:ILE:HG13	2.32	0.59
2:E:149:ARG:HB2	4:G:1068:PHE:CE1	2.37	0.59
6:J:196:LEU:HD23	6:J:208:CYS:SG	2.43	0.59
7:K:-37:DT:H2''	7:K:-36:DC:C5	2.38	0.59
4:G:767:LEU:HD23	4:G:1229:THR:HG21	1.84	0.59
10:N:44:LYS:HD3	13:S:115:LEU:HG	1.84	0.59
2:D:324:LEU:HD11	2:D:326:MET:HE3	1.84	0.59
8:L:28:DA:H5''	10:N:80:THR:HB	1.84	0.59
11:O:51:TYR:CZ	12:P:70:PHE:CD1	2.88	0.59
13:S:51:TYR:OH	12:T:70:PHE:CD1	2.55	0.59
7:K:-1:DT:H1'	7:K:0:DG:H5'	1.85	0.58
6:J:69:ARG:NH2	8:L:-29:DG:C8	2.70	0.58
4:G:605:ARG:HH12	8:L:-67:DA:P	2.26	0.58
8:L:-78:DC:H1'	8:L:-77:DG:H5'	1.85	0.58
1:C:256:ILE:HD11	4:G:1075:GLY:HA2	1.86	0.58
3:I:138:ASN:HD22	7:K:34:DG:H3'	1.67	0.58
8:L:-39:DT:H2'	8:L:-38:DT:C6	2.38	0.58
5:H:215:LYS:NZ	7:K:-16:DA:H62	2.01	0.58
8:L:-62:DG:H2'	8:L:-61:DT:H72	1.85	0.58
8:L:8:DT:H5''	10:N:45:ARG:HE	1.68	0.58
9:Q:78:PHE:CD1	10:R:67:ARG:CD	2.86	0.58
6:J:93:MET:HE1	8:L:-30:DC:O3'	2.03	0.58
7:K:13:DC:H2''	7:K:14:DG:OP2	2.02	0.58
8:L:-9:DT:H2''	8:L:-8:DT:C7	2.34	0.58
7:K:11:DC:H2'	7:K:12:DG:H8	1.69	0.58
3:I:139:ARG:CZ	7:K:33:DC:H3'	2.33	0.57
15:A:501:ATP:H5'1	15:A:501:ATP:H8	1.69	0.57
8:L:46:DT:H2''	8:L:47:DC:C5	2.38	0.57
7:K:-43:DT:H2''	7:K:-42:DA:H5'	1.86	0.57
7:K:10:DA:H5''	9:Q:40:ARG:HG3	1.86	0.57
7:K:55:DT:H3	8:L:-55:DA:H61	1.52	0.57
8:L:-65:DT:H2''	8:L:-64:DT:H5'	1.86	0.57
4:G:583:HIS:HB2	5:H:234:HIS:CE1	2.39	0.57
7:K:-6:DC:H4'	7:K:-5:DC:H5'	1.86	0.57
11:O:51:TYR:OH	12:P:70:PHE:HD1	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:24:DA:H5'	8:L:24:DA:C8	2.39	0.57
7:K:23:DC:H5'	7:K:23:DC:C6	2.40	0.56
3:I:184:LEU:HA	6:J:260:LEU:HD13	1.86	0.56
7:K:-13:DG:H1'	7:K:-12:DA:H5'	1.86	0.56
7:K:52:DC:C2	7:K:53:DT:H72	2.40	0.56
8:L:38:DT:OP1	11:O:44:VAL:HG13	2.05	0.56
11:O:20:ARG:NE	12:P:125:LYS:OXT	2.39	0.56
1:C:153:THR:HG22	5:H:285:SER:HB3	1.86	0.56
9:M:101:VAL:HG23	10:N:37:LEU:HD22	1.88	0.56
6:J:69:ARG:NH2	8:L:-29:DG:C5	2.73	0.56
1:B:71:PRO:HG2	1:B:74:THR:CG2	2.35	0.56
13:S:66:LEU:C	13:S:66:LEU:HD23	2.31	0.56
3:I:138:ASN:HD22	7:K:34:DG:C3'	2.19	0.55
11:O:51:TYR:C	11:O:51:TYR:CD2	2.84	0.55
13:S:78:ARG:HH21	12:T:45:LEU:HD13	1.71	0.55
7:K:75:DC:O2	8:L:-74:DG:N1	2.39	0.55
8:L:7:DA:H1'	8:L:8:DT:H5'	1.89	0.55
3:I:144:LEU:CD1	6:J:102:VAL:CG1	2.85	0.55
1:A:278:GLU:OE2	4:G:887:CYS:SG	2.55	0.55
7:K:2:DC:O2	8:L:-2:DG:N1	2.40	0.55
8:L:-54:DC:H4'	13:S:77:LYS:CE	2.37	0.55
7:K:-36:DC:H2''	7:K:-35:DT:C5	2.42	0.54
8:L:-47:DA:C8	8:L:-46:DG:C5	2.96	0.54
8:L:0:DC:H2''	8:L:1:DA:C8	2.42	0.54
3:I:200:ILE:HD11	2:D:167:GLU:O	2.07	0.54
7:K:51:DG:N2	8:L:-50:DT:O2	2.40	0.54
7:K:66:DT:H2'	7:K:67:DT:H71	1.89	0.54
1:B:333:ARG:HB3	1:B:336:CYS:SG	2.47	0.54
7:K:20:DC:H2''	7:K:21:DA:H8	1.70	0.54
8:L:-81:DT:H2'	8:L:-80:DG:C8	2.42	0.54
11:O:47:THR:HG22	12:P:91:SER:N	2.23	0.54
7:K:-3:DC:H1'	7:K:-2:DT:H5'	1.89	0.54
7:K:8:DA:OP1	10:R:45:ARG:HA	2.09	0.54
7:K:-6:DC:H1'	7:K:-5:DC:C4	2.43	0.53
1:A:263:LEU:HD11	1:B:260:MET:HE3	1.90	0.53
11:O:43:ARG:NH1	12:P:89:ILE:HG13	2.24	0.53
13:S:67:ALA:HB3	12:T:49:HIS:CE1	2.43	0.53
1:B:362:ARG:NH1	2:D:442:TYR:HB3	2.23	0.53
4:G:1199:ASN:ND2	7:K:74:DC:OP1	2.41	0.53
9:M:61:LEU:HD11	10:N:40:ARG:CZ	2.39	0.53
8:L:-46:DG:H2''	8:L:-45:DC:C5	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:52:DC:H4'	7:K:53:DT:H5'	1.91	0.53
8:L:-72:DC:H2''	8:L:-71:DG:N7	2.24	0.53
1:A:355:LEU:HD23	2:F:436:GLU:HG3	1.91	0.53
2:F:134:GLU:OE2	4:G:943:TYR:CD2	2.62	0.53
15:A:501:ATP:H5'1	15:A:501:ATP:C8	2.44	0.53
4:G:583:HIS:CB	5:H:234:HIS:HE1	2.22	0.52
7:K:-54:DT:H2''	7:K:-53:DG:C8	2.44	0.52
4:G:1157:ARG:NH2	5:H:234:HIS:ND1	2.51	0.52
11:O:34:LEU:HB3	11:O:43:ARG:CD	2.39	0.52
2:F:161:LEU:HD21	2:F:163:LEU:CD2	2.40	0.52
9:Q:78:PHE:CE1	10:R:67:ARG:HD3	2.45	0.52
10:R:71:THR:HG21	12:T:100:LEU:HD13	1.91	0.52
1:A:272:THR:HG21	2:F:261:PHE:HA	1.92	0.52
4:G:913:TRP:CD1	4:G:1049:CYS:SG	3.03	0.52
9:M:61:LEU:HD11	10:N:40:ARG:NH2	2.25	0.52
11:O:59:LEU:HD21	12:P:41:VAL:HG12	1.92	0.52
7:K:48:DA:H61	8:L:-49:DC:N4	2.02	0.51
13:S:47:THR:HG23	12:T:91:SER:HA	1.92	0.51
1:B:47:GLU:OE1	2:D:428:ARG:NH1	2.43	0.51
7:K:40:DG:N2	8:L:-39:DT:O2	2.44	0.51
8:L:-7:DT:H2''	8:L:-6:DA:C8	2.45	0.51
9:Q:78:PHE:CB	10:R:67:ARG:CZ	2.84	0.51
2:D:397:THR:O	2:D:398:SER:HB2	2.11	0.51
8:L:-62:DG:H2''	8:L:-61:DT:O5'	2.11	0.51
8:L:-54:DC:H4'	13:S:77:LYS:HE3	1.93	0.51
13:S:34:LEU:HD11	13:S:51:TYR:CD2	2.45	0.51
7:K:-3:DC:H42	8:L:3:DG:H1	1.59	0.51
1:C:454:TYR:HB3	2:F:331:GLY:N	2.25	0.50
7:K:34:DG:H1	8:L:-34:DC:H42	1.57	0.50
7:K:49:DG:N2	8:L:-47:DA:H2	2.09	0.50
2:F:27:HIS:CD2	2:F:374:ARG:HH21	2.29	0.50
6:J:69:ARG:NH1	8:L:-30:DC:C2	2.77	0.50
7:K:3:DG:H1	8:L:-3:DC:N4	2.04	0.50
8:L:-48:DT:H4'	8:L:-47:DA:C5'	2.42	0.50
9:M:82:LEU:HD12	10:N:81:VAL:HG23	1.92	0.50
4:G:742:PHE:O	4:G:743:MET:HB2	2.11	0.50
2:E:150:PRO:HA	5:H:272:MET:SD	2.52	0.50
13:S:58:TYR:CE2	12:T:69:ILE:HG21	2.46	0.50
3:I:139:ARG:NH2	7:K:33:DC:O5'	2.44	0.50
2:D:77:GLY:O	2:D:83:LYS:HE3	2.12	0.49
4:G:583:HIS:CG	5:H:234:HIS:CE1	3.00	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:451:ALA:HB3	6:J:452:PRO:HD3	1.94	0.49
7:K:6:DT:H4'	7:K:7:DA:OP1	2.11	0.49
8:L:53:DC:H2''	8:L:54:DA:N7	2.27	0.49
13:S:22:GLY:HA3	12:T:120:LYS:HE2	1.94	0.49
2:D:135:THR:HG23	4:G:1027:ASN:HD21	1.77	0.49
8:L:-3:DC:H2''	8:L:-2:DG:H8	1.77	0.49
3:I:136:LYS:HD2	8:L:-36:DA:N7	2.27	0.49
7:K:26:DG:O6	8:L:-27:DA:N6	2.45	0.49
8:L:-55:DA:H4'	8:L:-54:DC:OP1	2.13	0.49
4:G:1199:ASN:HD21	7:K:74:DC:P	2.35	0.49
3:I:224:THR:O	3:I:226:ILE:HG13	2.13	0.49
1:B:404:ARG:O	1:B:408:GLN:HG3	2.13	0.49
7:K:14:DG:C2	7:K:15:DG:C2	3.01	0.49
8:L:33:DT:H2''	8:L:34:DC:C6	2.48	0.48
10:N:71:THR:OG1	12:P:100:LEU:HD21	2.13	0.48
11:O:102:ILE:CG2	12:P:61:ILE:HD13	2.42	0.48
3:I:195:LEU:HB2	3:I:206:ILE:HD11	1.95	0.48
8:L:-31:DA:C6	8:L:-30:DC:N4	2.81	0.48
13:S:21:ALA:C	12:T:120:LYS:HE3	2.38	0.48
6:J:69:ARG:HH11	8:L:-30:DC:C1'	2.26	0.48
11:O:79:ILE:HG22	12:P:55:SER:CB	2.44	0.48
3:I:139:ARG:NH1	7:K:34:DG:C8	2.81	0.48
6:J:184:LEU:HD23	6:J:197:PRO:HA	1.96	0.48
8:L:-49:DC:C2'	8:L:-48:DT:H5'	2.44	0.48
8:L:-6:DA:H4'	9:Q:43:PRO:HG2	1.96	0.48
7:K:43:DG:N2	8:L:-42:DC:N3	2.62	0.48
11:O:34:LEU:HB3	11:O:43:ARG:HD2	1.96	0.48
13:S:43:ARG:CZ	12:T:89:ILE:HG13	2.43	0.48
7:K:5:DT:H2''	7:K:6:DT:C5	2.48	0.47
7:K:55:DT:H2''	7:K:56:DC:C5	2.48	0.47
1:C:256:ILE:CD1	4:G:1075:GLY:HA2	2.44	0.47
3:I:139:ARG:HE	7:K:34:DG:C5'	2.26	0.47
7:K:73:DG:H2''	7:K:74:DC:C6	2.50	0.47
11:O:15:VAL:HG12	11:O:16:SER:N	2.29	0.47
2:F:291:ILE:N	2:F:291:ILE:HD12	2.29	0.47
7:K:-21:DA:H2''	7:K:-20:DG:OP2	2.15	0.47
8:L:-3:DC:H2''	8:L:-2:DG:C8	2.50	0.47
11:O:79:ILE:HG22	12:P:55:SER:HB2	1.96	0.47
3:I:136:LYS:NZ	8:L:-36:DA:H2'	2.30	0.47
8:L:-62:DG:H2'	8:L:-61:DT:C7	2.44	0.47
2:F:370:ILE:HD11	14:F:501:ADP:C4	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:-30:DC:N3	8:L:30:DG:N2	2.61	0.47
7:K:56:DC:H1'	7:K:57:DT:C4	2.49	0.47
8:L:-47:DA:H4'	8:L:-46:DG:OP1	2.15	0.47
12:T:52:THR:HG22	12:T:53:GLY:N	2.30	0.47
3:I:171:SER:HA	6:J:470:GLU:OE1	2.14	0.47
11:O:51:TYR:OH	12:P:70:PHE:CD1	2.67	0.47
3:I:139:ARG:NH1	7:K:33:DC:C6	2.80	0.46
9:M:119:ILE:HG21	10:N:43:VAL:HG11	1.97	0.46
11:O:59:LEU:CD2	12:P:41:VAL:HG12	2.45	0.46
4:G:607:VAL:HG11	5:H:230:ARG:HD2	1.96	0.46
6:J:69:ARG:HE	8:L:-30:DC:C1'	2.14	0.46
7:K:-11:DG:H2''	7:K:-10:DT:C5'	2.45	0.46
8:L:-33:DG:C2	8:L:-32:DC:C2	3.03	0.46
9:Q:108:ASN:CG	10:R:43:VAL:CG1	2.84	0.46
2:F:174:LEU:CD1	2:F:179:ILE:CG1	2.93	0.46
4:G:1199:ASN:ND2	7:K:74:DC:P	2.88	0.46
7:K:-4:DC:N4	8:L:4:DG:H1	2.10	0.46
8:L:-29:DG:H1'	8:L:-28:DT:C5'	2.45	0.46
12:P:52:THR:HG22	12:P:53:GLY:N	2.31	0.46
1:B:105:GLU:C	2:D:111:LEU:HD22	2.40	0.46
2:F:170:THR:HG21	5:H:320:TYR:CG	2.50	0.46
7:K:44:DT:O4	8:L:-45:DC:N4	2.49	0.46
8:L:-60:DC:H5'	8:L:-60:DC:C6	2.50	0.46
7:K:55:DT:H3	8:L:-55:DA:N6	2.12	0.46
8:L:-2:DG:H2'	8:L:-1:DC:H6	1.79	0.46
11:O:50:VAL:HG23	12:P:114:GLY:CA	2.33	0.46
7:K:-10:DT:H2''	7:K:-9:DA:O5'	2.15	0.46
7:K:49:DG:H22	8:L:-47:DA:H2	1.63	0.46
7:K:39:DA:H61	8:L:-39:DT:H3	1.63	0.46
8:L:-54:DC:H4'	13:S:77:LYS:NZ	2.31	0.46
8:L:-50:DT:H2''	8:L:-49:DC:O4'	2.16	0.46
8:L:19:DT:H1'	8:L:20:DC:H5'	1.98	0.46
