Full wwPDB EM Validation Report

Nov 24, 2021 – 03:19 pm GMT

PDB ID	:	7PBX
EMDB ID	:	EMD-13308
Title	:	Cryo-EM structure of the GroEL-GroES complex with ADP bound to both rings ("tight" conformation).
Authors	:	Pichkur, E.B.; Stanishneva-Konovalova, T.B.
Deposited on	:	2021-08-02
Resolution	:	3.43 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 ⓘ symbol.

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

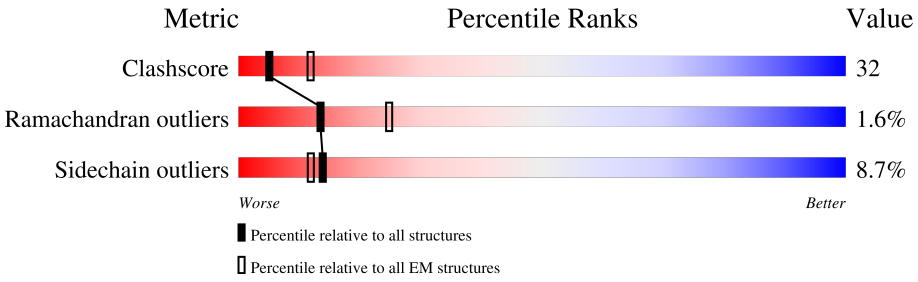
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4 (270009), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.43 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)
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	Ac	524	36% 88% 10% ·
1	Ad	524	8% 93% 6%
1	Ai	524	36% 88% 10% ·
1	Aj	524	9% 94% 6%
1	Ao	524	36% 88% 10% ·
1	Ap	524	8% 93% 6%
1	Au	524	37% 88% 10% ·
1	Av	524	8% 94% 6%

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Mol	Chain	Length	Quality of chain
1	Ba	524	36% 88% 10%
1	Bb	524	8% 94% 6%
1	Bg	524	36% 88% 10%
1	Bh	524	8% 94% 6%
1	Bm	524	36% 88% 10%
1	Bn	524	8% 94% 6%
2	Af	97	30% 65% 26% 5%
2	Al	97	30% 65% 26% 5%
2	Ar	97	30% 65% 26% 5%
2	Ax	97	31% 65% 26% 5%
2	Bd	97	30% 65% 26% 5%
2	Bj	97	30% 65% 26% 5%
2	Bp	97	30% 65% 26% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	Ad	601	X	-	-	-
3	ADP	Aj	601	X	-	-	-
3	ADP	Ap	601	X	-	-	-
3	ADP	Av	601	X	-	-	-
3	ADP	Bb	601	X	-	-	-
3	ADP	Bh	601	X	-	-	-
3	ADP	Bn	601	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 59472 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
1	Ac	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ad	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ai	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Aj	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ao	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ap	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Au	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Av	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ba	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bb	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bg	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bh	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bm	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bn	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		

- Molecule 2 is a protein called 10 kDa chaperonin.

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

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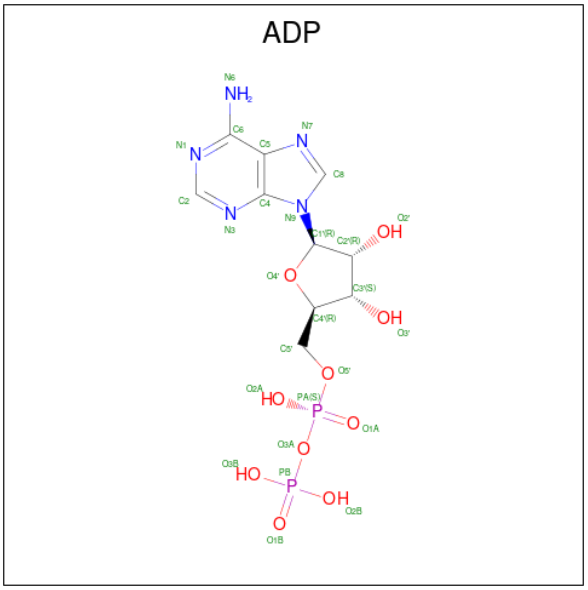
Mol	Chain	Residues	Atoms					AltConf	Trace
2	Al	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Ar	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Ax	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Bd	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Bj	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Bp	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

- 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
3	Ac	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ad	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ai	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Aj	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ao	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
3	Ap	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Au	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Av	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ba	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bb	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bg	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bh	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bm	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bn	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
4	Ac	1	Total	Mg	0
			1	1	
4	Ad	1	Total	Mg	0
			1	1	
4	Ai	1	Total	Mg	0
			1	1	
4	Aj	1	Total	Mg	0
			1	1	
4	Ao	1	Total	Mg	0
			1	1	
4	Ap	1	Total	Mg	0
			1	1	
4	Au	1	Total	Mg	0
			1	1	
4	Av	1	Total	Mg	0
			1	1	
4	Ba	1	Total	Mg	0
			1	1	
4	Bb	1	Total	Mg	0
			1	1	

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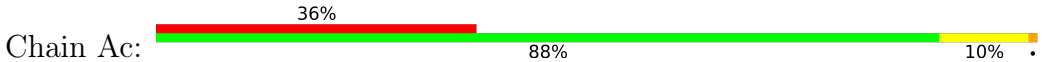
Mol	Chain	Residues	Atoms	AltConf
4	Bg	1	Total Mg 1 1	0
4	Bh	1	Total Mg 1 1	0
4	Bm	1	Total Mg 1 1	0
4	Bn	1	Total Mg 1 1	0

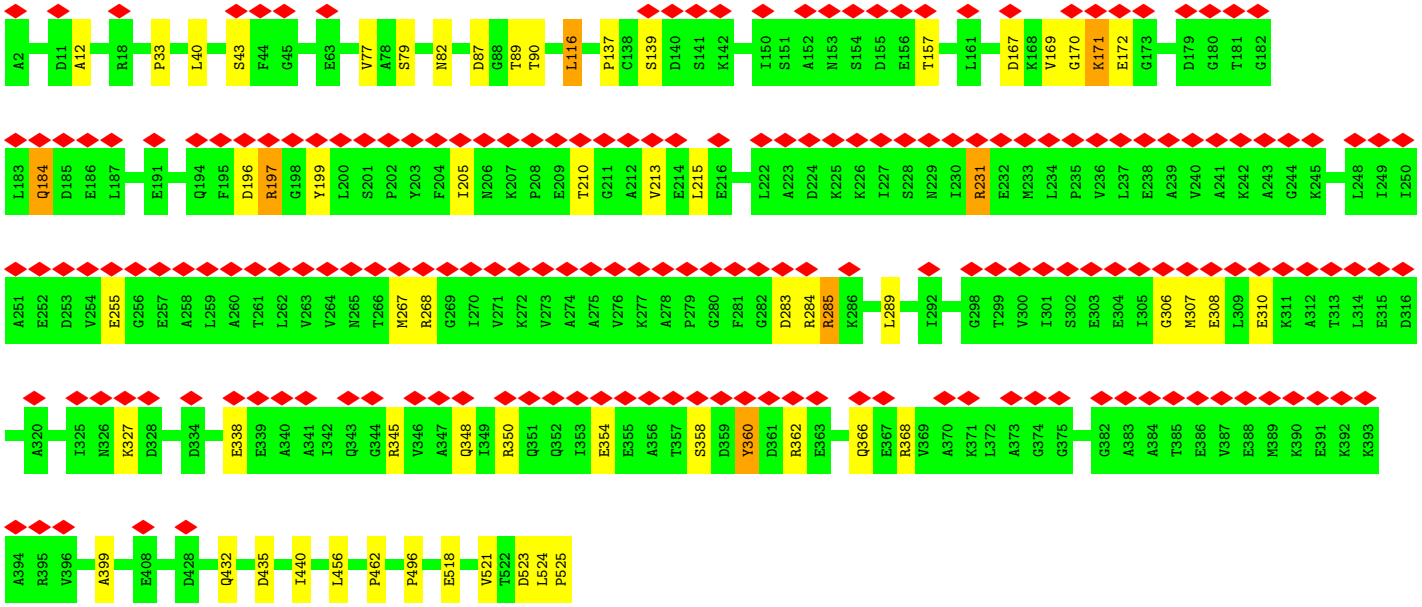
3 Residue-property plots (i)

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

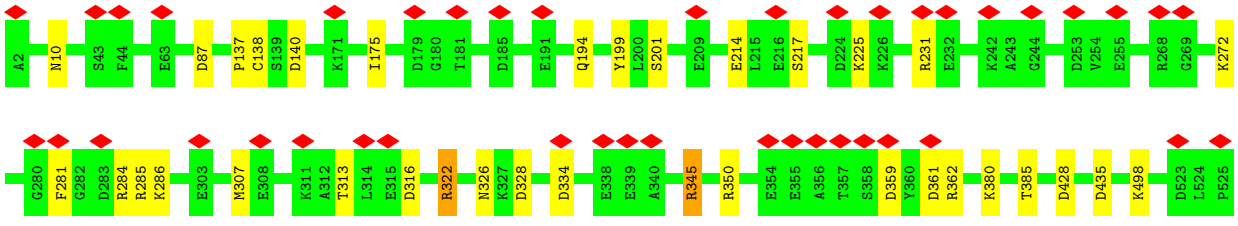
Chain Ac:





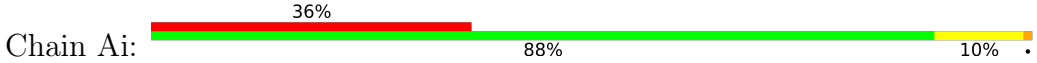
- Molecule 1: 60 kDa chaperonin

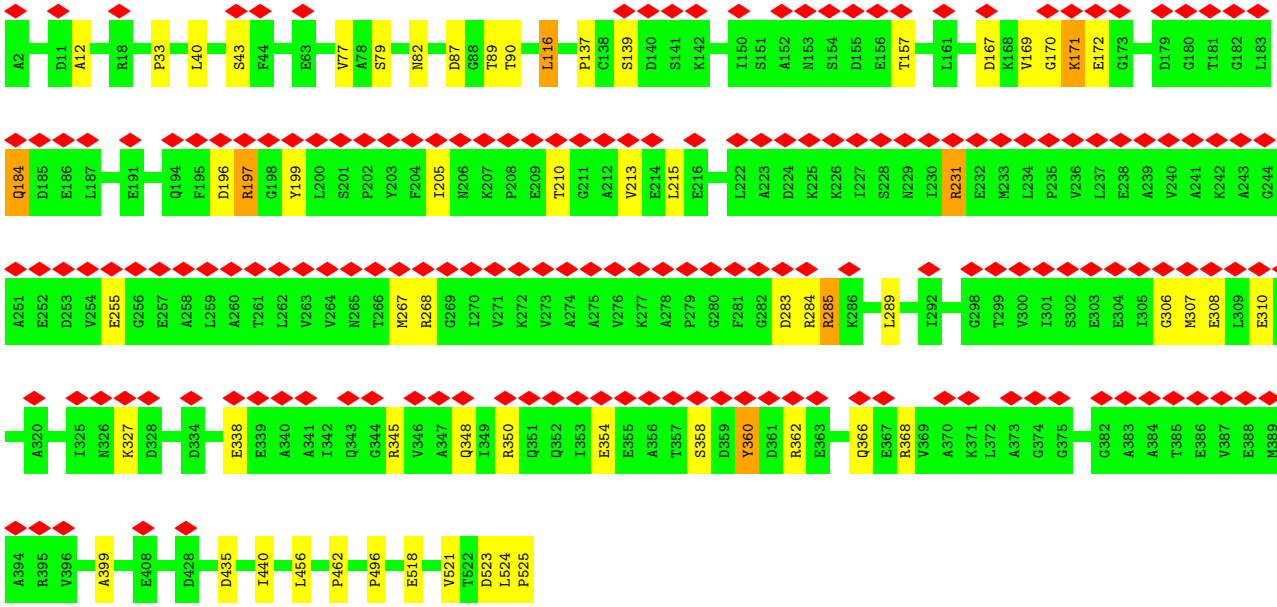
Chain Ad:



- Molecule 1: 60 kDa chaperonin

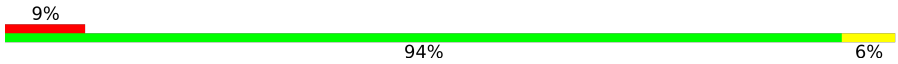
Chain Ai:

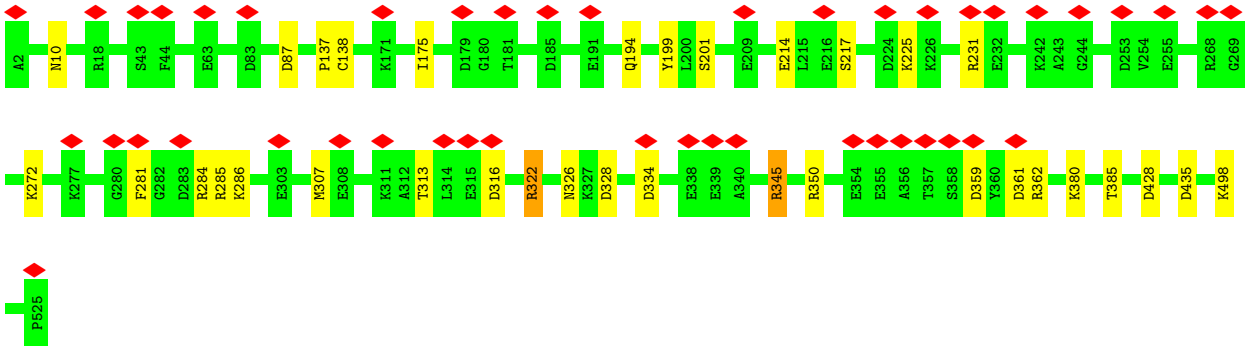




• Molecule 1: 60 kDa chaperonin

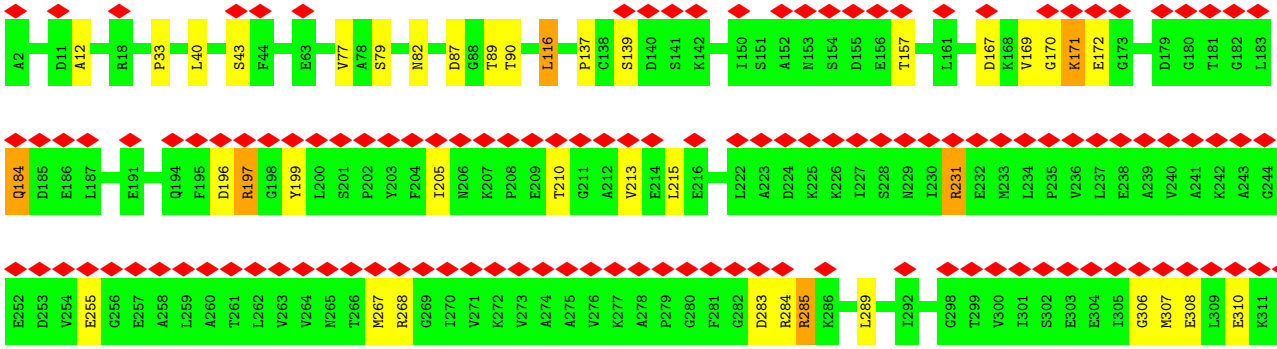
Chain Aj:

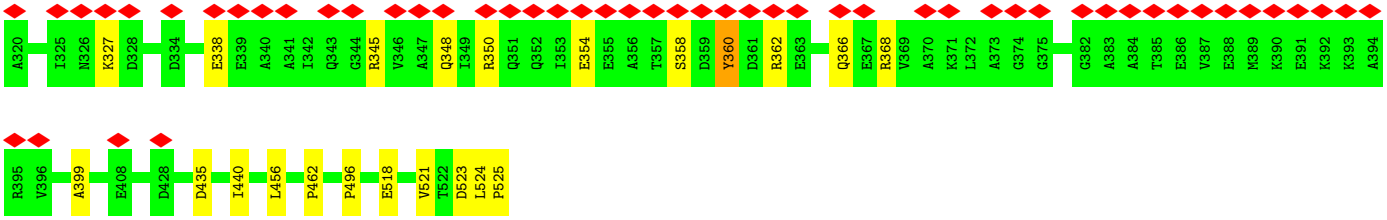




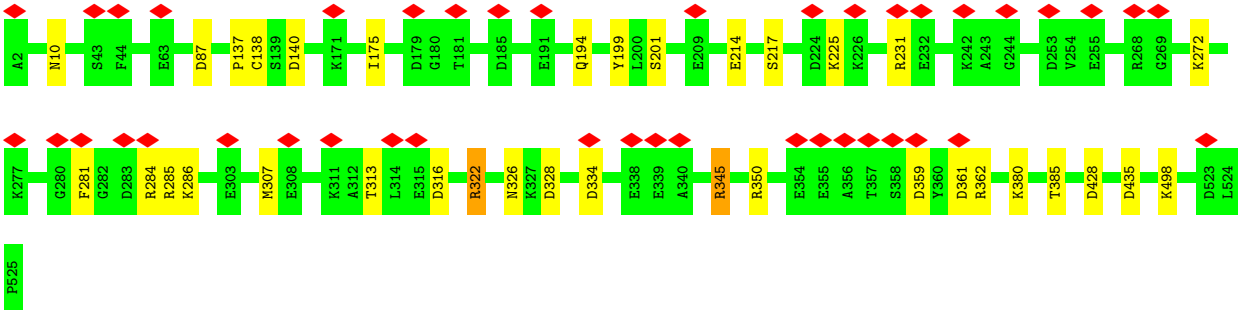
• Molecule 1: 60 kDa chaperonin

Chain Ao:

