Full wwPDB EM Validation Report (i)

Jul 7, 2024 – 02:33 pm BST

PDB ID	:	7PBJ
EMDB ID	:	EMD-13293
Title	:	Cryo-EM structure of the GroEL-GroES complex with ADP bound to both rings ("wide" conformation).
Authors	:	Pichkur, E.B.; Stanishneva-Konovalova, T.B.
Deposited on	:	2021-08-02
Resolution	:	3.40 Å(reported)
Based on initial model	:	1SX4

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 (i) 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 (1)) were used in the production of this report:

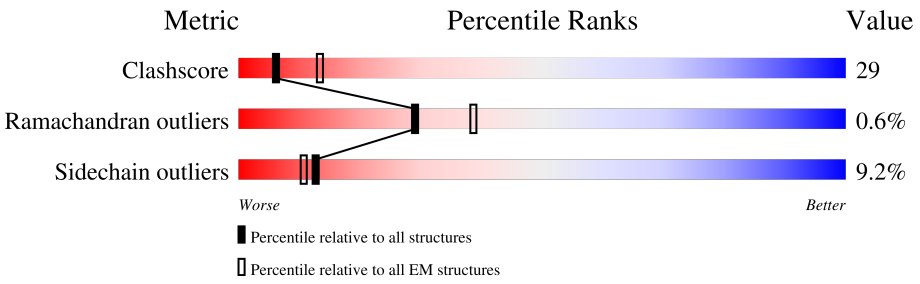
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	Ad	524	34% 85% 15% •
1	Ae	524	6% 95% 5%
1	Ak	524	34% 85% 15% •
1	Al	524	6% 95% 5%
1	Ar	524	34% 85% 15% •
1	As	524	6% 95% 5%
1	Ay	524	34% 85% 15% •
1	Az	524	6% 95% 5%

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Mol	Chain	Length	Quality of chain
1	Bf	524	34% 85% 15%
1	Bg	524	6% 95% 5%
1	Bm	524	34% 85% 15%
1	Bn	524	6% 95% 5%
1	Bt	524	34% 85% 15%
1	Bu	524	6% 95% 5%
2	Af	97	33% 89% 9%
2	Am	97	30% 89% 9%
2	At	97	30% 89% 9%
2	Ba	97	30% 89% 9%
2	Bh	97	30% 89% 9%
2	Bo	97	30% 89% 9%
2	Bv	97	30% 89% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 59486 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Ad	524	3856	2397	665	774	20	0	0
1	Ae	524	3856	2397	665	774	20	0	0
1	Ak	524	3856	2397	665	774	20	0	0
1	Al	524	3856	2397	665	774	20	0	0
1	Ar	524	3856	2397	665	774	20	0	0
1	As	524	3856	2397	665	774	20	0	0
1	Ay	524	3856	2397	665	774	20	0	0
1	Az	524	3856	2397	665	774	20	0	0
1	Bf	524	3856	2397	665	774	20	0	0
1	Bg	524	3856	2397	665	774	20	0	0
1	Bm	524	3856	2397	665	774	20	0	0
1	Bn	524	3856	2397	665	774	20	0	0
1	Bt	524	3856	2397	665	774	20	0	0
1	Bu	524	3856	2397	665	774	20	0	0

- Molecule 2 is a protein called 10 kDa chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Af	97	728	454	127	145	2	0	0

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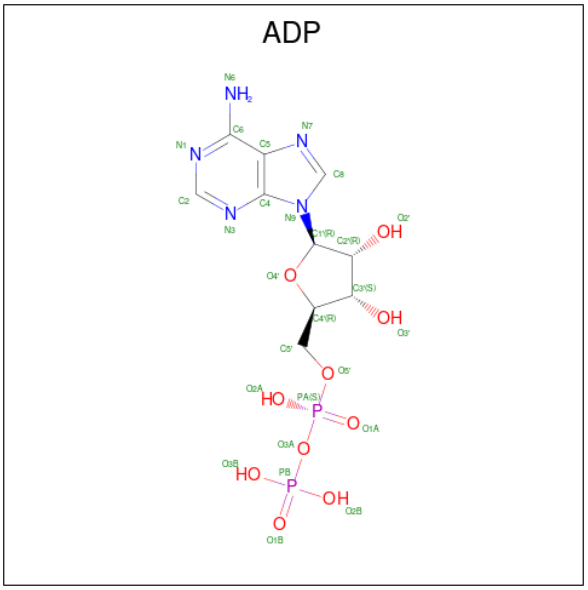
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Am	97	728	454	127	145	2	0	0
2	At	97	728	454	127	145	2	0	0
2	Ba	97	728	454	127	145	2	0	0
2	Bh	97	728	454	127	145	2	0	0
2	Bo	97	728	454	127	145	2	0	0
2	Bv	97	728	454	127	145	2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	Ad	1	27	10	5	10	2	0
3	Ae	1	27	10	5	10	2	0
3	Ak	1	27	10	5	10	2	0
3	Al	1	27	10	5	10	2	0
3	Ar	1	27	10	5	10	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	As	1	27	10	5	10	2	0
3	Ay	1	27	10	5	10	2	0
3	Az	1	27	10	5	10	2	0
3	Bf	1	27	10	5	10	2	0
3	Bg	1	27	10	5	10	2	0
3	Bm	1	27	10	5	10	2	0
3	Bn	1	27	10	5	10	2	0
3	Bt	1	27	10	5	10	2	0
3	Bu	1	27	10	5	10	2	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	Ad	1	1	1	0
4	Ae	1	1	1	0
4	Ak	1	1	1	0
4	Al	1	1	1	0
4	Ar	1	1	1	0
4	As	1	1	1	0
4	Ay	1	1	1	0
4	Az	1	1	1	0
4	Bf	1	1	1	0
4	Bg	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	Bm	1	1	1	0
4	Bn	1	1	1	0
4	Bt	1	1	1	0
4	Bu	1	1	1	0

- Molecule 5 is water.

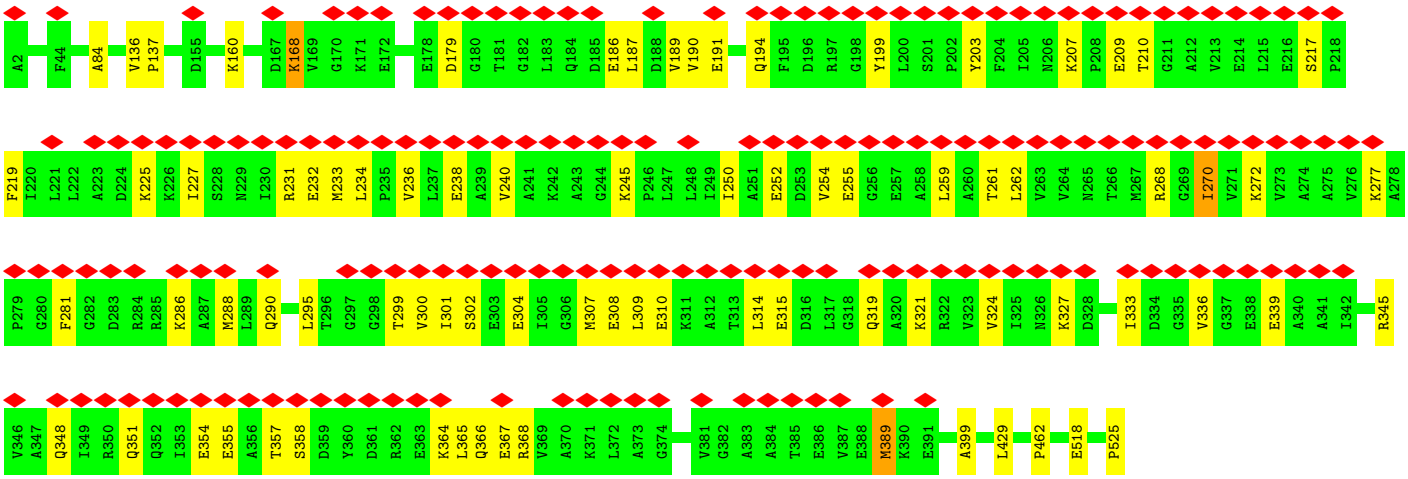
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	Ad	2	2	2	0
5	Ak	2	2	2	0
5	Ar	2	2	2	0
5	Ay	2	2	2	0
5	Bf	2	2	2	0
5	Bm	2	2	2	0
5	Bt	2	2	2	0

3 Residue-property plots (i)

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

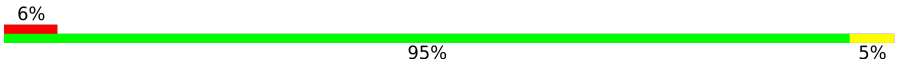
- Molecule 1: 60 kDa chaperonin

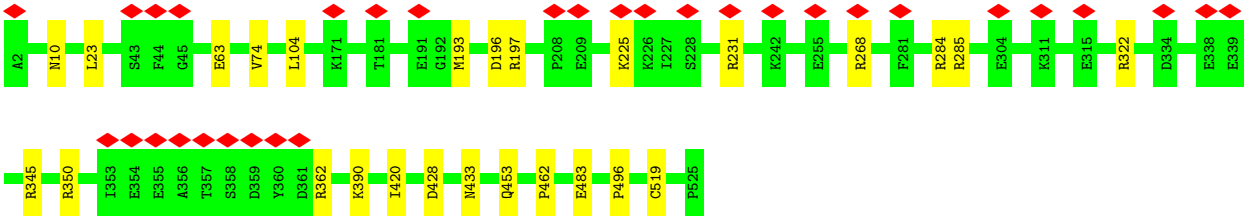
Chain Ad:



- Molecule 1: 60 kDa chaperonin

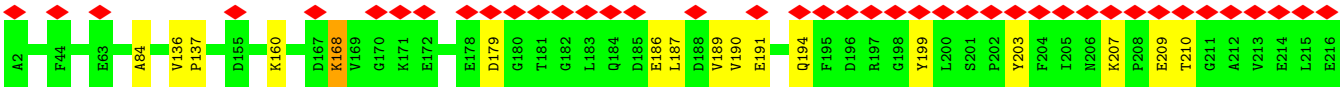
Chain Ae:

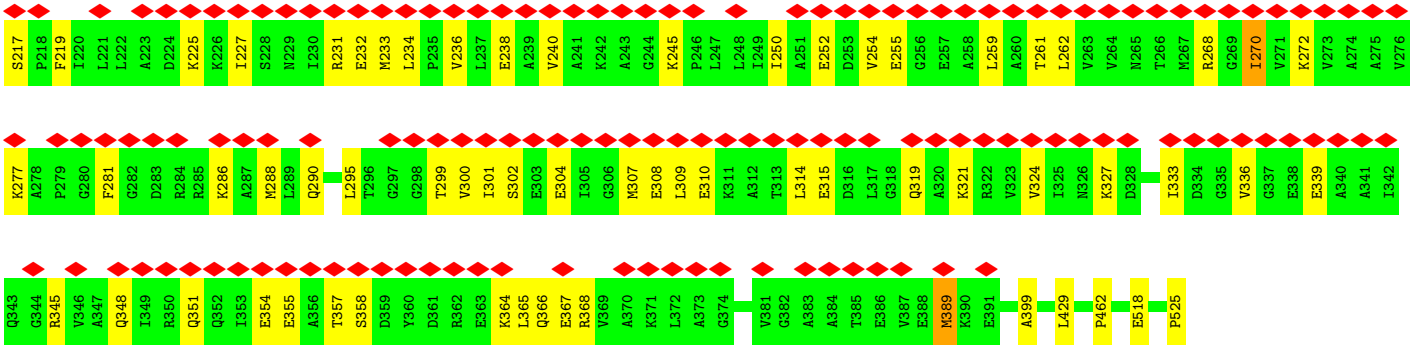




- Molecule 1: 60 kDa chaperonin

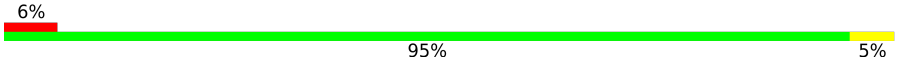
Chain Ak:

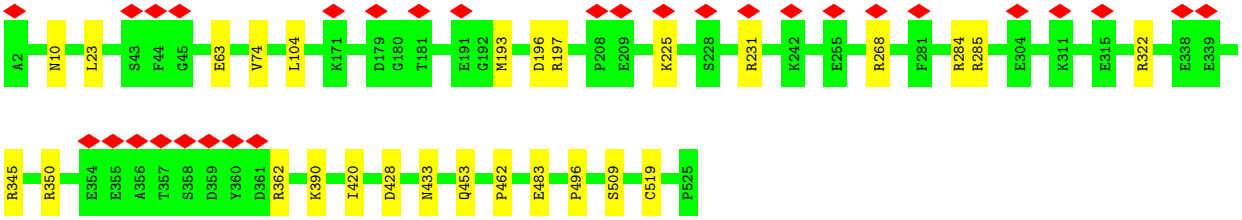




- Molecule 1: 60 kDa chaperonin

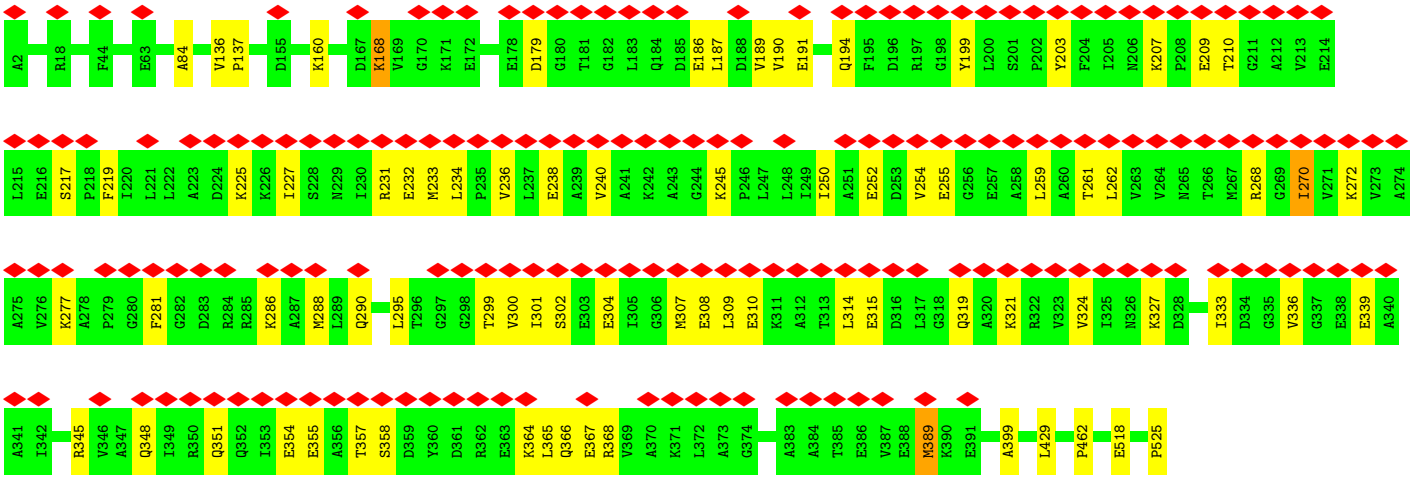
Chain Al:





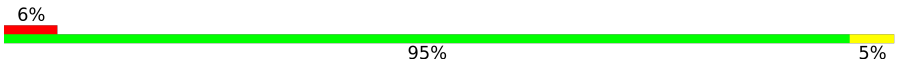
- Molecule 1: 60 kDa chaperonin

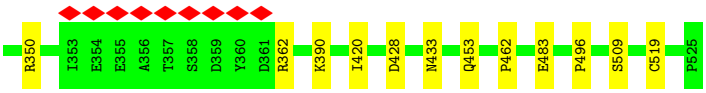
Chain Ar:



- Molecule 1: 60 kDa chaperonin

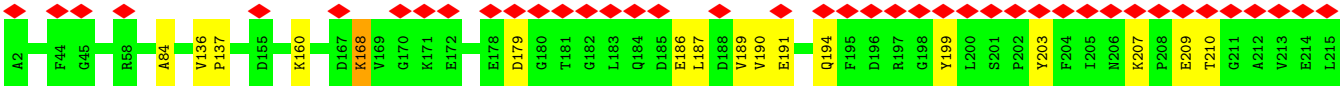
Chain As:

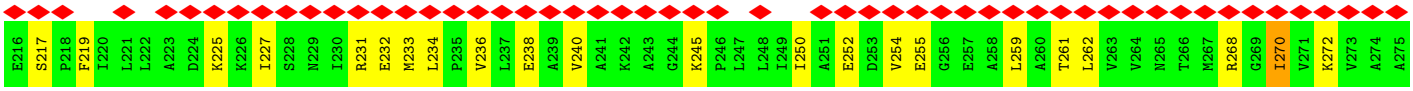


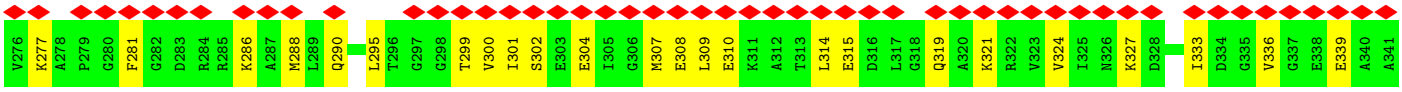


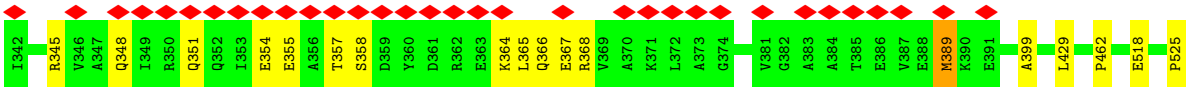
- Molecule 1: 60 kDa chaperonin

Chain Ay:



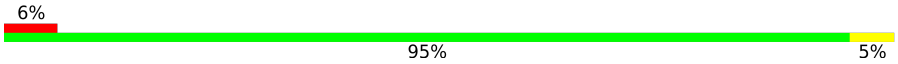


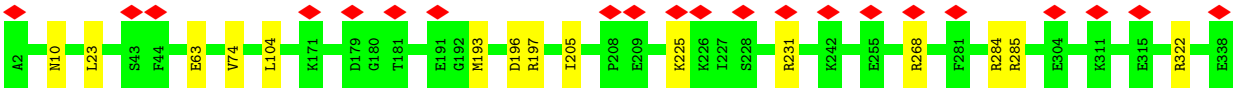


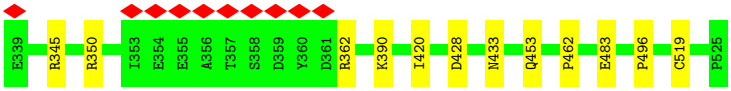


- Molecule 1: 60 kDa chaperonin

Chain Az:

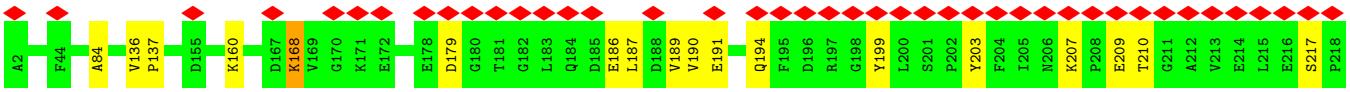


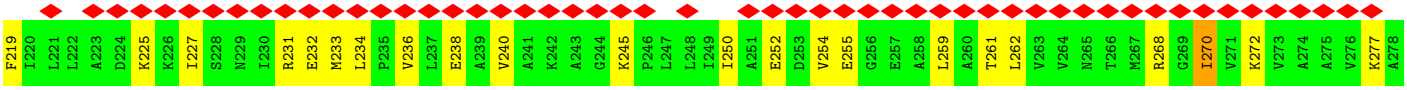


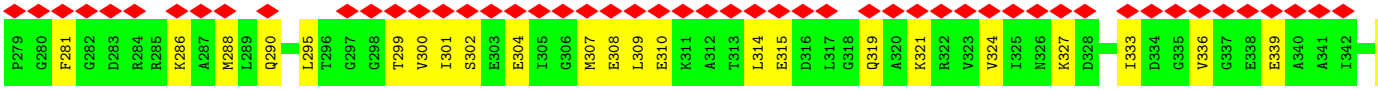


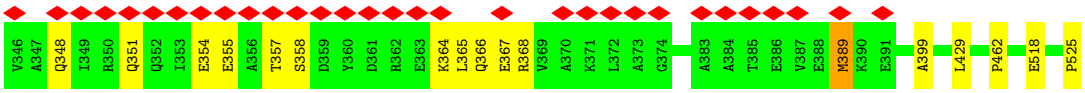
- Molecule 1: 60 kDa chaperonin

Chain Bf:



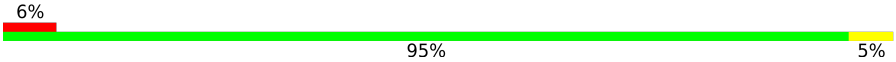


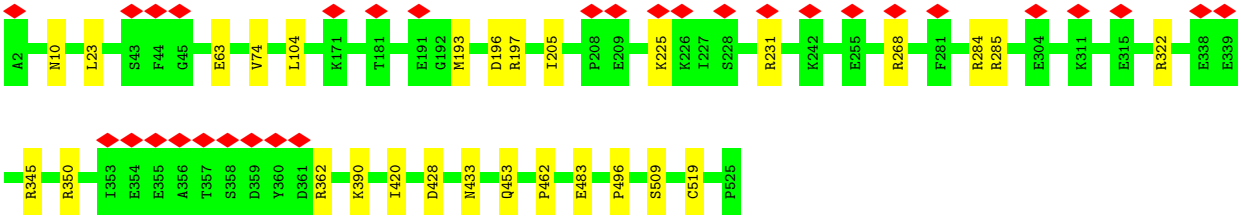




• Molecule 1: 60 kDa chaperonin

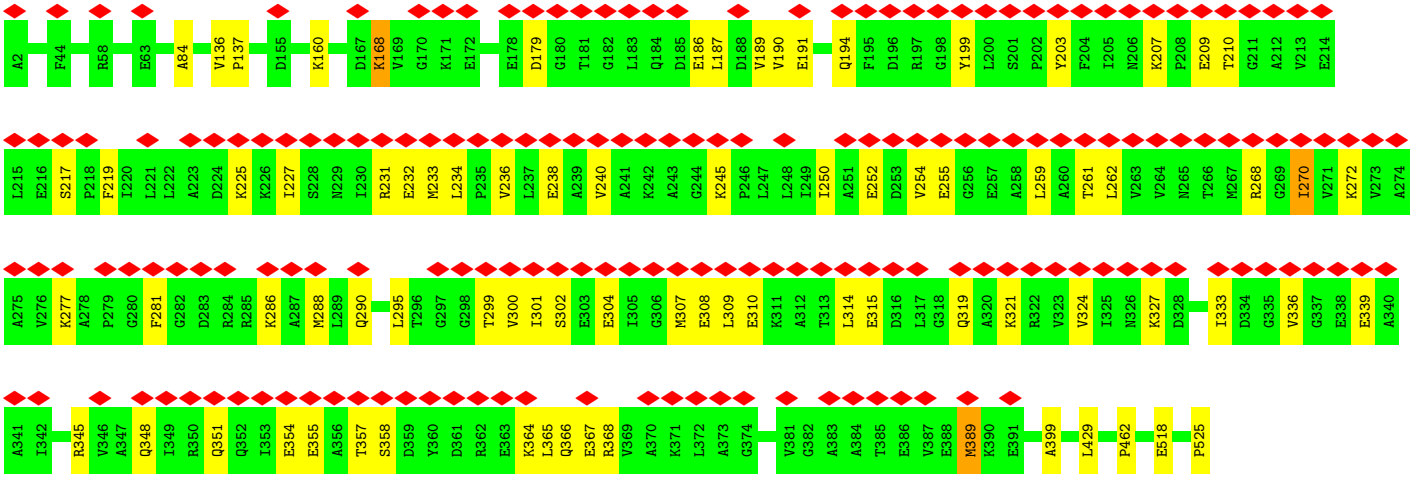
Chain Bg:





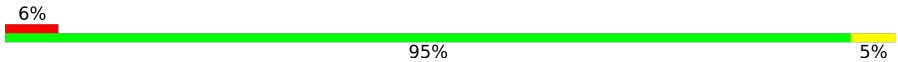
• Molecule 1: 60 kDa chaperonin

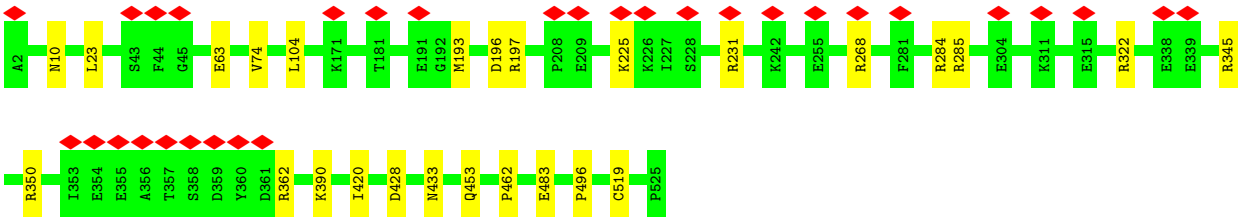
Chain Bm:



• Molecule 1: 60 kDa chaperonin

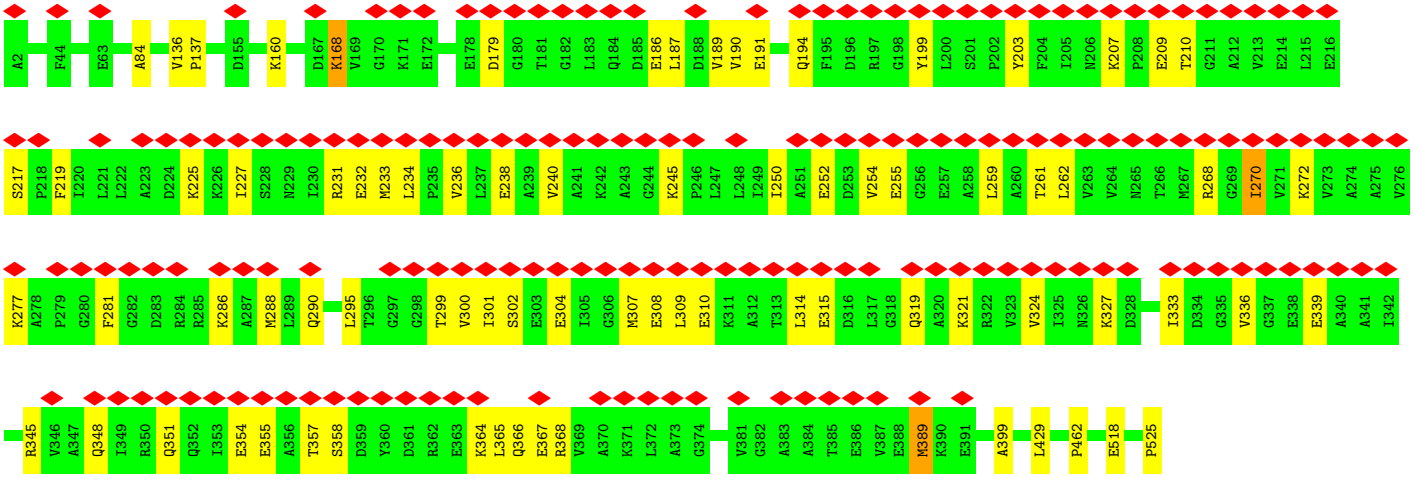
Chain Bn:





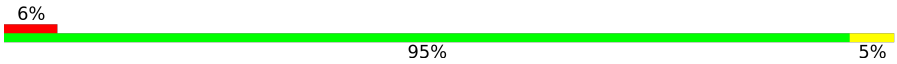
• Molecule 1: 60 kDa chaperonin

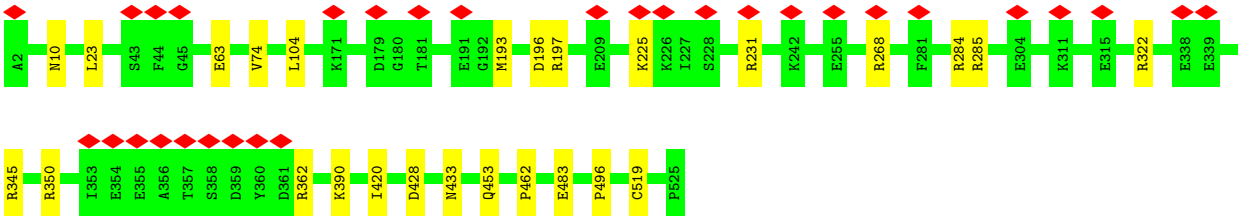
Chain Bt:



- Molecule 1: 60 kDa chaperonin

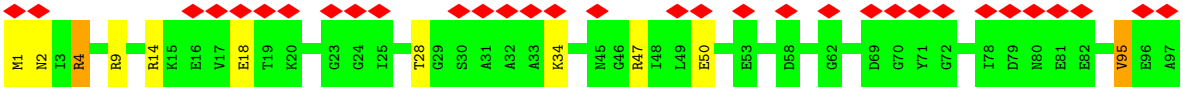
Chain Bu:





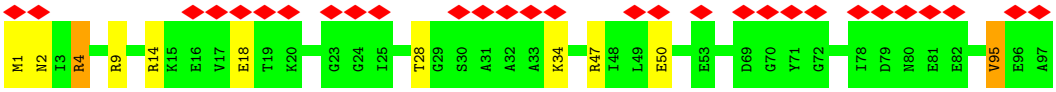
- Molecule 2: 10 kDa chaperonin

Chain Af:



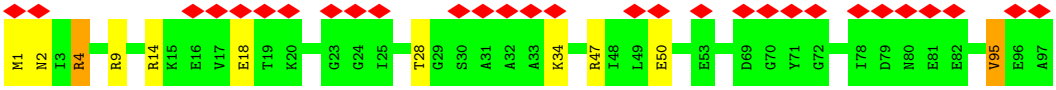
- Molecule 2: 10 kDa chaperonin

Chain Am:



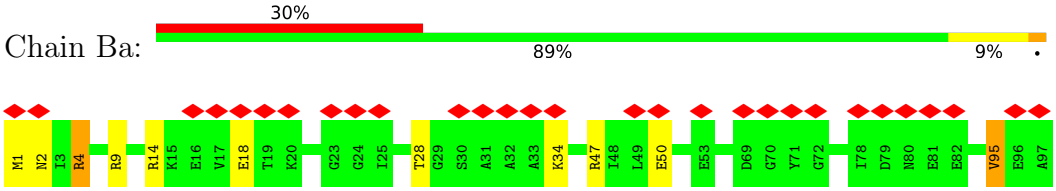
- Molecule 2: 10 kDa chaperonin

Chain At:



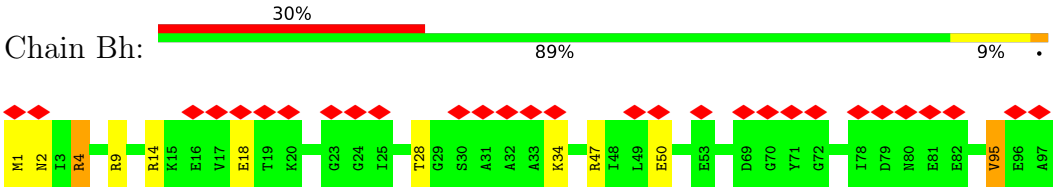
- Molecule 2: 10 kDa chaperonin

Chain Ba:



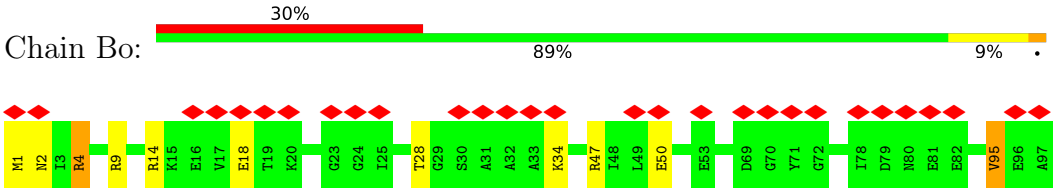
- Molecule 2: 10 kDa chaperonin

Chain Bh:



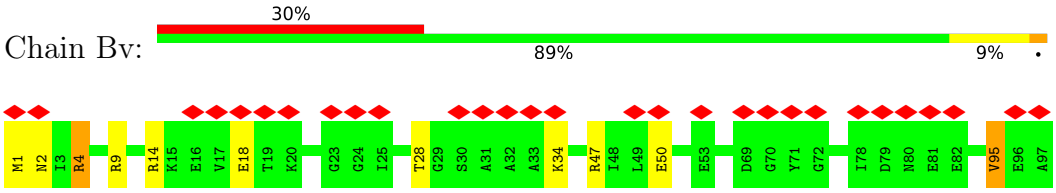
- Molecule 2: 10 kDa chaperonin

Chain Bo:



- Molecule 2: 10 kDa chaperonin

Chain Bv:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	41000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	6.071	Depositor
Minimum map value	-1.209	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	425.088, 425.088, 425.088	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.107, 1.107, 1.107	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	Ad	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	Ae	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
1	Ak	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	Al	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
1	Ar	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	As	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
1	Ay	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	Az	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
1	Bf	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	Bg	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
1	Bm	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	Bn	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
1	Bt	1.02	4/3884 (0.1%)	0.92	14/5243 (0.3%)
1	Bu	0.68	2/3884 (0.1%)	0.94	13/5243 (0.2%)
2	Af	0.77	0/732	1.25	5/983 (0.5%)
2	Am	0.77	0/732	1.25	5/983 (0.5%)
2	At	0.77	0/732	1.25	5/983 (0.5%)
2	Ba	0.77	0/732	1.25	5/983 (0.5%)
2	Bh	0.77	0/732	1.25	5/983 (0.5%)
2	Bo	0.77	0/732	1.25	5/983 (0.5%)
2	Bv	0.77	0/732	1.25	5/983 (0.5%)
All	All	0.86	42/59500 (0.1%)	0.96	224/80283 (0.3%)

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	Ad	0	1
1	Ae	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ak	0	1
1	Al	0	1
1	Ar	0	1
1	As	0	1
1	Ay	0	1
1	Az	0	1
1	Bf	0	1
1	Bg	0	1
1	Bm	0	1
1	Bn	0	1
1	Bt	0	1
1	Bu	0	1
2	Af	0	2
2	Am	0	2
2	At	0	2
2	Ba	0	2
2	Bh	0	2
2	Bo	0	2
2	Bv	0	2
All	All	0	28

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ay	525	PRO	C-O	49.36	2.21	1.23
1	Ad	525	PRO	C-O	49.35	2.21	1.23
1	Bt	525	PRO	C-O	49.35	2.21	1.23
1	Bm	525	PRO	C-O	49.35	2.21	1.23
1	Ak	525	PRO	C-O	49.34	2.21	1.23
1	Bf	525	PRO	C-O	49.34	2.21	1.23
1	Ar	525	PRO	C-O	49.32	2.21	1.23
1	Al	462	PRO	N-CD	-8.78	1.35	1.47
1	Bg	462	PRO	N-CD	-8.73	1.35	1.47
1	Az	462	PRO	N-CD	-8.73	1.35	1.47
1	Bn	462	PRO	N-CD	-8.72	1.35	1.47
1	Ae	462	PRO	N-CD	-8.72	1.35	1.47
1	Bu	462	PRO	N-CD	-8.71	1.35	1.47
1	As	462	PRO	N-CD	-8.70	1.35	1.47
1	Bn	496	PRO	N-CD	-8.16	1.36	1.47
1	Bg	496	PRO	N-CD	-8.15	1.36	1.47
1	Bu	496	PRO	N-CD	-8.13	1.36	1.47
1	Al	496	PRO	N-CD	-8.13	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	As	496	PRO	N-CD	-8.13	1.36	1.47
1	Ae	496	PRO	N-CD	-8.12	1.36	1.47
1	Az	496	PRO	N-CD	-8.11	1.36	1.47
1	Bf	189	VAL	C-N	6.86	1.49	1.34
1	Bm	189	VAL	C-N	6.83	1.49	1.34
1	Ad	189	VAL	C-N	6.83	1.49	1.34
1	Bt	189	VAL	C-N	6.82	1.49	1.34
1	Ak	189	VAL	C-N	6.82	1.49	1.34
1	Ay	189	VAL	C-N	6.82	1.49	1.34
1	Ar	189	VAL	C-N	6.81	1.49	1.34
1	Ar	137	PRO	N-CD	-6.72	1.38	1.47
1	Ad	137	PRO	N-CD	-6.67	1.38	1.47
1	Ak	137	PRO	N-CD	-6.67	1.38	1.47
1	Bf	137	PRO	N-CD	-6.67	1.38	1.47
1	Bt	137	PRO	N-CD	-6.65	1.38	1.47
1	Bm	137	PRO	N-CD	-6.63	1.38	1.47
1	Ay	137	PRO	N-CD	-6.63	1.38	1.47
1	Bf	462	PRO	N-CD	5.23	1.55	1.47
1	Ak	462	PRO	N-CD	5.21	1.55	1.47
1	Bt	462	PRO	N-CD	5.21	1.55	1.47
1	Ad	462	PRO	N-CD	5.19	1.55	1.47
1	Ar	462	PRO	N-CD	5.18	1.55	1.47
1	Ay	462	PRO	N-CD	5.15	1.55	1.47
1	Bm	462	PRO	N-CD	5.15	1.55	1.47