13:S:49:ALA:C	13:S:51:TYR:H	2.24	0.46
7:K:26:DG:O6	8:L:-27:DA:C6	2.69	0.45
8:L:8:DT:H1'	8:L:9:DT:H5'	1.97	0.45
6:J:69:ARG:NH1	8:L:-30:DC:C6	2.85	0.45
8:L:30:DG:H2'	8:L:31:DT:C6	2.52	0.45
8:L:57:DT:H2''	8:L:58:DA:N7	2.30	0.45
8:L:-20:DG:H8	8:L:-20:DG:OP2	2.00	0.45
3:I:195:LEU:HB2	3:I:206:ILE:CD1	2.46	0.45
2:D:161:LEU:HD13	2:D:163:LEU:HD11	1.93	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:109:PRO:HA	9:Q:55:GLN:HG2	1.99	0.45
2:D:279:LYS:HE3	4:G:853:PHE:CE1	2.52	0.45
7:K:53:DT:O2	7:K:53:DT:H2'	2.15	0.45
8:L:-32:DC:C2	8:L:-31:DA:C6	3.05	0.45
8:L:-29:DG:C8	8:L:-28:DT:C5	3.04	0.45
1:A:18:HIS:NE2	2:D:317:GLU:OE1	2.48	0.45
2:F:161:LEU:CD2	2:F:163:LEU:HD22	2.46	0.45
11:O:102:ILE:HG23	12:P:61:ILE:HD13	1.99	0.45
13:S:20:ARG:HH21	13:S:20:ARG:HG3	1.82	0.45
3:I:168:ALA:HB1	6:J:471:THR:HG22	1.99	0.45
3:I:168:ALA:HB1	6:J:471:THR:CG2	2.47	0.45
6:J:461:ILE:HG22	6:J:462:GLY:N	2.28	0.45
8:L:-27:DA:H1'	8:L:-26:DC:H5'	1.98	0.45
1:C:284:ASN:OD1	2:E:19:ILE:HG22	2.17	0.45
11:O:99:LYS:O	10:R:96:THR:CB	2.64	0.45
3:I:175:ALA:O	1:A:211:THR:HG21	2.16	0.45
1:A:284:ASN:ND2	2:F:19:ILE:HG22	2.32	0.45
7:K:15:DG:C2	7:K:16:DG:C2	3.05	0.45
10:N:71:THR:OG1	12:P:100:LEU:CD2	2.65	0.45
1:C:256:ILE:CD1	4:G:1075:GLY:C	2.88	0.44
2:D:405:LEU:HD22	2:D:429:VAL:HG12	1.99	0.44
3:I:223:ALA:O	3:I:224:THR:C	2.59	0.44
6:J:466:ALA:HB3	6:J:471:THR:HG23	1.99	0.44
9:M:70:LEU:HD21	10:N:62:LEU:HD22	1.99	0.44
2:D:75:ILE:HG22	2:D:83:LYS:HB2	1.99	0.44
8:L:32:DG:H1'	8:L:33:DT:C5'	2.46	0.44
11:O:50:VAL:O	11:O:50:VAL:HG22	2.17	0.44
1:C:357:ARG:C	2:E:404:GLN:HE22	2.25	0.44
6:J:69:ARG:HD2	8:L:-29:DG:O5'	2.17	0.44
7:K:15:DG:H4'	7:K:16:DG:OP1	2.18	0.44
1:C:274:LYS:NZ	4:G:981:SER:O	2.42	0.44
7:K:37:DT:H2''	7:K:38:DA:C8	2.53	0.44
11:O:43:ARG:NH2	12:P:89:ILE:HG13	2.28	0.44
4:G:739:LEU:HD22	4:G:743:MET:SD	2.58	0.44
7:K:67:DT:H2''	7:K:68:DG:O5'	2.18	0.44
1:C:336:CYS:SG	2:E:452:PHE:HB2	2.58	0.44
2:D:201:LYS:HD3	4:G:1025:TYR:CE1	2.52	0.44
7:K:-10:DT:H2''	7:K:-9:DA:C8	2.52	0.44
7:K:51:DG:H2''	7:K:53:DT:H6	1.83	0.44
13:S:55:ILE:HD13	13:S:55:ILE:HG21	1.71	0.44
1:C:124:ILE:HD11	4:G:967:LEU:CD2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:-30:DC:C2	8:L:30:DG:N2	2.82	0.44
8:L:-57:DA:H2''	8:L:-56:DG:C8	2.53	0.44
8:L:44:DC:H2''	8:L:45:DA:N7	2.33	0.44
9:Q:74:ILE:HG23	10:R:63:GLU:CD	2.43	0.44
1:A:20:HIS:HE1	15:A:501:ATP:N3	2.16	0.43
2:D:127:ILE:HD13	2:D:127:ILE:HG21	1.84	0.43
7:K:-6:DC:C4'	7:K:-5:DC:H5'	2.48	0.43
8:L:-5:DA:H2''	8:L:-4:DC:C5	2.53	0.43
8:L:-47:DA:H8	8:L:-46:DG:C5	2.36	0.43
2:D:275:GLN:HG3	4:G:850:ILE:HD11	2.00	0.43
7:K:58:DA:H2''	7:K:59:DC:OP2	2.17	0.43
2:D:333:THR:HG22	2:D:334:ARG:N	2.33	0.43
4:G:742:PHE:O	4:G:742:PHE:CD1	2.71	0.43
13:S:66:LEU:C	13:S:66:LEU:CD2	2.92	0.43
1:A:59:LYS:O	2:F:21:ARG:HD2	2.18	0.43
11:O:43:ARG:NH2	12:P:89:ILE:CG2	2.74	0.43
4:G:1157:ARG:HH22	5:H:234:HIS:CD2	2.35	0.43
7:K:-32:DC:H2''	7:K:-31:DA:H8	1.84	0.43
7:K:72:DG:H2''	7:K:73:DG:H5''	2.00	0.43
8:L:-58:DT:H4'	8:L:-57:DA:OP1	2.18	0.43
8:L:36:DG:H1'	8:L:37:DA:O4'	2.18	0.43
7:K:8:DA:OP2	10:R:35:ARG:NH1	2.33	0.43
7:K:15:DG:H1	8:L:-15:DC:N4	2.17	0.43
8:L:35:DA:H1'	8:L:36:DG:C5	2.51	0.43
11:O:76:VAL:HG12	11:O:77:LYS:H	1.83	0.43
3:I:139:ARG:NE	7:K:33:DC:H3'	2.33	0.43
3:I:139:ARG:HD2	7:K:34:DG:OP2	2.19	0.43
7:K:72:DG:H2''	7:K:73:DG:C5'	2.49	0.43
1:A:176:ILE:HD11	1:A:198:GLY:HA2	2.01	0.43
6:J:69:ARG:HD2	8:L:-29:DG:O4'	2.18	0.43
1:A:211:THR:HG22	1:A:211:THR:O	2.18	0.43
8:L:-29:DG:C8	8:L:-28:DT:C4	3.07	0.43
11:O:97:LEU:HD21	12:P:65:PHE:CE1	2.53	0.43
8:L:-47:DA:N7	8:L:-46:DG:C6	2.87	0.42
13:S:51:TYR:CE2	12:T:70:PHE:CE2	3.07	0.42
7:K:39:DA:C6	7:K:40:DG:C6	3.08	0.42
1:C:257:LEU:HB3	4:G:976:HIS:CE1	2.55	0.42
1:A:216:GLU:HA	1:A:216:GLU:OE1	2.18	0.42
7:K:42:DG:H2''	7:K:43:DG:C8	2.54	0.42
7:K:79:DG:H1	8:L:-79:DC:H42	1.66	0.42
8:L:5:DG:H4'	8:L:6:DG:OP1	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:121:PRO:HG2	10:R:49:LEU:HB3	2.00	0.42
6:J:188:SER:CB	6:J:193:THR:HG22	2.49	0.42
7:K:-25:DC:H42	8:L:25:DG:H1	1.66	0.42
13:S:78:ARG:NH2	12:T:45:LEU:HD13	2.34	0.42
2:F:19:ILE:HG21	2:F:19:ILE:HD13	1.82	0.42
7:K:-38:DA:H2'	7:K:-37:DT:C6	2.55	0.42
7:K:-24:DT:H1'	7:K:-23:DG:H5'	2.01	0.42
13:S:25:PHE:CZ	13:S:59:LEU:HD22	2.55	0.42
7:K:-1:DT:H2''	7:K:0:DG:OP2	2.20	0.42
7:K:56:DC:C4	8:L:-57:DA:C6	3.07	0.42
8:L:-20:DG:C8	8:L:-20:DG:H5'	2.54	0.42
7:K:-40:DA:C5	7:K:-39:DT:C4	3.08	0.42
7:K:3:DG:C2	8:L:-2:DG:C2	3.08	0.42
7:K:32:DG:H1'	7:K:33:DC:C6	2.54	0.42
11:O:59:LEU:N	11:O:59:LEU:CD1	2.82	0.42
1:C:192:TYR:CD2	4:G:928:GLN:HG2	2.55	0.42
1:A:397:ILE:HD13	1:A:397:ILE:HG21	1.88	0.42
8:L:-46:DG:H2''	8:L:-45:DC:C6	2.54	0.42
5:H:215:LYS:CE	7:K:-16:DA:H62	2.33	0.42
7:K:7:DA:N6	8:L:-8:DT:O4	2.53	0.42
8:L:34:DC:H1'	8:L:35:DA:N1	2.35	0.42
11:O:106:GLY:HA3	9:Q:58:THR:HG22	2.02	0.41
7:K:-27:DG:H2''	7:K:-26:DC:OP2	2.19	0.41
8:L:-17:DC:H2''	8:L:-16:DC:O5'	2.19	0.41
8:L:8:DT:OP1	10:N:45:ARG:HG2	2.21	0.41
1:B:72:PRO:HD2	2:D:449:ALA:O	2.19	0.41
6:J:69:ARG:NE	8:L:-30:DC:H1'	2.13	0.41
12:P:90:THR:O	12:P:91:SER:C	2.64	0.41
4:G:817:ASN:HB3	4:G:1129:MET:HE3	2.02	0.41
9:M:51:ILE:HD13	10:N:39:ARG:HD3	2.01	0.41
3:I:140:THR:CG2	6:J:106:LEU:H	2.34	0.41
2:D:279:LYS:HE3	4:G:853:PHE:CD1	2.55	0.41
6:J:196:LEU:CD2	6:J:208:CYS:SG	3.07	0.41
7:K:36:DT:H2''	7:K:37:DT:O5'	2.20	0.41
8:L:47:DC:H2''	8:L:48:DC:C6	2.55	0.41
2:D:326:MET:HE1	2:D:350:LEU:HD21	2.02	0.41
4:G:1157:ARG:HH22	5:H:234:HIS:CG	2.39	0.41
3:I:224:THR:O	3:I:225:SER:C	2.64	0.41
7:K:-6:DC:H6	7:K:-6:DC:H2'	1.69	0.41
12:T:41:VAL:CG2	12:T:59:MET:SD	3.09	0.41
3:I:144:LEU:CD1	6:J:102:VAL:HG12	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1199:ASN:ND2	7:K:74:DC:OP2	2.54	0.41
7:K:41:DC:O2	8:L:-41:DG:N1	2.54	0.41
8:L:-41:DG:H1'	8:L:-40:DC:H5'	2.02	0.41
9:Q:90:MET:HE2	9:Q:90:MET:HA	2.03	0.41
7:K:47:DT:H2''	7:K:48:DA:N7	2.34	0.41
10:N:84:MET:HE3	10:N:88:TYR:CZ	2.56	0.41
11:O:30:ILE:HG22	11:O:31:HIS:N	2.36	0.41
11:O:60:THR:HG23	12:P:44:VAL:CG1	2.52	0.41
1:B:119:ALA:HB3	1:B:325:PRO:HG3	2.02	0.40
2:F:170:THR:HG21	5:H:320:TYR:CD1	2.56	0.40
4:G:570:PHE:CZ	4:G:648:TYR:CD1	3.09	0.40
7:K:-11:DG:H2''	7:K:-10:DT:O5'	2.21	0.40
11:O:59:LEU:HG	12:P:62:MET:CE	2.51	0.40
2:E:292:ILE:HG13	2:E:292:ILE:O	2.21	0.40
1:B:201:LYS:HB2	4:G:1088:ILE:CD1	2.47	0.40
2:D:301:VAL:HG21	2:D:326:MET:HG2	2.04	0.40
4:G:767:LEU:CD2	4:G:1229:THR:HG21	2.50	0.40
7:K:64:DA:C2	7:K:65:DA:C5	3.10	0.40
8:L:-27:DA:H2''	8:L:-26:DC:O5'	2.22	0.40
13:S:53:ALA:C	13:S:55:ILE:H	2.30	0.40
1:C:175:SER:HB2	4:G:1069:PHE:CE2	2.56	0.40
2:E:235:ARG:HH11	4:G:989:HIS:CG	2.39	0.40
2:F:123:PHE:CZ	2:F:324:LEU:HD11	2.55	0.40
4:G:583:HIS:HB3	5:H:234:HIS:HE1	1.84	0.40
7:K:-23:DG:H2''	7:K:-22:DG:O5'	2.21	0.40
7:K:-9:DA:H2''	7:K:-8:DA:OP2	2.21	0.40
1:C:14:ARG:NH1	2:F:293:PRO:HB3	2.36	0.40
7:K:52:DC:H2''	7:K:53:DT:OP2	2.22	0.40
1:A:382:GLU:HG3	2:D:68:ILE:HD11	2.04	0.40
7:K:-10:DT:H2''	7:K:-9:DA:H8	1.85	0.40
7:K:5:DT:H2''	7:K:6:DT:C4	2.57	0.40
7:K:8:DA:H1'	7:K:9:DA:H5'	2.02	0.40
7:K:43:DG:H1	8:L:-43:DC:H42	1.68	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	430/456 (94%)	411 (96%)	18 (4%)	1 (0%)	43	73
1	B	443/456 (97%)	430 (97%)	12 (3%)	1 (0%)	43	73
1	C	441/456 (97%)	431 (98%)	10 (2%)	0	100	100
2	D	420/463 (91%)	410 (98%)	9 (2%)	1 (0%)	43	73
2	E	437/463 (94%)	429 (98%)	8 (2%)	0	100	100
2	F	430/463 (93%)	413 (96%)	14 (3%)	3 (1%)	18	50
3	I	105/192 (55%)	96 (91%)	8 (8%)	1 (1%)	12	42
4	G	674/1556 (43%)	633 (94%)	35 (5%)	6 (1%)	14	45
5	H	97/356 (27%)	93 (96%)	4 (4%)	0	100	100
6	J	406/607 (67%)	381 (94%)	20 (5%)	5 (1%)	10	38
9	M	89/136 (65%)	89 (100%)	0	0	100	100
9	Q	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
10	N	79/102 (78%)	73 (92%)	6 (8%)	0	100	100
10	R	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
11	O	104/127 (82%)	77 (74%)	24 (23%)	3 (3%)	3	23
12	P	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
12	T	90/125 (72%)	86 (96%)	3 (3%)	1 (1%)	11	40
13	S	106/127 (84%)	91 (86%)	14 (13%)	1 (1%)	14	45
All	All	4615/6448 (72%)	4396 (95%)	196 (4%)	23 (0%)	26	56