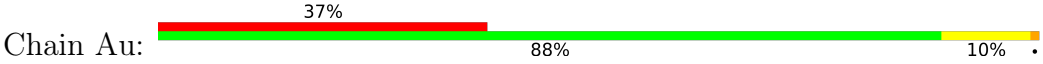


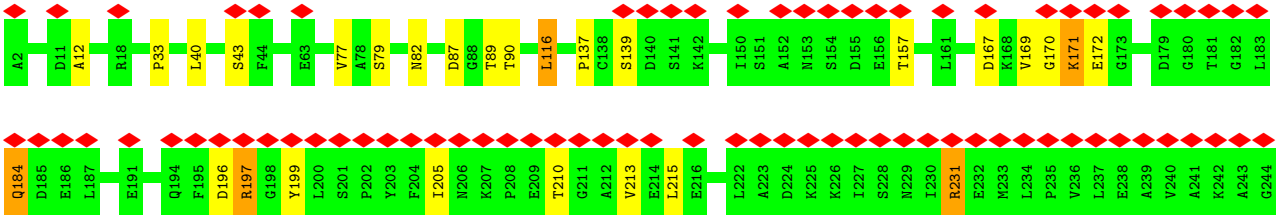


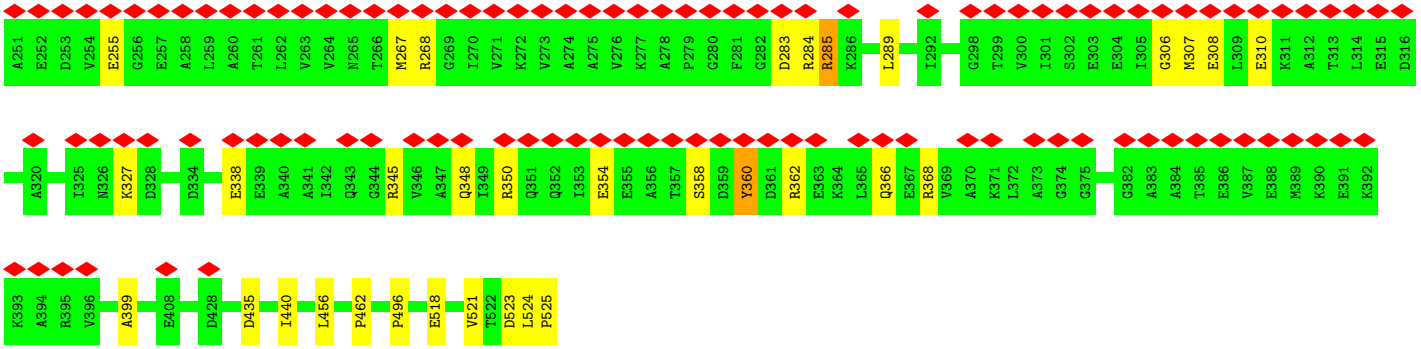
• Molecule 1: 60 kDa chaperonin



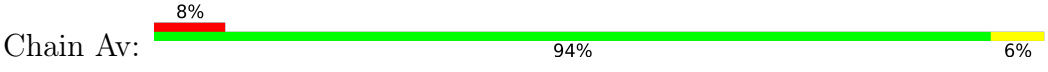
• Molecule 1: 60 kDa chaperonin

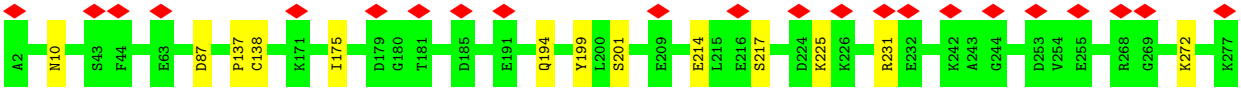


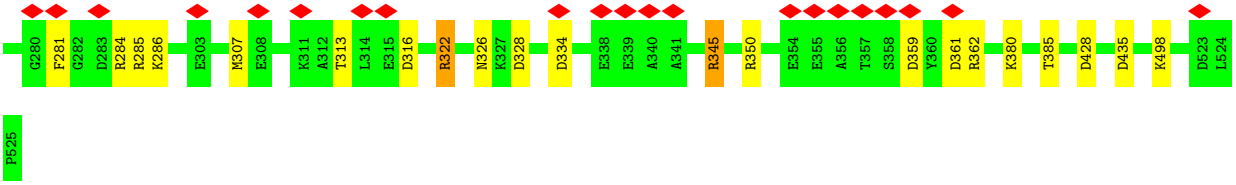




• Molecule 1: 60 kDa chaperonin





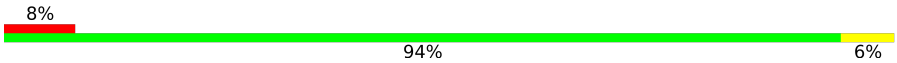


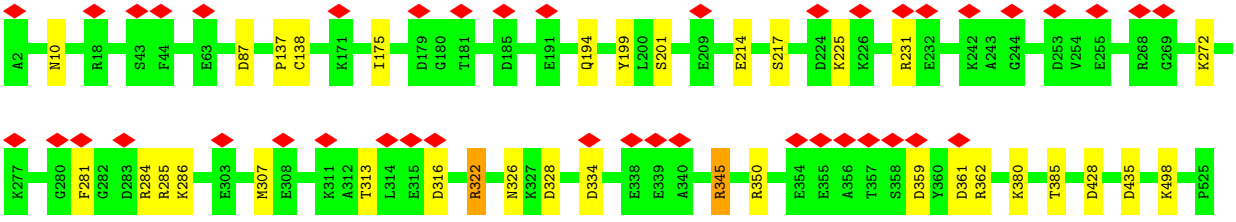
• Molecule 1: 60 kDa chaperonin

Chain Ba:

• Molecule 1: 60 kDa chaperonin

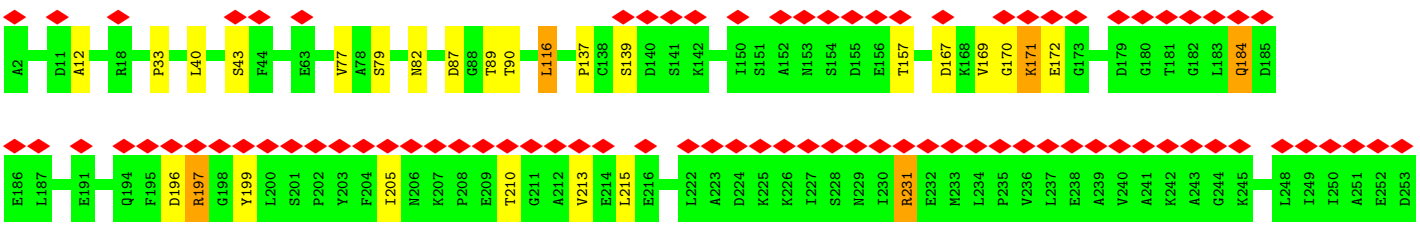
Chain Bb:

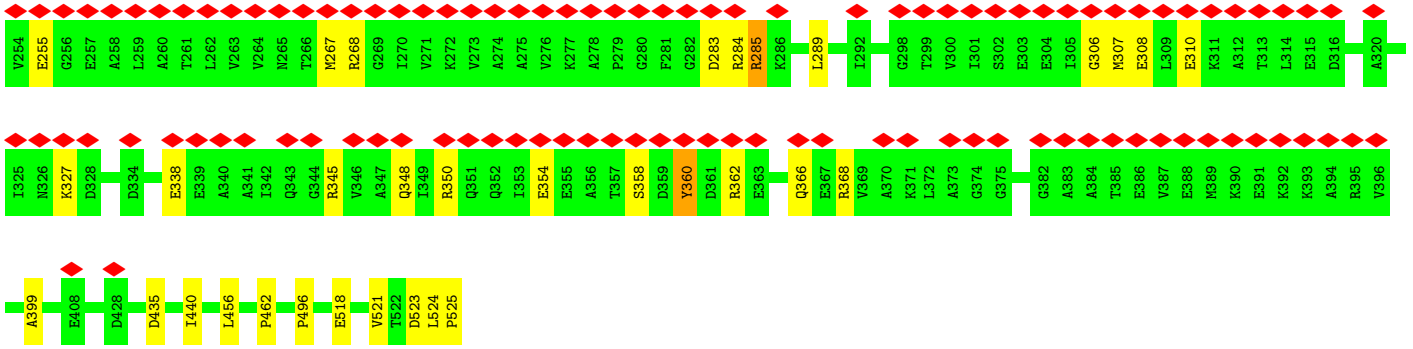




• Molecule 1: 60 kDa chaperonin

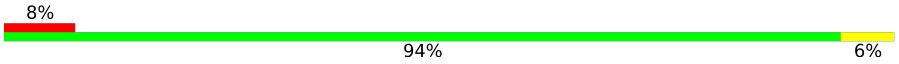
Chain Bg:

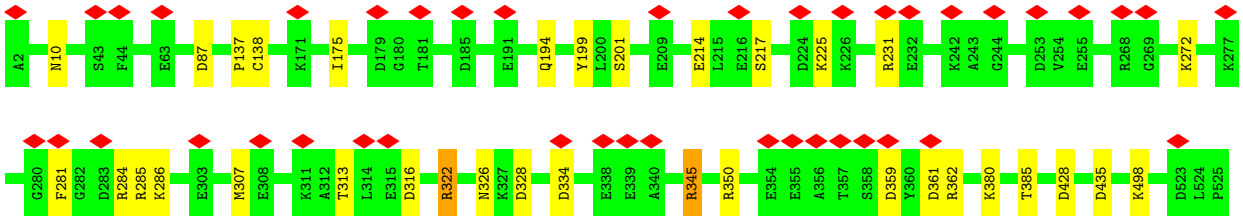




• Molecule 1: 60 kDa chaperonin

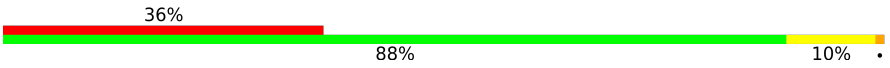
Chain Bh:

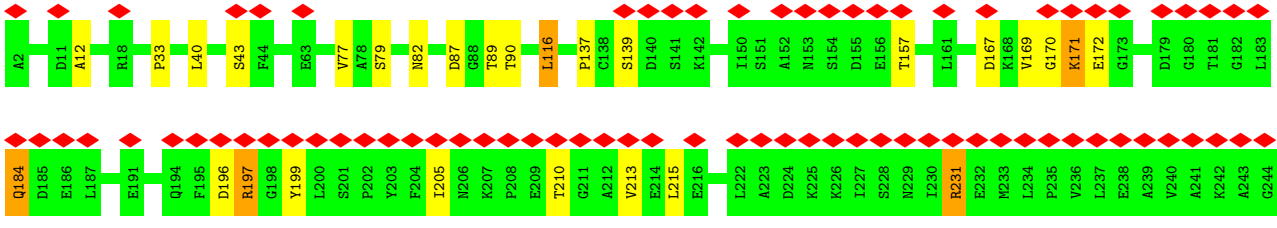




• Molecule 1: 60 kDa chaperonin

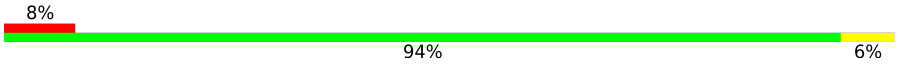
Chain Bm:

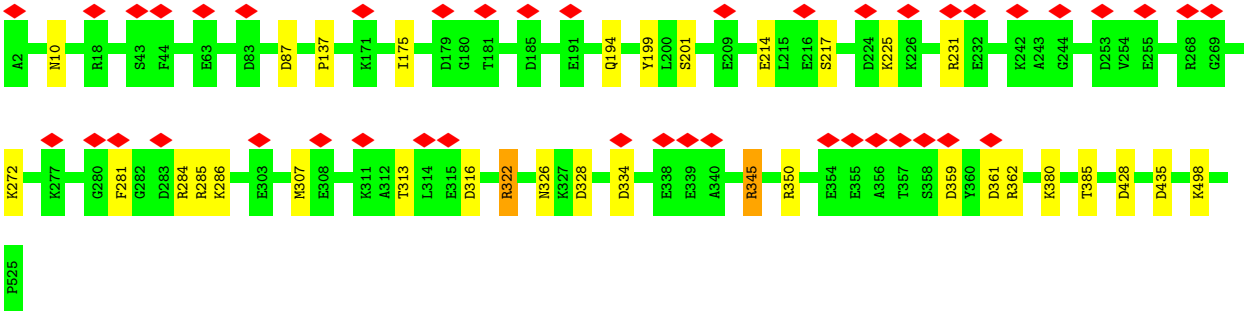




• Molecule 1: 60 kDa chaperonin

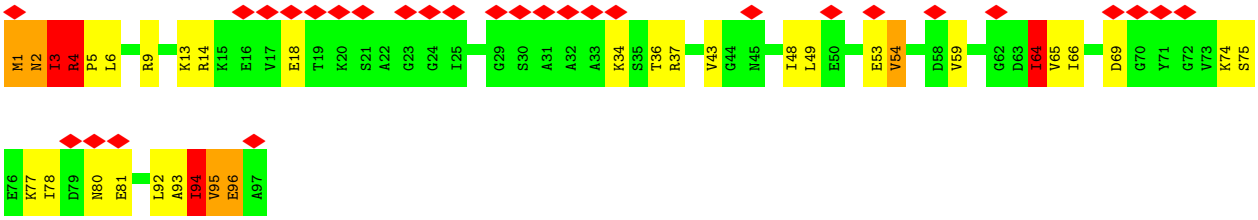
Chain Bn:





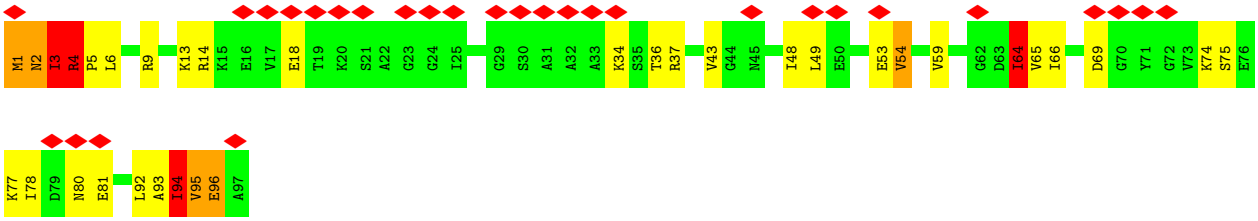
• Molecule 2: 10 kDa chaperonin

Chain Af:



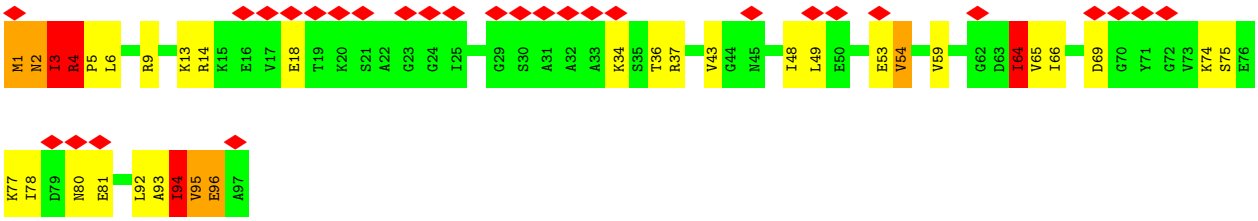
• Molecule 2: 10 kDa chaperonin

Chain Al:



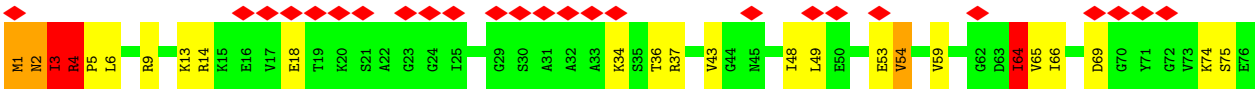
• Molecule 2: 10 kDa chaperonin

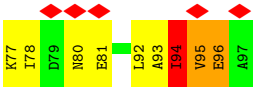
Chain Ar:



• Molecule 2: 10 kDa chaperonin

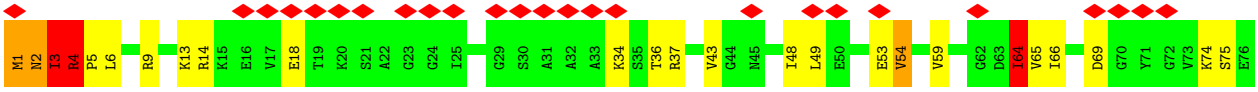
Chain Ax:

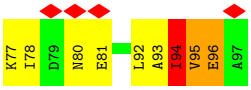




• Molecule 2: 10 kDa chaperonin

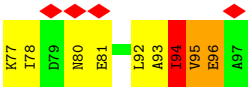
Chain Bd:





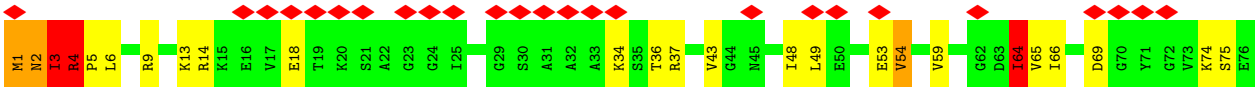
• Molecule 2: 10 kDa chaperonin

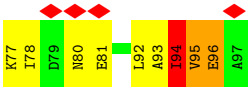
Chain Bj:



• Molecule 2: 10 kDa chaperonin

Chain Bp:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
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	5.566	Depositor
Minimum map value	-1.036	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.187	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: MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	Ac	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Ad	0.64	1/3884 (0.0%)	0.92	10/5243 (0.2%)
1	Ai	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Aj	0.64	1/3884 (0.0%)	0.92	9/5243 (0.2%)
1	Ao	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Ap	0.64	1/3884 (0.0%)	0.92	10/5243 (0.2%)
1	Au	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Av	0.64	1/3884 (0.0%)	0.92	9/5243 (0.2%)
1	Ba	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Bb	0.64	1/3884 (0.0%)	0.92	9/5243 (0.2%)
1	Bg	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Bh	0.64	1/3884 (0.0%)	0.92	9/5243 (0.2%)
1	Bm	1.35	5/3884 (0.1%)	1.15	31/5243 (0.6%)
1	Bn	0.64	1/3884 (0.0%)	0.92	8/5243 (0.2%)
2	Af	4.06	14/732 (1.9%)	2.02	34/983 (3.5%)
2	Al	4.06	14/732 (1.9%)	2.02	34/983 (3.5%)
2	Ar	4.06	14/732 (1.9%)	2.03	34/983 (3.5%)
2	Ax	4.06	14/732 (1.9%)	2.03	34/983 (3.5%)
2	Bd	4.06	14/732 (1.9%)	2.02	34/983 (3.5%)
2	Bj	4.06	14/732 (1.9%)	2.02	34/983 (3.5%)
2	Bp	4.06	14/732 (1.9%)	2.02	34/983 (3.5%)
All	All	1.56	140/59500 (0.2%)	1.16	519/80283 (0.6%)

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	Ac	0	5
1	Ad	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ai	0	5
1	Aj	0	1
1	Ao	0	5
1	Ap	0	1
1	Au	0	5
1	Av	0	1
1	Ba	0	5
1	Bb	0	1
1	Bg	0	5
1	Bh	0	1
1	Bm	0	5
1	Bn	0	1
2	Af	0	3
2	Al	0	3
2	Ar	0	3
2	Ax	0	3
2	Bd	0	3
2	Bj	0	3
2	Bp	0	3
All	All	0	63