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bt	525	PRO	CA-C-O	16.86	160.67	120.20
1	Ar	525	PRO	CA-C-O	16.86	160.66	120.20
1	Ad	525	PRO	CA-C-O	16.84	160.63	120.20
1	Ak	525	PRO	CA-C-O	16.84	160.62	120.20
1	Bf	525	PRO	CA-C-O	16.84	160.61	120.20
1	Bm	525	PRO	CA-C-O	16.83	160.60	120.20
1	Ay	525	PRO	CA-C-O	16.82	160.58	120.20
2	Bo	14	ARG	NE-CZ-NH1	12.18	126.39	120.30
2	At	14	ARG	NE-CZ-NH1	12.14	126.37	120.30
2	Am	14	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	Af	14	ARG	NE-CZ-NH1	12.09	126.35	120.30
2	Ba	14	ARG	NE-CZ-NH1	12.08	126.34	120.30
2	Bh	14	ARG	NE-CZ-NH1	12.08	126.34	120.30
2	Bv	14	ARG	NE-CZ-NH1	12.07	126.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Az	322	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	Al	322	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	Bg	322	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	Bu	322	ARG	NE-CZ-NH1	10.17	125.38	120.30
1	As	322	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	Ae	322	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	Bn	322	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	As	350	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	Az	350	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	Bu	350	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	Ae	350	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	Bn	350	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	Bg	350	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	Al	350	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	Bu	231	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	Az	231	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	Al	231	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	Ae	231	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	Bg	231	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	Bn	231	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	As	231	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	Ak	429	LEU	N-CA-C	-7.30	91.28	111.00
1	Bf	429	LEU	N-CA-C	-7.30	91.30	111.00
1	Bt	429	LEU	N-CA-C	-7.30	91.29	111.00
1	Ay	429	LEU	N-CA-C	-7.29	91.31	111.00
1	Ad	429	LEU	N-CA-C	-7.29	91.33	111.00
1	Ar	429	LEU	N-CA-C	-7.28	91.34	111.00
1	Bm	429	LEU	N-CA-C	-7.27	91.37	111.00
1	Ak	368	ARG	N-CA-CB	6.94	123.09	110.60
1	Ay	368	ARG	N-CA-CB	6.93	123.08	110.60
1	Bt	368	ARG	N-CA-CB	6.93	123.08	110.60
1	Ad	368	ARG	N-CA-CB	6.93	123.07	110.60
1	Ar	368	ARG	N-CA-CB	6.92	123.06	110.60
1	Bm	368	ARG	N-CA-CB	6.92	123.06	110.60
1	Bf	368	ARG	N-CA-CB	6.91	123.04	110.60
1	Az	496	PRO	N-CA-CB	-6.79	95.13	102.60
1	Bg	496	PRO	N-CA-CB	-6.77	95.15	102.60
1	Bu	496	PRO	N-CA-CB	-6.77	95.15	102.60
1	As	496	PRO	N-CA-CB	-6.77	95.16	102.60
1	Ae	496	PRO	N-CA-CB	-6.75	95.17	102.60
1	Al	496	PRO	N-CA-CB	-6.75	95.17	102.60
1	Bn	496	PRO	N-CA-CB	-6.74	95.19	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bu	496	PRO	CA-N-CD	6.65	121.02	111.70
1	Az	496	PRO	CA-N-CD	6.65	121.01	111.70
1	Bg	496	PRO	CA-N-CD	6.63	120.98	111.70
1	Ae	496	PRO	CA-N-CD	6.61	120.95	111.70
1	As	496	PRO	CA-N-CD	6.60	120.94	111.70
1	Al	496	PRO	CA-N-CD	6.59	120.93	111.70
1	Bn	496	PRO	CA-N-CD	6.59	120.93	111.70
1	Az	483	GLU	CB-CA-C	6.56	123.51	110.40
1	Al	483	GLU	CB-CA-C	6.54	123.48	110.40
1	Bn	483	GLU	CB-CA-C	6.54	123.48	110.40
1	Ae	483	GLU	CB-CA-C	6.54	123.47	110.40
1	Bg	483	GLU	CB-CA-C	6.53	123.46	110.40
1	Bu	483	GLU	CB-CA-C	6.52	123.44	110.40
1	As	483	GLU	CB-CA-C	6.52	123.44	110.40
1	Bg	462	PRO	CA-N-CD	6.42	120.69	111.70
1	Al	462	PRO	CA-N-CD	6.40	120.66	111.70
1	Bn	462	PRO	CA-N-CD	6.39	120.64	111.70
1	Ae	462	PRO	CA-N-CD	6.39	120.64	111.70
1	As	462	PRO	CA-N-CD	6.38	120.63	111.70
1	Az	462	PRO	CA-N-CD	6.36	120.61	111.70
1	Ak	366	GLN	N-CA-C	6.36	128.16	111.00
1	Ar	366	GLN	N-CA-C	6.36	128.17	111.00
1	Bf	366	GLN	N-CA-C	6.36	128.16	111.00
1	Ad	366	GLN	N-CA-C	6.35	128.14	111.00
1	Bm	366	GLN	N-CA-C	6.35	128.14	111.00
1	Bt	366	GLN	N-CA-C	6.35	128.14	111.00
1	Az	519	CYS	N-CA-CB	-6.35	99.17	110.60
1	Ay	366	GLN	N-CA-C	6.34	128.13	111.00
1	Bg	519	CYS	N-CA-CB	-6.34	99.19	110.60
1	Bu	462	PRO	CA-N-CD	6.34	120.58	111.70
1	Al	519	CYS	N-CA-CB	-6.33	99.20	110.60
1	Ae	519	CYS	N-CA-CB	-6.33	99.20	110.60
1	Bn	519	CYS	N-CA-CB	-6.33	99.21	110.60
1	As	519	CYS	N-CA-CB	-6.33	99.21	110.60
2	At	9	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	Bu	519	CYS	N-CA-CB	-6.32	99.23	110.60
2	Bh	9	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	Af	4	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	Am	9	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	Bh	4	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	Bv	4	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	Af	9	ARG	NE-CZ-NH1	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Ba	9	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	Am	4	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	Ba	4	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	Bv	9	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	Bo	9	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	Bo	4	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	Ay	364	LYS	N-CA-CB	6.16	121.69	110.60
1	Bf	364	LYS	N-CA-CB	6.15	121.68	110.60
1	Bm	364	LYS	N-CA-CB	6.15	121.68	110.60
1	Ak	364	LYS	N-CA-CB	6.15	121.67	110.60
1	Ad	364	LYS	N-CA-CB	6.14	121.66	110.60
1	Bt	364	LYS	N-CA-CB	6.14	121.66	110.60
1	Ar	364	LYS	N-CA-CB	6.13	121.63	110.60
2	At	4	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	Ak	399	ALA	N-CA-CB	6.00	118.50	110.10
1	Bt	399	ALA	N-CA-CB	6.00	118.49	110.10
1	Ad	399	ALA	N-CA-CB	5.98	118.47	110.10
1	Ar	399	ALA	N-CA-CB	5.98	118.47	110.10
1	Ay	399	ALA	N-CA-CB	5.96	118.45	110.10
1	Bf	399	ALA	N-CA-CB	5.96	118.44	110.10
1	Bm	399	ALA	N-CA-CB	5.96	118.44	110.10
1	Bu	285	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	Az	285	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	As	285	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	Bg	285	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	Bn	285	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	Ae	285	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	Al	285	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	Bv	47	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	Ba	47	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	Bo	47	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	Bt	365	LEU	N-CA-CB	-5.78	98.85	110.40
1	Ay	365	LEU	N-CA-CB	-5.77	98.86	110.40
1	Ar	365	LEU	N-CA-CB	-5.77	98.87	110.40
1	Bm	365	LEU	N-CA-CB	-5.77	98.86	110.40
1	Ak	365	LEU	N-CA-CB	-5.76	98.88	110.40
1	Ad	365	LEU	N-CA-CB	-5.75	98.90	110.40
1	Bf	365	LEU	N-CA-CB	-5.75	98.90	110.40
2	Af	47	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	Am	47	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	Bh	47	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	At	47	ARG	NE-CZ-NH2	-5.67	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Al	362	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	Bg	362	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	Ak	366	GLN	CB-CA-C	-5.57	99.27	110.40
1	Bf	366	GLN	CB-CA-C	-5.55	99.29	110.40
1	Bt	366	GLN	CB-CA-C	-5.55	99.30	110.40
1	Ad	366	GLN	CB-CA-C	-5.55	99.30	110.40
1	Ay	366	GLN	CB-CA-C	-5.54	99.31	110.40
1	As	362	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Ar	366	GLN	CB-CA-C	-5.53	99.34	110.40
1	Bm	366	GLN	CB-CA-C	-5.53	99.34	110.40
1	Ae	362	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Ak	367	GLU	N-CA-C	-5.50	96.15	111.00
1	Ay	168	LYS	N-CA-C	5.50	125.84	111.00
1	Bm	367	GLU	N-CA-C	-5.50	96.16	111.00
1	Bm	168	LYS	N-CA-C	5.50	125.84	111.00
1	Ar	367	GLU	N-CA-C	-5.49	96.17	111.00
1	Bf	367	GLU	N-CA-C	-5.49	96.18	111.00
1	Ad	168	LYS	N-CA-C	5.49	125.82	111.00
1	Ak	168	LYS	N-CA-C	5.49	125.82	111.00
1	Ad	367	GLU	N-CA-C	-5.49	96.19	111.00
1	Bt	168	LYS	N-CA-C	5.49	125.81	111.00
1	Bt	367	GLU	N-CA-C	-5.48	96.19	111.00
1	Bu	362	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	Ak	365	LEU	N-CA-C	5.48	125.80	111.00
1	Ar	168	LYS	N-CA-C	5.48	125.80	111.00
1	Bt	365	LEU	N-CA-C	5.48	125.80	111.00
1	Ar	365	LEU	N-CA-C	5.48	125.79	111.00
1	Bf	168	LYS	N-CA-C	5.48	125.79	111.00
1	Ay	365	LEU	N-CA-C	5.47	125.78	111.00
1	Ay	367	GLU	N-CA-C	-5.47	96.22	111.00
1	Ad	365	LEU	N-CA-C	5.47	125.77	111.00
1	Az	362	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	Bm	365	LEU	N-CA-C	5.47	125.76	111.00
1	Bf	365	LEU	N-CA-C	5.46	125.74	111.00
1	Bn	362	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	Al	345	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	As	345	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	Bg	345	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	Bg	428	ASP	CB-CA-C	-5.39	99.61	110.40
1	Bt	389	MET	N-CA-CB	5.39	120.31	110.60
1	Az	428	ASP	CB-CA-C	-5.39	99.62	110.40
1	Bu	428	ASP	CB-CA-C	-5.39	99.63	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ae	428	ASP	CB-CA-C	-5.38	99.64	110.40
1	As	428	ASP	CB-CA-C	-5.38	99.64	110.40
1	Bn	428	ASP	CB-CA-C	-5.38	99.64	110.40
1	Ae	345	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	Bu	345	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	Bf	389	MET	N-CA-CB	5.37	120.26	110.60
1	Az	345	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	Al	428	ASP	CB-CA-C	-5.37	99.67	110.40
1	Bm	389	MET	N-CA-CB	5.36	120.24	110.60
1	Ad	389	MET	N-CA-CB	5.36	120.24	110.60
1	Ay	389	MET	N-CA-CB	5.36	120.24	110.60
1	Ak	389	MET	N-CA-CB	5.35	120.23	110.60
1	Bg	197	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	Ar	389	MET	N-CA-CB	5.35	120.23	110.60
1	Bn	345	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	Bn	197	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Al	197	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	As	197	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	Ae	197	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	Az	197	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	Bt	84	ALA	N-CA-CB	5.25	117.46	110.10
1	Ak	84	ALA	N-CA-CB	5.25	117.44	110.10
1	Bm	84	ALA	N-CA-CB	5.24	117.44	110.10
1	Ad	84	ALA	N-CA-CB	5.23	117.42	110.10
1	Ar	84	ALA	N-CA-CB	5.23	117.42	110.10
1	Bu	197	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	Ay	84	ALA	N-CA-CB	5.23	117.42	110.10
1	Bf	84	ALA	N-CA-CB	5.22	117.41	110.10
2	At	95	VAL	N-CA-C	5.17	124.96	111.00
2	Bh	95	VAL	N-CA-C	5.17	124.95	111.00
2	Ba	95	VAL	N-CA-C	5.16	124.94	111.00
2	Bo	95	VAL	N-CA-C	5.16	124.93	111.00
2	Af	95	VAL	N-CA-C	5.16	124.93	111.00
2	Am	95	VAL	N-CA-C	5.16	124.93	111.00
2	Bv	95	VAL	N-CA-C	5.15	124.92	111.00
1	Ar	367	GLU	N-CA-CB	5.10	119.78	110.60
1	Ak	367	GLU	N-CA-CB	5.08	119.75	110.60
1	Ad	367	GLU	N-CA-CB	5.08	119.75	110.60
1	Bm	367	GLU	N-CA-CB	5.08	119.74	110.60
1	Ay	367	GLU	N-CA-CB	5.07	119.72	110.60
1	Bf	367	GLU	N-CA-CB	5.06	119.71	110.60
1	Bt	367	GLU	N-CA-CB	5.05	119.70	110.60

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Ad	136	VAL	Mainchain
1	Ae	268	ARG	Sidechain
2	Af	1	MET	Peptide
2	Af	4	ARG	Sidechain
1	Ak	136	VAL	Mainchain
1	Al	268	ARG	Sidechain
2	Am	1	MET	Peptide
2	Am	4	ARG	Sidechain
1	Ar	136	VAL	Mainchain
1	As	268	ARG	Sidechain
2	At	1	MET	Peptide
2	At	4	ARG	Sidechain
1	Ay	136	VAL	Mainchain
1	Az	268	ARG	Sidechain
2	Ba	1	MET	Peptide
2	Ba	4	ARG	Sidechain
1	Bf	136	VAL	Mainchain
1	Bg	268	ARG	Sidechain
2	Bh	1	MET	Peptide
2	Bh	4	ARG	Sidechain
1	Bm	136	VAL	Mainchain
1	Bn	268	ARG	Sidechain
2	Bo	1	MET	Peptide
2	Bo	4	ARG	Sidechain
1	Bt	136	VAL	Mainchain
1	Bu	268	ARG	Sidechain
2	Bv	1	MET	Peptide
2	Bv	4	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	Ad	3856	0	3976	0	0
1	Ae	3856	0	3976	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ak	3856	0	3976	0	0
1	Al	3856	0	3976	0	0
1	Ar	3856	0	3976	0	0
1	As	3856	0	3976	0	0
1	Ay	3856	0	3976	0	0
1	Az	3856	0	3976	0	0
1	Bf	3856	0	3976	0	0
1	Bg	3856	0	3976	0	0
1	Bm	3856	0	3976	0	0
1	Bn	3856	0	3976	0	0
1	Bt	3856	0	3976	0	0
1	Bu	3856	0	3976	0	0
2	Af	728	0	762	0	0
2	Am	728	0	762	0	0
2	At	728	0	762	0	0
2	Ba	728	0	762	0	0
2	Bh	728	0	762	0	0
2	Bo	728	0	762	0	0
2	Bv	728	0	762	0	0
3	Ad	27	0	11	0	0
3	Ae	27	0	11	0	0
3	Ak	27	0	11	0	0
3	Al	27	0	11	0	0
3	Ar	27	0	11	0	0
3	As	27	0	11	0	0
3	Ay	27	0	11	0	0
3	Az	27	0	11	0	0
3	Bf	27	0	11	0	0
3	Bg	27	0	11	0	0
3	Bm	27	0	11	0	0
3	Bn	27	0	11	0	0
3	Bt	27	0	11	0	0
3	Bu	27	0	11	0	0
4	Ad	1	0	0	0	0
4	Ae	1	0	0	0	0
4	Ak	1	0	0	0	0
4	Al	1	0	0	0	0
4	Ar	1	0	0	0	0
4	As	1	0	0	0	0
4	Ay	1	0	0	0	0
4	Az	1	0	0	0	0
4	Bf	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Bg	1	0	0	0	0
4	Bm	1	0	0	0	0
4	Bn	1	0	0	0	0
4	Bt	1	0	0	0	0
4	Bu	1	0	0	0	0
5	Ad	2	0	0	0	0
5	Ak	2	0	0	0	0
5	Ar	2	0	0	0	0
5	Ay	2	0	0	0	0
5	Bf	2	0	0	0	0
5	Bm	2	0	0	0	0
5	Bt	2	0	0	0	0
All	All	59486	0	61152	0	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 29.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Ad	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25 57
1	Ae	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	47 78
1	Ak	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25 57
1	Al	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	47 78
1	Ar	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25 57
1	As	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	47 78
1	Ay	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Az	522/524 (100%)	516 (99%)	4 (1%)	2 (0%)	34	67
1	Bf	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25	57
1	Bg	522/524 (100%)	516 (99%)	4 (1%)	2 (0%)	34	67
1	Bm	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25	57
1	Bn	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	47	78
1	Bt	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	25	57
1	Bu	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	47	78
2	Af	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
2	Am	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
2	At	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
2	Ba	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
2	Bh	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
2	Bo	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
2	Bv	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	4	22
All	All	7973/8015 (100%)	7723 (97%)	199 (2%)	51 (1%)	29	57

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Af	95	VAL
2	Am	95	VAL
2	At	95	VAL
2	Ba	95	VAL
2	Bh	95	VAL
2	Bo	95	VAL
2	Bv	95	VAL
1	Ad	270	ILE
1	Ak	270	ILE
1	Ar	270	ILE
1	Ay	270	ILE
1	Bf	270	ILE
1	Bm	270	ILE
1	Bt	270	ILE
1	Ad	272	LYS
1	Ak	272	LYS
1	Ar	272	LYS
1	Ay	272	LYS

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Mol	Chain	Res	Type
1	Bf	272	LYS
1	Bm	272	LYS
1	Bt	272	LYS
1	Ae	225	LYS
1	Al	225	LYS
1	As	225	LYS
1	Az	225	LYS
1	Bg	225	LYS
1	Bn	225	LYS
1	Bu	225	LYS
2	Af	18	GLU
2	Af	50	GLU
2	Am	18	GLU
2	Am	50	GLU
2	At	18	GLU
2	At	50	GLU
2	Ba	18	GLU
2	Ba	50	GLU
2	Bh	18	GLU
2	Bh	50	GLU
2	Bo	18	GLU
2	Bo	50	GLU
2	Bv	18	GLU
2	Bv	50	GLU
1	Ad	168	LYS
1	Ak	168	LYS
1	Ar	168	LYS
1	Ay	168	LYS
1	Bf	168	LYS
1	Bm	168	LYS
1	Bt	168	LYS
1	Az	205	ILE
1	Bg	205	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ad	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	Ae	404/404 (100%)	392 (97%)	12 (3%)	41	68
1	Ak	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	Al	404/404 (100%)	391 (97%)	13 (3%)	39	67
1	Ar	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	As	404/404 (100%)	391 (97%)	13 (3%)	39	67
1	Ay	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	Az	404/404 (100%)	392 (97%)	12 (3%)	41	68
1	Bf	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	Bg	404/404 (100%)	391 (97%)	13 (3%)	39	67
1	Bm	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	Bn	404/404 (100%)	392 (97%)	12 (3%)	41	68
1	Bt	404/404 (100%)	338 (84%)	66 (16%)	2	9
1	Bu	404/404 (100%)	392 (97%)	12 (3%)	41	68
2	Af	80/80 (100%)	77 (96%)	3 (4%)	33	61
2	Am	80/80 (100%)	77 (96%)	3 (4%)	33	61
2	At	80/80 (100%)	77 (96%)	3 (4%)	33	61
2	Ba	80/80 (100%)	77 (96%)	3 (4%)	33	61
2	Bh	80/80 (100%)	77 (96%)	3 (4%)	33	61
2	Bo	80/80 (100%)	77 (96%)	3 (4%)	33	61
2	Bv	80/80 (100%)	77 (96%)	3 (4%)	33	61
All	All	6216/6216 (100%)	5646 (91%)	570 (9%)	13	31

All (570) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ad	160	LYS
1	Ad	179	ASP
1	Ad	186	GLU
1	Ad	187	LEU
1	Ad	190	VAL
1	Ad	191	GLU
1	Ad	194	GLN
1	Ad	199	TYR
1	Ad	203	TYR
1	Ad	207	LYS

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Mol	Chain	Res	Type
1	Ad	209	GLU
1	Ad	210	THR
1	Ad	217	SER
1	Ad	219	PHE
1	Ad	225	LYS
1	Ad	227	ILE
1	Ad	231	ARG
1	Ad	232	GLU
1	Ad	233	MET
1	Ad	234	LEU
1	Ad	236	VAL
1	Ad	238	GLU
1	Ad	240	VAL
1	Ad	245	LYS
1	Ad	250	ILE
1	Ad	252	GLU
1	Ad	254	VAL
1	Ad	255	GLU
1	Ad	259	LEU
1	Ad	261	THR
1	Ad	262	LEU
1	Ad	268	ARG
1	Ad	270	ILE
1	Ad	277	LYS
1	Ad	281	PHE
1	Ad	286	LYS
1	Ad	288	MET
1	Ad	290	GLN
1	Ad	295	LEU
1	Ad	299	THR
1	Ad	300	VAL
1	Ad	301	ILE
1	Ad	302	SER
1	Ad	304	GLU
1	Ad	307	MET
1	Ad	308	GLU
1	Ad	309	LEU
1	Ad	310	GLU
1	Ad	314	LEU
1	Ad	315	GLU
1	Ad	319	GLN
1	Ad	321	LYS

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Mol	Chain	Res	Type
1	Ad	324	VAL
1	Ad	327	LYS
1	Ad	333	ILE
1	Ad	336	VAL
1	Ad	339	GLU
1	Ad	345	ARG
1	Ad	348	GLN
1	Ad	351	GLN
1	Ad	354	GLU
1	Ad	355	GLU
1	Ad	357	THR
1	Ad	358	SER
1	Ad	389	MET
1	Ad	518	GLU
1	Ae	10	ASN
1	Ae	23	LEU
1	Ae	63	GLU
1	Ae	74	VAL
1	Ae	104	LEU
1	Ae	193	MET
1	Ae	196	ASP
1	Ae	284	ARG
1	Ae	390	LYS
1	Ae	420	ILE
1	Ae	433	ASN
1	Ae	453	GLN
2	Af	2	ASN
2	Af	28	THR
2	Af	34	LYS
1	Ak	160	LYS
1	Ak	179	ASP
1	Ak	186	GLU
1	Ak	187	LEU
1	Ak	190	VAL
1	Ak	191	GLU
1	Ak	194	GLN
1	Ak	199	TYR
1	Ak	203	TYR
1	Ak	207	LYS
1	Ak	209	GLU
1	Ak	210	THR
1	Ak	217	SER

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Mol	Chain	Res	Type
1	Ak	219	PHE
1	Ak	225	LYS
1	Ak	227	ILE
1	Ak	231	ARG
1	Ak	232	GLU
1	Ak	233	MET
1	Ak	234	LEU
1	Ak	236	VAL
1	Ak	238	GLU
1	Ak	240	VAL
1	Ak	245	LYS
1	Ak	250	ILE
1	Ak	252	GLU
1	Ak	254	VAL
1	Ak	255	GLU
1	Ak	259	LEU
1	Ak	261	THR
1	Ak	262	LEU
1	Ak	268	ARG
1	Ak	270	ILE
1	Ak	277	LYS
1	Ak	281	PHE
1	Ak	286	LYS
1	Ak	288	MET
1	Ak	290	GLN
1	Ak	295	LEU
1	Ak	299	THR
1	Ak	300	VAL
1	Ak	301	ILE
1	Ak	302	SER
1	Ak	304	GLU
1	Ak	307	MET
1	Ak	308	GLU
1	Ak	309	LEU
1	Ak	310	GLU
1	Ak	314	LEU
1	Ak	315	GLU
1	Ak	319	GLN
1	Ak	321	LYS
1	Ak	324	VAL
1	Ak	327	LYS
1	Ak	333	ILE

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Mol	Chain	Res	Type
1	Ak	336	VAL
1	Ak	339	GLU
1	Ak	345	ARG
1	Ak	348	GLN
1	Ak	351	GLN
1	Ak	354	GLU
1	Ak	355	GLU
1	Ak	357	THR
1	Ak	358	SER
1	Ak	389	MET
1	Ak	518	GLU
1	Al	10	ASN
1	Al	23	LEU
1	Al	63	GLU
1	Al	74	VAL
1	Al	104	LEU
1	Al	193	MET
1	Al	196	ASP
1	Al	284	ARG
1	Al	390	LYS
1	Al	420	ILE
1	Al	433	ASN
1	Al	453	GLN
1	Al	509	SER
2	Am	2	ASN
2	Am	28	THR
2	Am	34	LYS
1	Ar	160	LYS
1	Ar	179	ASP
1	Ar	186	GLU
1	Ar	187	LEU
1	Ar	190	VAL
1	Ar	191	GLU
1	Ar	194	GLN
1	Ar	199	TYR
1	Ar	203	TYR
1	Ar	207	LYS
1	Ar	209	GLU
1	Ar	210	THR
1	Ar	217	SER
1	Ar	219	PHE
1	Ar	225	LYS

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Mol	Chain	Res	Type
1	Ar	227	ILE
1	Ar	231	ARG
1	Ar	232	GLU
1	Ar	233	MET
1	Ar	234	LEU
1	Ar	236	VAL
1	Ar	238	GLU
1	Ar	240	VAL
1	Ar	245	LYS
1	Ar	250	ILE
1	Ar	252	GLU
1	Ar	254	VAL
1	Ar	255	GLU
1	Ar	259	LEU
1	Ar	261	THR
1	Ar	262	LEU
1	Ar	268	ARG
1	Ar	270	ILE
1	Ar	277	LYS
1	Ar	281	PHE
1	Ar	286	LYS
1	Ar	288	MET
1	Ar	290	GLN
1	Ar	295	LEU
1	Ar	299	THR
1	Ar	300	VAL
1	Ar	301	ILE
1	Ar	302	SER
1	Ar	304	GLU
1	Ar	307	MET
1	Ar	308	GLU
1	Ar	309	LEU
1	Ar	310	GLU
1	Ar	314	LEU
1	Ar	315	GLU
1	Ar	319	GLN
1	Ar	321	LYS
1	Ar	324	VAL
1	Ar	327	LYS
1	Ar	333	ILE
1	Ar	336	VAL
1	Ar	339	GLU

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Mol	Chain	Res	Type
1	Ar	345	ARG
1	Ar	348	GLN
1	Ar	351	GLN
1	Ar	354	GLU
1	Ar	355	GLU
1	Ar	357	THR
1	Ar	358	SER
1	Ar	389	MET
1	Ar	518	GLU
1	As	10	ASN
1	As	23	LEU
1	As	63	GLU
1	As	74	VAL
1	As	104	LEU
1	As	193	MET
1	As	196	ASP
1	As	284	ARG
1	As	390	LYS
1	As	420	ILE
1	As	433	ASN
1	As	453	GLN
1	As	509	SER
2	At	2	ASN
2	At	28	THR
2	At	34	LYS
1	Ay	160	LYS
1	Ay	179	ASP
1	Ay	186	GLU
1	Ay	187	LEU
1	Ay	190	VAL
1	Ay	191	GLU
1	Ay	194	GLN
1	Ay	199	TYR
1	Ay	203	TYR
1	Ay	207	LYS
1	Ay	209	GLU
1	Ay	210	THR
1	Ay	217	SER
1	Ay	219	PHE
1	Ay	225	LYS
1	Ay	227	ILE
1	Ay	231	ARG