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	743	MET
6	J	123	SER
4	G	747	ILE
4	G	1230	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	J	124	SER
6	J	496	GLY
11	O	64	LEU
12	T	35	GLU
3	I	130	GLY
1	A	256	ILE
1	B	342	GLU
2	D	267	GLU
2	F	24	ALA
11	O	93	GLU
11	O	111	ILE
13	S	50	VAL
2	F	267	GLU
4	G	684	ILE
4	G	1143	THR
4	G	1200	PRO
6	J	106	LEU
6	J	125	GLN
2	F	452	PHE

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	367/387 (95%)	362 (99%)	5 (1%)	59	71
1	B	381/387 (98%)	377 (99%)	4 (1%)	68	75
1	C	374/387 (97%)	370 (99%)	4 (1%)	65	74
2	D	361/390 (93%)	353 (98%)	8 (2%)	45	65
2	E	369/390 (95%)	365 (99%)	4 (1%)	65	74
2	F	367/390 (94%)	358 (98%)	9 (2%)	42	63
3	I	92/158 (58%)	90 (98%)	2 (2%)	45	65
4	G	613/1359 (45%)	608 (99%)	5 (1%)	73	77
5	H	86/288 (30%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	351/520 (68%)	349 (99%)	2 (1%)	78	80
9	M	79/111 (71%)	77 (98%)	2 (2%)	42	63
9	Q	84/111 (76%)	82 (98%)	2 (2%)	43	64
10	N	66/78 (85%)	64 (97%)	2 (3%)	36	60
10	R	64/78 (82%)	64 (100%)	0	100	100
11	O	83/96 (86%)	81 (98%)	2 (2%)	43	64
12	P	80/105 (76%)	76 (95%)	4 (5%)	22	49
12	T	79/105 (75%)	73 (92%)	6 (8%)	12	38
13	S	85/96 (88%)	84 (99%)	1 (1%)	63	73
All	All	3981/5436 (73%)	3919 (98%)	62 (2%)	54	70

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	40	VAL
1	C	91	VAL
1	C	190	VAL
1	C	408	GLN
2	E	106	SER
2	E	161	LEU
2	E	270	SER
2	E	328	THR
3	I	185	LEU
3	I	189	THR
1	A	112	LEU
1	A	173	ASP
1	A	295	VAL
1	A	411	THR
1	A	450	GLN
1	B	40	VAL
1	B	109	THR
1	B	157	VAL
1	B	415	LEU
2	D	47	VAL
2	D	59	VAL
2	D	303	MET
2	D	313	ASN
2	D	324	LEU
2	D	328	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	399	LEU
2	D	453	ASN
2	F	165	THR
2	F	196	ASP
2	F	231	GLU
2	F	247	ILE
2	F	307	GLU
2	F	323	VAL
2	F	328	THR
2	F	333	THR
2	F	407	THR
4	G	560	LEU
4	G	662	SER
4	G	938	GLU
4	G	1088	ILE
4	G	1168	ASP
6	J	166	ASP
6	J	203	LEU
9	M	63	ARG
9	M	117	VAL
10	N	43	VAL
10	N	86	VAL
11	O	84	LEU
11	O	98	ILE
12	P	39	ILE
12	P	71	GLU
12	P	93	GLU
12	P	118	VAL
9	Q	90	MET
9	Q	121	PRO
13	S	47	THR
12	T	41	VAL
12	T	54	ILE
12	T	67	ASN
12	T	89	ILE
12	T	94	ILE
12	T	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	236	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	233	GLN
2	E	255	GLN
2	E	344	HIS
2	E	404	GLN
2	E	422	GLN
3	I	129	HIS
3	I	138	ASN
1	A	20	HIS
1	A	34	GLN
1	A	241	HIS
1	A	247	ASN
1	A	348	HIS
1	A	373	GLN
1	A	450	GLN
1	B	34	GLN
1	B	115	ASN
1	B	247	ASN
1	B	348	HIS
1	B	408	GLN
1	B	450	GLN
2	D	25	HIS
2	D	44	GLN
2	D	313	ASN
2	D	344	HIS
2	F	27	HIS
2	F	44	GLN
2	F	78	GLN
2	F	245	HIS
2	F	275	GLN
2	F	329	ASN
4	G	535	GLN
4	G	552	GLN
4	G	580	ASN
4	G	581	ASN
4	G	583	HIS
4	G	776	GLN
4	G	780	ASN
4	G	811	GLN
4	G	903	ASN
4	G	927	HIS
4	G	961	ASN
4	G	1027	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	1116	GLN
5	H	338	ASN
6	J	101	ASN
6	J	109	GLN
6	J	227	GLN
6	J	249	HIS
6	J	274	HIS
6	J	490	ASN
10	N	25	ASN
13	S	31	HIS
12	T	49	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is 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	$\# Z > 2$
14	ADP	J	701	-	28,29,29	0.68	0	43,45,45	1.15	3 (6%)
14	ADP	E	501	-	28,29,29	0.63	0	43,45,45	0.88	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	ADP	B	501	-	28,29,29	0.67	0	43,45,45	0.72	1 (2%)
15	ATP	A	501	-	32,33,33	0.83	1 (3%)	48,52,52	1.00	1 (2%)
14	ADP	F	501	-	28,29,29	0.71	0	43,45,45	0.65	0
14	ADP	D	501	-	28,29,29	0.71	0	43,45,45	0.69	0
14	ADP	G	1601	-	28,29,29	0.51	0	43,45,45	0.68	1 (2%)
14	ADP	C	501	-	28,29,29	0.79	1 (3%)	43,45,45	0.83	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ADP	J	701	-	-	0/16/32/32	0/3/3/3
14	ADP	E	501	-	-	2/16/32/32	0/3/3/3
14	ADP	B	501	-	-	2/16/32/32	0/3/3/3
15	ATP	A	501	-	-	3/22/38/38	0/3/3/3
14	ADP	F	501	-	-	0/16/32/32	0/3/3/3
14	ADP	D	501	-	-	4/16/32/32	0/3/3/3
14	ADP	G	1601	-	-	2/16/32/32	0/3/3/3
14	ADP	C	501	-	-	1/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	501	ADP	PB-O2B	-2.53	1.45	1.54
15	A	501	ATP	C8-N9	2.51	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	701	ADP	C2'-C3'-C4'	2.96	108.33	102.61
15	A	501	ATP	O4'-C4'-C3'	-2.56	100.08	105.15
14	C	501	ADP	O2A-PA-O3A	2.42	113.80	107.27
14	E	501	ADP	C2-N1-C6	-2.31	114.93	118.73
14	J	701	ADP	O3A-PB-O1B	-2.28	99.02	111.04
14	C	501	ADP	C5-C4-N3	-2.20	123.68	126.72
14	J	701	ADP	O2B-PB-O3A	2.16	111.89	104.64
14	G	1601	ADP	O2A-PA-O3A	2.03	112.76	107.27
14	B	501	ADP	O2A-PA-O3A	2.01	112.71	107.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