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Bp	96	GLU	CB-CG	82.59	3.09	1.52
2	Ar	96	GLU	CB-CG	82.57	3.09	1.52
2	Ax	96	GLU	CB-CG	82.57	3.09	1.52
2	Af	96	GLU	CB-CG	82.56	3.09	1.52
2	Bj	96	GLU	CB-CG	82.56	3.09	1.52
2	Bd	96	GLU	CB-CG	82.55	3.08	1.52
2	Al	96	GLU	CB-CG	82.52	3.08	1.52
1	Bm	525	PRO	C-O	69.08	2.61	1.23
1	Bg	525	PRO	C-O	69.07	2.61	1.23
1	Au	525	PRO	C-O	69.05	2.61	1.23
1	Ai	525	PRO	C-O	69.05	2.61	1.23
1	Ba	525	PRO	C-O	69.05	2.61	1.23
1	Ac	525	PRO	C-O	69.04	2.61	1.23
1	Ao	525	PRO	C-O	69.03	2.61	1.23
2	Bd	5	PRO	CA-CB	37.57	2.28	1.53
2	Ax	5	PRO	CA-CB	37.56	2.28	1.53
2	Bj	5	PRO	CA-CB	37.56	2.28	1.53
2	Bp	5	PRO	CA-CB	37.55	2.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Af	5	PRO	CA-CB	37.54	2.28	1.53
2	Ar	5	PRO	CA-CB	37.54	2.28	1.53
2	Al	5	PRO	CA-CB	37.53	2.28	1.53
2	Al	5	PRO	N-CD	35.89	1.98	1.47
2	Ar	5	PRO	N-CD	35.85	1.98	1.47
2	Ax	5	PRO	N-CD	35.82	1.98	1.47
2	Bp	5	PRO	N-CD	35.82	1.98	1.47
2	Af	5	PRO	N-CD	35.81	1.98	1.47
2	Bd	5	PRO	N-CD	35.81	1.98	1.47
2	Bj	5	PRO	N-CD	35.78	1.98	1.47
2	Ax	5	PRO	N-CA	31.92	2.01	1.47
2	Bj	5	PRO	N-CA	31.90	2.01	1.47
2	Af	5	PRO	N-CA	31.89	2.01	1.47
2	Bp	5	PRO	N-CA	31.88	2.01	1.47
2	Ar	5	PRO	N-CA	31.87	2.01	1.47
2	Bd	5	PRO	N-CA	31.87	2.01	1.47
2	Al	5	PRO	N-CA	31.86	2.01	1.47
2	Bp	5	PRO	CG-CD	19.70	2.15	1.50
2	Ar	5	PRO	CG-CD	19.70	2.15	1.50
2	Af	5	PRO	CG-CD	19.69	2.15	1.50
2	Bd	5	PRO	CG-CD	19.69	2.15	1.50
2	Ax	5	PRO	CG-CD	19.68	2.15	1.50
2	Al	5	PRO	CG-CD	19.68	2.15	1.50
2	Bj	5	PRO	CG-CD	19.68	2.15	1.50
1	Au	462	PRO	N-CD	-15.13	1.26	1.47
1	Ao	462	PRO	N-CD	-15.13	1.26	1.47
1	Ac	462	PRO	N-CD	-15.09	1.26	1.47
1	Bm	462	PRO	N-CD	-15.08	1.26	1.47
1	Ba	462	PRO	N-CD	-15.05	1.26	1.47
1	Ai	462	PRO	N-CD	-15.05	1.26	1.47
1	Bg	462	PRO	N-CD	-15.02	1.26	1.47
1	Ao	137	PRO	N-CD	13.73	1.67	1.47
1	Ai	137	PRO	N-CD	13.72	1.67	1.47
1	Bm	137	PRO	N-CD	13.72	1.67	1.47
1	Bg	137	PRO	N-CD	13.71	1.67	1.47
1	Ba	137	PRO	N-CD	13.71	1.67	1.47
1	Ac	137	PRO	N-CD	13.70	1.67	1.47
1	Au	137	PRO	N-CD	13.70	1.67	1.47
2	Bp	5	PRO	CB-CG	12.24	2.11	1.50
2	Af	5	PRO	CB-CG	12.24	2.11	1.50
2	Ar	5	PRO	CB-CG	12.24	2.11	1.50
2	Bj	5	PRO	CB-CG	12.24	2.11	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ax	5	PRO	CB-CG	12.24	2.11	1.50
2	Bd	5	PRO	CB-CG	12.24	2.11	1.50
2	Al	5	PRO	CB-CG	12.23	2.11	1.50
1	Ai	33	PRO	N-CD	-9.91	1.33	1.47
1	Ao	33	PRO	N-CD	-9.90	1.33	1.47
1	Bm	33	PRO	N-CD	-9.88	1.34	1.47
1	Ac	33	PRO	N-CD	-9.87	1.34	1.47
1	Ba	33	PRO	N-CD	-9.86	1.34	1.47
1	Bg	33	PRO	N-CD	-9.85	1.34	1.47
1	Au	33	PRO	N-CD	-9.84	1.34	1.47
2	Bd	95	VAL	N-CA	9.71	1.65	1.46
2	Af	95	VAL	N-CA	9.69	1.65	1.46
2	Al	95	VAL	N-CA	9.68	1.65	1.46
2	Bj	95	VAL	N-CA	9.68	1.65	1.46
2	Ax	95	VAL	N-CA	9.67	1.65	1.46
2	Bp	95	VAL	N-CA	9.67	1.65	1.46
2	Ar	95	VAL	N-CA	9.66	1.65	1.46
2	Al	3	ILE	CA-C	9.36	1.77	1.52
2	Bd	3	ILE	CA-C	9.36	1.77	1.52
2	Bp	3	ILE	CA-C	9.35	1.77	1.52
2	Ax	3	ILE	CA-C	9.34	1.77	1.52
2	Af	3	ILE	CA-C	9.34	1.77	1.52
2	Bj	3	ILE	CA-C	9.32	1.77	1.52
2	Ar	3	ILE	CA-C	9.31	1.77	1.52
2	Ar	95	VAL	CA-CB	8.41	1.72	1.54
2	Bp	95	VAL	CA-CB	8.40	1.72	1.54
2	Ax	95	VAL	CA-CB	8.38	1.72	1.54
2	Af	95	VAL	CA-CB	8.38	1.72	1.54
2	Al	95	VAL	CA-CB	8.37	1.72	1.54
2	Bj	95	VAL	CA-CB	8.36	1.72	1.54
2	Bd	95	VAL	CA-CB	8.35	1.72	1.54
2	Al	94	ILE	CA-C	8.21	1.74	1.52
2	Af	94	ILE	CA-C	8.20	1.74	1.52
2	Bd	94	ILE	CA-C	8.20	1.74	1.52
2	Bp	94	ILE	CA-C	8.19	1.74	1.52
2	Ar	94	ILE	CA-C	8.19	1.74	1.52
2	Bj	94	ILE	CA-C	8.18	1.74	1.52
2	Ax	94	ILE	CA-C	8.17	1.74	1.52
2	Bd	4	ARG	N-CA	7.85	1.62	1.46
2	Al	4	ARG	N-CA	7.85	1.62	1.46
2	Bp	4	ARG	N-CA	7.84	1.62	1.46
2	Ax	4	ARG	N-CA	7.84	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ar	4	ARG	N-CA	7.84	1.62	1.46
2	Af	4	ARG	N-CA	7.82	1.61	1.46
2	Bj	4	ARG	N-CA	7.81	1.61	1.46
2	Bj	3	ILE	C-N	7.66	1.51	1.34
2	Af	3	ILE	C-N	7.66	1.51	1.34
2	Ax	3	ILE	C-N	7.66	1.51	1.34
2	Ar	3	ILE	C-N	7.66	1.51	1.34
2	Bd	3	ILE	C-N	7.63	1.51	1.34
2	Bp	3	ILE	C-N	7.63	1.51	1.34
2	Al	3	ILE	C-N	7.63	1.51	1.34
2	Bj	94	ILE	C-N	7.17	1.50	1.34
2	Bd	94	ILE	C-N	7.16	1.50	1.34
2	Ar	94	ILE	C-N	7.14	1.50	1.34
2	Al	94	ILE	C-N	7.14	1.50	1.34
2	Ax	94	ILE	C-N	7.14	1.50	1.34
2	Af	94	ILE	C-N	7.13	1.50	1.34
2	Bp	94	ILE	C-N	7.13	1.50	1.34
2	Al	94	ILE	CA-CB	6.42	1.69	1.54
2	Ax	94	ILE	CA-CB	6.42	1.69	1.54
2	Bp	94	ILE	CA-CB	6.41	1.69	1.54
2	Bj	94	ILE	CA-CB	6.41	1.69	1.54
2	Ar	94	ILE	CA-CB	6.41	1.69	1.54
2	Bd	94	ILE	CA-CB	6.41	1.69	1.54
2	Af	94	ILE	CA-CB	6.40	1.69	1.54
1	Ai	496	PRO	N-CD	6.39	1.56	1.47
1	Au	496	PRO	N-CD	6.38	1.56	1.47
1	Ba	496	PRO	N-CD	6.38	1.56	1.47
1	Ac	496	PRO	N-CD	6.38	1.56	1.47
1	Bg	496	PRO	N-CD	6.38	1.56	1.47
1	Ao	496	PRO	N-CD	6.37	1.56	1.47
1	Bm	496	PRO	N-CD	6.36	1.56	1.47
1	Bn	137	PRO	N-CD	-5.10	1.40	1.47
1	Bh	137	PRO	N-CD	-5.09	1.40	1.47
1	Ad	137	PRO	N-CD	-5.07	1.40	1.47
1	Av	137	PRO	N-CD	-5.07	1.40	1.47
1	Bb	137	PRO	N-CD	-5.07	1.40	1.47
1	Aj	137	PRO	N-CD	-5.06	1.40	1.47
1	Ap	137	PRO	N-CD	-5.06	1.40	1.47