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Mol	Chain	Res	Type
1	Ay	232	GLU
1	Ay	233	MET
1	Ay	234	LEU
1	Ay	236	VAL
1	Ay	238	GLU
1	Ay	240	VAL
1	Ay	245	LYS
1	Ay	250	ILE
1	Ay	252	GLU
1	Ay	254	VAL
1	Ay	255	GLU
1	Ay	259	LEU
1	Ay	261	THR
1	Ay	262	LEU
1	Ay	268	ARG
1	Ay	270	ILE
1	Ay	277	LYS
1	Ay	281	PHE
1	Ay	286	LYS
1	Ay	288	MET
1	Ay	290	GLN
1	Ay	295	LEU
1	Ay	299	THR
1	Ay	300	VAL
1	Ay	301	ILE
1	Ay	302	SER
1	Ay	304	GLU
1	Ay	307	MET
1	Ay	308	GLU
1	Ay	309	LEU
1	Ay	310	GLU
1	Ay	314	LEU
1	Ay	315	GLU
1	Ay	319	GLN
1	Ay	321	LYS
1	Ay	324	VAL
1	Ay	327	LYS
1	Ay	333	ILE
1	Ay	336	VAL
1	Ay	339	GLU
1	Ay	345	ARG
1	Ay	348	GLN

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Mol	Chain	Res	Type
1	Ay	351	GLN
1	Ay	354	GLU
1	Ay	355	GLU
1	Ay	357	THR
1	Ay	358	SER
1	Ay	389	MET
1	Ay	518	GLU
1	Az	10	ASN
1	Az	23	LEU
1	Az	63	GLU
1	Az	74	VAL
1	Az	104	LEU
1	Az	193	MET
1	Az	196	ASP
1	Az	284	ARG
1	Az	390	LYS
1	Az	420	ILE
1	Az	433	ASN
1	Az	453	GLN
2	Ba	2	ASN
2	Ba	28	THR
2	Ba	34	LYS
1	Bf	160	LYS
1	Bf	179	ASP
1	Bf	186	GLU
1	Bf	187	LEU
1	Bf	190	VAL
1	Bf	191	GLU
1	Bf	194	GLN
1	Bf	199	TYR
1	Bf	203	TYR
1	Bf	207	LYS
1	Bf	209	GLU
1	Bf	210	THR
1	Bf	217	SER
1	Bf	219	PHE
1	Bf	225	LYS
1	Bf	227	ILE
1	Bf	231	ARG
1	Bf	232	GLU
1	Bf	233	MET
1	Bf	234	LEU

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Mol	Chain	Res	Type
1	Bf	236	VAL
1	Bf	238	GLU
1	Bf	240	VAL
1	Bf	245	LYS
1	Bf	250	ILE
1	Bf	252	GLU
1	Bf	254	VAL
1	Bf	255	GLU
1	Bf	259	LEU
1	Bf	261	THR
1	Bf	262	LEU
1	Bf	268	ARG
1	Bf	270	ILE
1	Bf	277	LYS
1	Bf	281	PHE
1	Bf	286	LYS
1	Bf	288	MET
1	Bf	290	GLN
1	Bf	295	LEU
1	Bf	299	THR
1	Bf	300	VAL
1	Bf	301	ILE
1	Bf	302	SER
1	Bf	304	GLU
1	Bf	307	MET
1	Bf	308	GLU
1	Bf	309	LEU
1	Bf	310	GLU
1	Bf	314	LEU
1	Bf	315	GLU
1	Bf	319	GLN
1	Bf	321	LYS
1	Bf	324	VAL
1	Bf	327	LYS
1	Bf	333	ILE
1	Bf	336	VAL
1	Bf	339	GLU
1	Bf	345	ARG
1	Bf	348	GLN
1	Bf	351	GLN
1	Bf	354	GLU
1	Bf	355	GLU

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Mol	Chain	Res	Type
1	Bf	357	THR
1	Bf	358	SER
1	Bf	389	MET
1	Bf	518	GLU
1	Bg	10	ASN
1	Bg	23	LEU
1	Bg	63	GLU
1	Bg	74	VAL
1	Bg	104	LEU
1	Bg	193	MET
1	Bg	196	ASP
1	Bg	284	ARG
1	Bg	390	LYS
1	Bg	420	ILE
1	Bg	433	ASN
1	Bg	453	GLN
1	Bg	509	SER
2	Bh	2	ASN
2	Bh	28	THR
2	Bh	34	LYS
1	Bm	160	LYS
1	Bm	179	ASP
1	Bm	186	GLU
1	Bm	187	LEU
1	Bm	190	VAL
1	Bm	191	GLU
1	Bm	194	GLN
1	Bm	199	TYR
1	Bm	203	TYR
1	Bm	207	LYS
1	Bm	209	GLU
1	Bm	210	THR
1	Bm	217	SER
1	Bm	219	PHE
1	Bm	225	LYS
1	Bm	227	ILE
1	Bm	231	ARG
1	Bm	232	GLU
1	Bm	233	MET
1	Bm	234	LEU
1	Bm	236	VAL
1	Bm	238	GLU

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Mol	Chain	Res	Type
1	Bm	240	VAL
1	Bm	245	LYS
1	Bm	250	ILE
1	Bm	252	GLU
1	Bm	254	VAL
1	Bm	255	GLU
1	Bm	259	LEU
1	Bm	261	THR
1	Bm	262	LEU
1	Bm	268	ARG
1	Bm	270	ILE
1	Bm	277	LYS
1	Bm	281	PHE
1	Bm	286	LYS
1	Bm	288	MET
1	Bm	290	GLN
1	Bm	295	LEU
1	Bm	299	THR
1	Bm	300	VAL
1	Bm	301	ILE
1	Bm	302	SER
1	Bm	304	GLU
1	Bm	307	MET
1	Bm	308	GLU
1	Bm	309	LEU
1	Bm	310	GLU
1	Bm	314	LEU
1	Bm	315	GLU
1	Bm	319	GLN
1	Bm	321	LYS
1	Bm	324	VAL
1	Bm	327	LYS
1	Bm	333	ILE
1	Bm	336	VAL
1	Bm	339	GLU
1	Bm	345	ARG
1	Bm	348	GLN
1	Bm	351	GLN
1	Bm	354	GLU
1	Bm	355	GLU
1	Bm	357	THR
1	Bm	358	SER

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Mol	Chain	Res	Type
1	Bm	389	MET
1	Bm	518	GLU
1	Bn	10	ASN
1	Bn	23	LEU
1	Bn	63	GLU
1	Bn	74	VAL
1	Bn	104	LEU
1	Bn	193	MET
1	Bn	196	ASP
1	Bn	284	ARG
1	Bn	390	LYS
1	Bn	420	ILE
1	Bn	433	ASN
1	Bn	453	GLN
2	Bo	2	ASN
2	Bo	28	THR
2	Bo	34	LYS
1	Bt	160	LYS
1	Bt	179	ASP
1	Bt	186	GLU
1	Bt	187	LEU
1	Bt	190	VAL
1	Bt	191	GLU
1	Bt	194	GLN
1	Bt	199	TYR
1	Bt	203	TYR
1	Bt	207	LYS
1	Bt	209	GLU
1	Bt	210	THR
1	Bt	217	SER
1	Bt	219	PHE
1	Bt	225	LYS
1	Bt	227	ILE
1	Bt	231	ARG
1	Bt	232	GLU
1	Bt	233	MET
1	Bt	234	LEU
1	Bt	236	VAL
1	Bt	238	GLU
1	Bt	240	VAL
1	Bt	245	LYS
1	Bt	250	ILE

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Mol	Chain	Res	Type
1	Bt	252	GLU
1	Bt	254	VAL
1	Bt	255	GLU
1	Bt	259	LEU
1	Bt	261	THR
1	Bt	262	LEU
1	Bt	268	ARG
1	Bt	270	ILE
1	Bt	277	LYS
1	Bt	281	PHE
1	Bt	286	LYS
1	Bt	288	MET
1	Bt	290	GLN
1	Bt	295	LEU
1	Bt	299	THR
1	Bt	300	VAL
1	Bt	301	ILE
1	Bt	302	SER
1	Bt	304	GLU
1	Bt	307	MET
1	Bt	308	GLU
1	Bt	309	LEU
1	Bt	310	GLU
1	Bt	314	LEU
1	Bt	315	GLU
1	Bt	319	GLN
1	Bt	321	LYS
1	Bt	324	VAL
1	Bt	327	LYS
1	Bt	333	ILE
1	Bt	336	VAL
1	Bt	339	GLU
1	Bt	345	ARG
1	Bt	348	GLN
1	Bt	351	GLN
1	Bt	354	GLU
1	Bt	355	GLU
1	Bt	357	THR
1	Bt	358	SER
1	Bt	389	MET
1	Bt	518	GLU
1	Bu	10	ASN

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Mol	Chain	Res	Type
1	Bu	23	LEU
1	Bu	63	GLU
1	Bu	74	VAL
1	Bu	104	LEU
1	Bu	193	MET
1	Bu	196	ASP
1	Bu	284	ARG
1	Bu	390	LYS
1	Bu	420	ILE
1	Bu	433	ASN
1	Bu	453	GLN
2	Bv	2	ASN
2	Bv	28	THR
2	Bv	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ad	37	ASN
1	Ad	112	ASN
1	Ad	146	GLN
1	Ad	348	GLN
1	Ad	366	GLN
1	Ad	453	GLN
1	Ae	21	ASN
1	Ae	82	ASN
1	Ae	146	GLN
2	Af	2	ASN
1	Ak	37	ASN
1	Ak	112	ASN
1	Ak	146	GLN
1	Ak	348	GLN
1	Ak	366	GLN
1	Ak	453	GLN
1	Al	21	ASN
1	Al	82	ASN
1	Al	146	GLN
2	Am	2	ASN
1	Ar	37	ASN
1	Ar	112	ASN
1	Ar	146	GLN
1	Ar	348	GLN

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Mol	Chain	Res	Type
1	Ar	366	GLN
1	Ar	453	GLN
1	As	21	ASN
1	As	82	ASN
1	As	146	GLN
1	Ay	37	ASN
1	Ay	112	ASN
1	Ay	146	GLN
1	Ay	348	GLN
1	Ay	366	GLN
1	Ay	453	GLN
1	Az	21	ASN
1	Az	82	ASN
1	Az	146	GLN
1	Bf	37	ASN
1	Bf	112	ASN
1	Bf	146	GLN
1	Bf	348	GLN
1	Bf	366	GLN
1	Bf	453	GLN
1	Bg	21	ASN
1	Bg	82	ASN
1	Bg	146	GLN
1	Bm	37	ASN
1	Bm	112	ASN
1	Bm	146	GLN
1	Bm	348	GLN
1	Bm	366	GLN
1	Bm	453	GLN
1	Bn	21	ASN
1	Bn	82	ASN
1	Bn	146	GLN
2	Bo	2	ASN
1	Bt	37	ASN
1	Bt	112	ASN
1	Bt	146	GLN
1	Bt	348	GLN
1	Bt	366	GLN
1	Bt	453	GLN
1	Bu	21	ASN
1	Bu	82	ASN
1	Bu	146	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	ADP	Bu	601	4	24,29,29	4.22	7 (29%)	29,45,45	1.43	3 (10%)
3	ADP	Ae	601	4	24,29,29	4.22	7 (29%)	29,45,45	1.42	3 (10%)
3	ADP	Ar	601	4	24,29,29	4.25	7 (29%)	29,45,45	1.31	2 (6%)
3	ADP	Bg	601	4	24,29,29	4.22	7 (29%)	29,45,45	1.42	3 (10%)
3	ADP	Az	601	4	24,29,29	4.22	7 (29%)	29,45,45	1.42	3 (10%)
3	ADP	Ak	601	4	24,29,29	4.25	7 (29%)	29,45,45	1.30	2 (6%)
3	ADP	As	601	4	24,29,29	4.23	7 (29%)	29,45,45	1.43	3 (10%)
3	ADP	Bf	601	4	24,29,29	4.26	7 (29%)	29,45,45	1.30	2 (6%)
3	ADP	Bm	601	4	24,29,29	4.23	7 (29%)	29,45,45	1.31	2 (6%)
3	ADP	Bt	601	4	24,29,29	4.25	7 (29%)	29,45,45	1.30	2 (6%)
3	ADP	Bn	601	4	24,29,29	4.22	7 (29%)	29,45,45	1.42	3 (10%)
3	ADP	Ay	601	4	24,29,29	4.26	7 (29%)	29,45,45	1.30	2 (6%)
3	ADP	Al	601	4	24,29,29	4.22	7 (29%)	29,45,45	1.43	3 (10%)
3	ADP	Ad	601	4	24,29,29	4.25	7 (29%)	29,45,45	1.30	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
3	ADP	Bu	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Ae	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Ar	601	4	-	3/12/32/32	0/3/3/3
3	ADP	Bg	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Az	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Ak	601	4	-	3/12/32/32	0/3/3/3
3	ADP	As	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Bf	601	4	-	3/12/32/32	0/3/3/3
3	ADP	Bm	601	4	-	3/12/32/32	0/3/3/3
3	ADP	Bt	601	4	-	3/12/32/32	0/3/3/3
3	ADP	Bn	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Ay	601	4	-	3/12/32/32	0/3/3/3
3	ADP	Al	601	4	-	6/12/32/32	0/3/3/3
3	ADP	Ad	601	4	-	3/12/32/32	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Bf	601	ADP	O4'-C1'	13.65	1.60	1.41
3	Ay	601	ADP	O4'-C1'	13.63	1.60	1.41
3	Ad	601	ADP	O4'-C1'	13.62	1.60	1.41
3	Ar	601	ADP	O4'-C1'	13.61	1.60	1.41
3	Ak	601	ADP	O4'-C1'	13.57	1.60	1.41
3	Bt	601	ADP	O4'-C1'	13.57	1.60	1.41
3	Bm	601	ADP	O4'-C1'	13.57	1.60	1.41
3	As	601	ADP	O4'-C1'	13.52	1.59	1.41
3	Bu	601	ADP	O4'-C1'	13.51	1.59	1.41
3	Az	601	ADP	O4'-C1'	13.51	1.59	1.41
3	Al	601	ADP	O4'-C1'	13.49	1.59	1.41
3	Ae	601	ADP	O4'-C1'	13.48	1.59	1.41
3	Bg	601	ADP	O4'-C1'	13.48	1.59	1.41
3	Bn	601	ADP	O4'-C1'	13.48	1.59	1.41
3	Ak	601	ADP	C2'-C1'	-13.01	1.34	1.53
3	Ay	601	ADP	C2'-C1'	-13.01	1.34	1.53
3	Bf	601	ADP	C2'-C1'	-13.01	1.34	1.53
3	Ar	601	ADP	C2'-C1'	-13.00	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Bt	601	ADP	C2'-C1'	-13.00	1.34	1.53
3	Ad	601	ADP	C2'-C1'	-12.97	1.34	1.53
3	Bm	601	ADP	C2'-C1'	-12.90	1.34	1.53
3	As	601	ADP	C2'-C1'	-12.80	1.34	1.53
3	Az	601	ADP	C2'-C1'	-12.79	1.34	1.53
3	Ae	601	ADP	C2'-C1'	-12.76	1.34	1.53
3	Bg	601	ADP	C2'-C1'	-12.75	1.34	1.53
3	Bn	601	ADP	C2'-C1'	-12.75	1.34	1.53
3	Al	601	ADP	C2'-C1'	-12.74	1.34	1.53
3	Bu	601	ADP	C2'-C1'	-12.73	1.34	1.53
3	Al	601	ADP	O4'-C4'	-5.67	1.32	1.45
3	Ae	601	ADP	O4'-C4'	-5.65	1.32	1.45
3	Bg	601	ADP	O4'-C4'	-5.65	1.32	1.45
3	Bn	601	ADP	O4'-C4'	-5.65	1.32	1.45
3	Bu	601	ADP	O4'-C4'	-5.65	1.32	1.45
3	Az	601	ADP	O4'-C4'	-5.64	1.32	1.45
3	As	601	ADP	O4'-C4'	-5.63	1.32	1.45
3	Ar	601	ADP	O4'-C4'	-5.55	1.32	1.45
3	Ay	601	ADP	O4'-C4'	-5.55	1.32	1.45
3	Ad	601	ADP	O4'-C4'	-5.54	1.32	1.45
3	Bt	601	ADP	O4'-C4'	-5.54	1.32	1.45
3	Ak	601	ADP	O4'-C4'	-5.53	1.32	1.45
3	Bf	601	ADP	O4'-C4'	-5.52	1.32	1.45
3	Bm	601	ADP	O4'-C4'	-5.51	1.32	1.45
3	Ar	601	ADP	C6-N6	3.78	1.47	1.34
3	Bm	601	ADP	C6-N6	3.77	1.47	1.34
3	Ad	601	ADP	C6-N6	3.76	1.47	1.34
3	Ak	601	ADP	C6-N6	3.75	1.47	1.34
3	Bt	601	ADP	C6-N6	3.75	1.47	1.34
3	Bf	601	ADP	C6-N6	3.74	1.47	1.34
3	Ay	601	ADP	C6-N6	3.74	1.47	1.34
3	Al	601	ADP	C6-N6	3.72	1.47	1.34
3	Bn	601	ADP	C6-N6	3.71	1.47	1.34
3	Ae	601	ADP	C6-N6	3.71	1.47	1.34
3	Bg	601	ADP	C6-N6	3.70	1.47	1.34
3	Bu	601	ADP	C6-N6	3.70	1.47	1.34
3	As	601	ADP	C6-N6	3.70	1.47	1.34
3	Az	601	ADP	C6-N6	3.70	1.47	1.34
3	Bf	601	ADP	O3'-C3'	-3.36	1.35	1.43
3	Ak	601	ADP	O3'-C3'	-3.35	1.35	1.43
3	Bt	601	ADP	O3'-C3'	-3.35	1.35	1.43
3	Bm	601	ADP	O3'-C3'	-3.33	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Ad	601	ADP	O3'-C3'	-3.33	1.35	1.43
3	Ar	601	ADP	O3'-C3'	-3.32	1.35	1.43
3	Ay	601	ADP	O3'-C3'	-3.32	1.35	1.43
3	Az	601	ADP	O3'-C3'	-3.31	1.35	1.43
3	As	601	ADP	O3'-C3'	-3.30	1.35	1.43
3	Bn	601	ADP	O3'-C3'	-3.29	1.35	1.43
3	Ae	601	ADP	O3'-C3'	-3.28	1.35	1.43
3	Al	601	ADP	O3'-C3'	-3.28	1.35	1.43
3	Bu	601	ADP	O3'-C3'	-3.25	1.35	1.43
3	Bg	601	ADP	O3'-C3'	-3.25	1.35	1.43
3	Bn	601	ADP	O2'-C2'	2.51	1.48	1.43
3	Al	601	ADP	O2'-C2'	2.49	1.48	1.43
3	Bu	601	ADP	O2'-C2'	2.49	1.48	1.43
3	As	601	ADP	O2'-C2'	2.48	1.48	1.43
3	Ae	601	ADP	O2'-C2'	2.48	1.48	1.43
3	Az	601	ADP	O2'-C2'	2.47	1.48	1.43
3	Bg	601	ADP	O2'-C2'	2.47	1.48	1.43
3	Bf	601	ADP	O2'-C2'	2.37	1.48	1.43
3	Ak	601	ADP	O2'-C2'	2.35	1.48	1.43
3	Ad	601	ADP	O2'-C2'	2.34	1.48	1.43
3	Ar	601	ADP	O2'-C2'	2.34	1.48	1.43
3	Ay	601	ADP	O2'-C2'	2.33	1.48	1.43
3	Bm	601	ADP	O2'-C2'	2.33	1.48	1.43
3	Bt	601	ADP	O2'-C2'	2.32	1.48	1.43
3	Ay	601	ADP	PA-O5'	2.25	1.68	1.59
3	Bm	601	ADP	PA-O5'	2.23	1.68	1.59
3	Bt	601	ADP	PA-O5'	2.22	1.68	1.59
3	Bf	601	ADP	PA-O5'	2.22	1.68	1.59
3	Ad	601	ADP	PA-O5'	2.22	1.68	1.59
3	Ar	601	ADP	PA-O5'	2.22	1.68	1.59
3	Ak	601	ADP	PA-O5'	2.22	1.68	1.59
3	As	601	ADP	PA-O5'	2.13	1.67	1.59
3	Bn	601	ADP	PA-O5'	2.12	1.67	1.59
3	Ae	601	ADP	PA-O5'	2.11	1.67	1.59
3	Az	601	ADP	PA-O5'	2.11	1.67	1.59
3	Bu	601	ADP	PA-O5'	2.11	1.67	1.59
3	Al	601	ADP	PA-O5'	2.10	1.67	1.59
3	Bg	601	ADP	PA-O5'	2.10	1.67	1.59