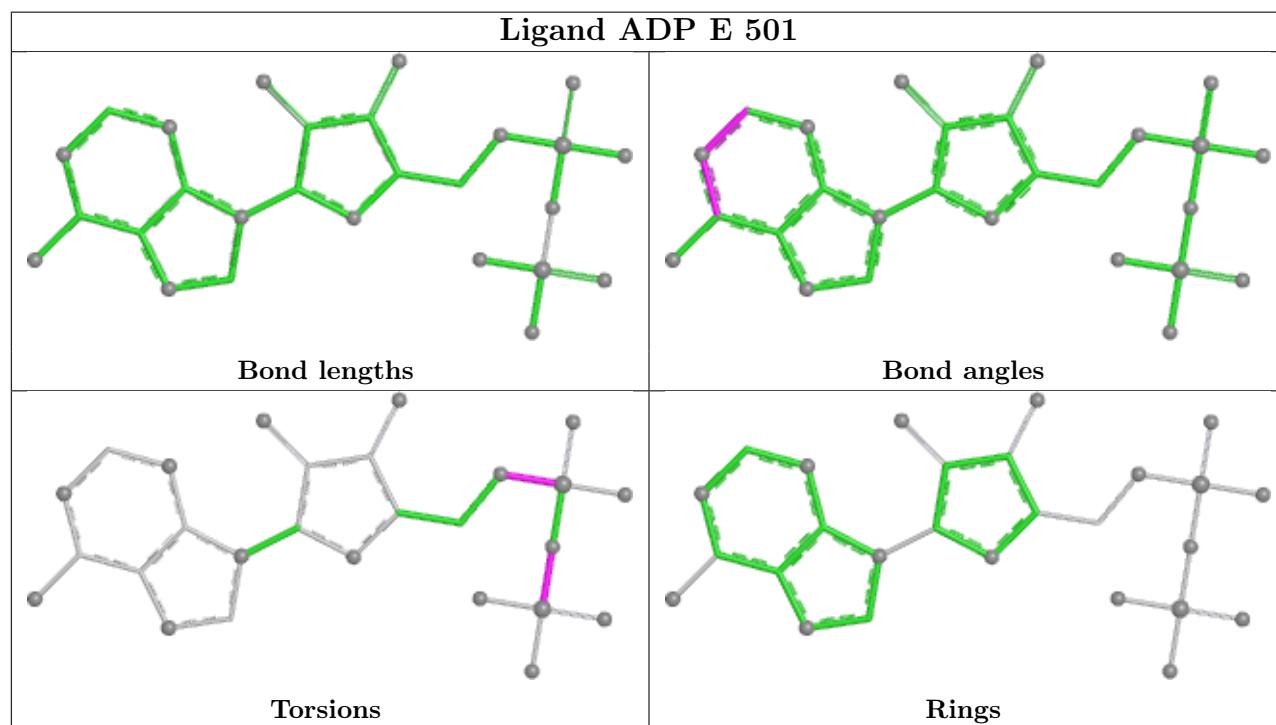
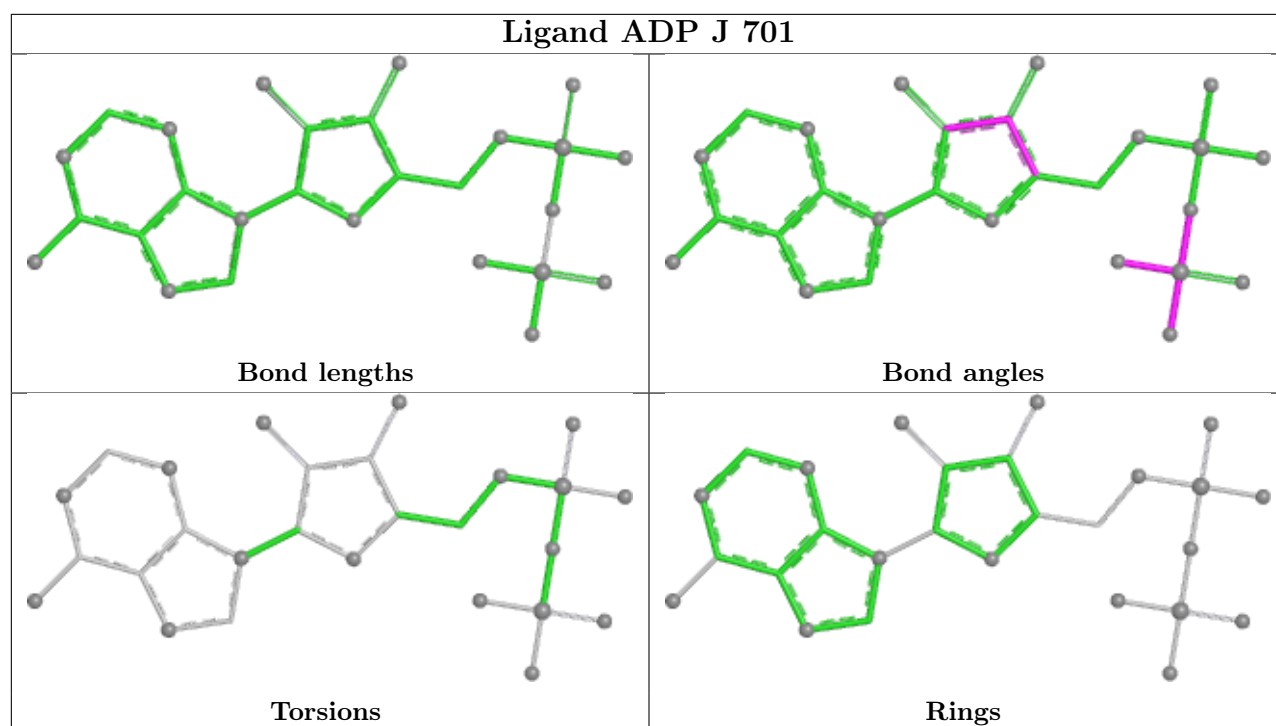
Mol	Chain	Res	Type	Atoms
14	D	501	ADP	C5'-O5'-PA-O2A
15	A	501	ATP	C5'-O5'-PA-O3A
14	G	1601	ADP	PB-O3A-PA-O1A
15	A	501	ATP	O4'-C4'-C5'-O5'
14	E	501	ADP	PA-O3A-PB-O2B
14	E	501	ADP	C5'-O5'-PA-O1A
14	D	501	ADP	C5'-O5'-PA-O1A
14	D	501	ADP	C5'-O5'-PA-O3A
15	A	501	ATP	C5'-O5'-PA-O1A
14	C	501	ADP	PA-O3A-PB-O2B
14	B	501	ADP	PA-O3A-PB-O2B
14	B	501	ADP	PA-O3A-PB-O3B
14	D	501	ADP	PB-O3A-PA-O2A
14	G	1601	ADP	PB-O3A-PA-O2A

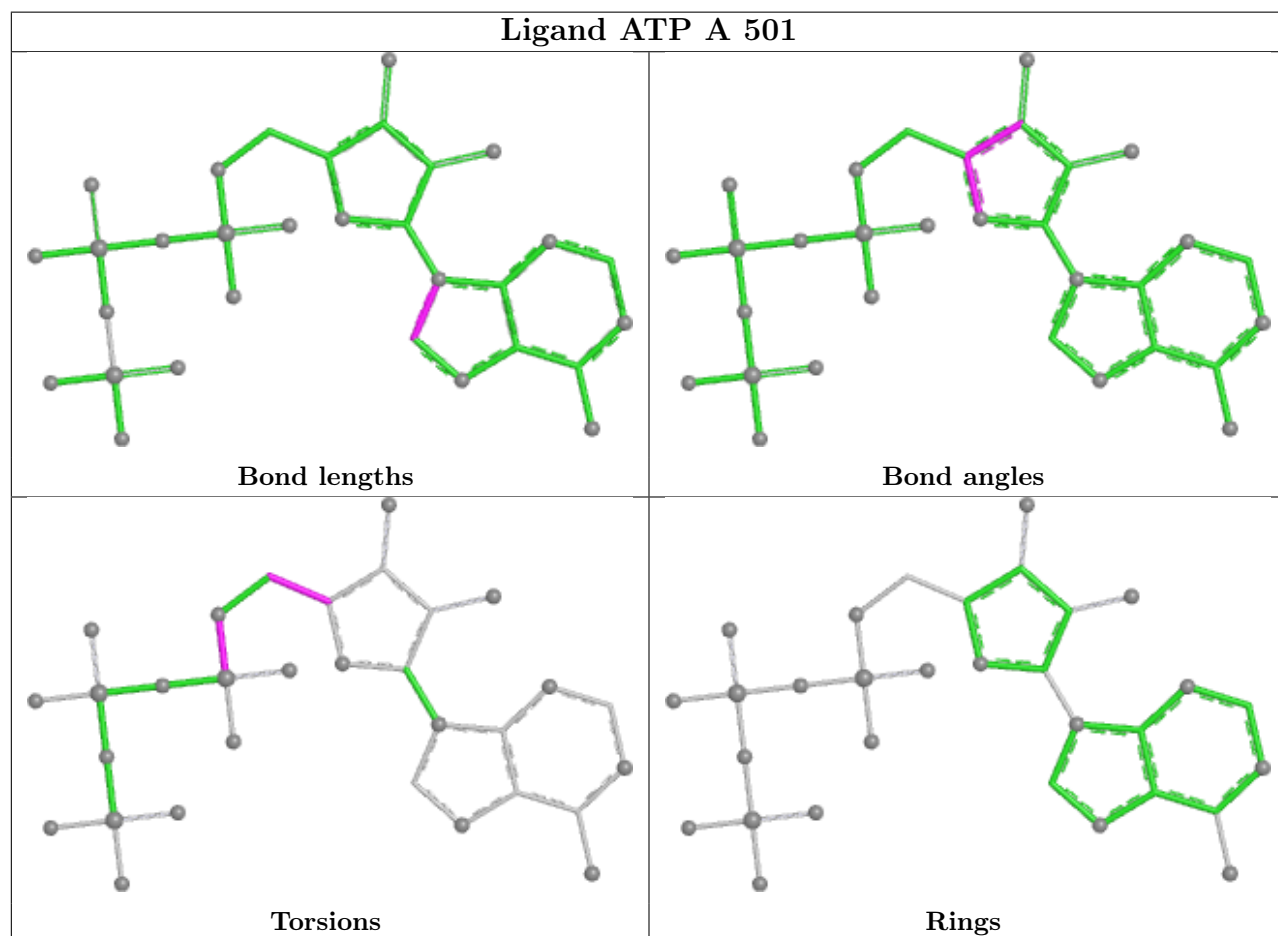
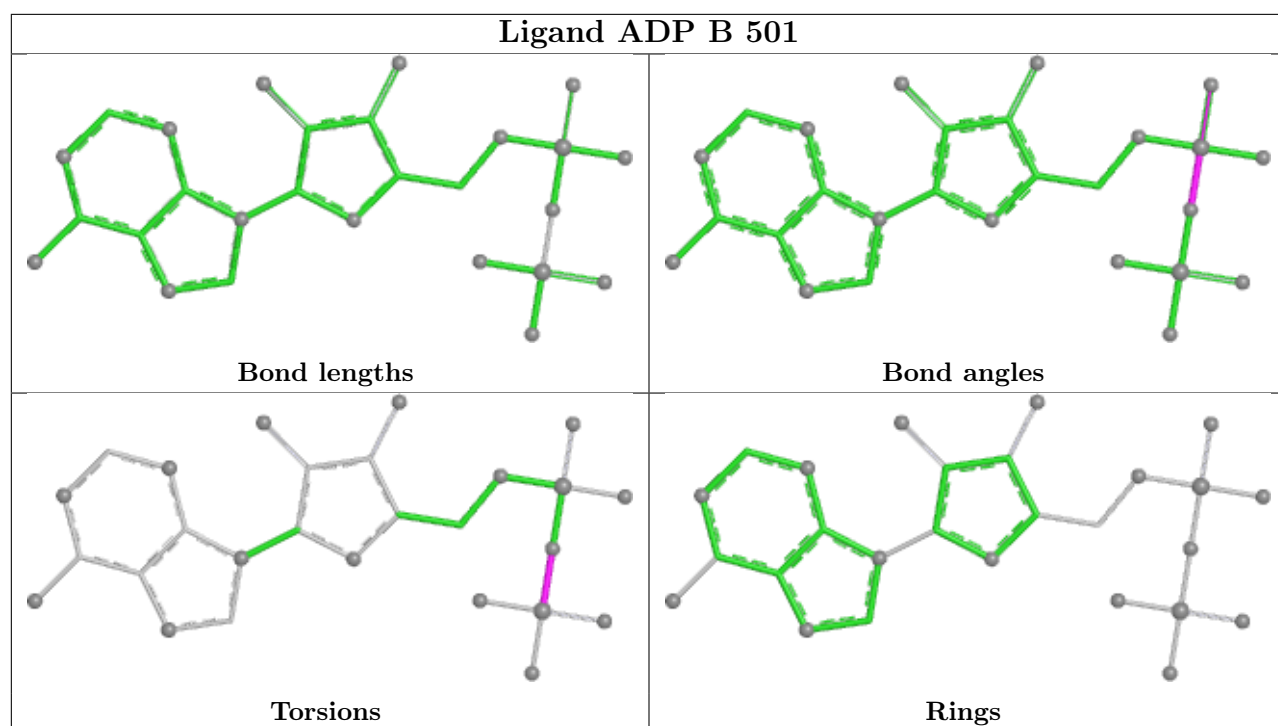
There are no ring outliers.