All (519) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Ar	94	ILE	CB-CA-C	14.60	140.79	111.60
2	Bj	94	ILE	CB-CA-C	14.59	140.78	111.60
2	Af	94	ILE	CB-CA-C	14.59	140.78	111.60
2	Bd	94	ILE	CB-CA-C	14.59	140.78	111.60
2	Al	94	ILE	CB-CA-C	14.59	140.78	111.60
2	Ax	94	ILE	CB-CA-C	14.59	140.77	111.60
2	Bp	94	ILE	CB-CA-C	14.58	140.76	111.60
2	Ax	3	ILE	C-N-CA	13.87	156.36	121.70
2	Ar	3	ILE	C-N-CA	13.86	156.35	121.70
2	Al	3	ILE	C-N-CA	13.85	156.32	121.70
2	Af	3	ILE	C-N-CA	13.85	156.31	121.70
2	Bd	3	ILE	C-N-CA	13.84	156.29	121.70
2	Bp	3	ILE	C-N-CA	13.84	156.29	121.70
2	Bj	3	ILE	C-N-CA	13.83	156.27	121.70
2	Ar	95	VAL	N-CA-CB	13.40	140.98	111.50
2	Ax	95	VAL	N-CA-CB	13.40	140.98	111.50
2	Bd	95	VAL	N-CA-CB	13.39	140.96	111.50
2	Bj	95	VAL	N-CA-CB	13.39	140.96	111.50
2	Bp	95	VAL	N-CA-CB	13.39	140.96	111.50
2	Af	95	VAL	N-CA-CB	13.39	140.95	111.50
2	Al	95	VAL	N-CA-CB	13.38	140.94	111.50
2	Bj	94	ILE	C-N-CA	12.97	154.12	121.70
2	Af	94	ILE	C-N-CA	12.96	154.10	121.70
2	Bp	94	ILE	C-N-CA	12.96	154.10	121.70
2	Ar	94	ILE	C-N-CA	12.96	154.09	121.70
2	Al	94	ILE	C-N-CA	12.95	154.07	121.70
2	Ax	94	ILE	C-N-CA	12.95	154.07	121.70
2	Bd	94	ILE	C-N-CA	12.95	154.06	121.70
2	Ax	14	ARG	NE-CZ-NH1	12.62	126.61	120.30
2	Bp	14	ARG	NE-CZ-NH1	12.60	126.60	120.30
2	Ar	14	ARG	NE-CZ-NH1	12.57	126.59	120.30
2	Bj	14	ARG	NE-CZ-NH1	12.53	126.57	120.30
2	Af	14	ARG	NE-CZ-NH1	12.53	126.56	120.30
2	Bd	14	ARG	NE-CZ-NH1	12.50	126.55	120.30
2	Ax	94	ILE	CA-CB-CG1	12.38	134.52	111.00
2	Bp	94	ILE	CA-CB-CG1	12.37	134.51	111.00
2	Al	14	ARG	NE-CZ-NH1	12.37	126.48	120.30
2	Al	94	ILE	CA-CB-CG1	12.37	134.50	111.00
2	Af	94	ILE	CA-CB-CG1	12.36	134.49	111.00
2	Ar	94	ILE	CA-CB-CG1	12.36	134.49	111.00
2	Bd	94	ILE	CA-CB-CG1	12.35	134.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bj	94	ILE	CA-CB-CG1	12.35	134.47	111.00
1	Ao	197	ARG	NE-CZ-NH1	12.29	126.45	120.30
1	Ai	197	ARG	NE-CZ-NH1	12.28	126.44	120.30
2	Bj	3	ILE	O-C-N	-12.26	103.08	122.70
2	Af	3	ILE	O-C-N	-12.24	103.12	122.70
1	Bm	197	ARG	NE-CZ-NH1	12.24	126.42	120.30
2	Ar	3	ILE	O-C-N	-12.23	103.13	122.70
2	Al	3	ILE	O-C-N	-12.23	103.13	122.70
1	Ac	197	ARG	NE-CZ-NH1	12.23	126.41	120.30
2	Ax	3	ILE	O-C-N	-12.23	103.14	122.70
2	Bd	3	ILE	O-C-N	-12.23	103.14	122.70
2	Bp	3	ILE	O-C-N	-12.22	103.14	122.70
1	Au	197	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	Ba	197	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	Bg	197	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	Al	95	VAL	CA-CB-CG1	11.78	128.57	110.90
2	Bd	95	VAL	CA-CB-CG1	11.78	128.57	110.90
2	Bj	95	VAL	CA-CB-CG1	11.78	128.57	110.90
2	Af	95	VAL	CA-CB-CG1	11.76	128.54	110.90
2	Ar	95	VAL	CA-CB-CG1	11.75	128.53	110.90
2	Ax	95	VAL	CA-CB-CG1	11.73	128.50	110.90
2	Bp	95	VAL	CA-CB-CG1	11.73	128.50	110.90
2	Bj	3	ILE	CA-C-N	11.72	142.98	117.20
2	Al	3	ILE	CA-C-N	11.71	142.95	117.20
2	Af	3	ILE	CA-C-N	11.70	142.94	117.20
2	Bd	3	ILE	CA-C-N	11.70	142.93	117.20
2	Bp	3	ILE	CA-C-N	11.69	142.92	117.20
2	Ax	3	ILE	CA-C-N	11.69	142.91	117.20
2	Ar	3	ILE	CA-C-N	11.68	142.91	117.20
2	Ax	94	ILE	CA-C-N	11.58	142.68	117.20
2	Bp	94	ILE	CA-C-N	11.58	142.68	117.20
2	Al	94	ILE	CA-C-N	11.57	142.65	117.20
2	Bd	94	ILE	CA-C-N	11.57	142.66	117.20
2	Af	94	ILE	CA-C-N	11.57	142.65	117.20
2	Ar	94	ILE	CA-C-N	11.57	142.65	117.20
2	Bj	94	ILE	CA-C-N	11.55	142.61	117.20
1	Aj	345	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	Bh	345	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	Bb	345	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	Bn	345	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	Ad	345	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	Av	345	ARG	NE-CZ-NH1	11.34	125.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ap	345	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	Ao	462	PRO	CA-N-CD	10.90	126.96	111.70
1	Bm	462	PRO	CA-N-CD	10.89	126.95	111.70
1	Ai	462	PRO	CA-N-CD	10.88	126.94	111.70
1	Ac	462	PRO	CA-N-CD	10.88	126.93	111.70
1	Ba	462	PRO	CA-N-CD	10.87	126.91	111.70
1	Au	462	PRO	CA-N-CD	10.86	126.90	111.70
1	Bg	462	PRO	CA-N-CD	10.86	126.90	111.70
2	Bj	4	ARG	N-CA-C	10.40	139.07	111.00
2	Af	4	ARG	N-CA-C	10.39	139.05	111.00
2	Bd	4	ARG	N-CA-C	10.39	139.06	111.00
2	Bp	4	ARG	N-CA-C	10.39	139.05	111.00
2	Ax	4	ARG	N-CA-C	10.38	139.04	111.00
2	Al	4	ARG	N-CA-C	10.37	139.00	111.00
2	Ar	4	ARG	N-CA-C	10.37	139.00	111.00
2	Al	64	ILE	CB-CA-C	10.35	132.30	111.60
2	Ax	64	ILE	CB-CA-C	10.35	132.30	111.60
2	Bp	64	ILE	CB-CA-C	10.34	132.29	111.60
2	Ar	64	ILE	CB-CA-C	10.34	132.28	111.60
2	Bd	64	ILE	CB-CA-C	10.34	132.28	111.60
2	Af	64	ILE	CB-CA-C	10.33	132.26	111.60
2	Bj	64	ILE	CB-CA-C	10.32	132.25	111.60
1	Ai	345	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	Bg	345	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	Ao	345	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	Au	345	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	Ac	345	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	Bm	345	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	Ba	345	ARG	NE-CZ-NH2	-10.12	115.24	120.30
2	Ax	95	VAL	CA-CB-CG2	10.04	125.95	110.90
1	Ai	345	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	Bg	345	ARG	NE-CZ-NH1	10.03	125.31	120.30
2	Al	95	VAL	CA-CB-CG2	10.02	125.93	110.90
2	Bd	95	VAL	CA-CB-CG2	10.02	125.92	110.90
2	Bp	95	VAL	CA-CB-CG2	10.01	125.92	110.90
2	Bj	95	VAL	CA-CB-CG2	10.01	125.92	110.90
2	Af	95	VAL	CA-CB-CG2	10.01	125.91	110.90
2	Ar	95	VAL	CA-CB-CG2	9.99	125.88	110.90
1	Au	345	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	Ac	345	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	Ao	345	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	Bm	345	ARG	NE-CZ-NH1	9.82	125.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ba	345	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	Ax	94	ILE	O-C-N	-9.29	107.84	122.70
2	Ar	94	ILE	O-C-N	-9.28	107.85	122.70
2	Bd	94	ILE	O-C-N	-9.28	107.86	122.70
2	Al	94	ILE	O-C-N	-9.26	107.88	122.70
2	Af	94	ILE	O-C-N	-9.26	107.89	122.70
2	Bj	94	ILE	O-C-N	-9.25	107.89	122.70
2	Bp	94	ILE	O-C-N	-9.25	107.90	122.70
1	Ba	268	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	Ao	268	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	Bm	268	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	Ac	268	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	Au	268	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	Bg	268	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	Ai	268	ARG	NE-CZ-NH1	9.12	124.86	120.30
2	Al	96	GLU	CA-CB-CG	8.49	132.08	113.40
2	Bj	96	GLU	CA-CB-CG	8.48	132.06	113.40
2	Af	96	GLU	CA-CB-CG	8.48	132.05	113.40
2	Bp	96	GLU	CA-CB-CG	8.47	132.04	113.40
2	Ar	96	GLU	CA-CB-CG	8.47	132.03	113.40
2	Ax	96	GLU	CA-CB-CG	8.47	132.03	113.40
2	Bd	96	GLU	CA-CB-CG	8.47	132.03	113.40
1	Bh	350	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	Bn	350	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	Ad	350	ARG	NE-CZ-NH1	8.25	124.42	120.30
2	Al	96	GLU	CB-CG-CD	8.25	136.47	114.20
1	Aj	350	ARG	NE-CZ-NH1	8.24	124.42	120.30
2	Af	96	GLU	CB-CG-CD	8.23	136.43	114.20
2	Ar	96	GLU	CB-CG-CD	8.23	136.42	114.20
2	Ax	96	GLU	CB-CG-CD	8.23	136.42	114.20
2	Bj	96	GLU	CB-CG-CD	8.23	136.42	114.20
2	Bp	96	GLU	CB-CG-CD	8.23	136.42	114.20
2	Bd	96	GLU	CB-CG-CD	8.22	136.41	114.20
1	Bb	350	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	Ap	350	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	Av	350	ARG	NE-CZ-NH1	8.07	124.33	120.30
2	Ar	3	ILE	N-CA-C	7.92	132.39	111.00
2	Ax	3	ILE	N-CA-C	7.92	132.39	111.00
2	Bd	3	ILE	N-CA-C	7.91	132.37	111.00
2	Af	3	ILE	N-CA-C	7.91	132.35	111.00
2	Bp	3	ILE	N-CA-C	7.91	132.35	111.00
2	Al	3	ILE	N-CA-C	7.90	132.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bj	3	ILE	N-CA-C	7.89	132.31	111.00
1	Bb	322	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	Bh	322	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	Aj	322	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	Ap	322	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	Ad	322	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	Av	322	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	Bn	322	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	Ba	368	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	Ai	368	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	Ac	368	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	Bm	368	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	Bg	368	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	Ao	368	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	Bg	231	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	Bm	231	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	Au	368	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	Ac	231	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	Ao	231	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	Au	231	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	Ba	231	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	Bh	285	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	Ai	231	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	Ai	197	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	Ap	285	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	Bb	285	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	Aj	285	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	Ad	285	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	Ac	197	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	Bg	197	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	Ao	197	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	Bn	285	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	Bm	197	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	Ba	197	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	Au	197	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	Ao	285	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	Av	285	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	Au	285	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	Bm	462	PRO	N-CA-CB	-6.94	94.96	102.60
1	Bm	285	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	Ao	462	PRO	N-CA-CB	-6.92	94.98	102.60
1	Ac	462	PRO	N-CA-CB	-6.92	94.99	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ba	137	PRO	N-CA-CB	6.91	111.60	103.30
1	Ai	462	PRO	N-CA-CB	-6.91	95.00	102.60
1	Au	137	PRO	N-CA-CB	6.91	111.59	103.30
1	Ac	285	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	Bg	285	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	Ba	462	PRO	N-CA-CB	-6.89	95.02	102.60
1	Ai	285	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	Au	462	PRO	N-CA-CB	-6.88	95.03	102.60
1	Ba	285	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	Au	362	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	Bh	345	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	Ac	137	PRO	N-CA-CB	6.87	111.55	103.30
1	Bg	137	PRO	N-CA-CB	6.87	111.55	103.30
1	Ai	137	PRO	N-CA-CB	6.87	111.54	103.30
1	Bg	462	PRO	N-CA-CB	-6.87	95.05	102.60
1	Bm	137	PRO	N-CA-CB	6.87	111.54	103.30
1	Ac	362	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	Ba	362	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	Ao	137	PRO	N-CA-CB	6.83	111.50	103.30
1	Ai	362	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	Bn	345	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	Aj	345	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	Ao	362	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	Ap	345	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	Bb	345	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	Bg	362	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	Ad	345	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	Av	345	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	Ba	525	PRO	CA-C-O	-6.73	104.05	120.20
1	Bm	362	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	Au	525	PRO	CA-C-O	-6.72	104.06	120.20
1	Bm	525	PRO	CA-C-O	-6.72	104.06	120.20
1	Ac	525	PRO	CA-C-O	-6.72	104.08	120.20
1	Bg	525	PRO	CA-C-O	-6.71	104.09	120.20
1	Ai	525	PRO	CA-C-O	-6.71	104.10	120.20
1	Ao	525	PRO	CA-C-O	-6.71	104.11	120.20
1	Au	137	PRO	CA-N-CD	-6.64	102.20	111.50
2	Bd	95	VAL	CG1-CB-CG2	-6.63	100.30	110.90
2	Al	95	VAL	CG1-CB-CG2	-6.62	100.30	110.90
2	Bj	95	VAL	CG1-CB-CG2	-6.62	100.31	110.90
1	Bm	137	PRO	CA-N-CD	-6.61	102.25	111.50
2	Ax	95	VAL	CG1-CB-CG2	-6.61	100.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ba	167	ASP	N-CA-C	-6.60	93.17	111.00
1	Ac	167	ASP	N-CA-C	-6.60	93.17	111.00
2	Af	95	VAL	CG1-CB-CG2	-6.60	100.33	110.90
1	Ai	167	ASP	N-CA-C	-6.60	93.17	111.00
1	Ba	137	PRO	CA-N-CD	-6.60	102.26	111.50
1	Ao	137	PRO	CA-N-CD	-6.60	102.26	111.50
1	Bg	167	ASP	N-CA-C	-6.60	93.18	111.00
1	Au	167	ASP	N-CA-C	-6.60	93.19	111.00
1	Ac	137	PRO	CA-N-CD	-6.59	102.27	111.50
1	Ao	167	ASP	N-CA-C	-6.59	93.20	111.00
2	Ar	95	VAL	CG1-CB-CG2	-6.59	100.35	110.90
1	Bm	167	ASP	N-CA-C	-6.59	93.20	111.00
2	Bp	4	ARG	O-C-N	-6.59	108.59	121.10
2	Bd	4	ARG	O-C-N	-6.58	108.59	121.10
2	Bj	4	ARG	O-C-N	-6.58	108.60	121.10
1	Ai	137	PRO	CA-N-CD	-6.58	102.29	111.50
2	Ar	4	ARG	CA-CB-CG	6.58	127.87	113.40
1	Bg	137	PRO	CA-N-CD	-6.58	102.29	111.50
2	Bp	95	VAL	CG1-CB-CG2	-6.58	100.37	110.90
2	Al	4	ARG	O-C-N	-6.57	108.61	121.10
2	Af	4	ARG	O-C-N	-6.57	108.62	121.10
2	Al	4	ARG	CA-CB-CG	6.57	127.85	113.40
2	Ar	4	ARG	O-C-N	-6.57	108.62	121.10
1	Ai	267	MET	CG-SD-CE	-6.56	89.70	100.20
2	Af	4	ARG	CA-CB-CG	6.56	127.83	113.40
2	Bj	4	ARG	CA-CB-CG	6.56	127.82	113.40
2	Ax	4	ARG	O-C-N	-6.55	108.65	121.10
2	Ax	4	ARG	CA-CB-CG	6.55	127.82	113.40
1	Ba	267	MET	CG-SD-CE	-6.55	89.72	100.20
2	Bp	4	ARG	CA-CB-CG	6.55	127.82	113.40
1	Au	267	MET	CG-SD-CE	-6.55	89.72	100.20
1	Bg	267	MET	CG-SD-CE	-6.55	89.72	100.20
1	Ac	267	MET	CG-SD-CE	-6.55	89.73	100.20
1	Bm	267	MET	CG-SD-CE	-6.55	89.72	100.20
2	Bd	4	ARG	CA-CB-CG	6.54	127.79	113.40
1	Ao	267	MET	CG-SD-CE	-6.53	89.76	100.20
1	Ao	399	ALA	N-CA-C	6.34	128.13	111.00
1	Bm	399	ALA	N-CA-C	6.34	128.11	111.00
1	Ac	399	ALA	N-CA-C	6.33	128.10	111.00
1	Bg	399	ALA	N-CA-C	6.33	128.09	111.00
1	Ba	399	ALA	N-CA-C	6.33	128.09	111.00
1	Ai	399	ALA	N-CA-C	6.32	128.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Au	399	ALA	N-CA-C	6.32	128.07	111.00
1	Bg	435	ASP	N-CA-CB	6.32	121.97	110.60
2	Bp	5	PRO	CB-CA-C	6.32	127.79	112.00
2	Bj	5	PRO	CB-CA-C	6.31	127.78	112.00
2	Af	5	PRO	CB-CA-C	6.31	127.77	112.00
1	Ai	435	ASP	N-CA-CB	6.31	121.96	110.60
2	Ax	5	PRO	CB-CA-C	6.31	127.78	112.00
1	Ba	435	ASP	N-CA-CB	6.31	121.95	110.60
2	Ar	5	PRO	CB-CA-C	6.31	127.77	112.00
2	Al	5	PRO	CB-CA-C	6.30	127.76	112.00
1	Ao	435	ASP	N-CA-CB	6.30	121.95	110.60
2	Bd	5	PRO	CB-CA-C	6.30	127.76	112.00
1	Au	435	ASP	N-CA-CB	6.30	121.94	110.60
1	Bm	435	ASP	N-CA-CB	6.30	121.94	110.60
1	Ac	435	ASP	N-CA-CB	6.29	121.93	110.60
1	Ap	362	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Av	362	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Bg	12	ALA	N-CA-CB	-6.25	101.35	110.10
1	Aj	362	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	Ad	362	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	Ba	12	ALA	N-CA-CB	-6.23	101.37	110.10
1	Ao	12	ALA	N-CA-CB	-6.22	101.39	110.10
1	Au	12	ALA	N-CA-CB	-6.22	101.40	110.10
1	Ac	12	ALA	N-CA-CB	-6.21	101.40	110.10
1	Bm	12	ALA	N-CA-CB	-6.21	101.40	110.10
1	Bb	362	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	Bn	362	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	Ai	12	ALA	N-CA-CB	-6.18	101.45	110.10
1	Bh	362	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	Ar	95	VAL	CB-CA-C	-6.17	99.67	111.40
1	Ba	184	GLN	N-CA-CB	6.17	121.70	110.60
2	Al	95	VAL	CB-CA-C	-6.16	99.70	111.40
1	Au	184	GLN	N-CA-CB	6.16	121.68	110.60
2	Ax	95	VAL	CB-CA-C	-6.16	99.71	111.40
2	Bp	95	VAL	CB-CA-C	-6.16	99.70	111.40
1	Bm	184	GLN	N-CA-CB	6.15	121.68	110.60
2	Bj	95	VAL	CB-CA-C	-6.15	99.71	111.40
2	Af	95	VAL	CB-CA-C	-6.15	99.72	111.40
1	Bg	184	GLN	N-CA-CB	6.15	121.67	110.60
1	Ac	184	GLN	N-CA-CB	6.14	121.66	110.60
1	Ao	184	GLN	N-CA-CB	6.14	121.65	110.60
1	Ai	184	GLN	N-CA-CB	6.14	121.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bd	95	VAL	CB-CA-C	-6.14	99.74	111.40
2	Bd	14	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	Bg	350	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	Bm	350	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	Ax	14	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	Ac	368	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	Ai	350	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	Ai	368	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	Ao	368	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	Ba	368	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	Ar	14	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	Ac	350	ARG	NE-CZ-NH1	6.01	123.31	120.30
2	Bj	14	ARG	NE-CZ-NH2	-6.01	117.30	120.30
2	Af	14	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	Bp	14	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	Bm	368	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	Ba	350	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	Au	368	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	Al	14	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	Bg	368	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	Au	350	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	Bg	169	VAL	N-CA-CB	-5.91	98.51	111.50
1	Ao	172	GLU	N-CA-C	5.90	126.94	111.00
1	Ac	169	VAL	N-CA-CB	-5.90	98.52	111.50
1	Ao	350	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	Ai	172	GLU	N-CA-C	5.90	126.93	111.00
1	Ao	169	VAL	N-CA-CB	-5.90	98.53	111.50
1	Au	169	VAL	N-CA-CB	-5.90	98.53	111.50
1	Ac	172	GLU	N-CA-C	5.89	126.91	111.00
1	Ba	172	GLU	N-CA-C	5.89	126.91	111.00
1	Bg	172	GLU	N-CA-C	5.89	126.91	111.00
1	Au	172	GLU	N-CA-C	5.89	126.90	111.00
1	Ai	169	VAL	N-CA-CB	-5.89	98.55	111.50
1	Ba	169	VAL	N-CA-CB	-5.89	98.55	111.50
1	Bm	172	GLU	N-CA-C	5.88	126.89	111.00
1	Bm	169	VAL	N-CA-CB	-5.88	98.56	111.50
2	Al	9	ARG	NE-CZ-NH1	5.83	123.22	120.30
2	Ax	9	ARG	NE-CZ-NH1	5.81	123.21	120.30
2	Bd	4	ARG	CA-C-N	5.79	133.32	117.10
2	Bp	4	ARG	CA-C-N	5.79	133.32	117.10
2	Bj	4	ARG	CA-C-N	5.78	133.28	117.10
2	Af	4	ARG	CA-C-N	5.78	133.28	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Ar	4	ARG	CA-C-N	5.78	133.28	117.10
2	Ax	4	ARG	CA-C-N	5.78	133.27	117.10
2	Bd	9	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	Al	4	ARG	CA-C-N	5.77	133.25	117.10
2	Af	9	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	Ar	9	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	Ar	64	ILE	CA-CB-CG2	5.75	122.40	110.90
2	Bd	64	ILE	CA-CB-CG2	5.75	122.40	110.90
2	Bj	64	ILE	CA-CB-CG2	5.75	122.40	110.90
2	Af	64	ILE	CA-CB-CG2	5.75	122.39	110.90
2	Al	64	ILE	CA-CB-CG2	5.74	122.39	110.90
2	Bp	9	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	Bp	64	ILE	CA-CB-CG2	5.73	122.36	110.90
2	Ax	64	ILE	CA-CB-CG2	5.72	122.34	110.90
2	Bj	9	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	Bp	94	ILE	CG1-CB-CG2	-5.66	98.95	111.40
2	Af	94	ILE	CG1-CB-CG2	-5.66	98.96	111.40
2	Bd	94	ILE	CG1-CB-CG2	-5.66	98.96	111.40
2	Ax	94	ILE	CG1-CB-CG2	-5.65	98.96	111.40
2	Bj	94	ILE	CG1-CB-CG2	-5.65	98.96	111.40
2	Al	94	ILE	CG1-CB-CG2	-5.65	98.97	111.40
2	Ar	94	ILE	CG1-CB-CG2	-5.65	98.98	111.40
1	Bn	316	ASP	CB-CG-OD1	5.60	123.34	118.30
1	Av	316	ASP	CB-CG-OD1	5.59	123.33	118.30
1	Ap	316	ASP	CB-CG-OD1	5.57	123.31	118.30
1	Ba	171	LYS	N-CA-CB	5.56	120.61	110.60
1	Bb	316	ASP	CB-CG-OD1	5.56	123.30	118.30
1	Aj	316	ASP	CB-CG-OD1	5.55	123.30	118.30
1	Ai	171	LYS	N-CA-CB	5.55	120.58	110.60
1	Ac	171	LYS	N-CA-CB	5.54	120.57	110.60
1	Bm	171	LYS	N-CA-CB	5.53	120.56	110.60
1	Ad	316	ASP	CB-CG-OD1	5.53	123.28	118.30
1	Au	171	LYS	N-CA-CB	5.53	120.55	110.60
1	Ao	171	LYS	N-CA-CB	5.52	120.54	110.60
1	Ba	284	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	Ar	2	ASN	C-N-CA	5.52	135.49	121.70
2	Ax	2	ASN	C-N-CA	5.52	135.49	121.70
1	Au	284	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	Bg	171	LYS	N-CA-CB	5.51	120.52	110.60
1	Bm	284	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Bh	316	ASP	CB-CG-OD1	5.50	123.25	118.30
2	Bp	2	ASN	C-N-CA	5.50	135.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ac	284	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	Af	2	ASN	C-N-CA	5.49	135.44	121.70
2	Bd	2	ASN	C-N-CA	5.49	135.44	121.70
2	Al	2	ASN	C-N-CA	5.49	135.42	121.70
2	Bj	2	ASN	C-N-CA	5.49	135.41	121.70
1	Ai	284	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	Ao	284	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	Bg	284	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	Bm	399	ALA	N-CA-CB	-5.42	102.52	110.10
1	Ac	399	ALA	N-CA-CB	-5.41	102.53	110.10
1	Ai	399	ALA	N-CA-CB	-5.41	102.53	110.10
1	Bg	399	ALA	N-CA-CB	-5.41	102.53	110.10
1	Ao	399	ALA	N-CA-CB	-5.41	102.53	110.10
1	Ba	399	ALA	N-CA-CB	-5.40	102.55	110.10
1	Au	399	ALA	N-CA-CB	-5.39	102.55	110.10
1	Ai	43	SER	N-CA-CB	-5.36	102.46	110.50
1	Ao	43	SER	N-CA-CB	-5.34	102.49	110.50
1	Au	43	SER	N-CA-CB	-5.34	102.49	110.50
1	Ac	43	SER	N-CA-CB	-5.33	102.51	110.50
1	Ba	43	SER	N-CA-CB	-5.32	102.52	110.50
1	Bg	43	SER	N-CA-CB	-5.32	102.51	110.50
2	Ar	4	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Ba	268	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	Bm	43	SER	N-CA-CB	-5.31	102.53	110.50
1	Bm	268	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	Ba	116	LEU	N-CA-C	-5.28	96.74	111.00
1	Ai	116	LEU	N-CA-C	-5.28	96.75	111.00
2	Bd	4	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	Ac	116	LEU	N-CA-C	-5.27	96.76	111.00
1	Bm	116	LEU	N-CA-C	-5.27	96.77	111.00
1	Ao	116	LEU	N-CA-C	-5.27	96.78	111.00
2	Ax	4	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	Au	116	LEU	N-CA-C	-5.26	96.79	111.00
1	Bg	116	LEU	N-CA-C	-5.26	96.79	111.00
1	Ac	268	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	Bd	92	LEU	CB-CA-C	-5.26	100.21	110.20
1	Ao	268	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	Af	4	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	Ax	92	LEU	CB-CA-C	-5.25	100.22	110.20
2	Ar	92	LEU	CB-CA-C	-5.25	100.23	110.20
2	Af	92	LEU	CB-CA-C	-5.25	100.23	110.20
1	Au	268	ARG	NE-CZ-NH2	-5.25	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Al	92	LEU	CB-CA-C	-5.24	100.24	110.20
2	Bj	4	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	Bp	92	LEU	CB-CA-C	-5.24	100.24	110.20
2	Bp	4	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	Bj	92	LEU	CB-CA-C	-5.23	100.26	110.20
2	Al	4	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	Bh	428	ASP	CB-CA-C	-5.22	99.95	110.40
1	Av	428	ASP	CB-CA-C	-5.21	99.97	110.40
1	Bn	428	ASP	CB-CA-C	-5.21	99.98	110.40
1	Bg	268	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	Ad	428	ASP	CB-CA-C	-5.20	100.00	110.40
1	Ap	428	ASP	CB-CA-C	-5.20	100.01	110.40
1	Bb	428	ASP	CB-CA-C	-5.20	100.01	110.40
1	Aj	428	ASP	CB-CA-C	-5.19	100.02	110.40
1	Ai	268	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	Bp	94	ILE	CA-C-O	-5.17	109.25	120.10
2	Af	94	ILE	CA-C-O	-5.14	109.30	120.10
2	Al	94	ILE	CA-C-O	-5.14	109.30	120.10
2	Ax	94	ILE	CA-C-O	-5.14	109.31	120.10
2	Bd	94	ILE	CA-C-O	-5.13	109.32	120.10
2	Ar	94	ILE	CA-C-O	-5.13	109.33	120.10
2	Bj	94	ILE	CA-C-O	-5.13	109.33	120.10
2	Bj	5	PRO	CA-C-N	5.12	128.46	117.20
2	Al	5	PRO	CA-C-N	5.12	128.45	117.20
2	Bp	5	PRO	CA-C-N	5.11	128.45	117.20
2	Ar	1	MET	CG-SD-CE	5.11	108.37	100.20
2	Bd	5	PRO	CA-C-N	5.11	128.44	117.20
2	Af	94	ILE	N-CA-C	-5.11	97.21	111.00
2	Bj	1	MET	CG-SD-CE	5.11	108.37	100.20
2	Al	94	ILE	N-CA-C	-5.11	97.21	111.00
2	Bd	1	MET	CG-SD-CE	5.10	108.36	100.20
2	Bd	94	ILE	N-CA-C	-5.10	97.22	111.00
2	Af	1	MET	CG-SD-CE	5.10	108.36	100.20
2	Ar	94	ILE	N-CA-C	-5.10	97.23	111.00
1	Ba	170	GLY	N-CA-C	-5.10	100.35	113.10
2	Bj	94	ILE	N-CA-C	-5.10	97.23	111.00
2	Bp	94	ILE	N-CA-C	-5.10	97.23	111.00
2	Al	1	MET	CG-SD-CE	5.10	108.36	100.20
2	Ax	1	MET	CG-SD-CE	5.10	108.36	100.20
2	Ax	94	ILE	N-CA-C	-5.09	97.24	111.00
2	Af	5	PRO	CA-C-N	5.09	128.40	117.20
2	Bp	1	MET	CG-SD-CE	5.09	108.34	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ai	170	GLY	N-CA-C	-5.08	100.39	113.10
2	Ax	5	PRO	CA-C-N	5.08	128.38	117.20
1	Au	170	GLY	N-CA-C	-5.08	100.40	113.10
1	Ac	170	GLY	N-CA-C	-5.07	100.42	113.10
2	Ar	5	PRO	CA-C-N	5.07	128.35	117.20
1	Bg	170	GLY	N-CA-C	-5.07	100.42	113.10
1	Bm	170	GLY	N-CA-C	-5.06	100.45	113.10
1	Ao	170	GLY	N-CA-C	-5.05	100.46	113.10
1	Av	138	CYS	CB-CA-C	-5.02	100.36	110.40
1	Ap	138	CYS	CB-CA-C	-5.02	100.36	110.40
1	Aj	138	CYS	CB-CA-C	-5.01	100.37	110.40
1	Bh	138	CYS	CB-CA-C	-5.01	100.37	110.40
1	Ad	138	CYS	CB-CA-C	-5.01	100.37	110.40
1	Bb	138	CYS	CB-CA-C	-5.01	100.39	110.40
1	Ap	140	ASP	N-CA-C	-5.00	97.49	111.00
1	Ad	140	ASP	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Ac	213	VAL	Peptide
1	Ac	255	GLU	Peptide
1	Ac	285	ARG	Sidechain
1	Ac	354	GLU	Peptide
1	Ac	360	TYR	Sidechain
1	Ad	345	ARG	Sidechain
2	Af	3	ILE	Peptide
2	Af	93	ALA	Peptide
2	Af	96	GLU	Peptide
1	Ai	213	VAL	Peptide
1	Ai	255	GLU	Peptide
1	Ai	285	ARG	Sidechain
1	Ai	354	GLU	Peptide
1	Ai	360	TYR	Sidechain
1	Aj	345	ARG	Sidechain
2	Al	3	ILE	Peptide
2	Al	93	ALA	Peptide
2	Al	96	GLU	Peptide
1	Ao	213	VAL	Peptide
1	Ao	255	GLU	Peptide
1	Ao	285	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	Ao	354	GLU	Peptide
1	Ao	360	TYR	Sidechain
1	Ap	345	ARG	Sidechain
2	Ar	3	ILE	Peptide
2	Ar	93	ALA	Peptide
2	Ar	96	GLU	Peptide
1	Au	213	VAL	Peptide
1	Au	255	GLU	Peptide
1	Au	285	ARG	Sidechain
1	Au	354	GLU	Peptide
1	Au	360	TYR	Sidechain
1	Av	345	ARG	Sidechain
2	Ax	3	ILE	Peptide
2	Ax	93	ALA	Peptide
2	Ax	96	GLU	Peptide
1	Ba	213	VAL	Peptide
1	Ba	255	GLU	Peptide
1	Ba	285	ARG	Sidechain
1	Ba	354	GLU	Peptide
1	Ba	360	TYR	Sidechain
1	Bb	345	ARG	Sidechain
2	Bd	3	ILE	Peptide
2	Bd	93	ALA	Peptide
2	Bd	96	GLU	Peptide
1	Bg	213	VAL	Peptide
1	Bg	255	GLU	Peptide
1	Bg	285	ARG	Sidechain
1	Bg	354	GLU	Peptide
1	Bg	360	TYR	Sidechain
1	Bh	345	ARG	Sidechain
2	Bj	3	ILE	Peptide
2	Bj	93	ALA	Peptide
2	Bj	96	GLU	Peptide
1	Bm	213	VAL	Peptide
1	Bm	255	GLU	Peptide
1	Bm	285	ARG	Sidechain
1	Bm	354	GLU	Peptide
1	Bm	360	TYR	Sidechain
1	Bn	345	ARG	Sidechain
2	Bp	3	ILE	Peptide
2	Bp	93	ALA	Peptide
2	Bp	96	GLU	Peptide