All (35) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Al	601	ADP	N3-C2-N1	-4.44	121.74	128.68
3	As	601	ADP	N3-C2-N1	-4.44	121.75	128.68
3	Bn	601	ADP	N3-C2-N1	-4.42	121.77	128.68
3	Bu	601	ADP	N3-C2-N1	-4.41	121.78	128.68
3	Ae	601	ADP	N3-C2-N1	-4.40	121.80	128.68
3	Bm	601	ADP	N3-C2-N1	-4.40	121.81	128.68
3	Az	601	ADP	N3-C2-N1	-4.40	121.81	128.68
3	Bg	601	ADP	N3-C2-N1	-4.40	121.81	128.68
3	Ar	601	ADP	N3-C2-N1	-4.39	121.82	128.68
3	Bf	601	ADP	N3-C2-N1	-4.39	121.82	128.68
3	Ad	601	ADP	N3-C2-N1	-4.37	121.85	128.68
3	Ak	601	ADP	N3-C2-N1	-4.37	121.85	128.68
3	Ay	601	ADP	N3-C2-N1	-4.35	121.87	128.68
3	Bt	601	ADP	N3-C2-N1	-4.35	121.88	128.68
3	Bu	601	ADP	PA-O3A-PB	-3.30	121.51	132.83
3	Al	601	ADP	PA-O3A-PB	-3.30	121.52	132.83
3	Ae	601	ADP	PA-O3A-PB	-3.29	121.54	132.83
3	Bn	601	ADP	PA-O3A-PB	-3.29	121.55	132.83
3	Bg	601	ADP	PA-O3A-PB	-3.28	121.57	132.83
3	As	601	ADP	PA-O3A-PB	-3.28	121.57	132.83
3	Az	601	ADP	PA-O3A-PB	-3.28	121.58	132.83
3	Bt	601	ADP	PA-O3A-PB	-2.23	125.18	132.83
3	Bm	601	ADP	PA-O3A-PB	-2.22	125.19	132.83
3	Ak	601	ADP	PA-O3A-PB	-2.22	125.20	132.83
3	Bf	601	ADP	PA-O3A-PB	-2.22	125.21	132.83
3	Ad	601	ADP	PA-O3A-PB	-2.22	125.21	132.83
3	Ar	601	ADP	PA-O3A-PB	-2.22	125.21	132.83
3	Ay	601	ADP	PA-O3A-PB	-2.21	125.23	132.83
3	Az	601	ADP	C4-C5-N7	-2.11	107.20	109.40
3	Al	601	ADP	C4-C5-N7	-2.11	107.20	109.40
3	Bn	601	ADP	C4-C5-N7	-2.11	107.20	109.40
3	As	601	ADP	C4-C5-N7	-2.10	107.21	109.40
3	Ae	601	ADP	C4-C5-N7	-2.10	107.21	109.40
3	Bu	601	ADP	C4-C5-N7	-2.10	107.22	109.40
3	Bg	601	ADP	C4-C5-N7	-2.09	107.22	109.40

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Ae	601	ADP	C5'-O5'-PA-O1A
3	Ae	601	ADP	C5'-O5'-PA-O2A
3	Ae	601	ADP	C5'-O5'-PA-O3A
3	Ae	601	ADP	C3'-C4'-C5'-O5'
3	Al	601	ADP	C5'-O5'-PA-O1A
3	Al	601	ADP	C5'-O5'-PA-O2A
3	Al	601	ADP	C5'-O5'-PA-O3A
3	Al	601	ADP	C3'-C4'-C5'-O5'
3	As	601	ADP	C5'-O5'-PA-O1A
3	As	601	ADP	C5'-O5'-PA-O2A
3	As	601	ADP	C5'-O5'-PA-O3A
3	As	601	ADP	C3'-C4'-C5'-O5'
3	Az	601	ADP	C5'-O5'-PA-O1A
3	Az	601	ADP	C5'-O5'-PA-O2A
3	Az	601	ADP	C5'-O5'-PA-O3A
3	Az	601	ADP	C3'-C4'-C5'-O5'
3	Bg	601	ADP	C5'-O5'-PA-O1A
3	Bg	601	ADP	C5'-O5'-PA-O2A
3	Bg	601	ADP	C5'-O5'-PA-O3A
3	Bg	601	ADP	C3'-C4'-C5'-O5'
3	Bn	601	ADP	C5'-O5'-PA-O1A
3	Bn	601	ADP	C5'-O5'-PA-O2A
3	Bn	601	ADP	C5'-O5'-PA-O3A
3	Bn	601	ADP	C3'-C4'-C5'-O5'
3	Bu	601	ADP	C5'-O5'-PA-O1A
3	Bu	601	ADP	C5'-O5'-PA-O2A
3	Bu	601	ADP	C5'-O5'-PA-O3A
3	Bu	601	ADP	C3'-C4'-C5'-O5'
3	Ae	601	ADP	O4'-C4'-C5'-O5'
3	Al	601	ADP	O4'-C4'-C5'-O5'
3	As	601	ADP	O4'-C4'-C5'-O5'
3	Az	601	ADP	O4'-C4'-C5'-O5'
3	Bg	601	ADP	O4'-C4'-C5'-O5'
3	Bn	601	ADP	O4'-C4'-C5'-O5'
3	Bu	601	ADP	O4'-C4'-C5'-O5'
3	Ad	601	ADP	C3'-C4'-C5'-O5'
3	Ak	601	ADP	C3'-C4'-C5'-O5'
3	Ar	601	ADP	C3'-C4'-C5'-O5'
3	Ay	601	ADP	C3'-C4'-C5'-O5'
3	Bf	601	ADP	C3'-C4'-C5'-O5'
3	Bm	601	ADP	C3'-C4'-C5'-O5'
3	Bt	601	ADP	C3'-C4'-C5'-O5'
3	Ae	601	ADP	PB-O3A-PA-O5'

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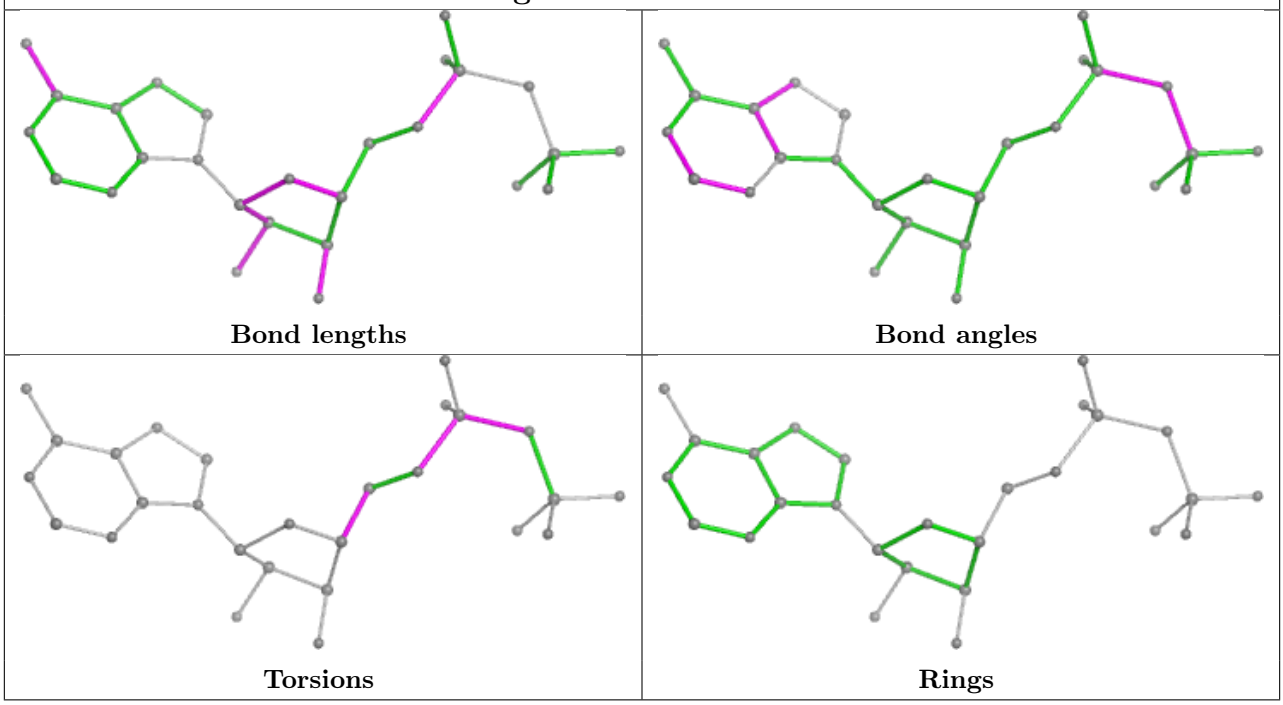
Mol	Chain	Res	Type	Atoms
3	Al	601	ADP	PB-O3A-PA-O5'
3	As	601	ADP	PB-O3A-PA-O5'
3	Az	601	ADP	PB-O3A-PA-O5'
3	Bg	601	ADP	PB-O3A-PA-O5'
3	Bn	601	ADP	PB-O3A-PA-O5'
3	Bu	601	ADP	PB-O3A-PA-O5'
3	Bm	601	ADP	O4'-C4'-C5'-O5'
3	Ad	601	ADP	O4'-C4'-C5'-O5'
3	Ak	601	ADP	O4'-C4'-C5'-O5'
3	Ar	601	ADP	O4'-C4'-C5'-O5'
3	Ay	601	ADP	O4'-C4'-C5'-O5'
3	Bf	601	ADP	O4'-C4'-C5'-O5'
3	Bt	601	ADP	O4'-C4'-C5'-O5'
3	Ad	601	ADP	PB-O3A-PA-O2A
3	Ak	601	ADP	PB-O3A-PA-O2A
3	Ar	601	ADP	PB-O3A-PA-O2A
3	Ay	601	ADP	PB-O3A-PA-O2A
3	Bf	601	ADP	PB-O3A-PA-O2A
3	Bm	601	ADP	PB-O3A-PA-O2A
3	Bt	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

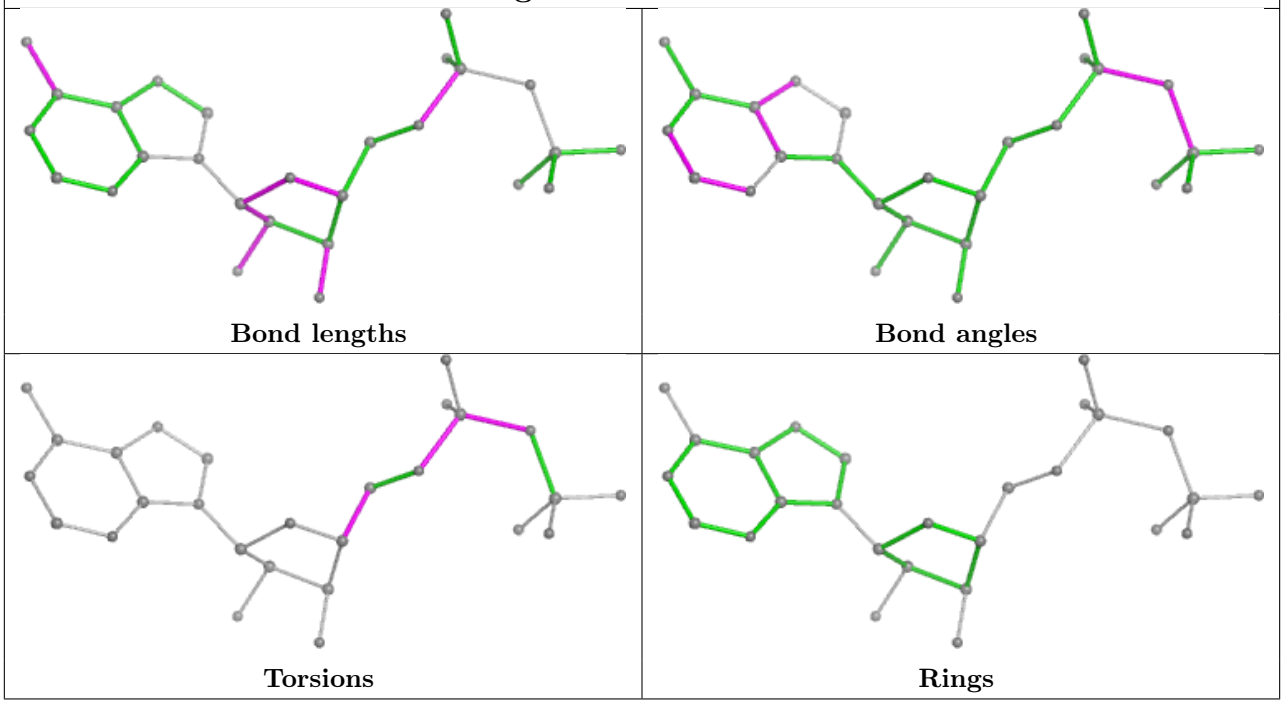
No monomer is involved in short contacts.

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

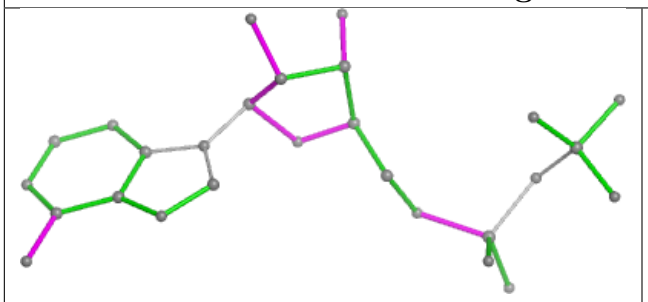
Ligand ADP Bu 601



Ligand ADP Ae 601



Ligand ADP Ar 601



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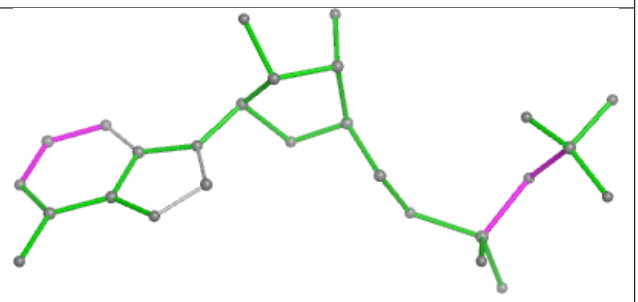
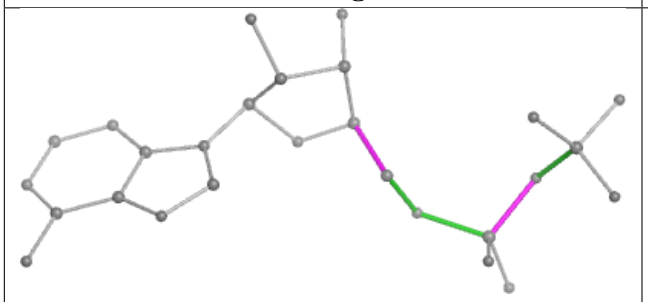
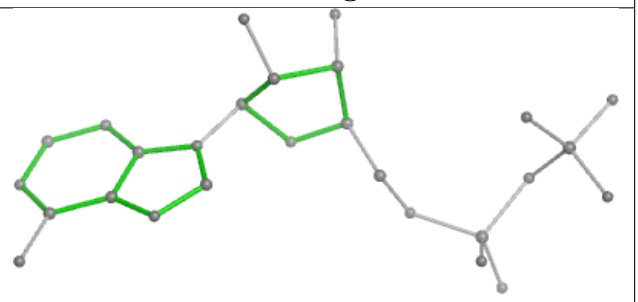


Bond angles

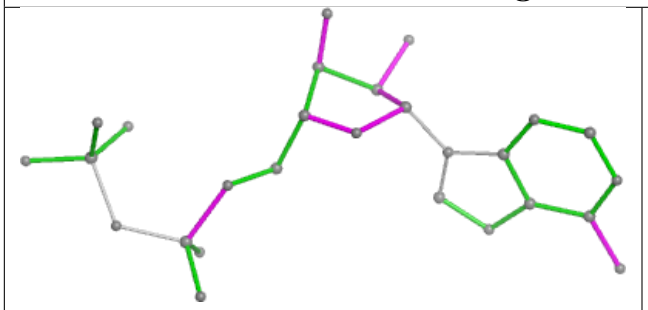


Torsions

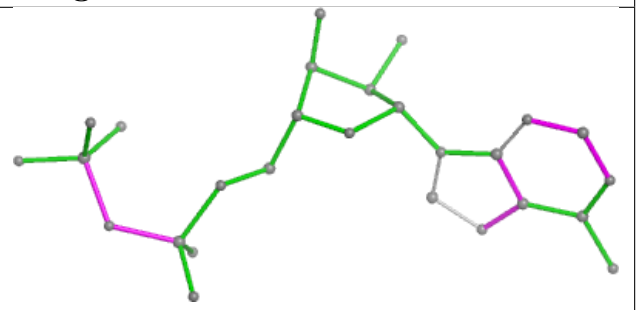


Rings

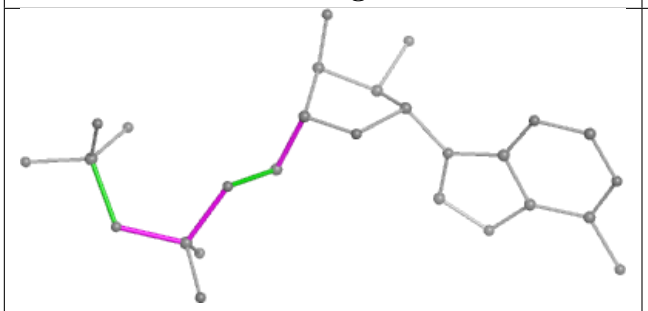
Ligand ADP Bg 601



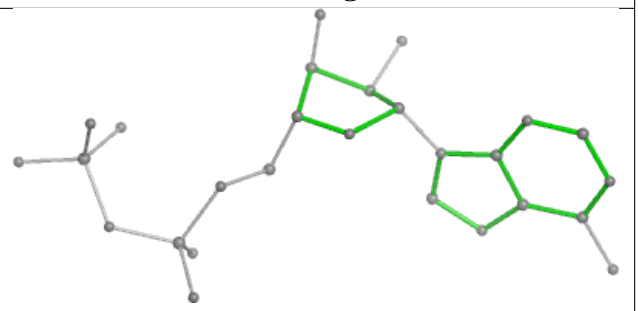
Bond lengths



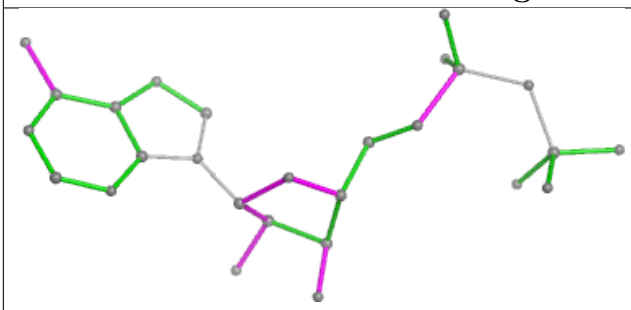
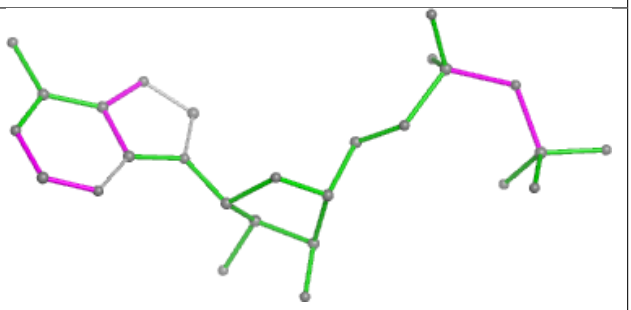
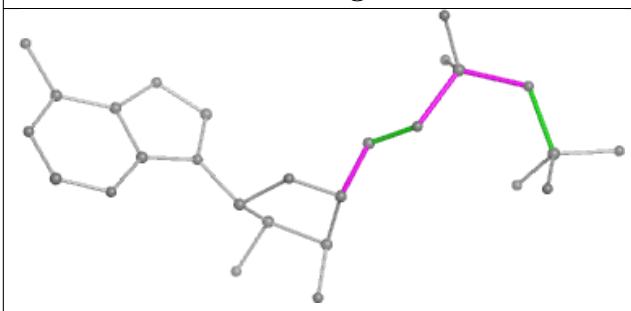
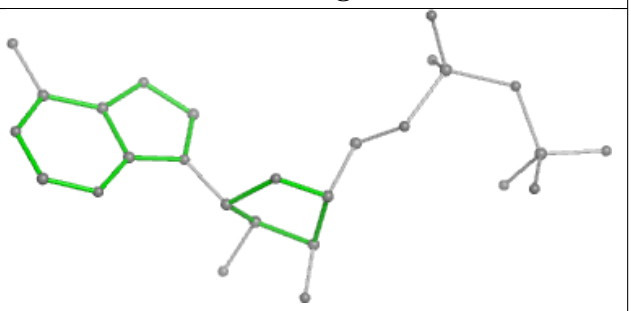
Bond angles