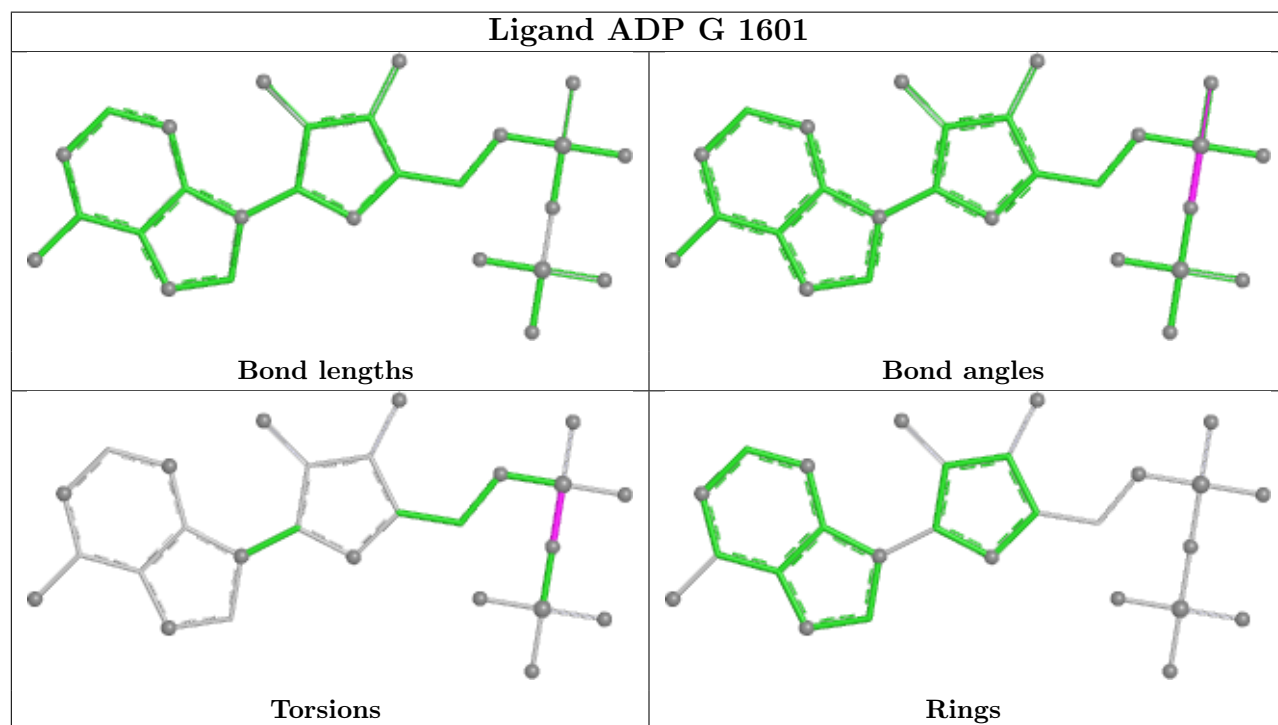
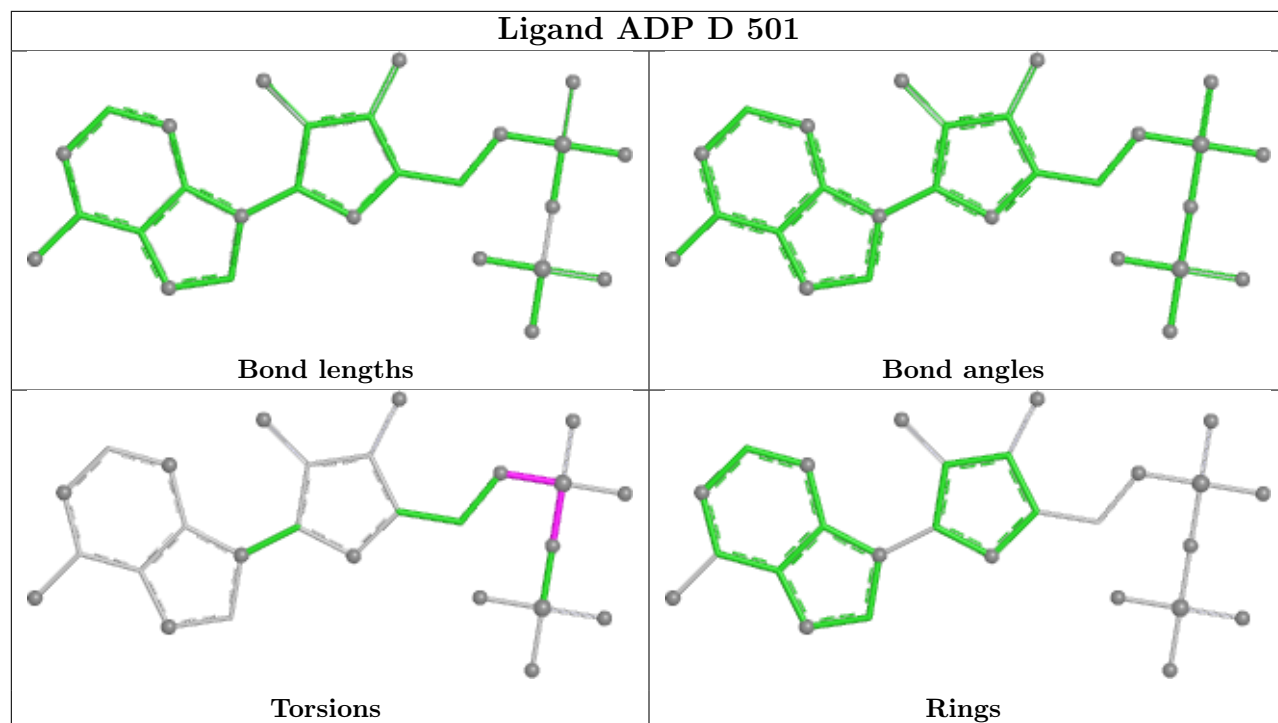
2 monomers are involved in 4 short contacts:

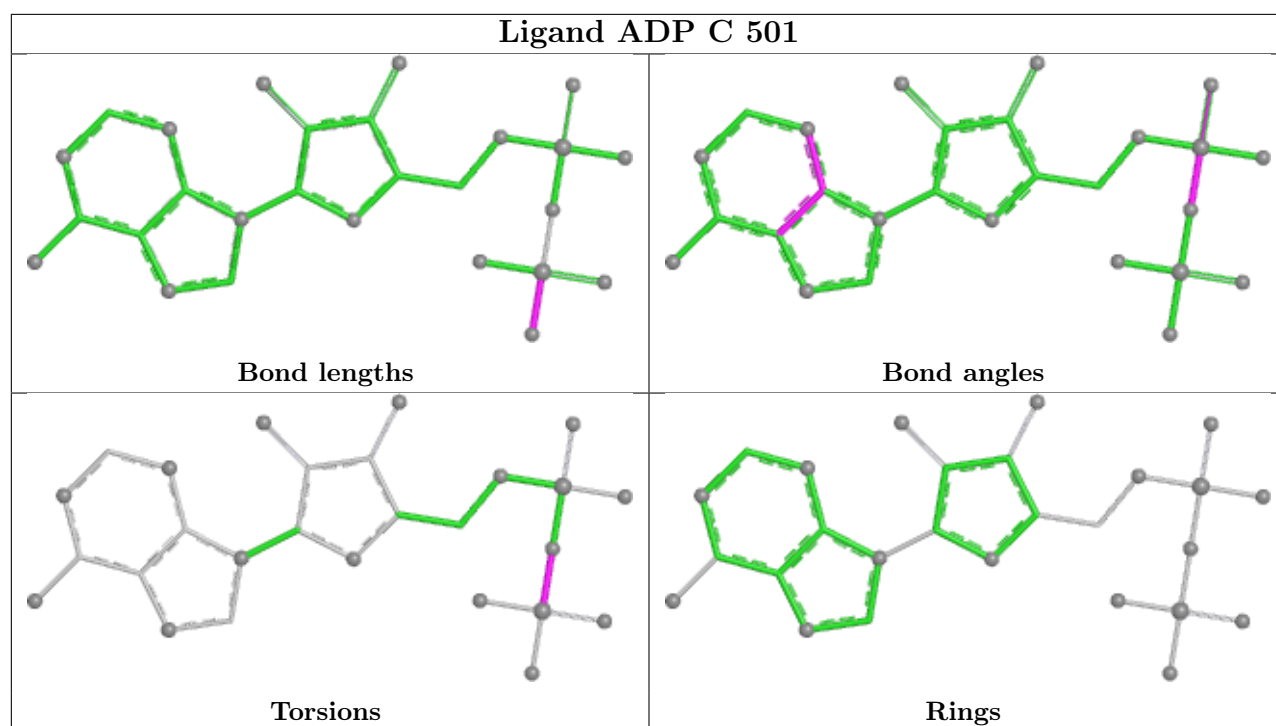
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	501	ATP	3	0
14	F	501	ADP	1	0

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.









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.

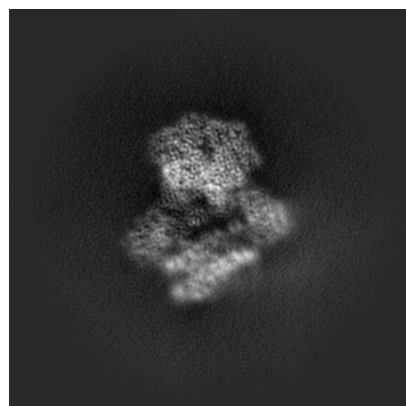
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51229. These allow visual inspection of the internal detail of the map and identification of artifacts.

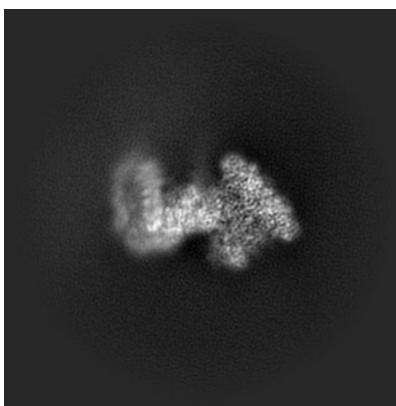
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