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	Ac	3856	0	3975	0	0
1	Ad	3856	0	3976	0	0
1	Ai	3856	0	3975	0	0
1	Aj	3856	0	3976	0	0
1	Ao	3856	0	3975	0	0
1	Ap	3856	0	3976	0	0
1	Au	3856	0	3975	0	0
1	Av	3856	0	3976	0	0
1	Ba	3856	0	3975	0	0
1	Bb	3856	0	3976	0	0
1	Bg	3856	0	3975	0	0
1	Bh	3856	0	3976	0	0
1	Bm	3856	0	3975	0	0
1	Bn	3856	0	3976	0	0
2	Af	728	0	761	0	0
2	Al	728	0	761	0	0
2	Ar	728	0	761	0	0
2	Ax	728	0	761	0	0
2	Bd	728	0	761	0	0
2	Bj	728	0	761	0	0
2	Bp	728	0	761	0	0
3	Ac	27	0	11	0	0
3	Ad	27	0	11	0	0
3	Ai	27	0	11	0	0
3	Aj	27	0	11	0	0
3	Ao	27	0	11	0	0
3	Ap	27	0	11	0	0
3	Au	27	0	11	0	0
3	Av	27	0	11	0	0
3	Ba	27	0	11	0	0
3	Bb	27	0	11	0	0
3	Bg	27	0	11	0	0
3	Bh	27	0	11	0	0
3	Bm	27	0	11	0	0
3	Bn	27	0	11	0	0
4	Ac	1	0	0	0	0
4	Ad	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ai	1	0	0	0	0
4	Aj	1	0	0	0	0
4	Ao	1	0	0	0	0
4	Ap	1	0	0	0	0
4	Au	1	0	0	0	0
4	Av	1	0	0	0	0
4	Ba	1	0	0	0	0
4	Bb	1	0	0	0	0
4	Bg	1	0	0	0	0
4	Bh	1	0	0	0	0
4	Bm	1	0	0	0	0
4	Bn	1	0	0	0	0
All	All	59472	0	61138	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 32.

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	Ac	522/524 (100%)	494 (95%)	22 (4%)	6 (1%)	14	50
1	Ad	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
1	Ai	522/524 (100%)	494 (95%)	22 (4%)	6 (1%)	14	50
1	Aj	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
1	Ao	522/524 (100%)	493 (94%)	23 (4%)	6 (1%)	14	50
1	Ap	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
1	Au	522/524 (100%)	494 (95%)	22 (4%)	6 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Av	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
1	Ba	522/524 (100%)	493 (94%)	23 (4%)	6 (1%)	14	50
1	Bb	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
1	Bg	522/524 (100%)	493 (94%)	23 (4%)	6 (1%)	14	50
1	Bh	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
1	Bm	522/524 (100%)	494 (95%)	22 (4%)	6 (1%)	14	50
1	Bn	522/524 (100%)	510 (98%)	7 (1%)	5 (1%)	15	52
2	Af	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
2	Al	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
2	Ar	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
2	Ax	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
2	Bd	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
2	Bj	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
2	Bp	95/97 (98%)	82 (86%)	6 (6%)	7 (7%)	1	10
All	All	7973/8015 (100%)	7599 (95%)	248 (3%)	126 (2%)	13	42

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ac	171	LYS
2	Af	4	ARG
2	Af	95	VAL
1	Ai	171	LYS
2	Al	4	ARG
2	Al	95	VAL
1	Ao	171	LYS
2	Ar	4	ARG
2	Ar	95	VAL
1	Au	171	LYS
2	Ax	4	ARG
2	Ax	95	VAL
1	Ba	171	LYS
2	Bd	4	ARG
2	Bd	95	VAL
1	Bg	171	LYS
2	Bj	4	ARG
2	Bj	95	VAL

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Mol	Chain	Res	Type
1	Bm	171	LYS
2	Bp	4	ARG
2	Bp	95	VAL
1	Ac	205	ILE
1	Ad	231	ARG
2	Af	18	GLU
2	Af	54	VAL
2	Af	64	ILE
2	Af	94	ILE
1	Ai	205	ILE
1	Aj	231	ARG
2	Al	18	GLU
2	Al	54	VAL
2	Al	64	ILE
2	Al	94	ILE
1	Ao	205	ILE
1	Ap	231	ARG
2	Ar	18	GLU
2	Ar	54	VAL
2	Ar	64	ILE
2	Ar	94	ILE
1	Au	205	ILE
1	Av	231	ARG
2	Ax	18	GLU
2	Ax	54	VAL
2	Ax	64	ILE
2	Ax	94	ILE
1	Ba	205	ILE
1	Bb	231	ARG
2	Bd	18	GLU
2	Bd	54	VAL
2	Bd	64	ILE
2	Bd	94	ILE
1	Bg	205	ILE
1	Bh	231	ARG
2	Bj	18	GLU
2	Bj	54	VAL
2	Bj	64	ILE
2	Bj	94	ILE
1	Bm	205	ILE
1	Bn	231	ARG
2	Bp	18	GLU

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Mol	Chain	Res	Type
2	Bp	54	VAL
2	Bp	64	ILE
2	Bp	94	ILE
1	Ac	87	ASP
1	Ac	306	GLY
1	Ac	308	GLU
1	Ad	225	LYS
1	Ad	334	ASP
1	Ai	87	ASP
1	Ai	306	GLY
1	Ai	308	GLU
1	Aj	225	LYS
1	Aj	334	ASP
1	Ao	87	ASP
1	Ao	306	GLY
1	Ao	308	GLU
1	Ap	225	LYS
1	Ap	334	ASP
1	Au	87	ASP
1	Au	306	GLY
1	Au	308	GLU
1	Av	225	LYS
1	Av	334	ASP
1	Ba	87	ASP
1	Ba	306	GLY
1	Ba	308	GLU
1	Bb	225	LYS
1	Bb	334	ASP
1	Bg	87	ASP
1	Bg	306	GLY
1	Bg	308	GLU
1	Bh	225	LYS
1	Bh	334	ASP
1	Bm	87	ASP
1	Bm	306	GLY
1	Bm	308	GLU
1	Bn	225	LYS
1	Bn	334	ASP
1	Ac	210	THR
1	Ai	210	THR
1	Ao	210	THR
1	Au	210	THR

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Mol	Chain	Res	Type
1	Ba	210	THR
1	Bg	210	THR
1	Bm	210	THR
1	Ad	322	ARG
1	Aj	322	ARG
1	Ap	322	ARG
1	Av	322	ARG
1	Bb	322	ARG
1	Bh	322	ARG
1	Bn	322	ARG
2	Af	59	VAL
2	Al	59	VAL
2	Ar	59	VAL
2	Ax	59	VAL
2	Bd	59	VAL
2	Bj	59	VAL
2	Bp	59	VAL
1	Ad	217	SER
1	Aj	217	SER
1	Ap	217	SER
1	Av	217	SER
1	Bb	217	SER
1	Bh	217	SER
1	Bn	217	SER

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	Ac	404/404 (100%)	372 (92%)	32 (8%)	12	41
1	Ad	404/404 (100%)	383 (95%)	21 (5%)	23	55
1	Ai	404/404 (100%)	373 (92%)	31 (8%)	13	42
1	Aj	404/404 (100%)	383 (95%)	21 (5%)	23	55
1	Ao	404/404 (100%)	373 (92%)	31 (8%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Ap	404/404 (100%)	383 (95%)	21 (5%)	23 55
1	Au	404/404 (100%)	373 (92%)	31 (8%)	13 42
1	Av	404/404 (100%)	383 (95%)	21 (5%)	23 55
1	Ba	404/404 (100%)	372 (92%)	32 (8%)	12 41
1	Bb	404/404 (100%)	383 (95%)	21 (5%)	23 55
1	Bg	404/404 (100%)	373 (92%)	31 (8%)	13 42
1	Bh	404/404 (100%)	383 (95%)	21 (5%)	23 55
1	Bm	404/404 (100%)	372 (92%)	32 (8%)	12 41
1	Bn	404/404 (100%)	383 (95%)	21 (5%)	23 55
2	Af	80/80 (100%)	55 (69%)	25 (31%)	0 2
2	Al	80/80 (100%)	55 (69%)	25 (31%)	0 2
2	Ar	80/80 (100%)	55 (69%)	25 (31%)	0 2
2	Ax	80/80 (100%)	55 (69%)	25 (31%)	0 2
2	Bd	80/80 (100%)	55 (69%)	25 (31%)	0 2
2	Bj	80/80 (100%)	55 (69%)	25 (31%)	0 2
2	Bp	80/80 (100%)	55 (69%)	25 (31%)	0 2
All	All	6216/6216 (100%)	5674 (91%)	542 (9%)	14 37

All (542) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ac	40	LEU
1	Ac	77	VAL
1	Ac	79	SER
1	Ac	82	ASN
1	Ac	89	THR
1	Ac	90	THR
1	Ac	116	LEU
1	Ac	139	SER
1	Ac	157	THR
1	Ac	184	GLN
1	Ac	196	ASP
1	Ac	197	ARG
1	Ac	199	TYR
1	Ac	215	LEU
1	Ac	231	ARG

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Mol	Chain	Res	Type
1	Ac	283	ASP
1	Ac	289	LEU
1	Ac	307	MET
1	Ac	310	GLU
1	Ac	327	LYS
1	Ac	338	GLU
1	Ac	348	GLN
1	Ac	358	SER
1	Ac	360	TYR
1	Ac	366	GLN
1	Ac	432	GLN
1	Ac	440	ILE
1	Ac	456	LEU
1	Ac	518	GLU
1	Ac	521	VAL
1	Ac	523	ASP
1	Ac	524	LEU
1	Ad	10	ASN
1	Ad	87	ASP
1	Ad	175	ILE
1	Ad	194	GLN
1	Ad	199	TYR
1	Ad	201	SER
1	Ad	214	GLU
1	Ad	272	LYS
1	Ad	281	PHE
1	Ad	284	ARG
1	Ad	286	LYS
1	Ad	307	MET
1	Ad	313	THR
1	Ad	326	ASN
1	Ad	328	ASP
1	Ad	359	ASP
1	Ad	361	ASP
1	Ad	380	LYS
1	Ad	385	THR
1	Ad	435	ASP
1	Ad	498	LYS
2	Af	1	MET
2	Af	2	ASN
2	Af	3	ILE
2	Af	4	ARG

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Mol	Chain	Res	Type
2	Af	6	LEU
2	Af	13	LYS
2	Af	34	LYS
2	Af	36	THR
2	Af	37	ARG
2	Af	43	VAL
2	Af	48	ILE
2	Af	49	LEU
2	Af	53	GLU
2	Af	54	VAL
2	Af	64	ILE
2	Af	65	VAL
2	Af	66	ILE
2	Af	69	ASP
2	Af	74	LYS
2	Af	75	SER
2	Af	77	LYS
2	Af	78	ILE
2	Af	80	ASN
2	Af	81	GLU
2	Af	94	ILE
1	Ai	40	LEU
1	Ai	77	VAL
1	Ai	79	SER
1	Ai	82	ASN
1	Ai	89	THR
1	Ai	90	THR
1	Ai	116	LEU
1	Ai	139	SER
1	Ai	157	THR
1	Ai	184	GLN
1	Ai	196	ASP
1	Ai	197	ARG
1	Ai	199	TYR
1	Ai	215	LEU
1	Ai	231	ARG
1	Ai	283	ASP
1	Ai	289	LEU
1	Ai	307	MET
1	Ai	310	GLU
1	Ai	327	LYS
1	Ai	338	GLU

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Mol	Chain	Res	Type
1	Ai	348	GLN
1	Ai	358	SER
1	Ai	360	TYR
1	Ai	366	GLN
1	Ai	440	ILE
1	Ai	456	LEU
1	Ai	518	GLU
1	Ai	521	VAL
1	Ai	523	ASP
1	Ai	524	LEU
1	Aj	10	ASN
1	Aj	87	ASP
1	Aj	175	ILE
1	Aj	194	GLN
1	Aj	199	TYR
1	Aj	201	SER
1	Aj	214	GLU
1	Aj	272	LYS
1	Aj	281	PHE
1	Aj	284	ARG
1	Aj	286	LYS
1	Aj	307	MET
1	Aj	313	THR
1	Aj	326	ASN
1	Aj	328	ASP
1	Aj	359	ASP
1	Aj	361	ASP
1	Aj	380	LYS
1	Aj	385	THR
1	Aj	435	ASP
1	Aj	498	LYS
2	Al	1	MET
2	Al	2	ASN
2	Al	3	ILE
2	Al	4	ARG
2	Al	6	LEU
2	Al	13	LYS
2	Al	34	LYS
2	Al	36	THR
2	Al	37	ARG
2	Al	43	VAL
2	Al	48	ILE

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Mol	Chain	Res	Type
2	Al	49	LEU
2	Al	53	GLU
2	Al	54	VAL
2	Al	64	ILE
2	Al	65	VAL
2	Al	66	ILE
2	Al	69	ASP
2	Al	74	LYS
2	Al	75	SER
2	Al	77	LYS
2	Al	78	ILE
2	Al	80	ASN
2	Al	81	GLU
2	Al	94	ILE
1	Ao	40	LEU
1	Ao	77	VAL
1	Ao	79	SER
1	Ao	82	ASN
1	Ao	89	THR
1	Ao	90	THR
1	Ao	116	LEU
1	Ao	139	SER
1	Ao	157	THR
1	Ao	184	GLN
1	Ao	196	ASP
1	Ao	197	ARG
1	Ao	199	TYR
1	Ao	215	LEU
1	Ao	231	ARG
1	Ao	283	ASP
1	Ao	289	LEU
1	Ao	307	MET
1	Ao	310	GLU
1	Ao	327	LYS
1	Ao	338	GLU
1	Ao	348	GLN
1	Ao	358	SER
1	Ao	360	TYR
1	Ao	366	GLN
1	Ao	440	ILE
1	Ao	456	LEU
1	Ao	518	GLU

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Mol	Chain	Res	Type
1	Ao	521	VAL
1	Ao	523	ASP
1	Ao	524	LEU
1	Ap	10	ASN
1	Ap	87	ASP
1	Ap	175	ILE
1	Ap	194	GLN
1	Ap	199	TYR
1	Ap	201	SER
1	Ap	214	GLU
1	Ap	272	LYS
1	Ap	281	PHE
1	Ap	284	ARG
1	Ap	286	LYS
1	Ap	307	MET
1	Ap	313	THR
1	Ap	326	ASN
1	Ap	328	ASP
1	Ap	359	ASP
1	Ap	361	ASP
1	Ap	380	LYS
1	Ap	385	THR
1	Ap	435	ASP
1	Ap	498	LYS
2	Ar	1	MET
2	Ar	2	ASN
2	Ar	3	ILE
2	Ar	4	ARG
2	Ar	6	LEU
2	Ar	13	LYS
2	Ar	34	LYS
2	Ar	36	THR
2	Ar	37	ARG
2	Ar	43	VAL
2	Ar	48	ILE
2	Ar	49	LEU
2	Ar	53	GLU
2	Ar	54	VAL
2	Ar	64	ILE
2	Ar	65	VAL
2	Ar	66	ILE
2	Ar	69	ASP

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Mol	Chain	Res	Type
2	Ar	74	LYS
2	Ar	75	SER
2	Ar	77	LYS
2	Ar	78	ILE
2	Ar	80	ASN
2	Ar	81	GLU
2	Ar	94	ILE
1	Au	40	LEU
1	Au	77	VAL
1	Au	79	SER
1	Au	82	ASN
1	Au	89	THR
1	Au	90	THR
1	Au	116	LEU
1	Au	139	SER
1	Au	157	THR
1	Au	184	GLN
1	Au	196	ASP
1	Au	197	ARG
1	Au	199	TYR
1	Au	215	LEU
1	Au	231	ARG
1	Au	283	ASP
1	Au	289	LEU
1	Au	307	MET
1	Au	310	GLU
1	Au	327	LYS
1	Au	338	GLU
1	Au	348	GLN
1	Au	358	SER
1	Au	360	TYR
1	Au	366	GLN
1	Au	440	ILE
1	Au	456	LEU
1	Au	518	GLU
1	Au	521	VAL
1	Au	523	ASP
1	Au	524	LEU
1	Av	10	ASN
1	Av	87	ASP
1	Av	175	ILE
1	Av	194	GLN