Torsions



Rings

Ligand ADP Az 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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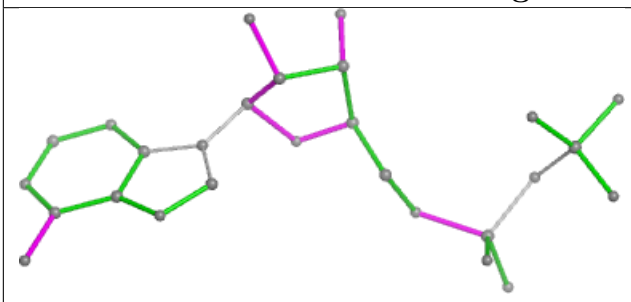
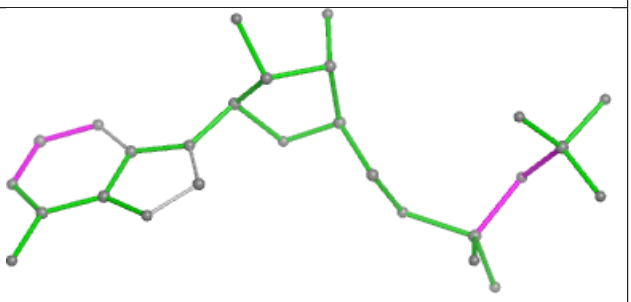
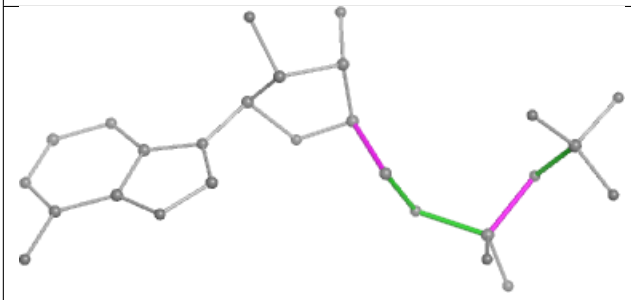
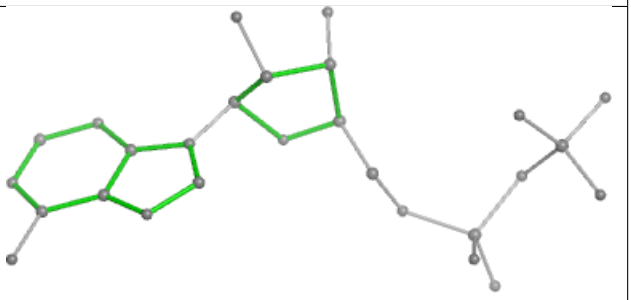
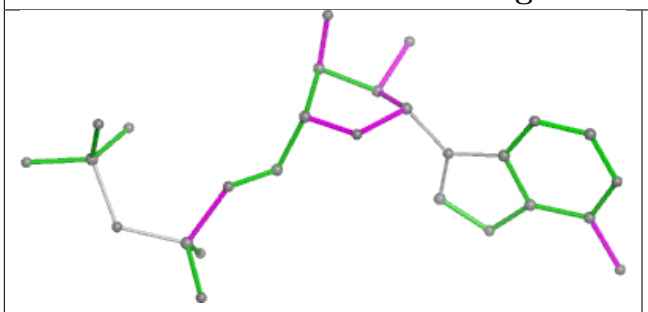
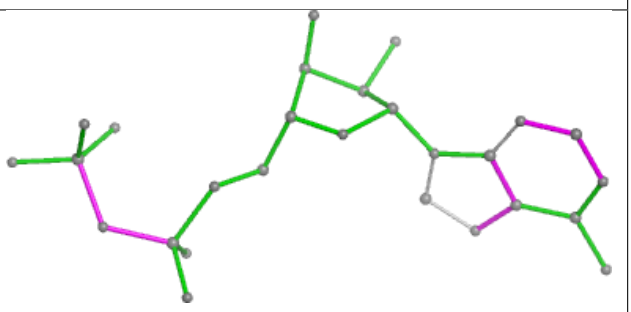
 Bond lengths	 Bond angles
 Torsions	 Rings

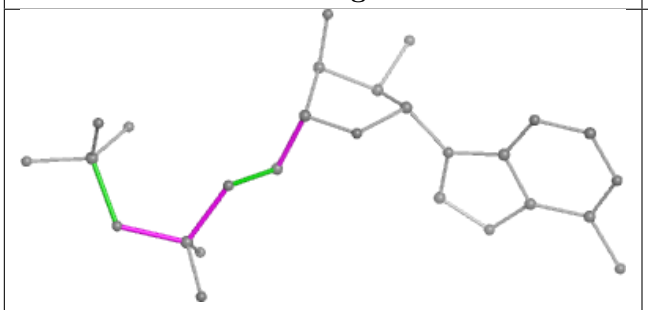
Ligand ADP As 601



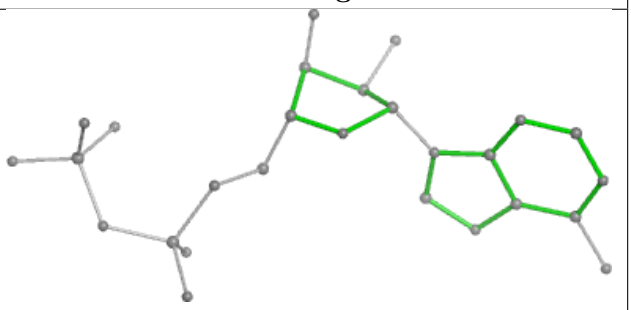
Bond lengths



Bond angles

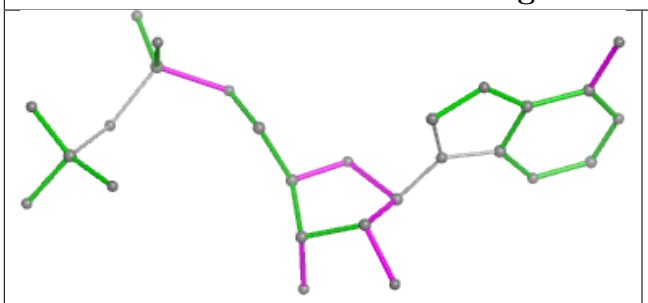


Torsions



Rings

Ligand ADP Bf 601



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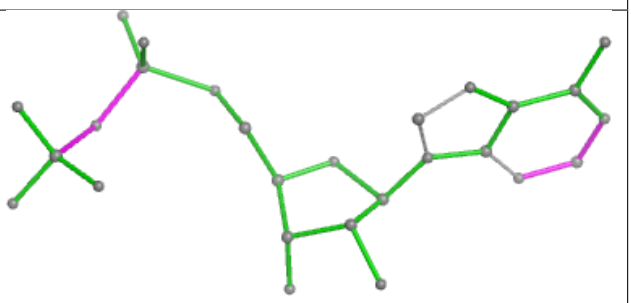
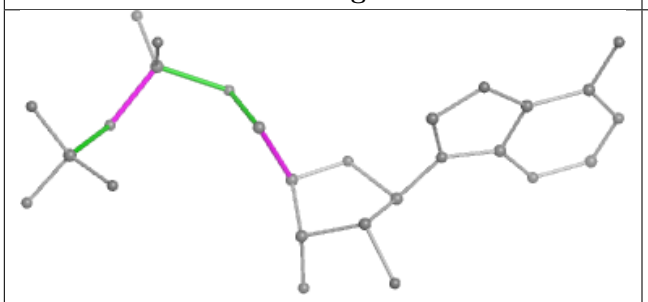


Bond angles



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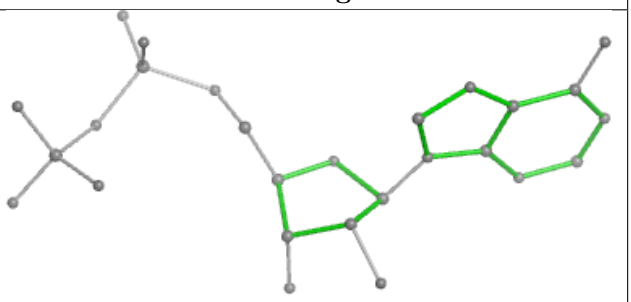
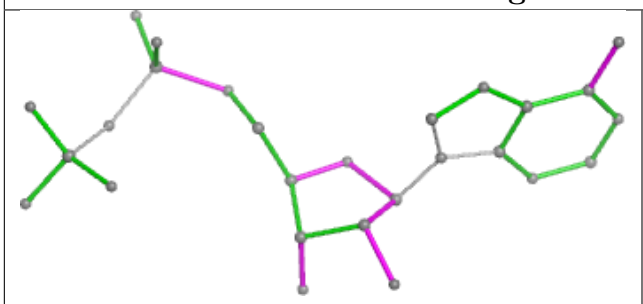
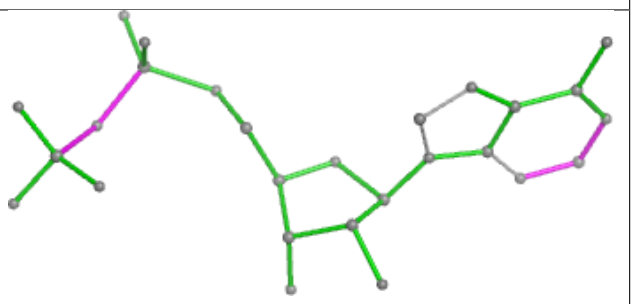
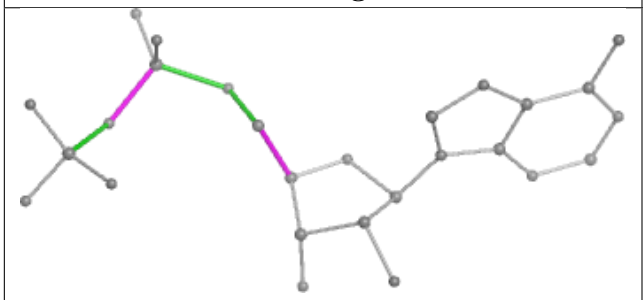
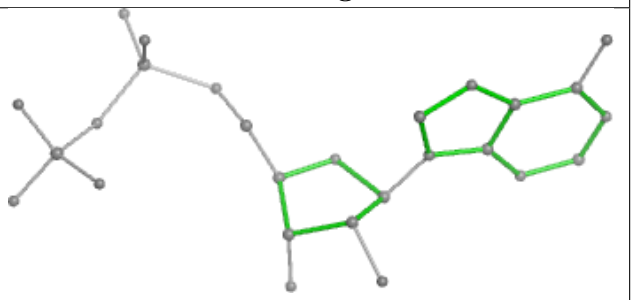
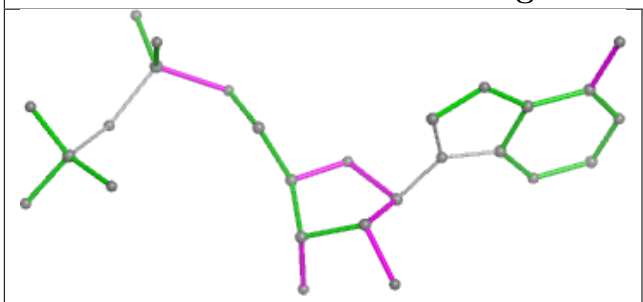
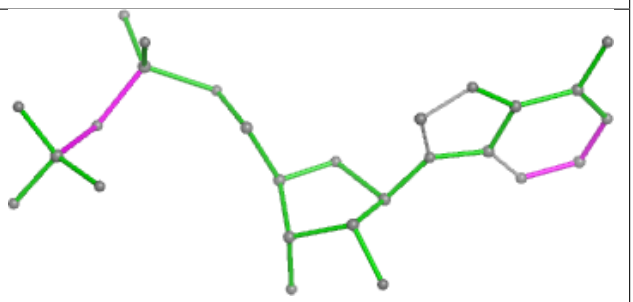
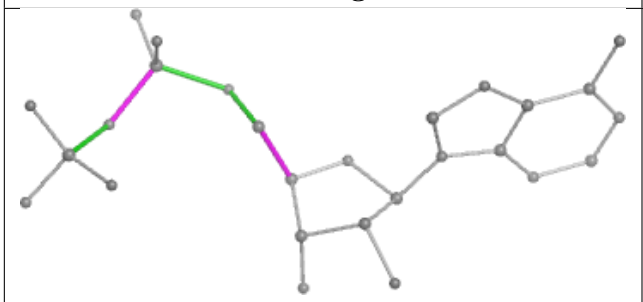
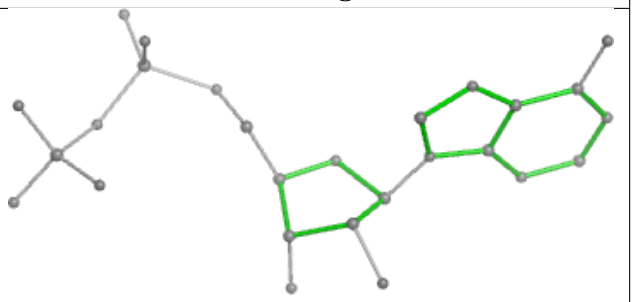
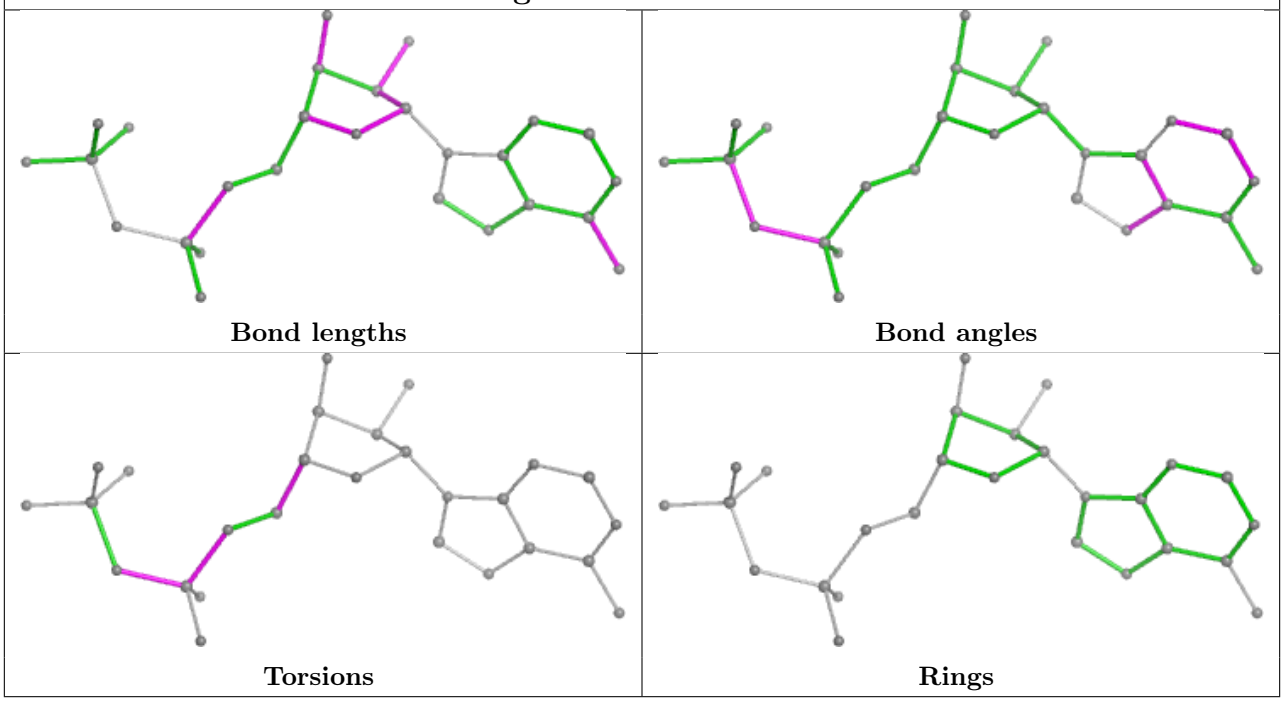


Rings

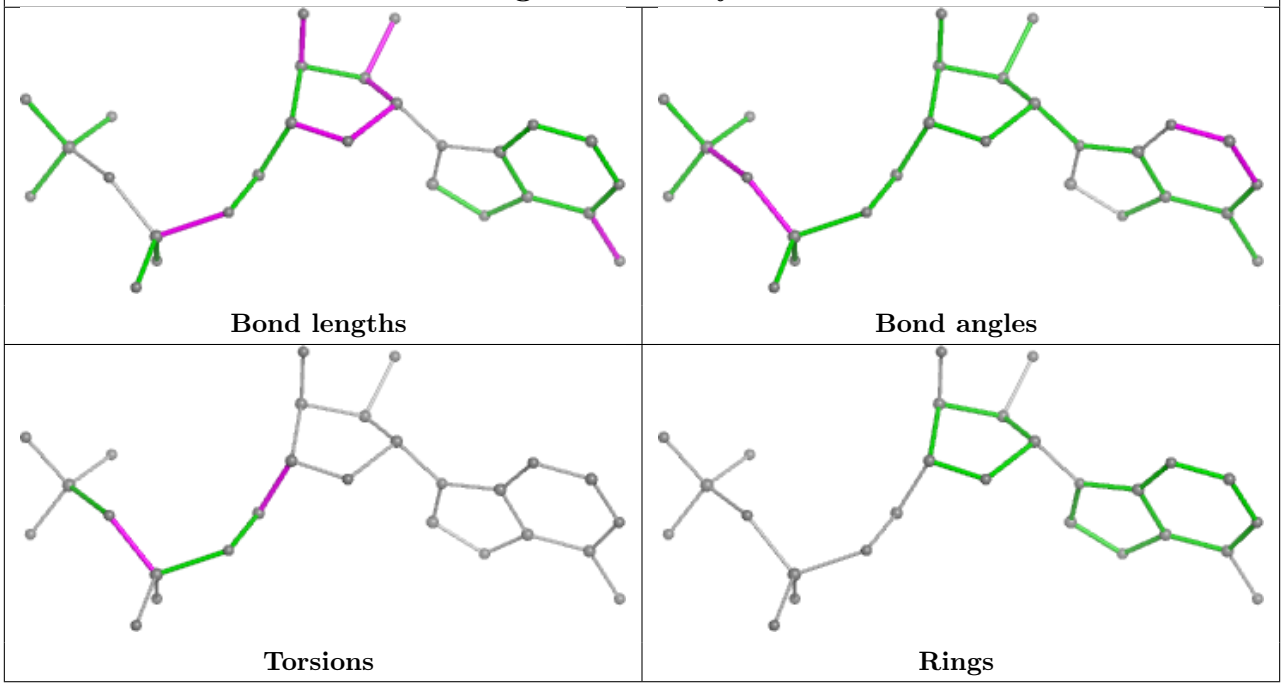
Ligand ADP Bm 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

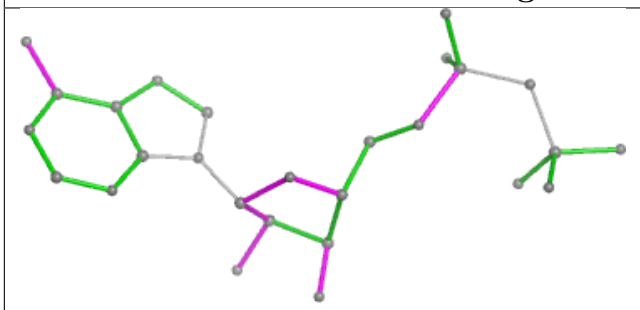
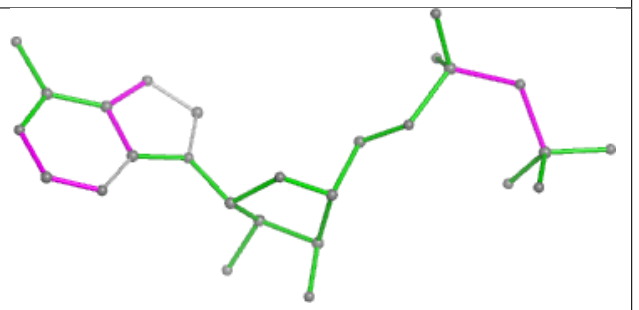
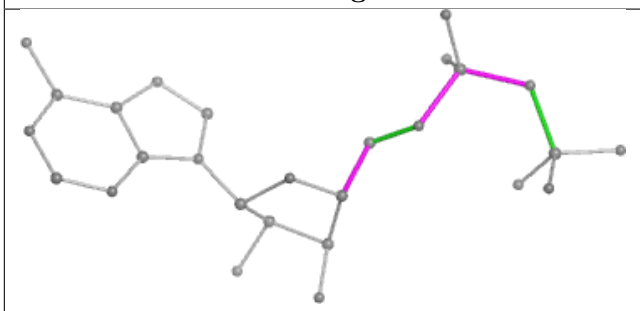
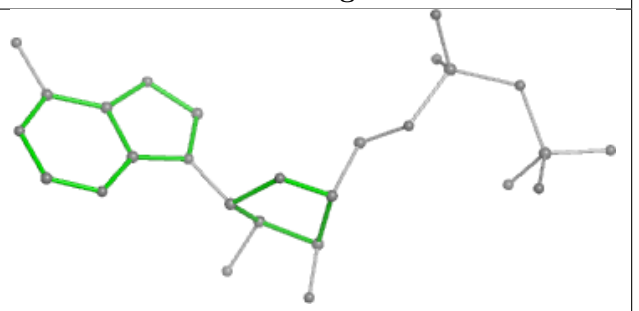
Ligand ADP Bt 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

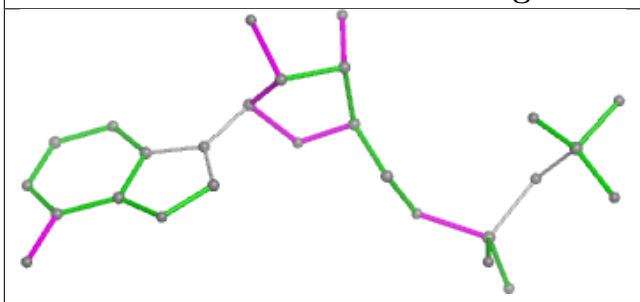
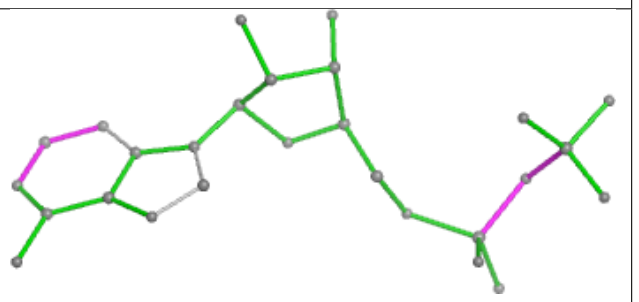
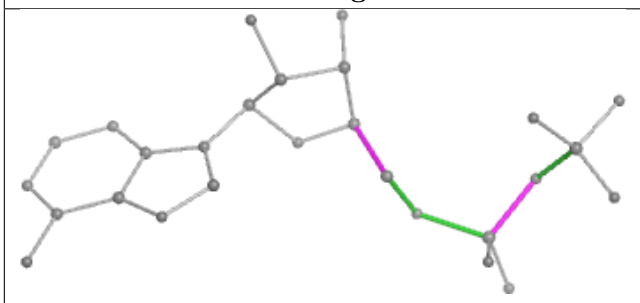
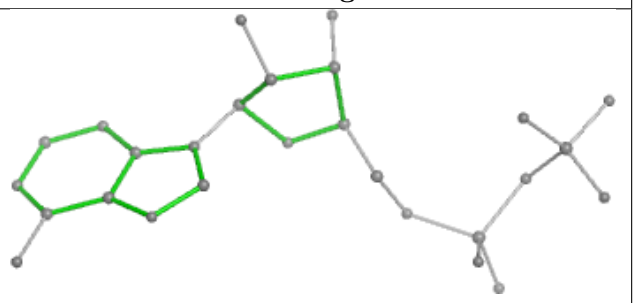
Ligand ADP Bn 601



Ligand ADP Ay 601



Ligand ADP Al 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Ad 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

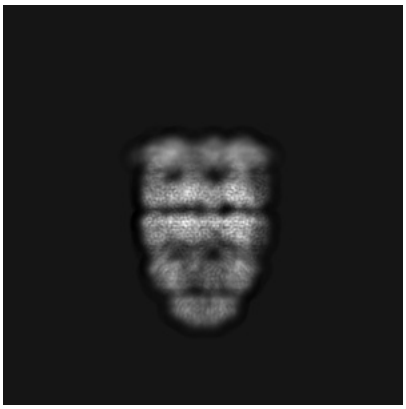
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13293. These allow visual inspection of the internal detail of the map and identification of artifacts.