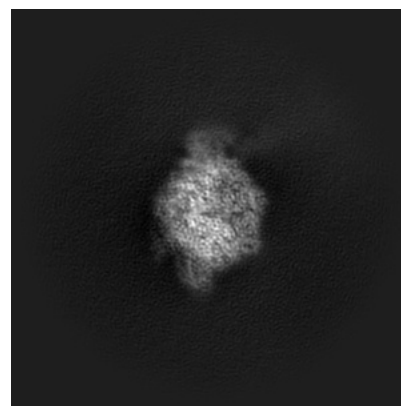
6.1.1 Primary map



X

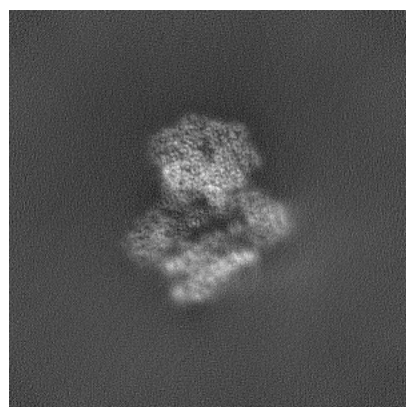


Y

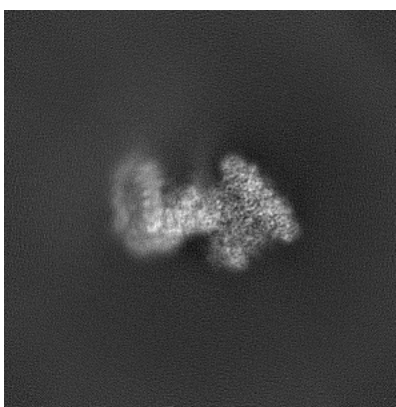


Z

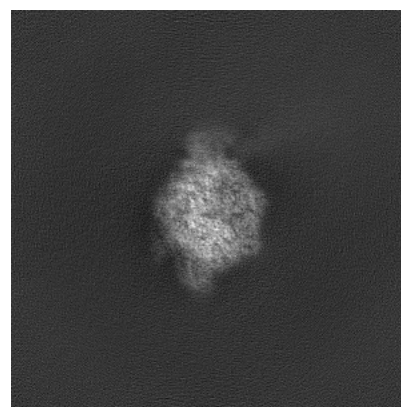
6.1.2 Raw map



X



Y

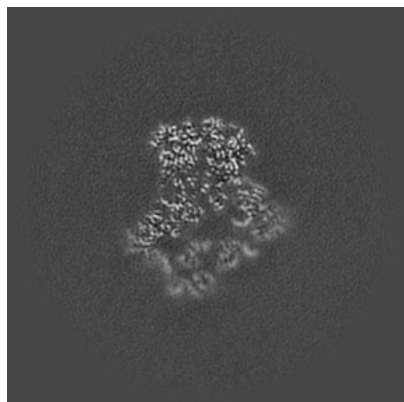


Z

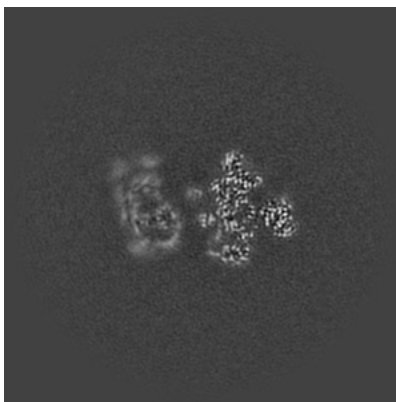
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

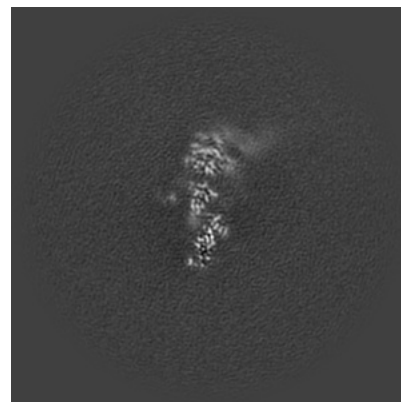
6.2.1 Primary map



X Index: 220

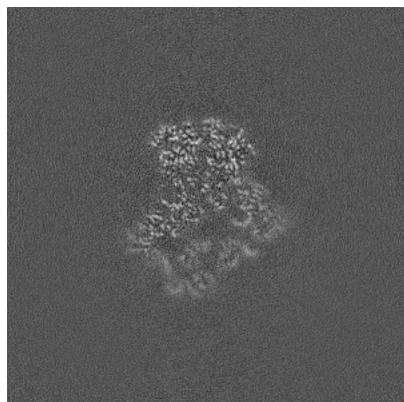


Y Index: 220

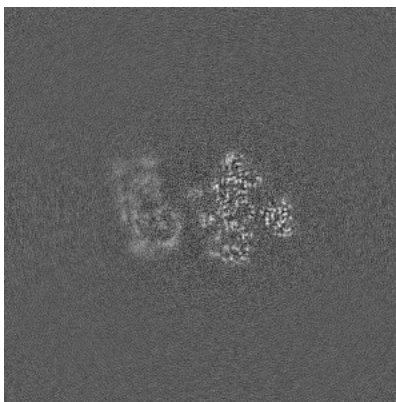


Z Index: 220

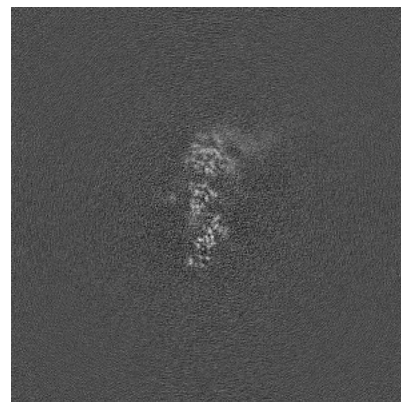
6.2.2 Raw map



X Index: 220



Y Index: 220

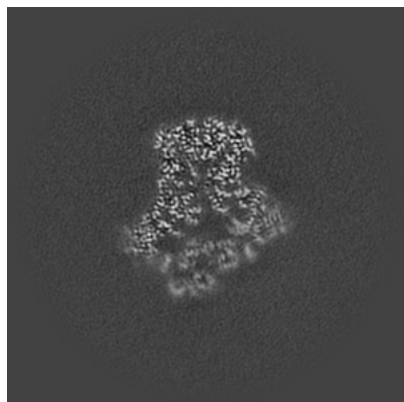


Z Index: 220

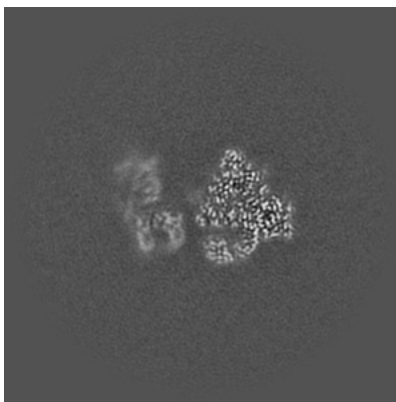
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

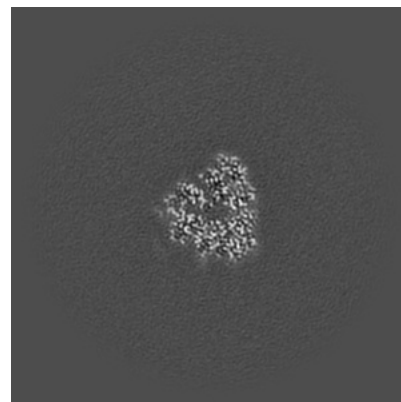
6.3.1 Primary map



X Index: 216

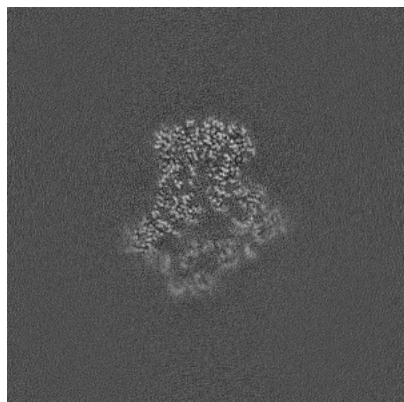


Y Index: 228

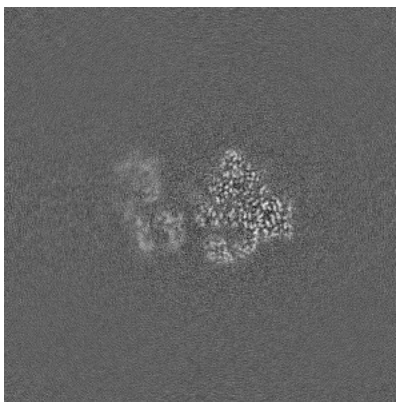


Z Index: 270

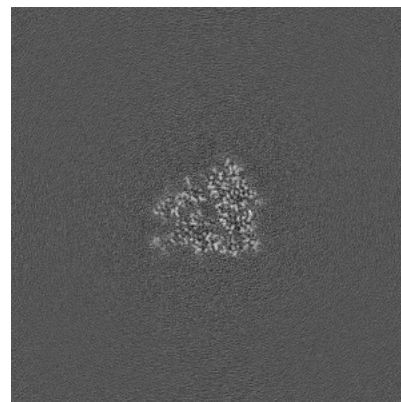
6.3.2 Raw map



X Index: 217



Y Index: 228

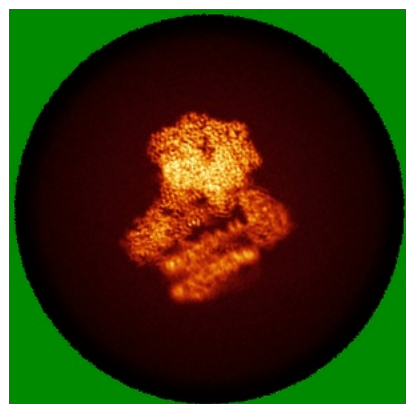


Z Index: 265

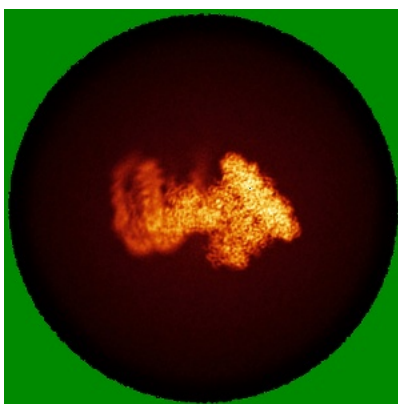
The images above show the largest variance slices of the map in three orthogonal directions.

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

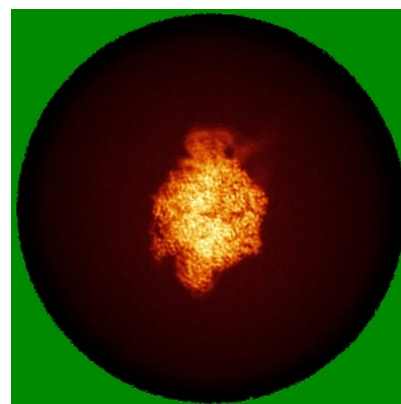
6.4.1 Primary map



X

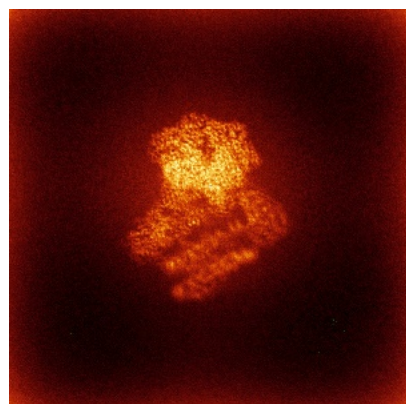


Y

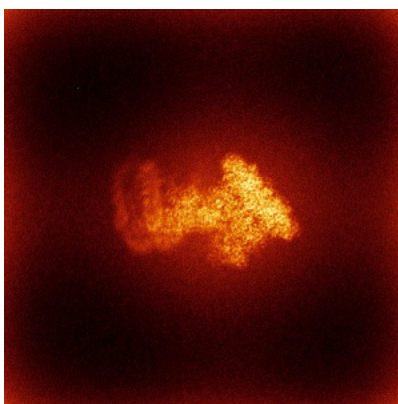


Z

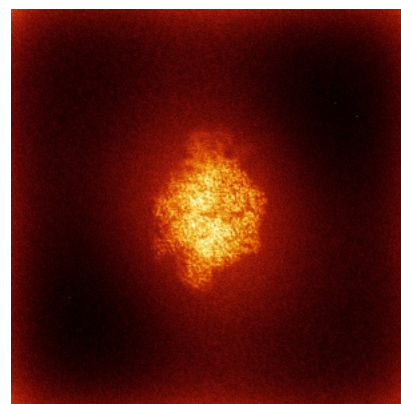
6.4.2 Raw map



X



Y

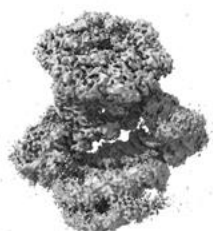


Z

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



X



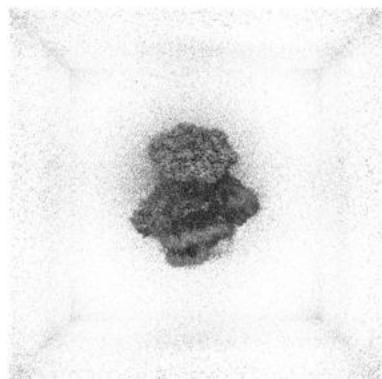
Y



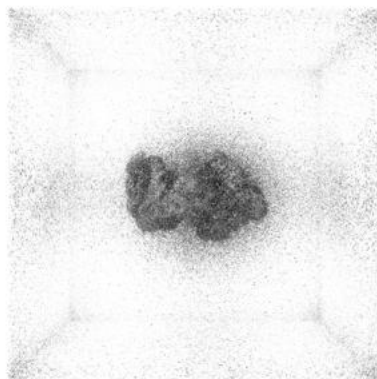
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

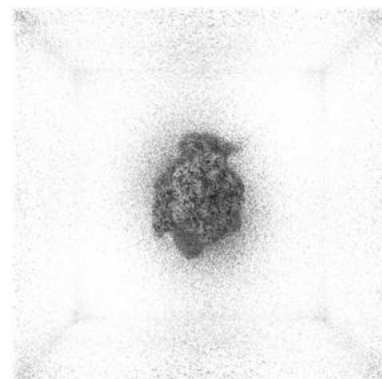
6.5.2 Raw map



X



Y



Z

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.