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Mol	Chain	Res	Type
1	Av	199	TYR
1	Av	201	SER
1	Av	214	GLU
1	Av	272	LYS
1	Av	281	PHE
1	Av	284	ARG
1	Av	286	LYS
1	Av	307	MET
1	Av	313	THR
1	Av	326	ASN
1	Av	328	ASP
1	Av	359	ASP
1	Av	361	ASP
1	Av	380	LYS
1	Av	385	THR
1	Av	435	ASP
1	Av	498	LYS
2	Ax	1	MET
2	Ax	2	ASN
2	Ax	3	ILE
2	Ax	4	ARG
2	Ax	6	LEU
2	Ax	13	LYS
2	Ax	34	LYS
2	Ax	36	THR
2	Ax	37	ARG
2	Ax	43	VAL
2	Ax	48	ILE
2	Ax	49	LEU
2	Ax	53	GLU
2	Ax	54	VAL
2	Ax	64	ILE
2	Ax	65	VAL
2	Ax	66	ILE
2	Ax	69	ASP
2	Ax	74	LYS
2	Ax	75	SER
2	Ax	77	LYS
2	Ax	78	ILE
2	Ax	80	ASN
2	Ax	81	GLU
2	Ax	94	ILE

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Mol	Chain	Res	Type
1	Ba	40	LEU
1	Ba	77	VAL
1	Ba	79	SER
1	Ba	82	ASN
1	Ba	89	THR
1	Ba	90	THR
1	Ba	116	LEU
1	Ba	139	SER
1	Ba	157	THR
1	Ba	184	GLN
1	Ba	196	ASP
1	Ba	197	ARG
1	Ba	199	TYR
1	Ba	215	LEU
1	Ba	231	ARG
1	Ba	283	ASP
1	Ba	289	LEU
1	Ba	307	MET
1	Ba	310	GLU
1	Ba	327	LYS
1	Ba	338	GLU
1	Ba	348	GLN
1	Ba	358	SER
1	Ba	360	TYR
1	Ba	366	GLN
1	Ba	432	GLN
1	Ba	440	ILE
1	Ba	456	LEU
1	Ba	518	GLU
1	Ba	521	VAL
1	Ba	523	ASP
1	Ba	524	LEU
1	Bb	10	ASN
1	Bb	87	ASP
1	Bb	175	ILE
1	Bb	194	GLN
1	Bb	199	TYR
1	Bb	201	SER
1	Bb	214	GLU
1	Bb	272	LYS
1	Bb	281	PHE
1	Bb	284	ARG

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Mol	Chain	Res	Type
1	Bb	286	LYS
1	Bb	307	MET
1	Bb	313	THR
1	Bb	326	ASN
1	Bb	328	ASP
1	Bb	359	ASP
1	Bb	361	ASP
1	Bb	380	LYS
1	Bb	385	THR
1	Bb	435	ASP
1	Bb	498	LYS
2	Bd	1	MET
2	Bd	2	ASN
2	Bd	3	ILE
2	Bd	4	ARG
2	Bd	6	LEU
2	Bd	13	LYS
2	Bd	34	LYS
2	Bd	36	THR
2	Bd	37	ARG
2	Bd	43	VAL
2	Bd	48	ILE
2	Bd	49	LEU
2	Bd	53	GLU
2	Bd	54	VAL
2	Bd	64	ILE
2	Bd	65	VAL
2	Bd	66	ILE
2	Bd	69	ASP
2	Bd	74	LYS
2	Bd	75	SER
2	Bd	77	LYS
2	Bd	78	ILE
2	Bd	80	ASN
2	Bd	81	GLU
2	Bd	94	ILE
1	Bg	40	LEU
1	Bg	77	VAL
1	Bg	79	SER
1	Bg	82	ASN
1	Bg	89	THR
1	Bg	90	THR

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Mol	Chain	Res	Type
1	Bg	116	LEU
1	Bg	139	SER
1	Bg	157	THR
1	Bg	184	GLN
1	Bg	196	ASP
1	Bg	197	ARG
1	Bg	199	TYR
1	Bg	215	LEU
1	Bg	231	ARG
1	Bg	283	ASP
1	Bg	289	LEU
1	Bg	307	MET
1	Bg	310	GLU
1	Bg	327	LYS
1	Bg	338	GLU
1	Bg	348	GLN
1	Bg	358	SER
1	Bg	360	TYR
1	Bg	366	GLN
1	Bg	440	ILE
1	Bg	456	LEU
1	Bg	518	GLU
1	Bg	521	VAL
1	Bg	523	ASP
1	Bg	524	LEU
1	Bh	10	ASN
1	Bh	87	ASP
1	Bh	175	ILE
1	Bh	194	GLN
1	Bh	199	TYR
1	Bh	201	SER
1	Bh	214	GLU
1	Bh	272	LYS
1	Bh	281	PHE
1	Bh	284	ARG
1	Bh	286	LYS
1	Bh	307	MET
1	Bh	313	THR
1	Bh	326	ASN
1	Bh	328	ASP
1	Bh	359	ASP
1	Bh	361	ASP

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Mol	Chain	Res	Type
1	Bh	380	LYS
1	Bh	385	THR
1	Bh	435	ASP
1	Bh	498	LYS
2	Bj	1	MET
2	Bj	2	ASN
2	Bj	3	ILE
2	Bj	4	ARG
2	Bj	6	LEU
2	Bj	13	LYS
2	Bj	34	LYS
2	Bj	36	THR
2	Bj	37	ARG
2	Bj	43	VAL
2	Bj	48	ILE
2	Bj	49	LEU
2	Bj	53	GLU
2	Bj	54	VAL
2	Bj	64	ILE
2	Bj	65	VAL
2	Bj	66	ILE
2	Bj	69	ASP
2	Bj	74	LYS
2	Bj	75	SER
2	Bj	77	LYS
2	Bj	78	ILE
2	Bj	80	ASN
2	Bj	81	GLU
2	Bj	94	ILE
1	Bm	40	LEU
1	Bm	77	VAL
1	Bm	79	SER
1	Bm	82	ASN
1	Bm	89	THR
1	Bm	90	THR
1	Bm	116	LEU
1	Bm	139	SER
1	Bm	157	THR
1	Bm	184	GLN
1	Bm	196	ASP
1	Bm	197	ARG
1	Bm	199	TYR

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Mol	Chain	Res	Type
1	Bm	215	LEU
1	Bm	231	ARG
1	Bm	283	ASP
1	Bm	289	LEU
1	Bm	307	MET
1	Bm	310	GLU
1	Bm	327	LYS
1	Bm	338	GLU
1	Bm	348	GLN
1	Bm	358	SER
1	Bm	360	TYR
1	Bm	366	GLN
1	Bm	432	GLN
1	Bm	440	ILE
1	Bm	456	LEU
1	Bm	518	GLU
1	Bm	521	VAL
1	Bm	523	ASP
1	Bm	524	LEU
1	Bn	10	ASN
1	Bn	87	ASP
1	Bn	175	ILE
1	Bn	194	GLN
1	Bn	199	TYR
1	Bn	201	SER
1	Bn	214	GLU
1	Bn	272	LYS
1	Bn	281	PHE
1	Bn	284	ARG
1	Bn	286	LYS
1	Bn	307	MET
1	Bn	313	THR
1	Bn	326	ASN
1	Bn	328	ASP
1	Bn	359	ASP
1	Bn	361	ASP
1	Bn	380	LYS
1	Bn	385	THR
1	Bn	435	ASP
1	Bn	498	LYS
2	Bp	1	MET
2	Bp	2	ASN

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Mol	Chain	Res	Type
2	Bp	3	ILE
2	Bp	4	ARG
2	Bp	6	LEU
2	Bp	13	LYS
2	Bp	34	LYS
2	Bp	36	THR
2	Bp	37	ARG
2	Bp	43	VAL
2	Bp	48	ILE
2	Bp	49	LEU
2	Bp	53	GLU
2	Bp	54	VAL
2	Bp	64	ILE
2	Bp	65	VAL
2	Bp	66	ILE
2	Bp	69	ASP
2	Bp	74	LYS
2	Bp	75	SER
2	Bp	77	LYS
2	Bp	78	ILE
2	Bp	80	ASN
2	Bp	81	GLU
2	Bp	94	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ac	21	ASN
1	Ac	366	GLN
1	Ac	401	HIS
1	Ac	437	ASN
1	Ac	467	ASN
1	Ac	479	ASN
1	Ad	21	ASN
1	Ad	82	ASN
1	Ad	146	GLN
1	Ad	351	GLN
1	Ai	21	ASN
1	Ai	366	GLN
1	Ai	401	HIS
1	Ai	437	ASN
1	Ai	467	ASN

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Mol	Chain	Res	Type
1	Ai	479	ASN
1	Aj	21	ASN
1	Aj	82	ASN
1	Aj	146	GLN
1	Aj	351	GLN
1	Ao	21	ASN
1	Ao	366	GLN
1	Ao	401	HIS
1	Ao	437	ASN
1	Ao	467	ASN
1	Ao	479	ASN
1	Ap	21	ASN
1	Ap	82	ASN
1	Ap	146	GLN
1	Ap	351	GLN
1	Au	21	ASN
1	Au	366	GLN
1	Au	401	HIS
1	Au	437	ASN
1	Au	467	ASN
1	Au	479	ASN
1	Av	21	ASN
1	Av	82	ASN
1	Av	146	GLN
1	Av	351	GLN
1	Ba	21	ASN
1	Ba	366	GLN
1	Ba	401	HIS
1	Ba	437	ASN
1	Ba	467	ASN
1	Ba	479	ASN
1	Bb	21	ASN
1	Bb	82	ASN
1	Bb	146	GLN
1	Bb	351	GLN
1	Bg	21	ASN
1	Bg	366	GLN
1	Bg	401	HIS
1	Bg	437	ASN
1	Bg	467	ASN
1	Bg	479	ASN
1	Bh	21	ASN

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Mol	Chain	Res	Type
1	Bh	82	ASN
1	Bh	146	GLN
1	Bh	351	GLN
1	Bm	21	ASN
1	Bm	366	GLN
1	Bm	401	HIS
1	Bm	437	ASN
1	Bm	467	ASN
1	Bm	479	ASN
1	Bn	21	ASN
1	Bn	82	ASN
1	Bn	146	GLN
1	Bn	351	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

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	Ad	601	4	1/1/6/6	-	-
3	ADP	Bh	601	4	1/1/6/6	-	-
3	ADP	Av	601	4	1/1/6/6	-	-
3	ADP	Ap	601	4	1/1/6/6	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	Bn	601	4	1/1/6/6	-	-
3	ADP	Aj	601	4	1/1/6/6	-	-
3	ADP	Bb	601	4	1/1/6/6	-	-

There are no bond length outliers.

There are no bond angle outliers.

All (7) chirality outliers are listed below:

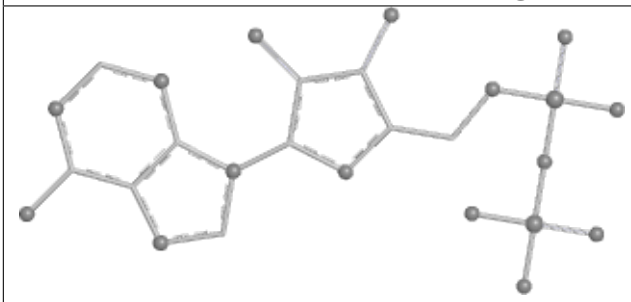
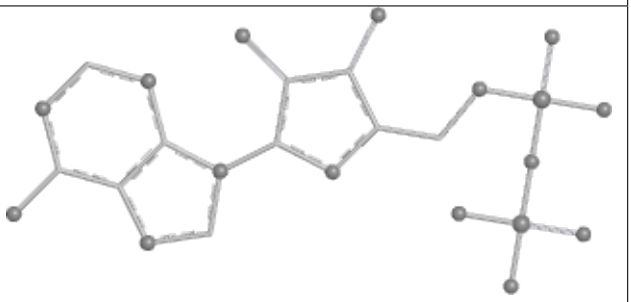
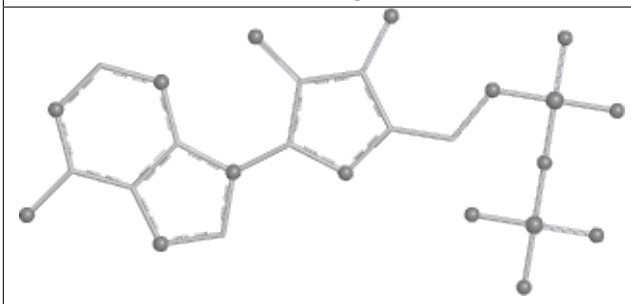
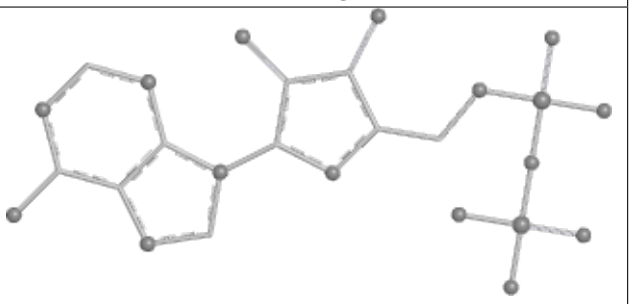
Mol	Chain	Res	Type	Atom
3	Ad	601	ADP	C1'
3	Aj	601	ADP	C1'
3	Ap	601	ADP	C1'
3	Av	601	ADP	C1'
3	Bb	601	ADP	C1'
3	Bh	601	ADP	C1'
3	Bn	601	ADP	C1'

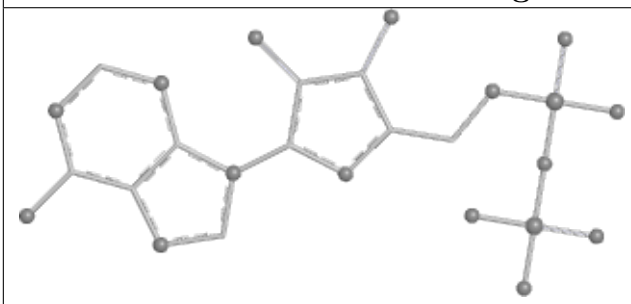
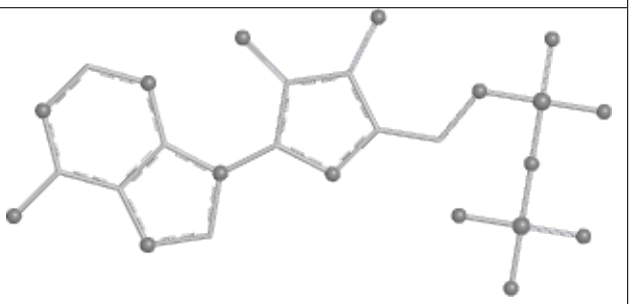
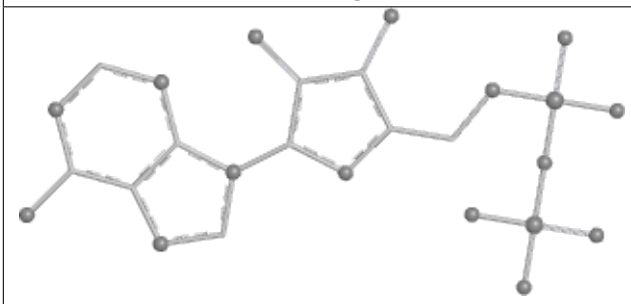
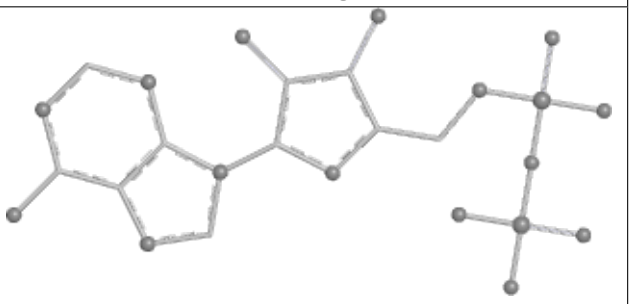
There are no torsion outliers.

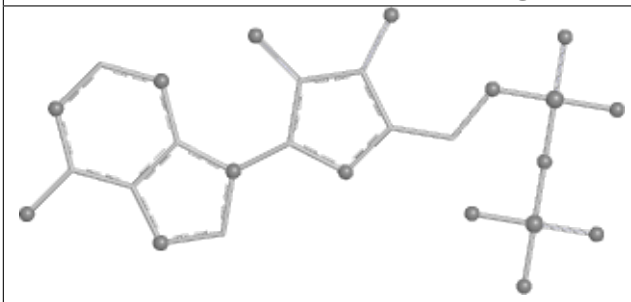
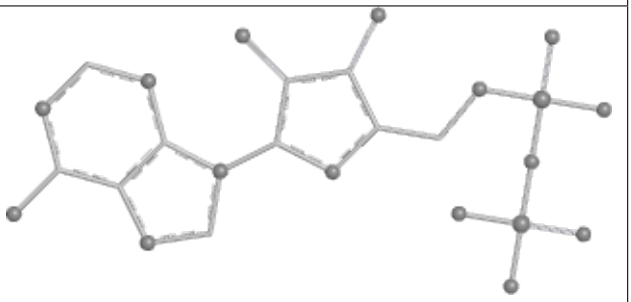
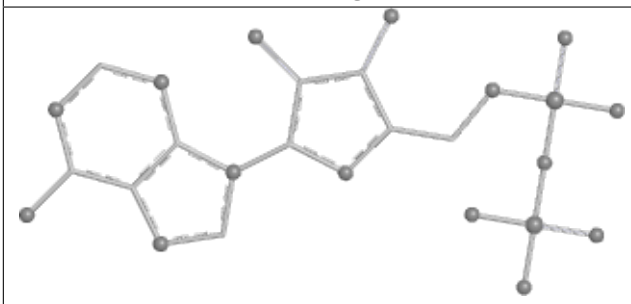
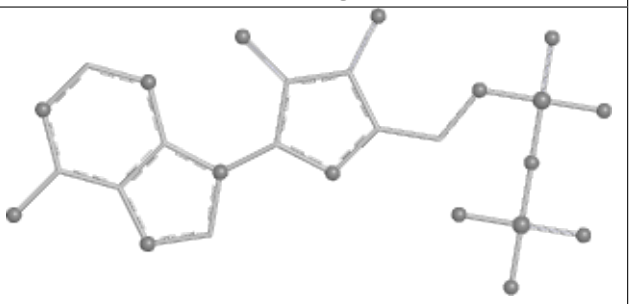
There are no ring outliers.