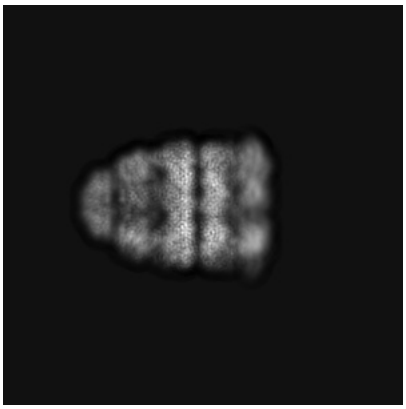
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

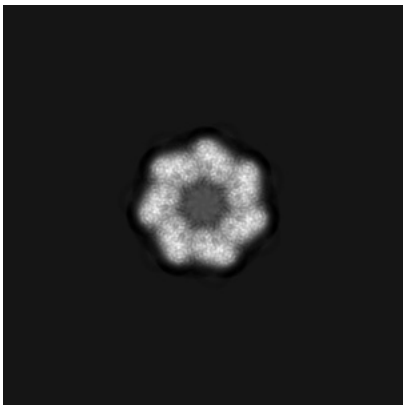
6.1.1 Primary map



X

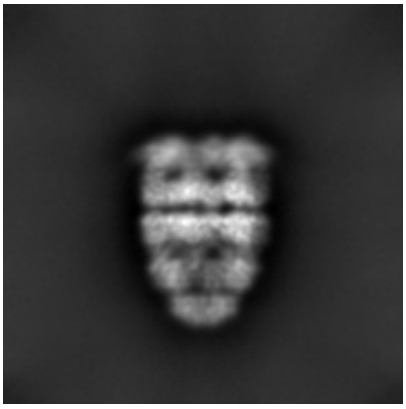


Y

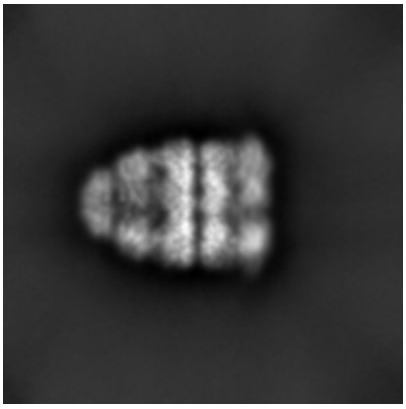


Z

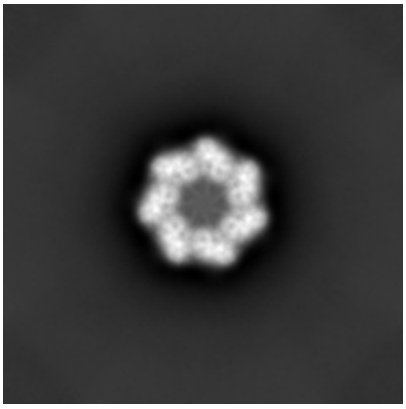
6.1.2 Raw map



X



Y

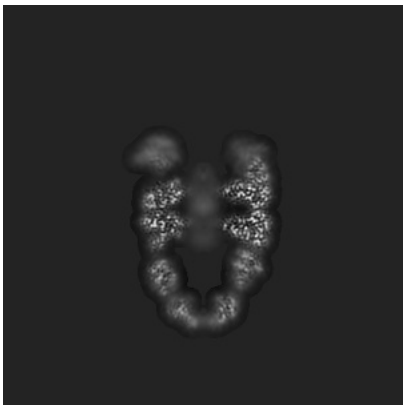


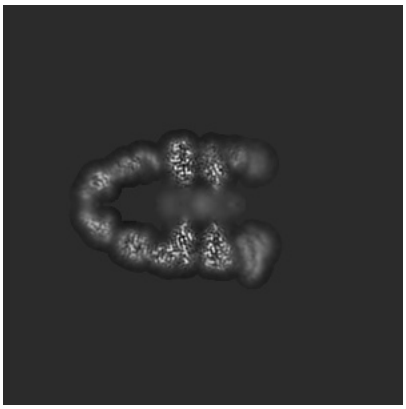
Z

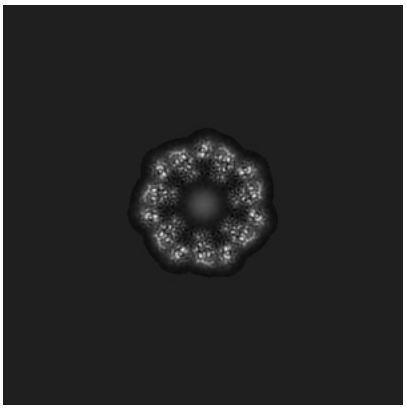
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

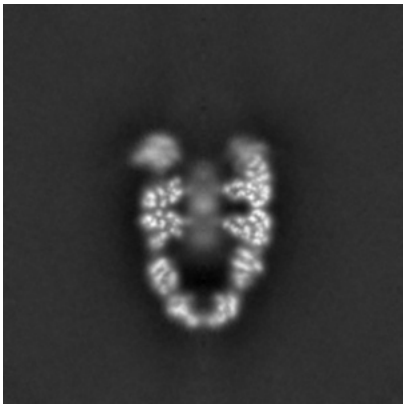
6.2.1 Primary map

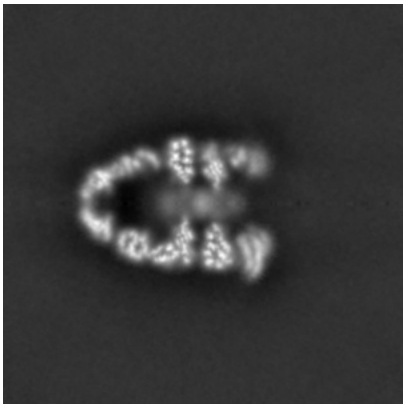

X Index: 192

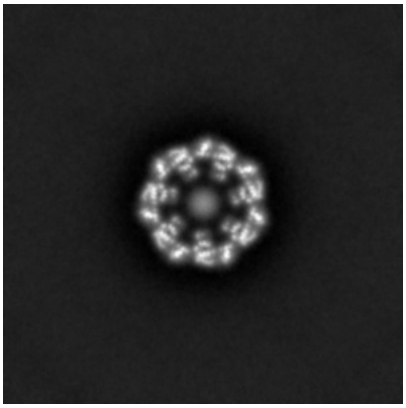

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

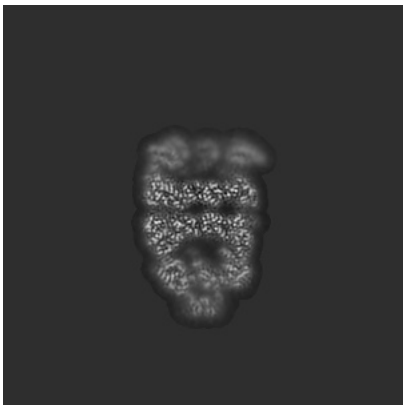

Y Index: 192

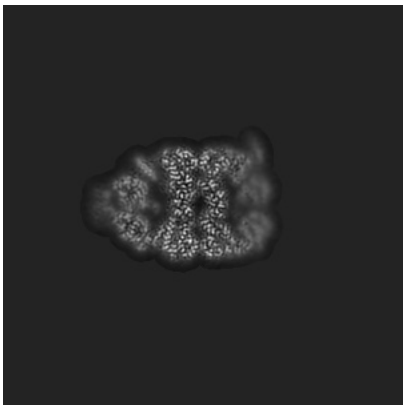

Z Index: 192

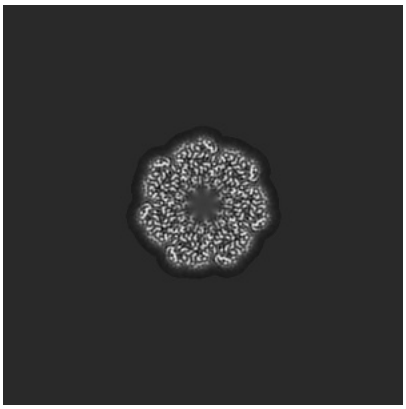
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

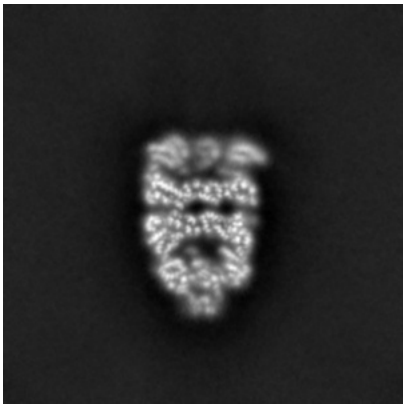
6.3.1 Primary map

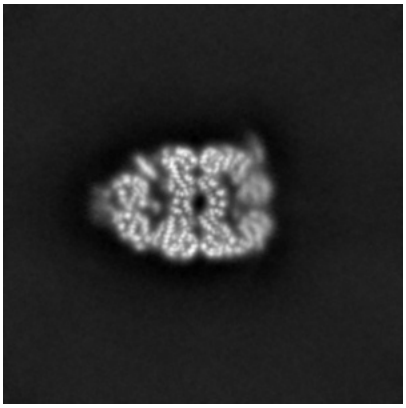

X Index: 162

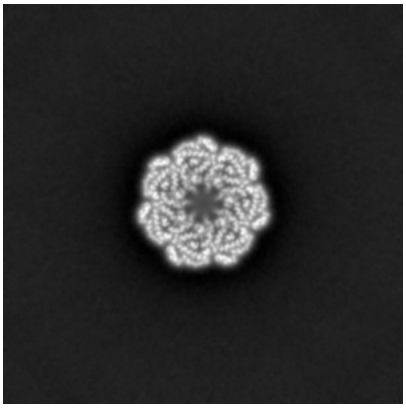

Y Index: 225


Z Index: 175

6.3.2 Raw map


X Index: 161

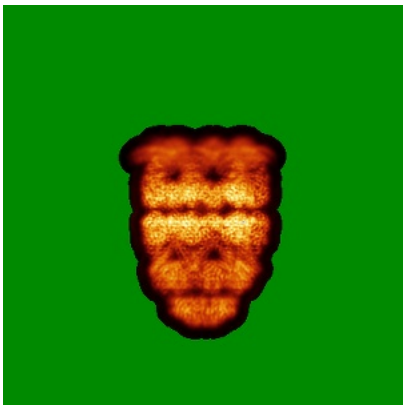

Y Index: 226

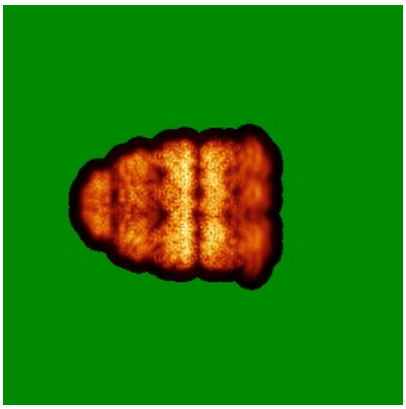

Z Index: 175

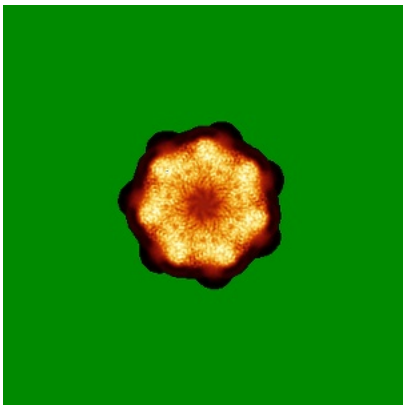
The images above show the largest variance slices of the map in three orthogonal directions.

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

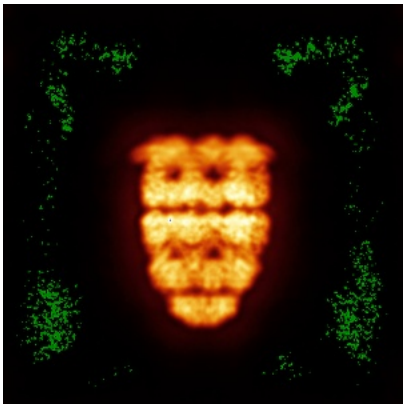
6.4.1 Primary map

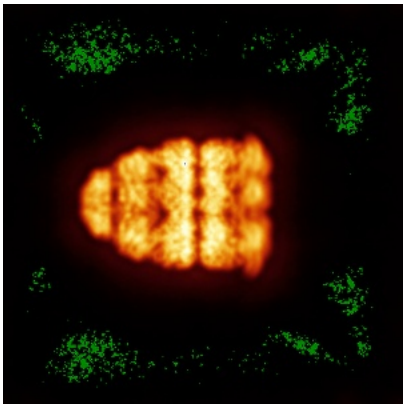

X

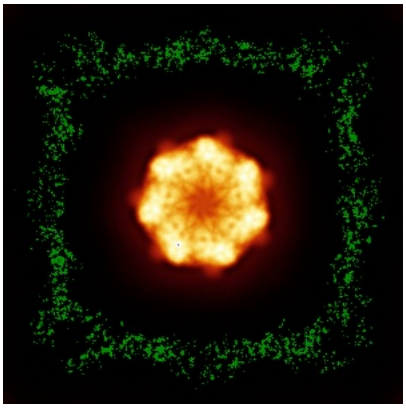

Y


Z

6.4.2 Raw map


X

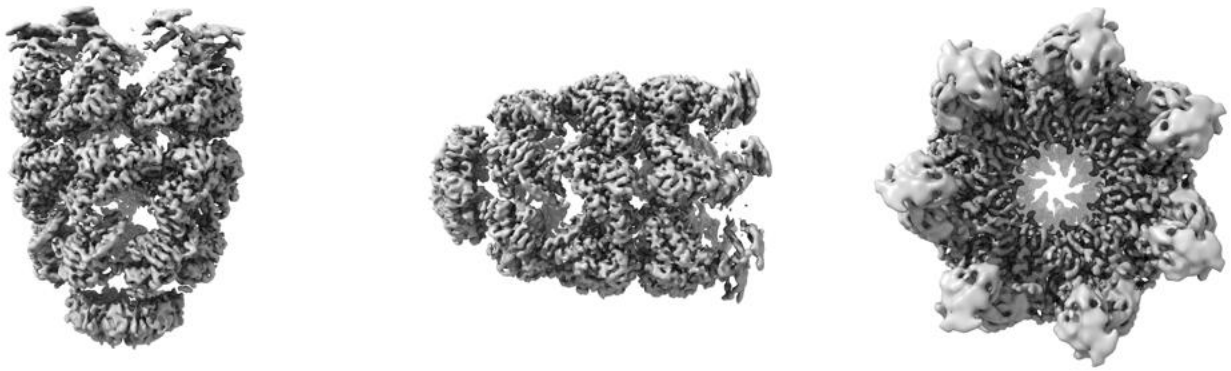

Y


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)

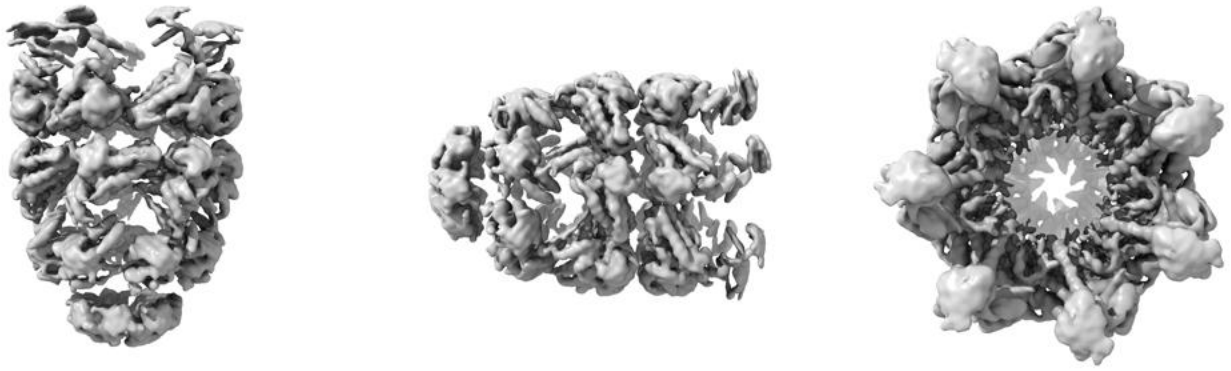
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. 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.

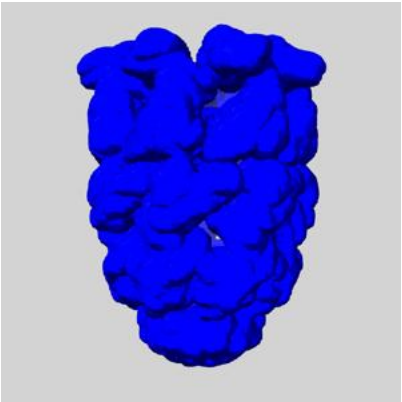
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

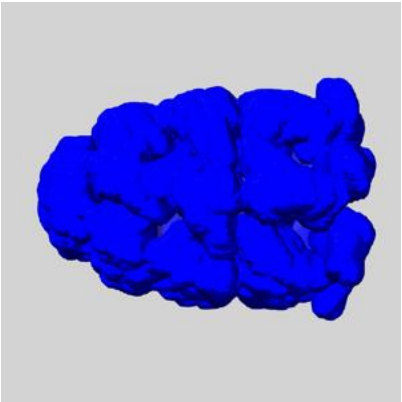
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

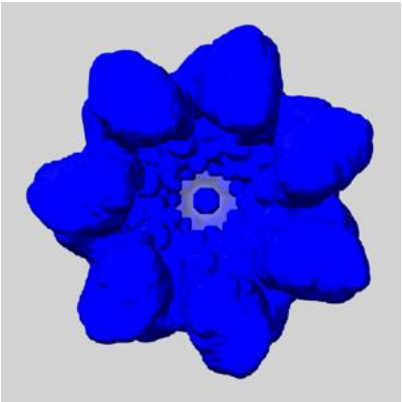
6.6.1 emd_13293_msk_1.map (i)