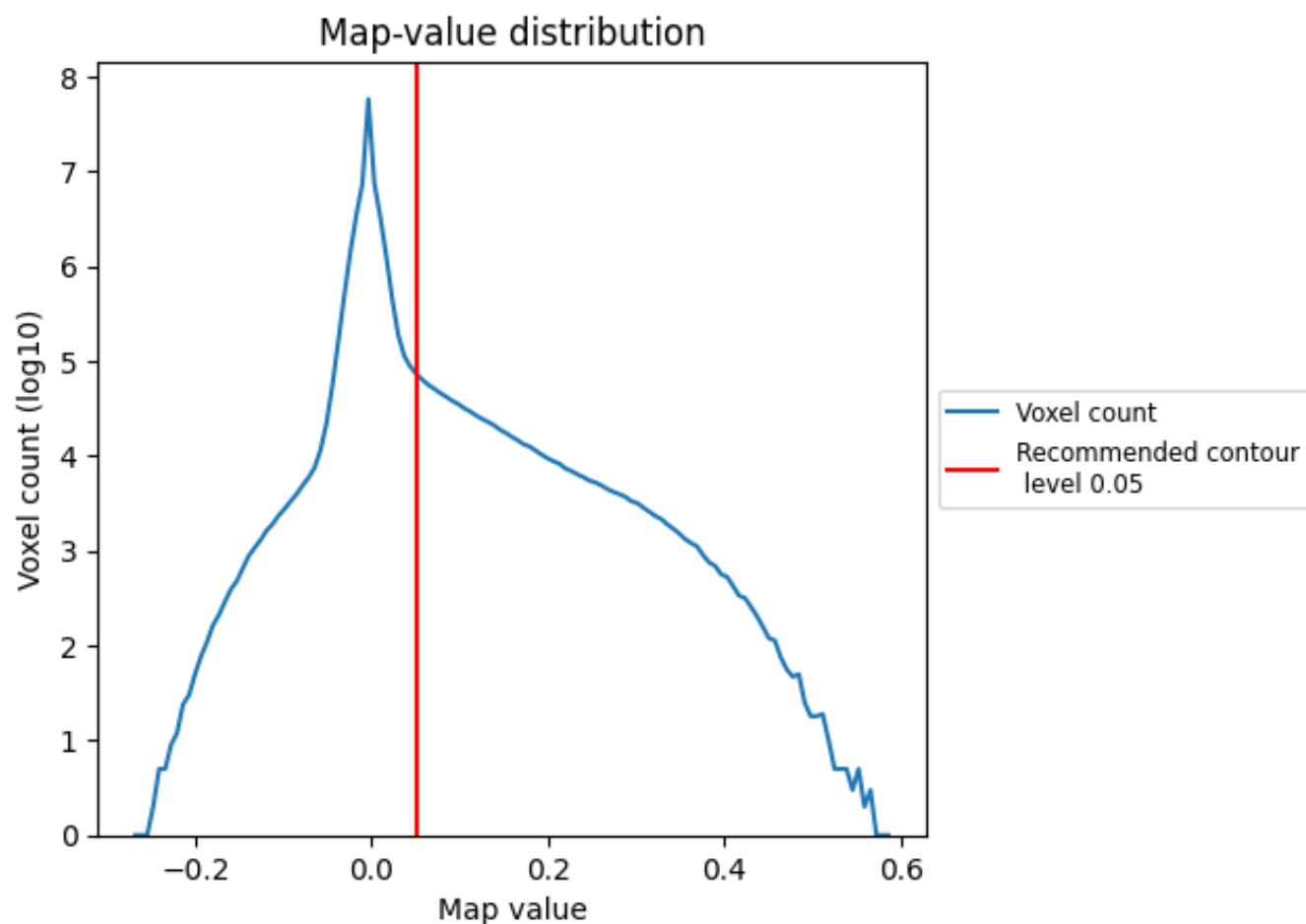
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

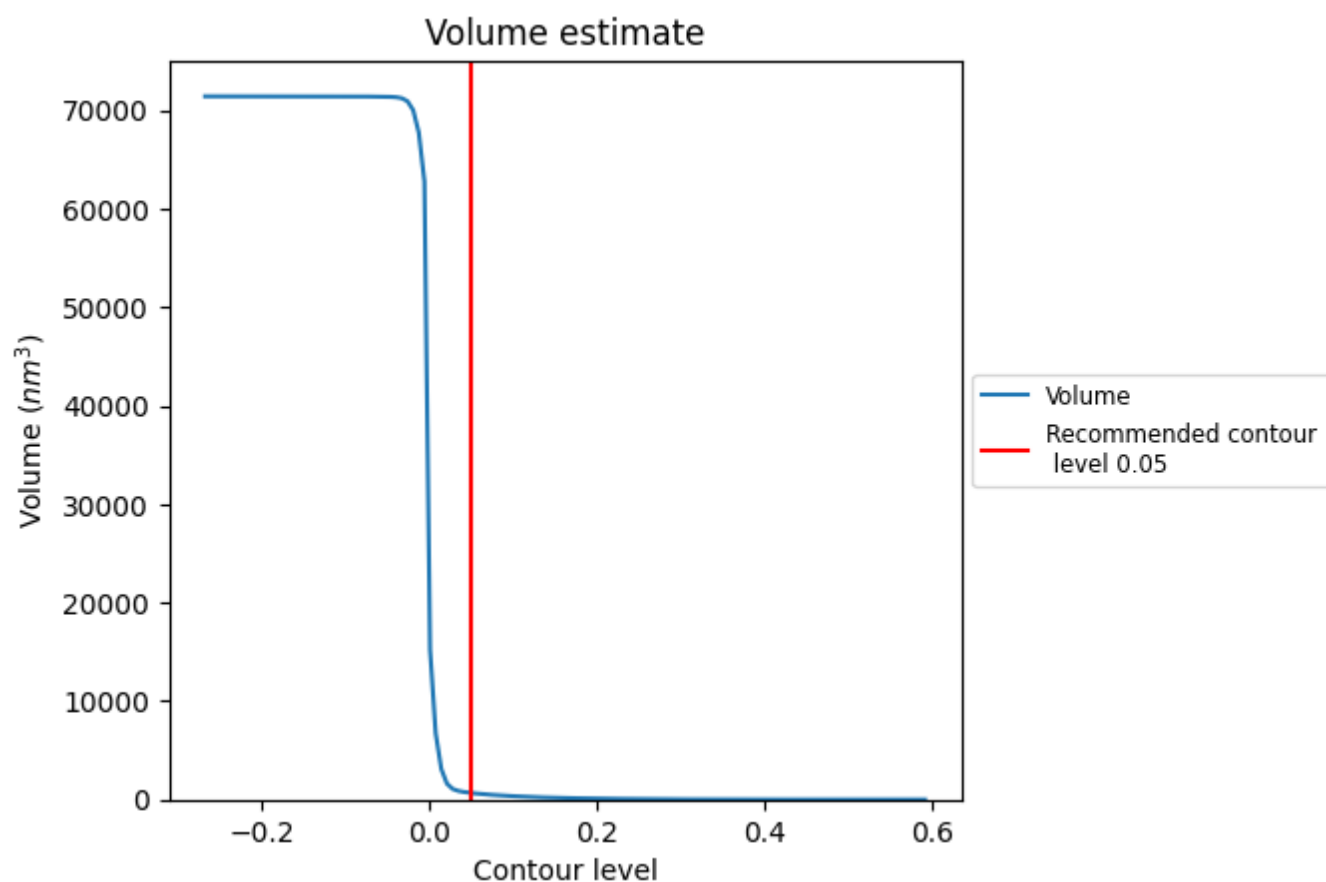
This section contains the results of statistical analysis of the map.

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.

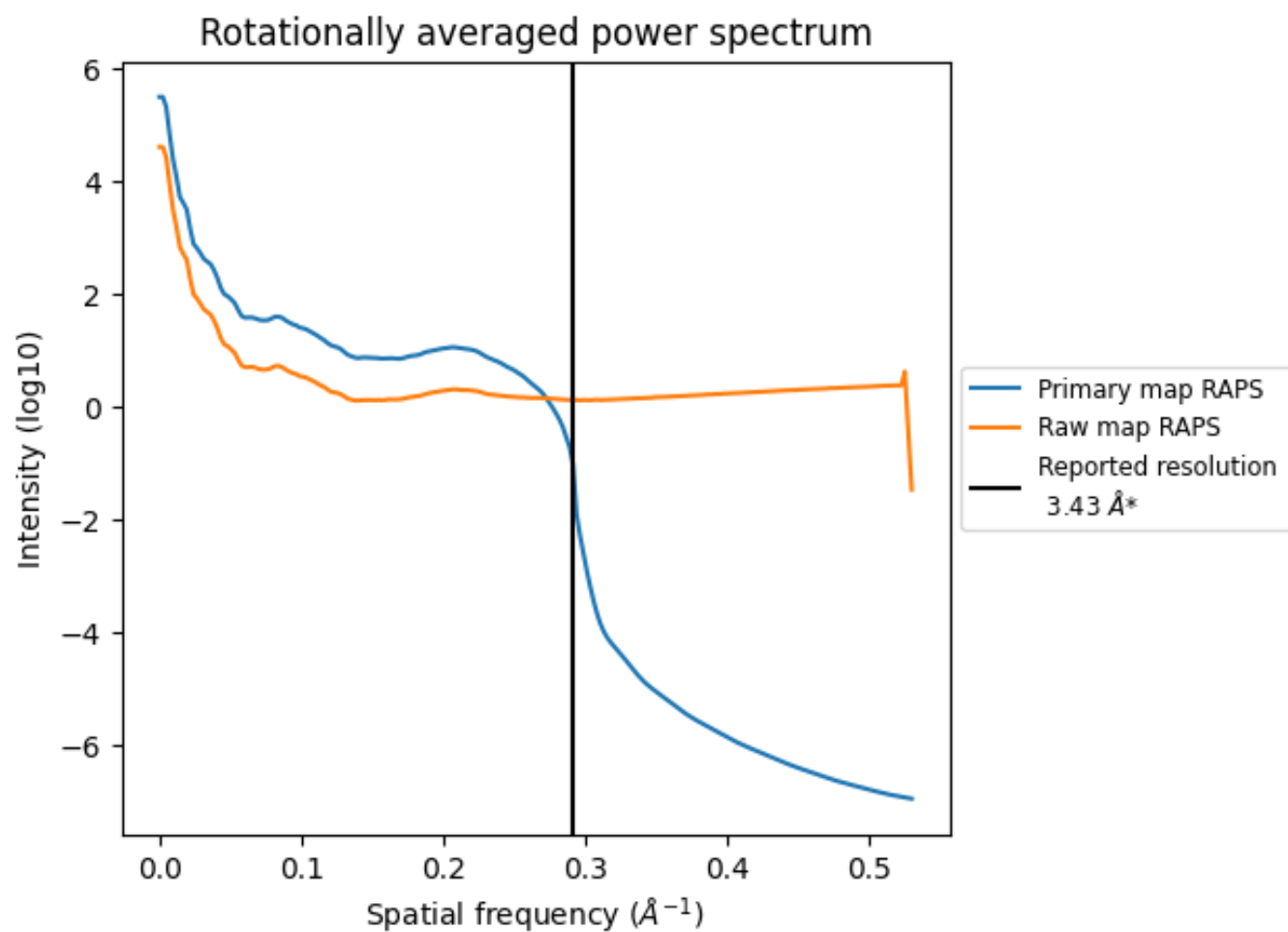
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 672 nm³; this corresponds to an approximate mass of 607 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 ⓘ