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 Ad 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Bh 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Av 601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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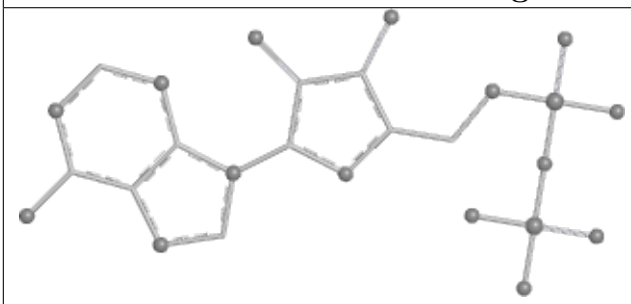
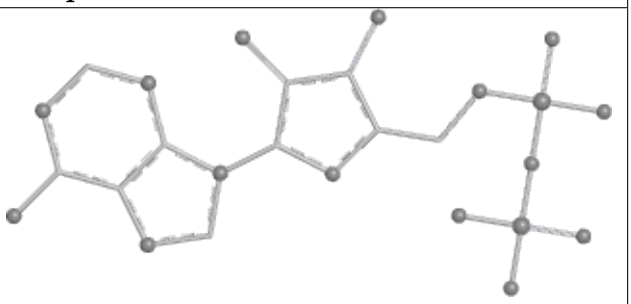
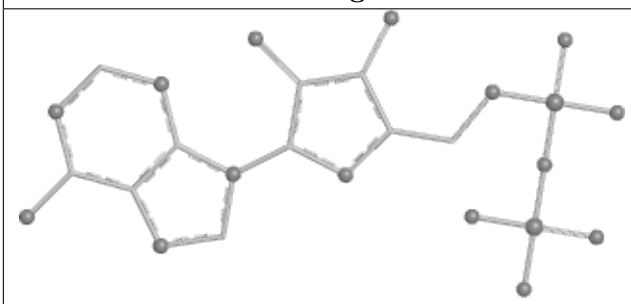
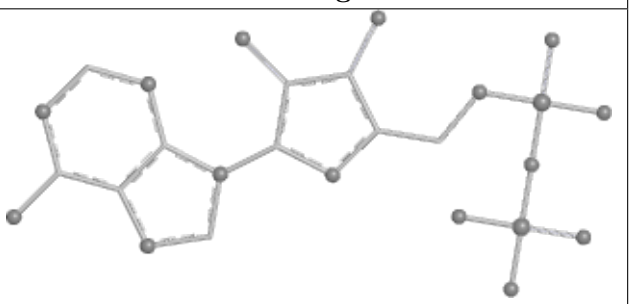
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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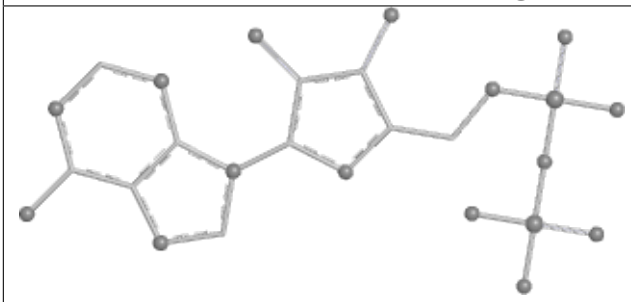
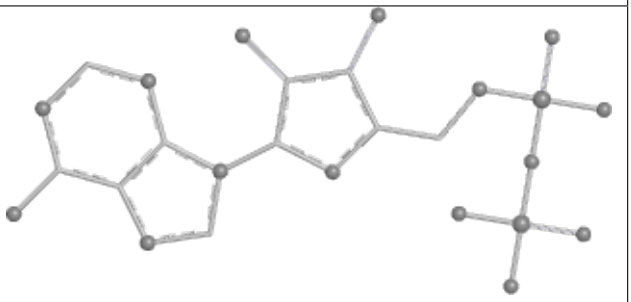
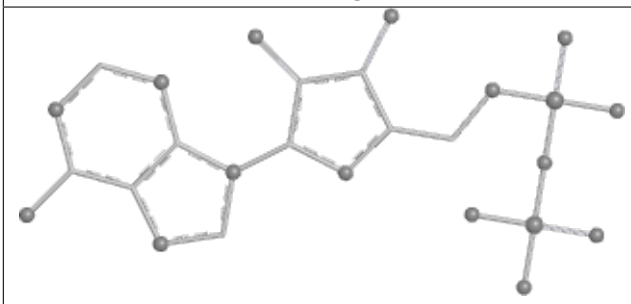
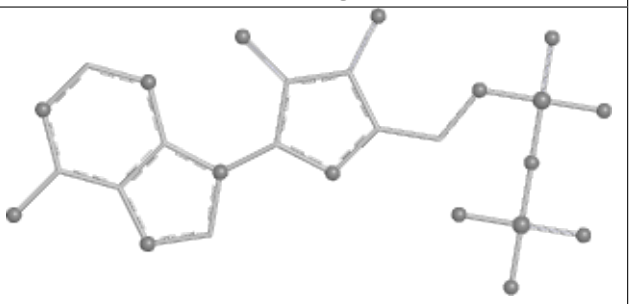
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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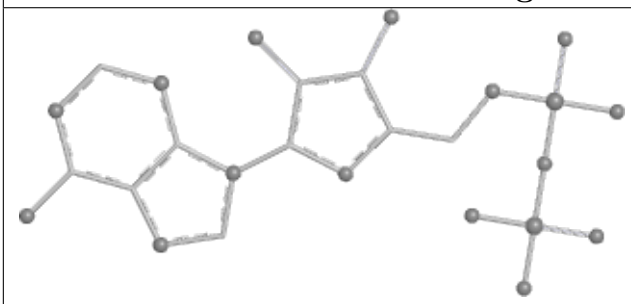
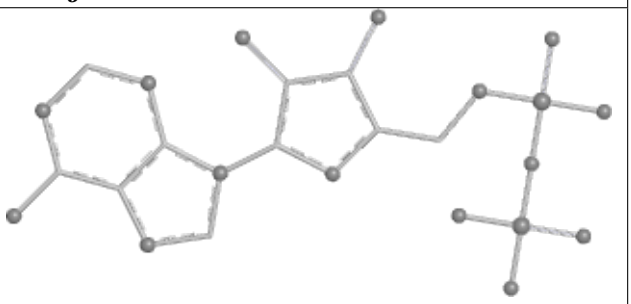
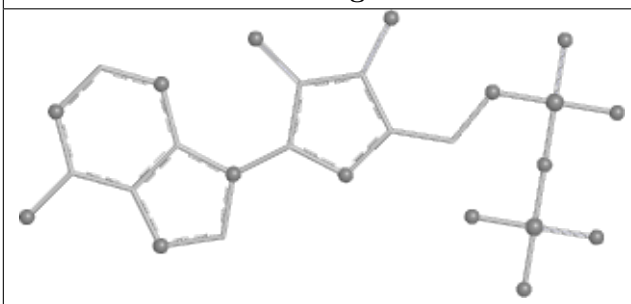
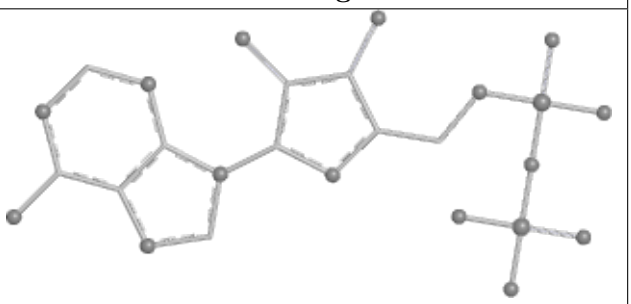
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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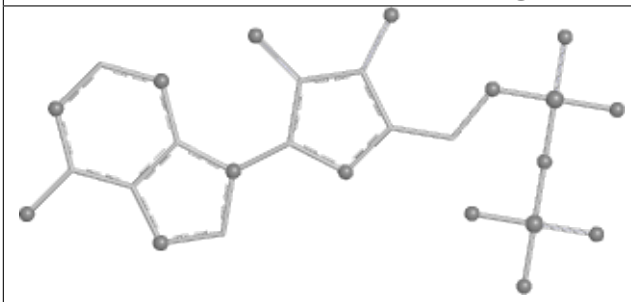
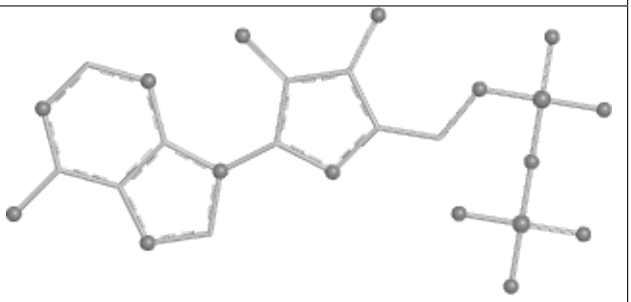
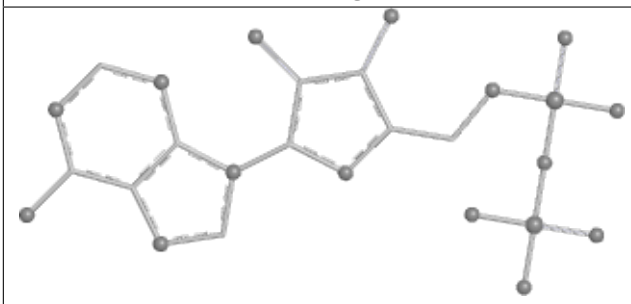
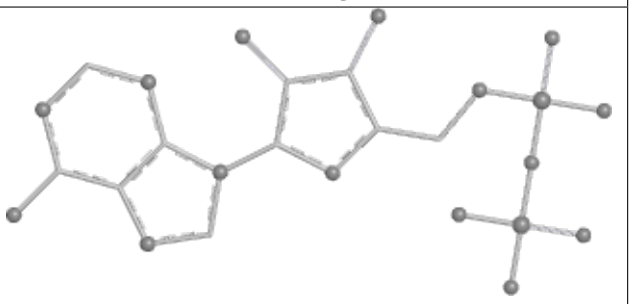
 Bond lengths	 Bond angles
 Torsions	 Rings

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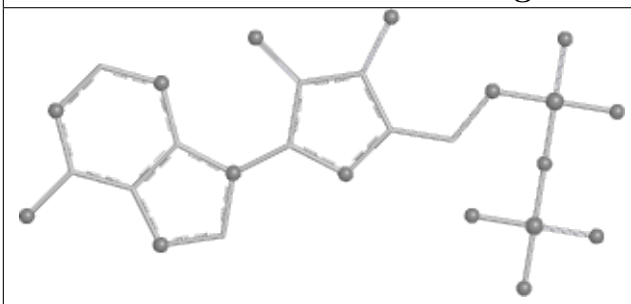
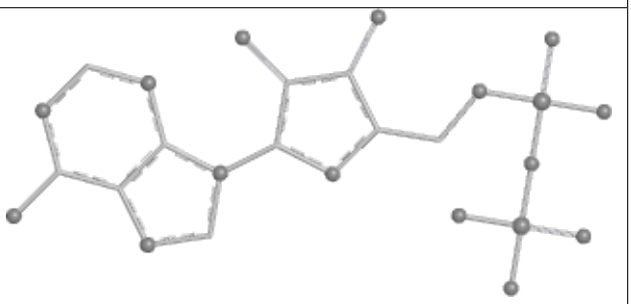
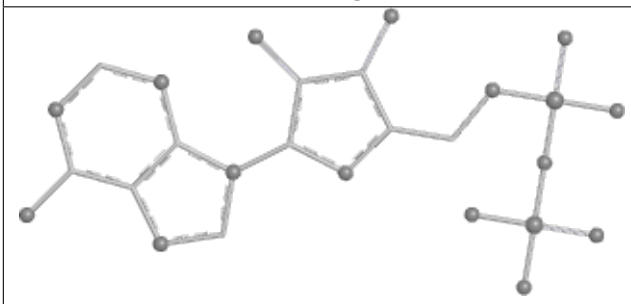
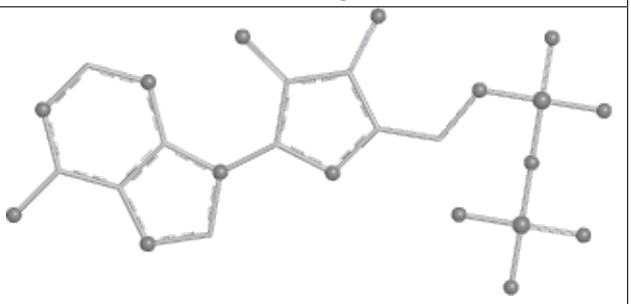
 Bond lengths	 Bond angles
 Torsions	 Rings

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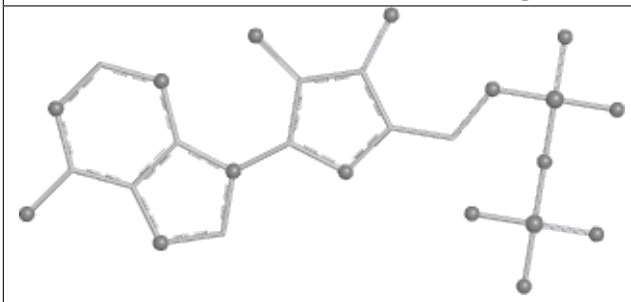
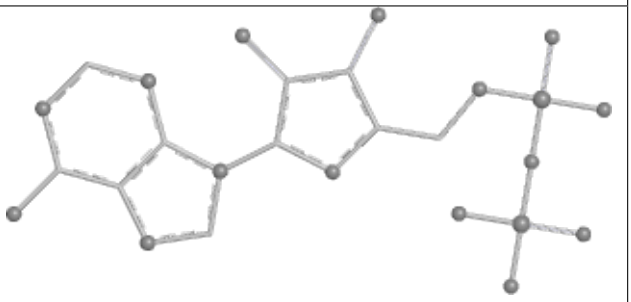
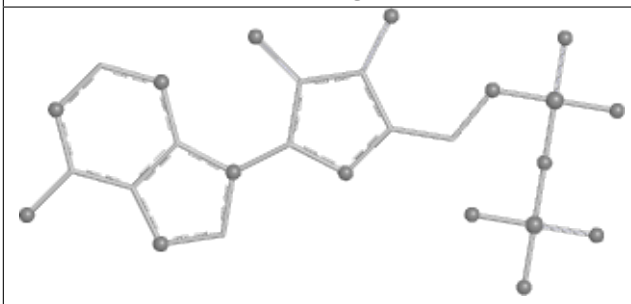
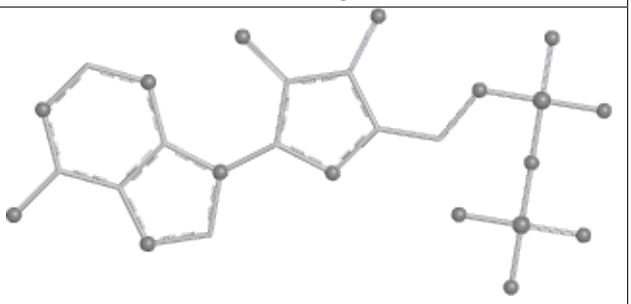
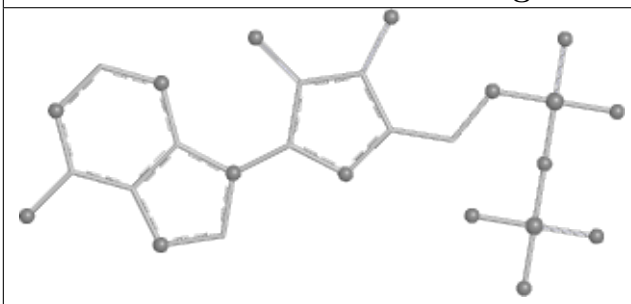
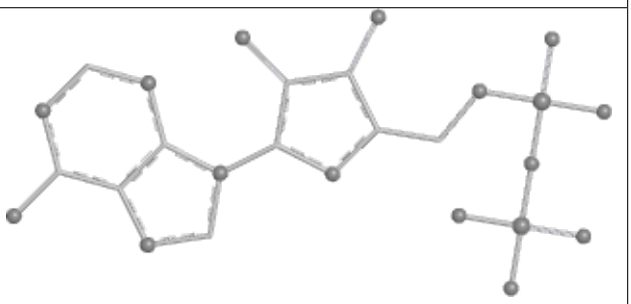
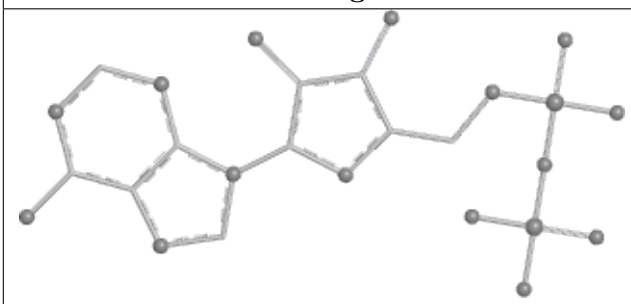
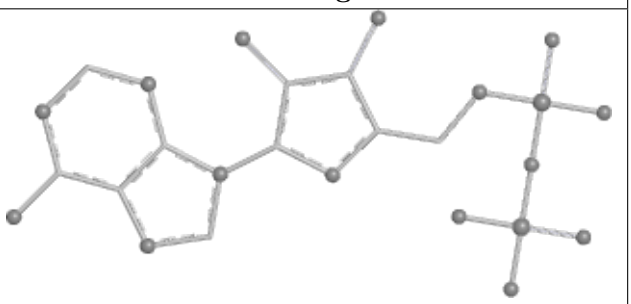
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand ADP Ao 601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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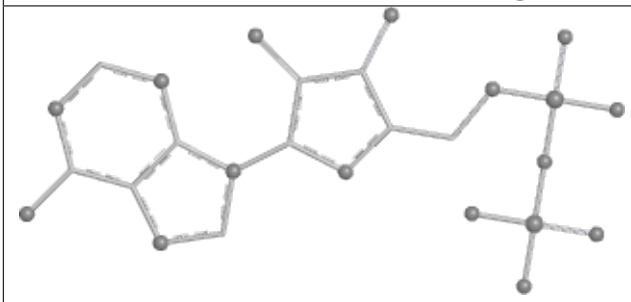
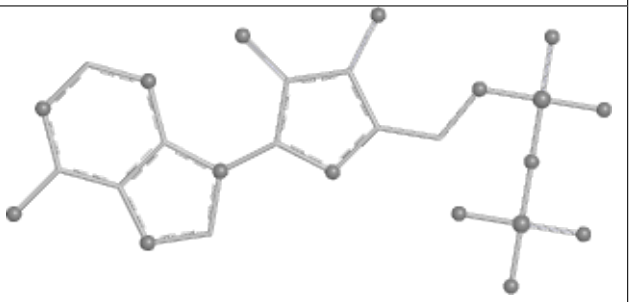
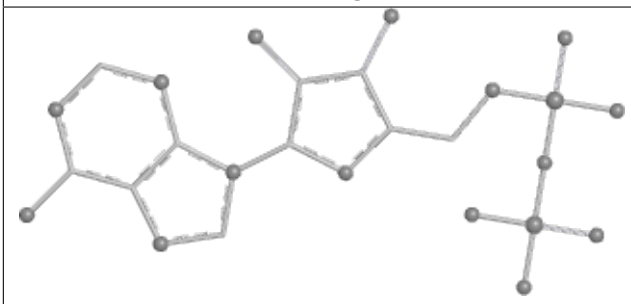
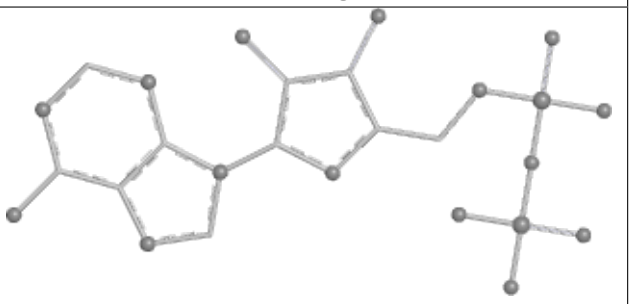
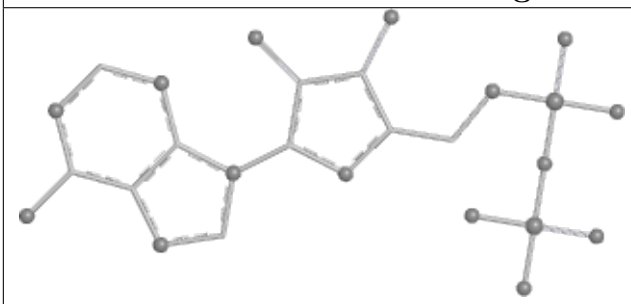
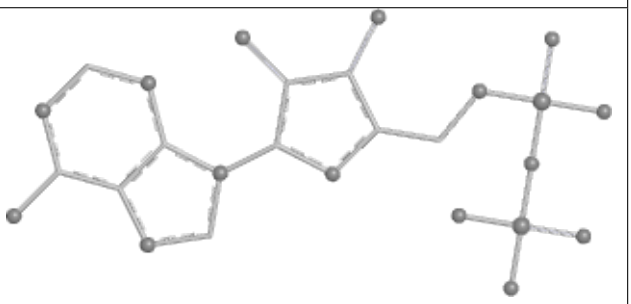
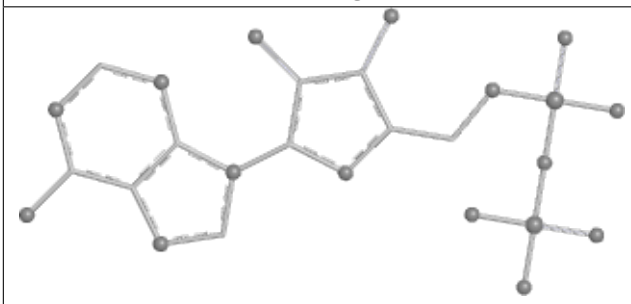
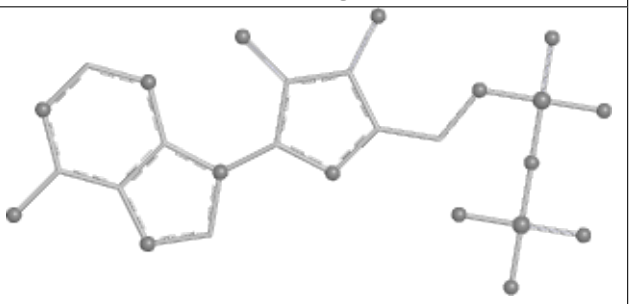
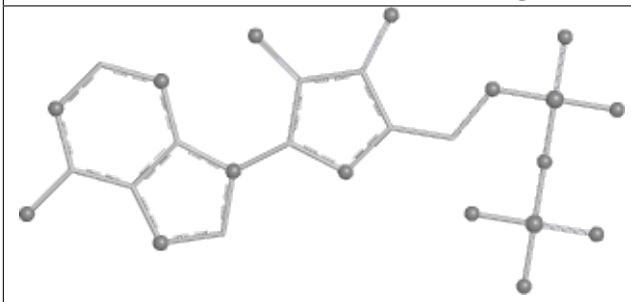
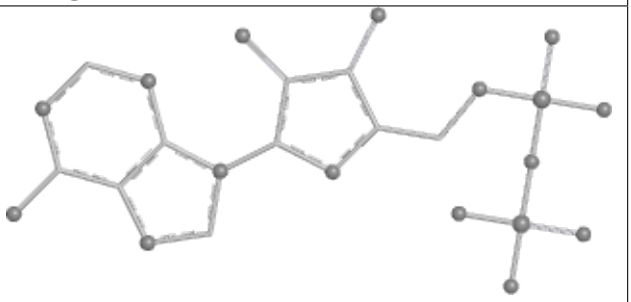
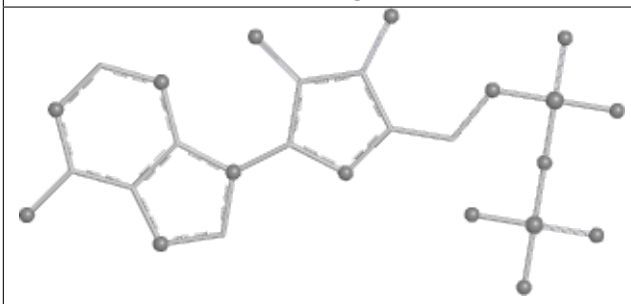
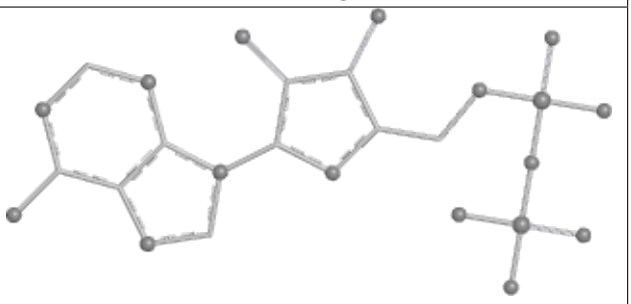
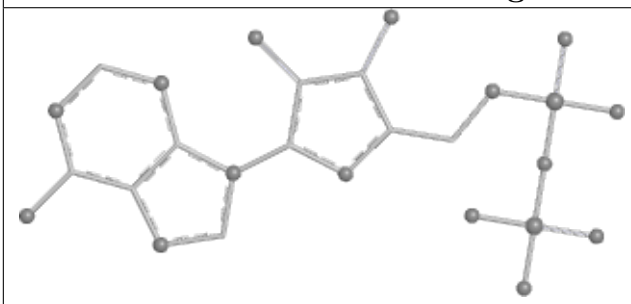
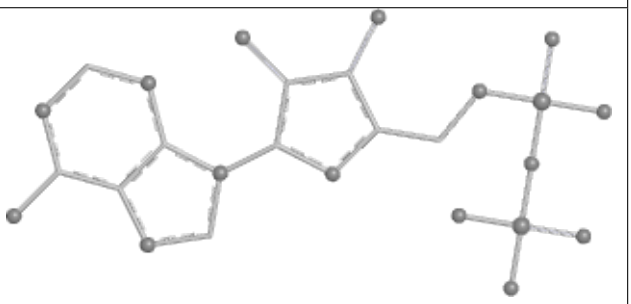
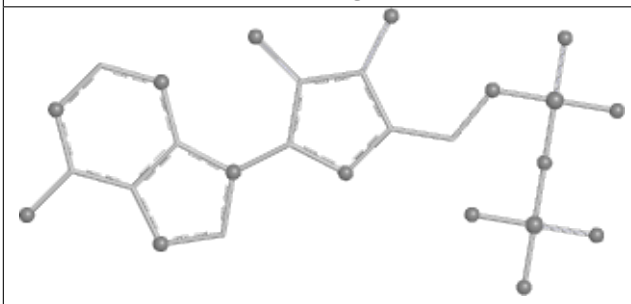
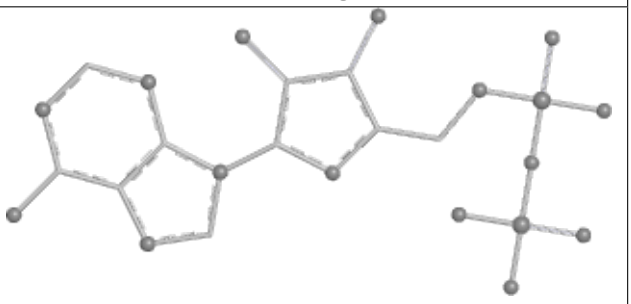
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Ba 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Bg 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Bm 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