X



Y

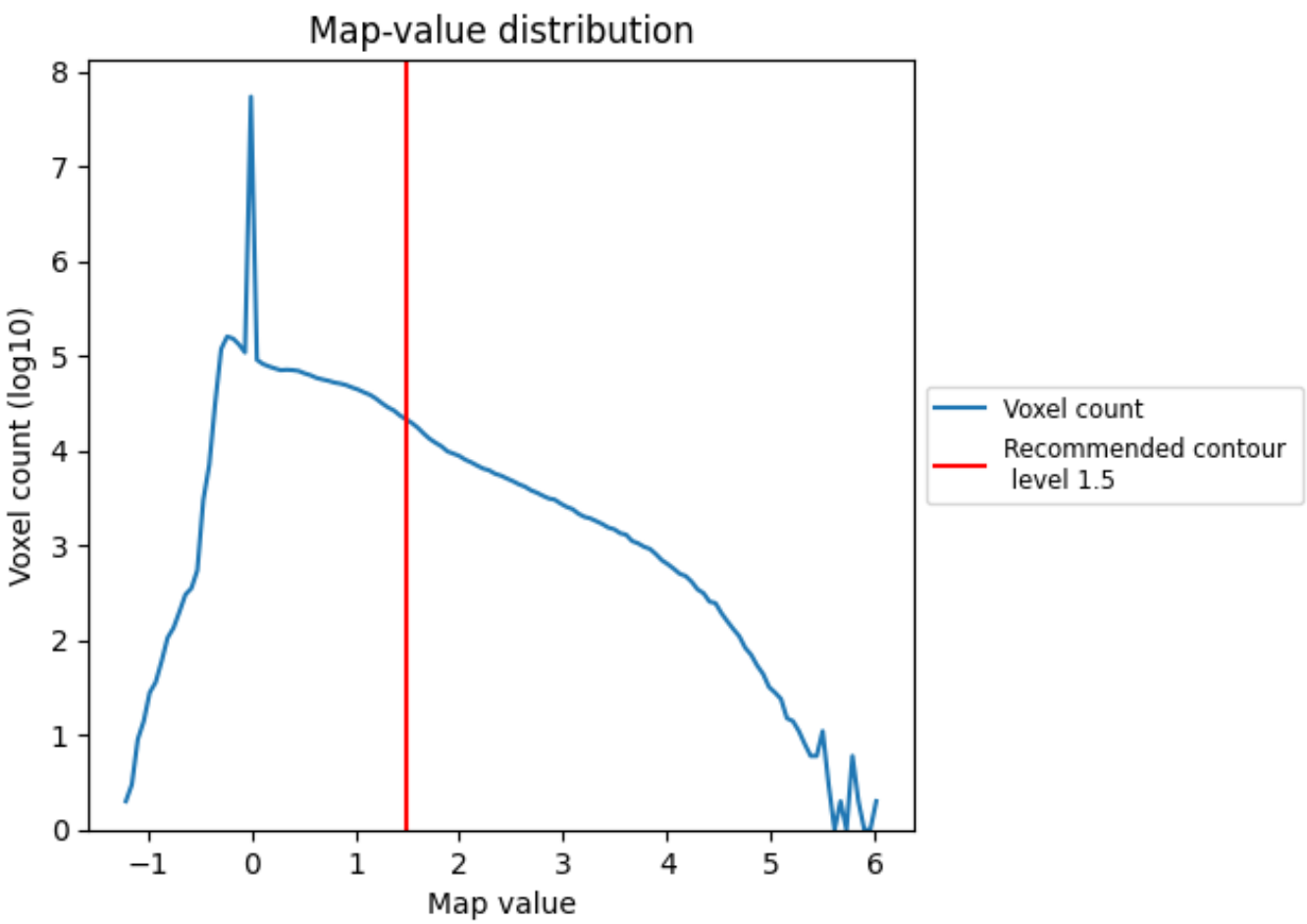


Z

7 Map analysis (i)

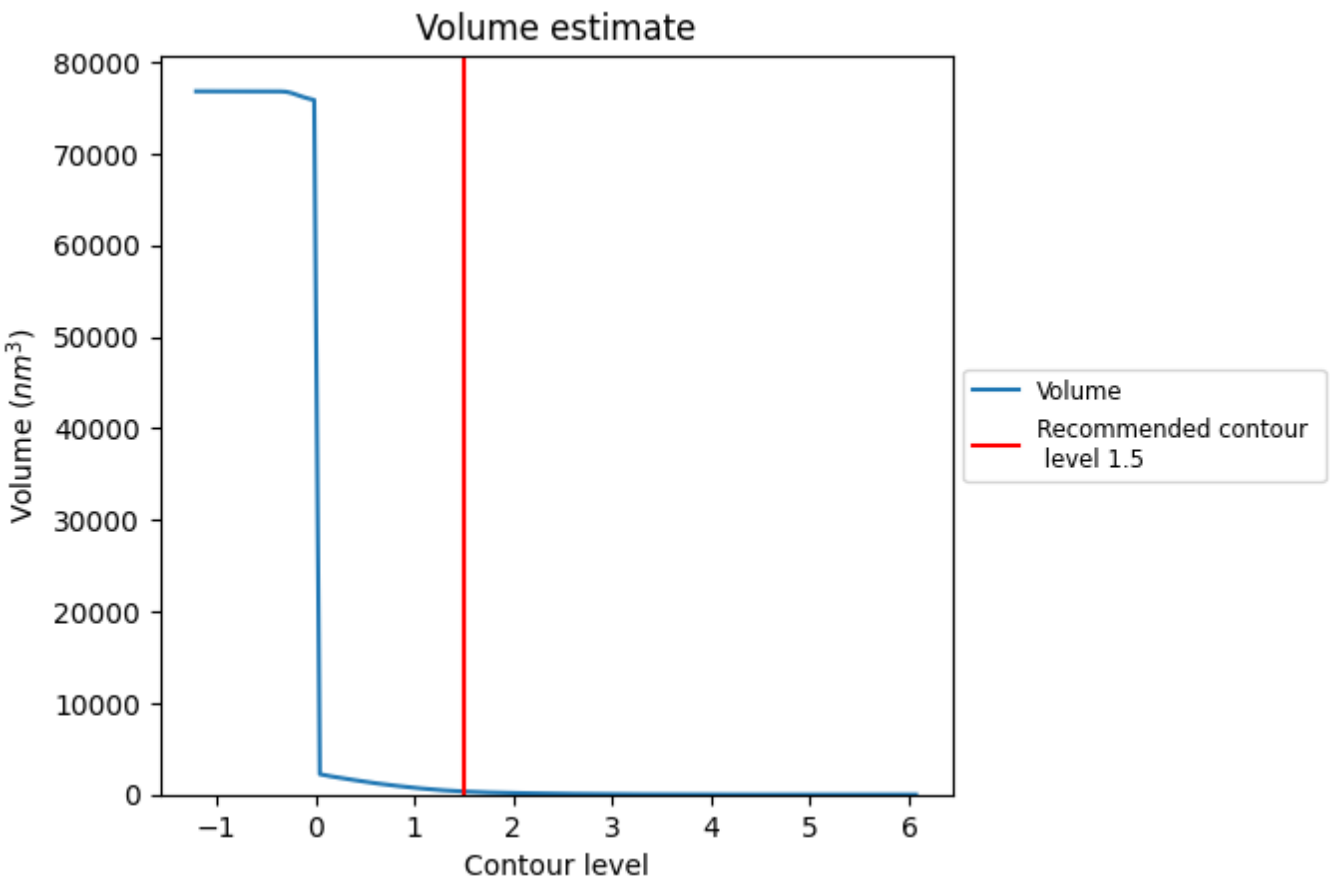
This section contains the results of statistical analysis of the map.

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.

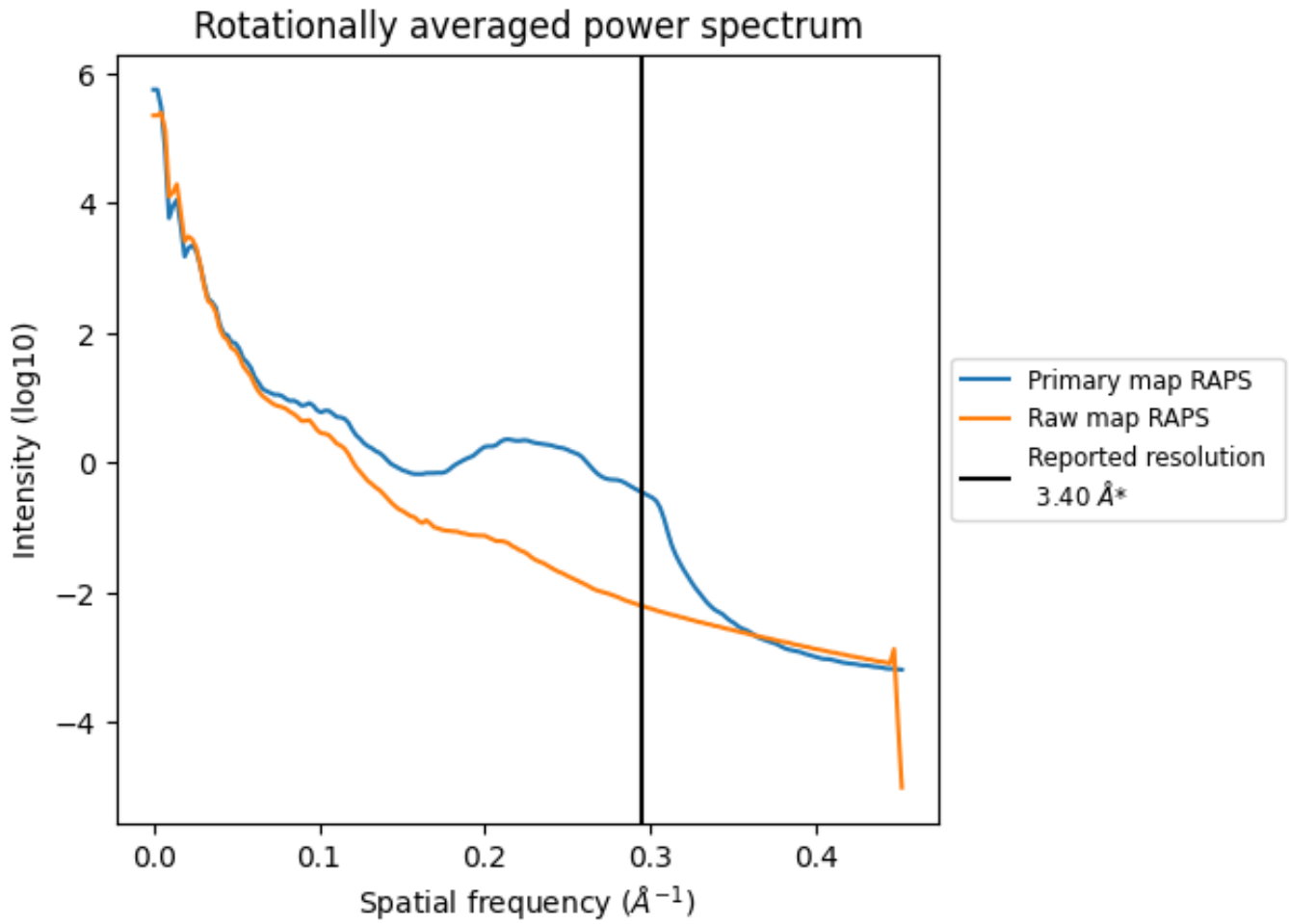
7.2 Volume estimate (i)



The volume at the recommended contour level is 336 nm^3; this corresponds to an approximate mass of 303 kDa.

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

7.3 Rotationally averaged power spectrum (i)

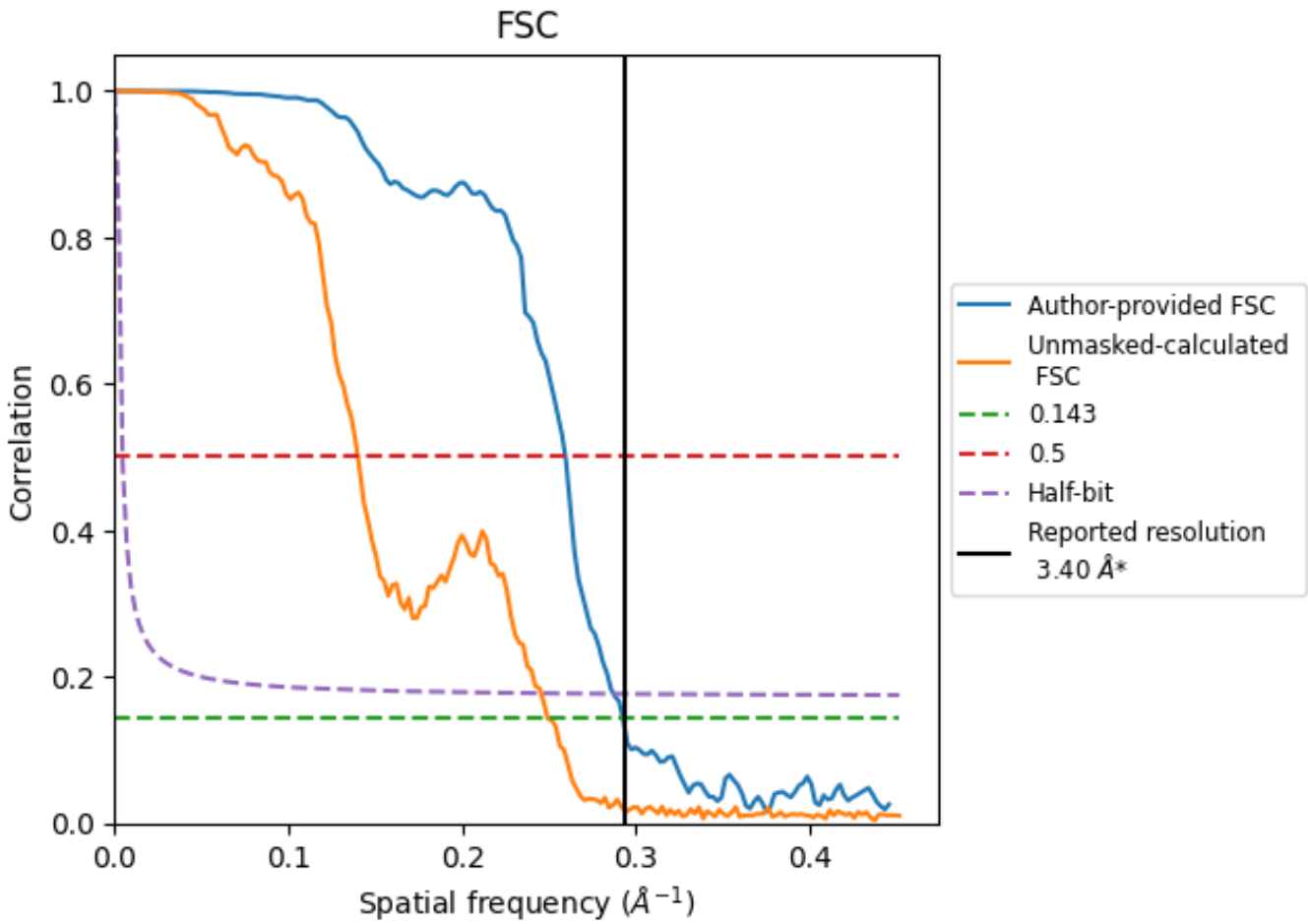


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

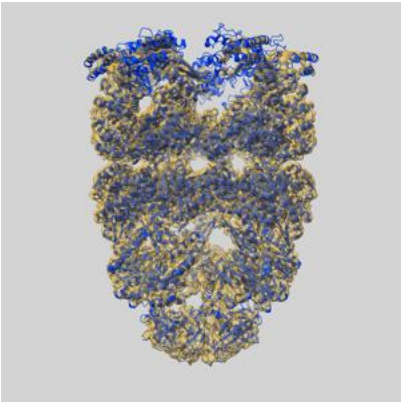
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.85	3.48
Unmasked-calculated*	4.01	7.14	4.07

*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 4.01 differs from the reported value 3.4 by more than 10 %

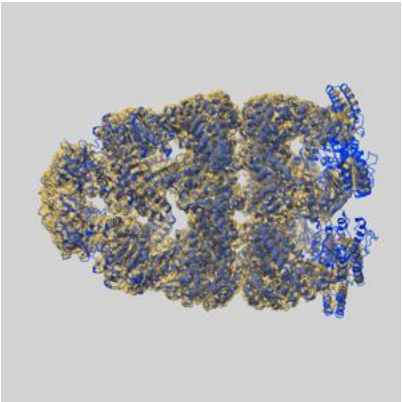
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13293 and PDB model 7PBJ. Per-residue inclusion information can be found in section 3 on page 8.

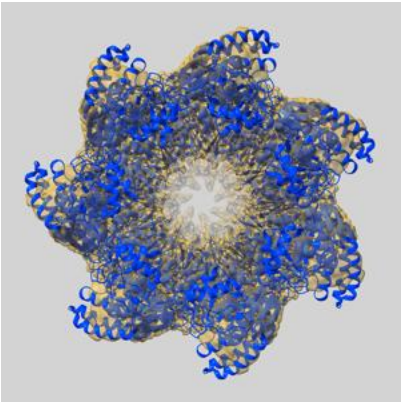
9.1 Map-model overlay (i)



X



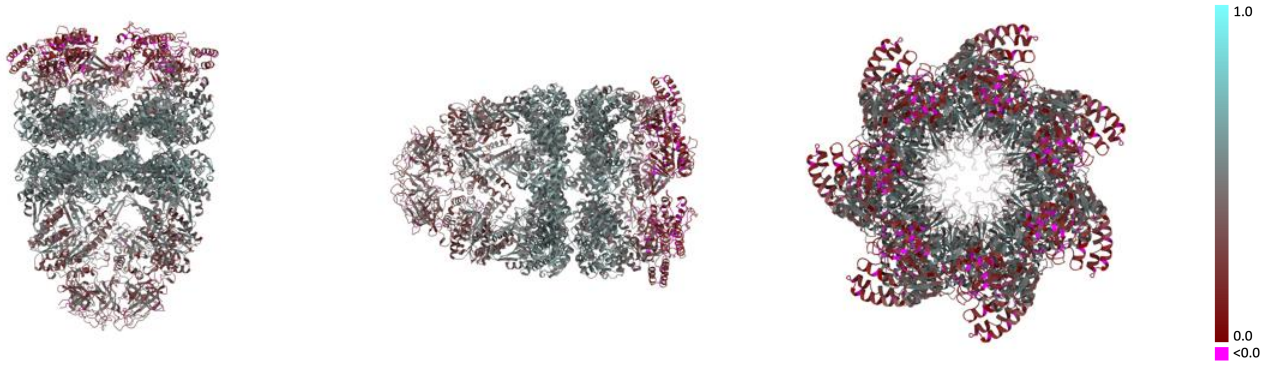
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

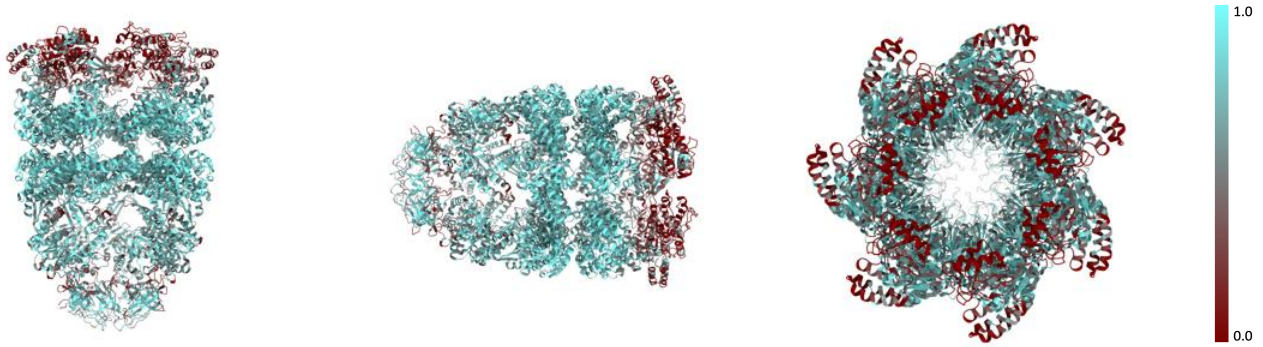
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

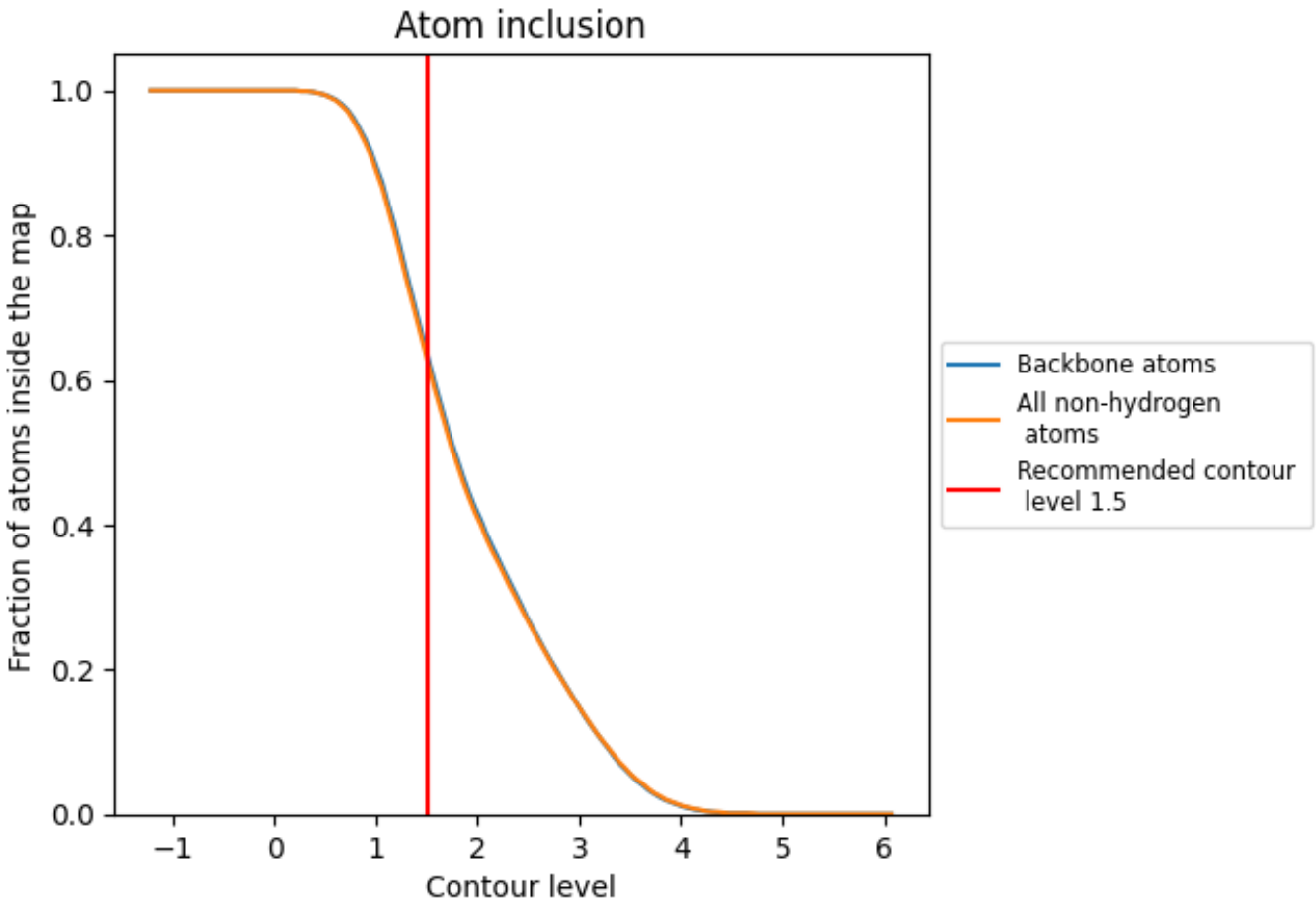
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.4050
Ad	0.5420	0.3630
Ae	0.7500	0.4650
Af	0.5440	0.3120
Ak	0.5390	0.3620
Al	0.7520	0.4650
Am	0.5540	0.3100
Ar	0.5410	0.3630
As	0.7520	0.4640
At	0.5520	0.3100
Ay	0.5400	0.3610
Az	0.7540	0.4640
Ba	0.5480	0.3130
Bf	0.5410	0.3620
Bg	0.7540	0.4660
Bh	0.5580	0.3130
Bm	0.5420	0.3630
Bn	0.7570	0.4640
Bo	0.5520	0.3130
Bt	0.5420	0.3630
Bu	0.7520	0.4660
Bv	0.5520	0.3130