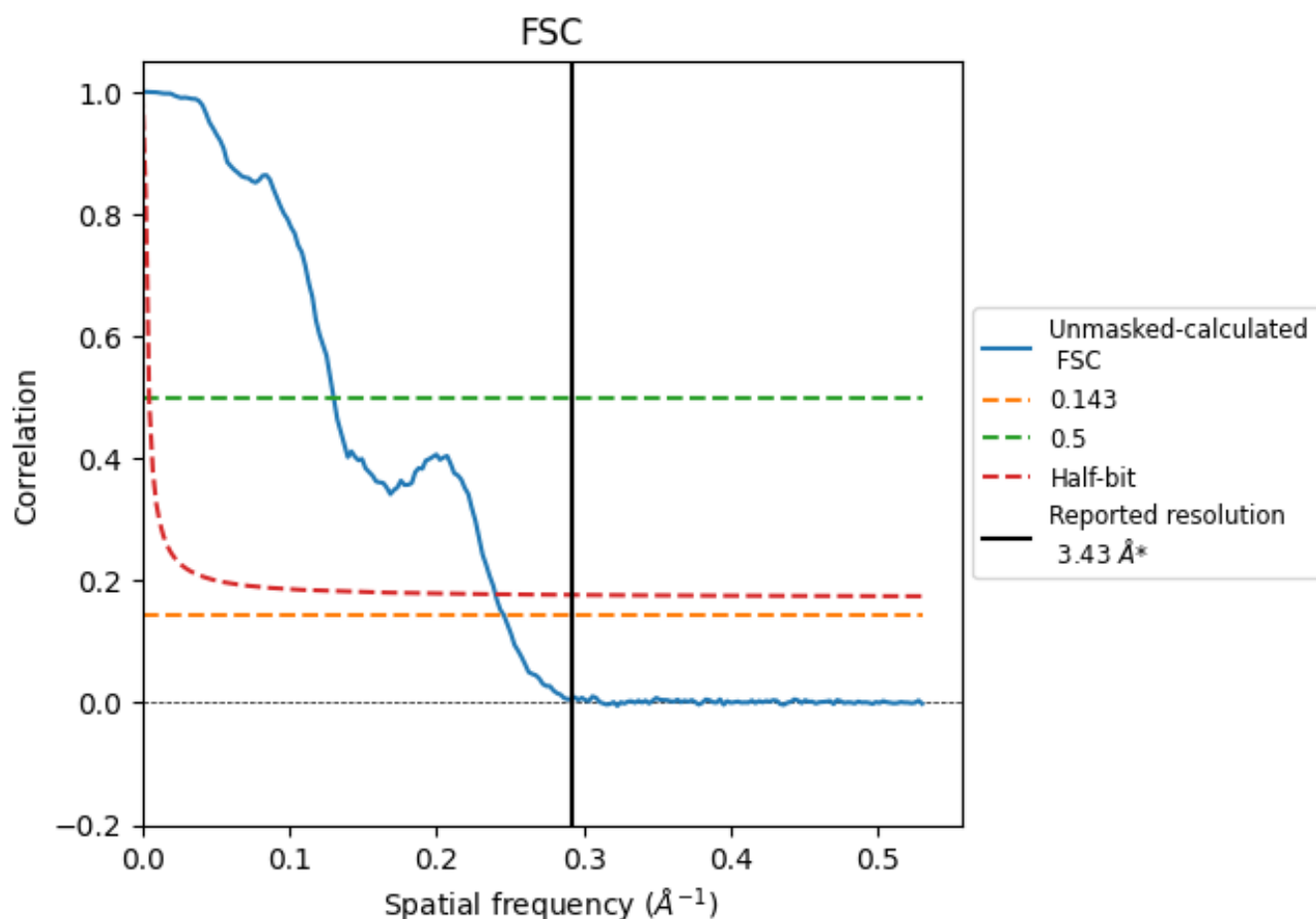


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

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 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

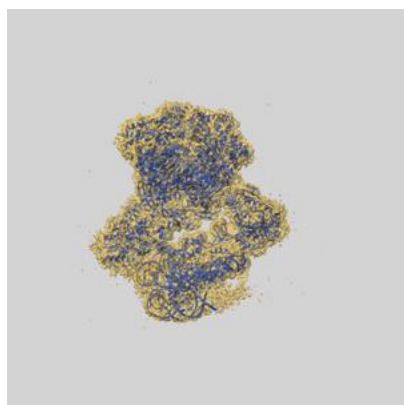
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	7.69	4.16

*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 4.07 differs from the reported value 3.43 by more than 10 %

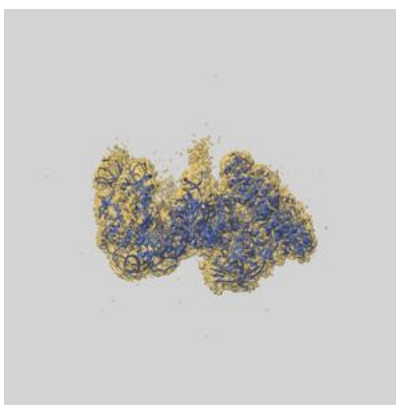
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51229 and PDB model 9GCG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

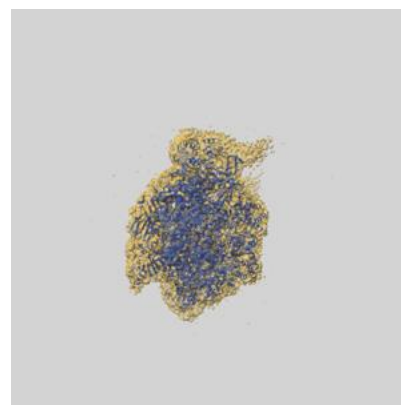
9.1 Map-model overlay [i](#)



X



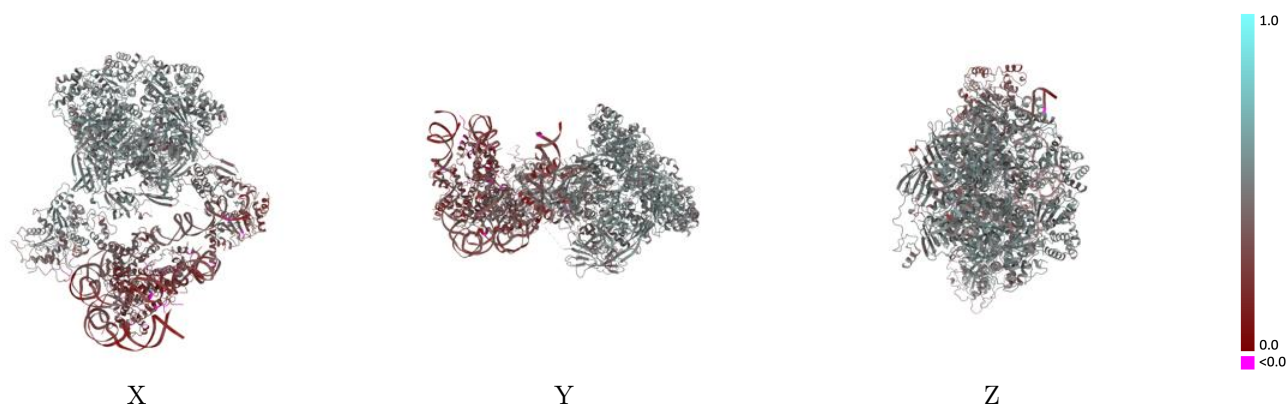
Y



Z

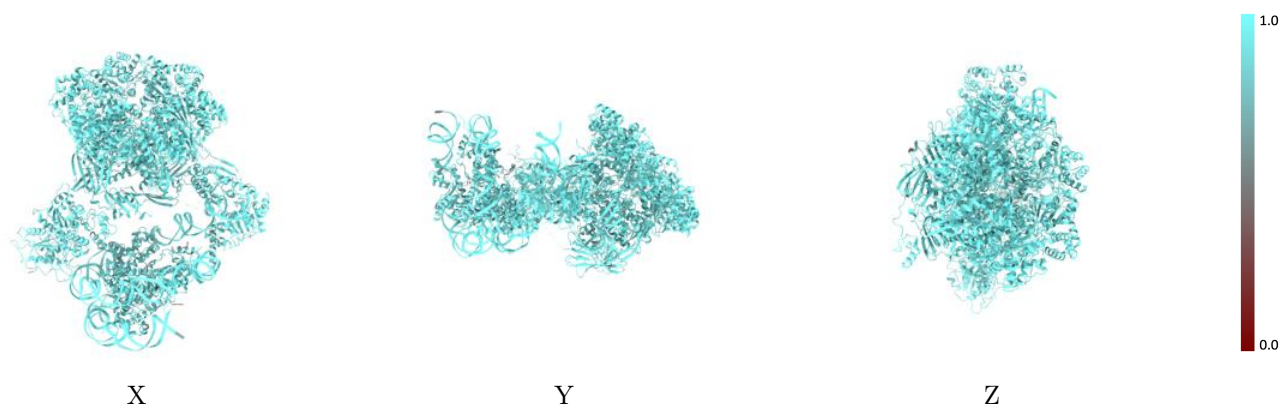
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



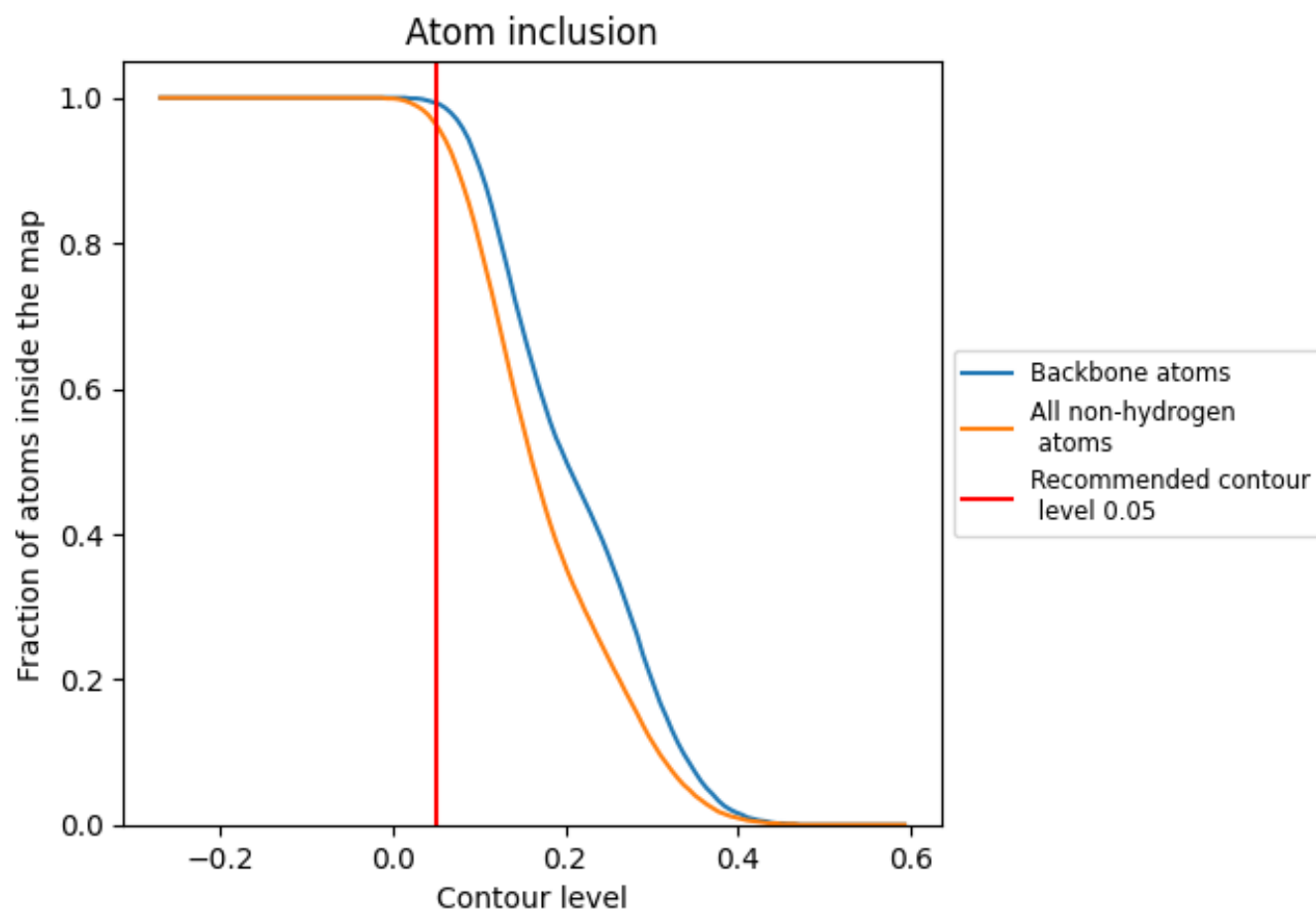
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.9640	 0.4240
A	 0.9760	 0.5130
B	 0.9760	 0.5000
C	 0.9780	 0.5050
D	 0.9780	 0.5040
E	 0.9710	 0.4980
F	 0.9760	 0.5090
G	 0.9630	 0.4200
H	 0.9590	 0.3790
I	 0.9390	 0.4440
J	 0.9650	 0.4490
K	 0.9840	 0.2780
L	 0.9910	 0.2830
M	 0.9330	 0.3190
N	 0.9320	 0.3060
O	 0.8720	 0.2420
P	 0.9150	 0.2720
Q	 0.8910	 0.2100
R	 0.9190	 0.2590
S	 0.8600	 0.3420
T	 0.9270	 0.3750