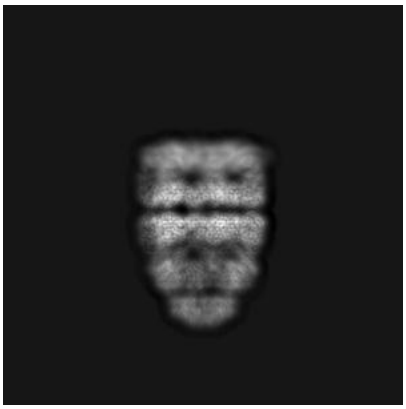
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13308. These allow visual inspection of the internal detail of the map and identification of artifacts.

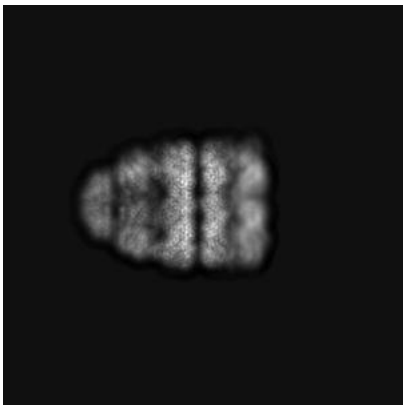
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

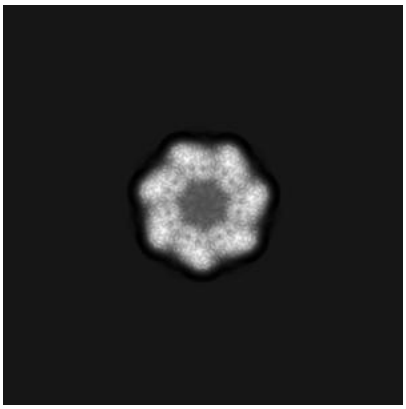
6.1.1 Primary map



X

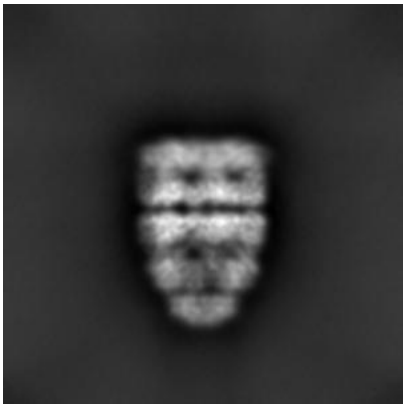


Y

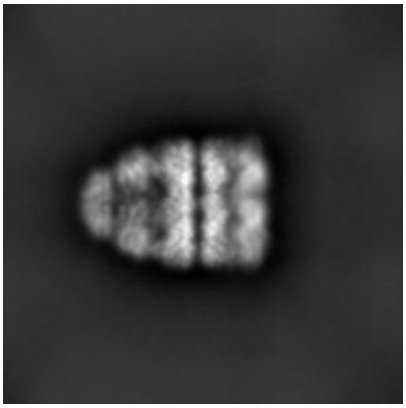


Z

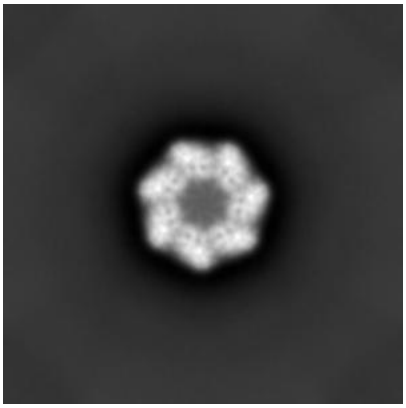
6.1.2 Raw map



X



Y

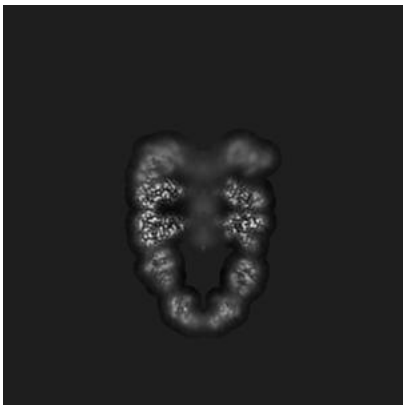


Z

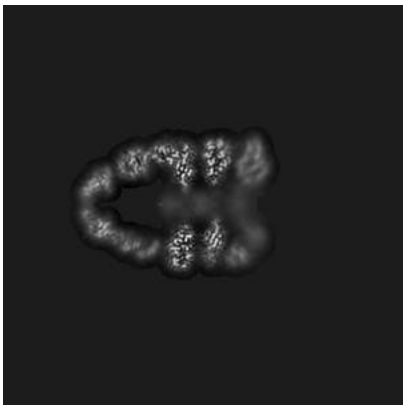
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

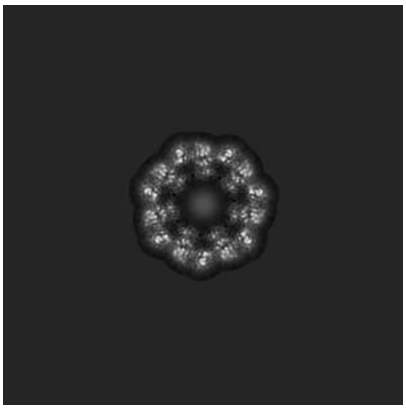
6.2.1 Primary map



X Index: 192

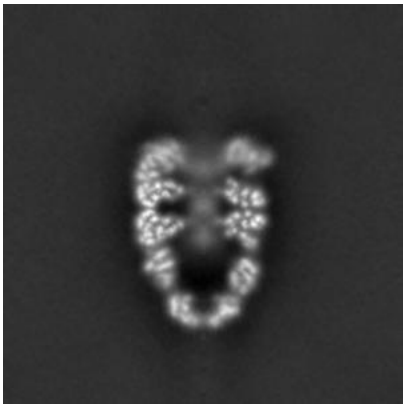


Y Index: 192

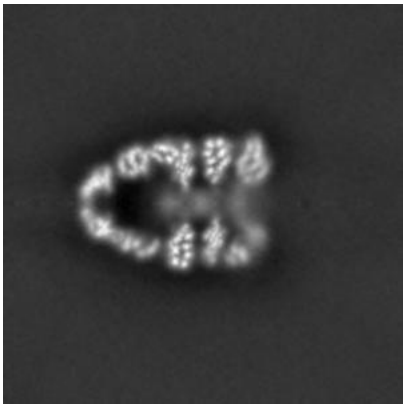


Z Index: 192

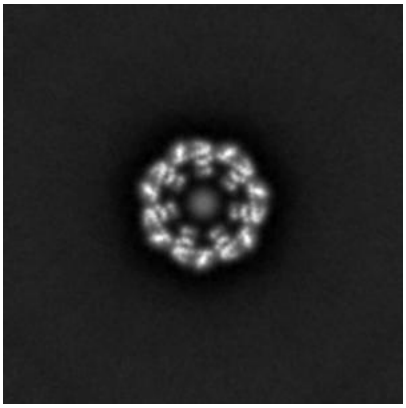
6.2.2 Raw map



X Index: 192



Y Index: 192

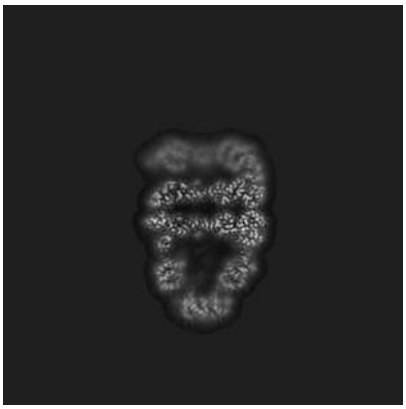


Z Index: 192

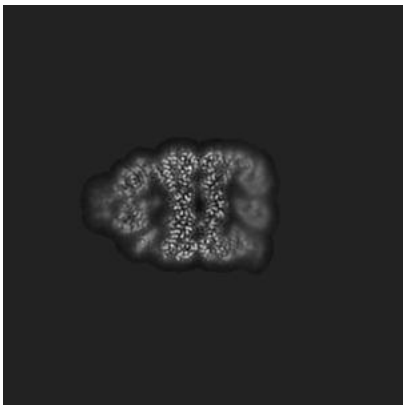
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

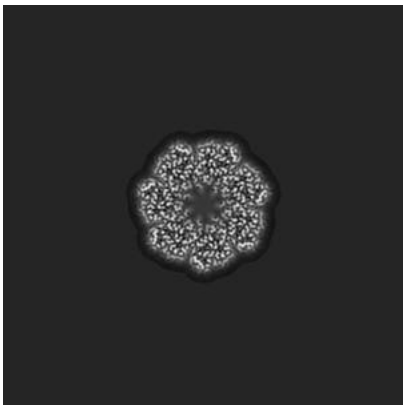
6.3.1 Primary map



X Index: 215

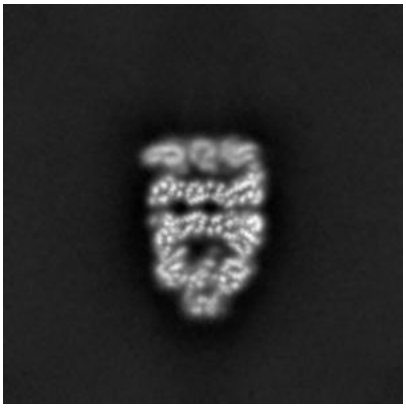


Y Index: 159

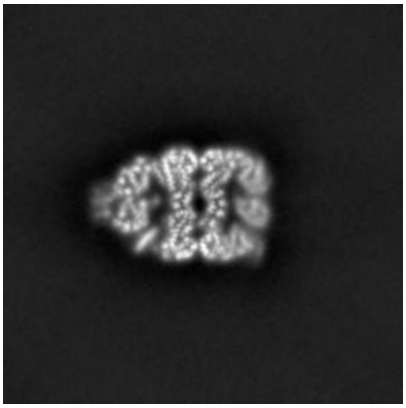


Z Index: 175

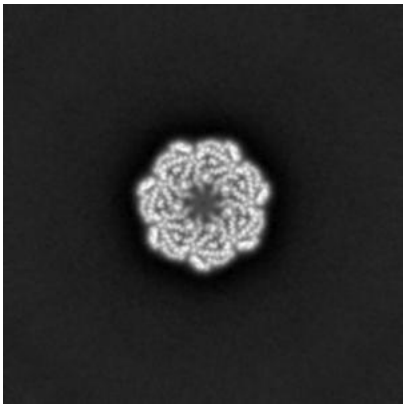
6.3.2 Raw map



X Index: 222



Y Index: 159

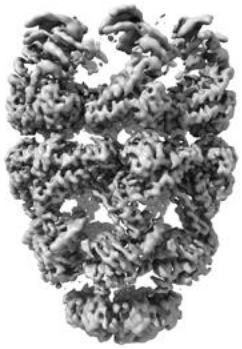


Z Index: 175

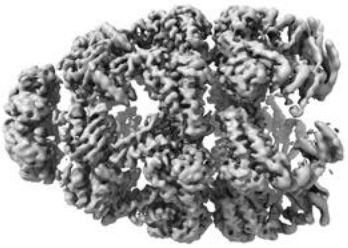
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

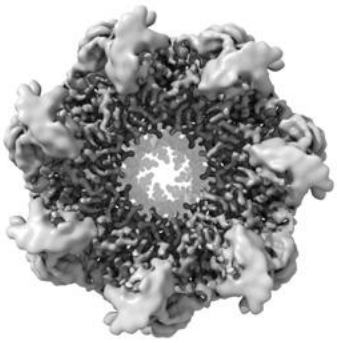
6.4.1 Primary map



X



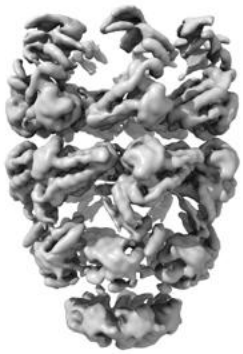
Y



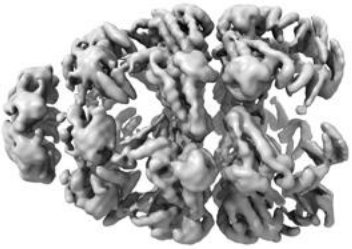
Z

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.

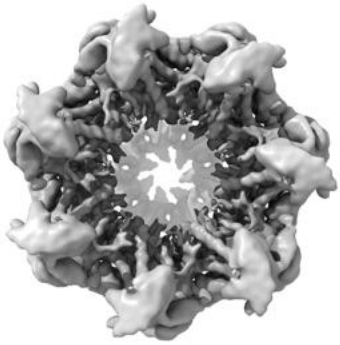
6.4.2 Raw map



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.

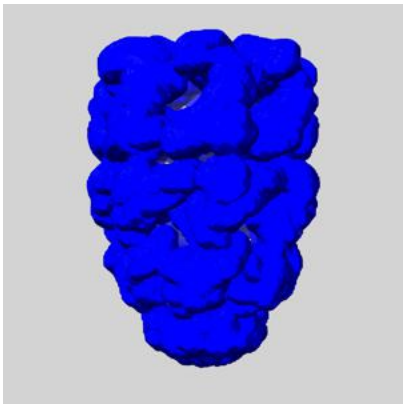
6.5 Mask visualisation (i)

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

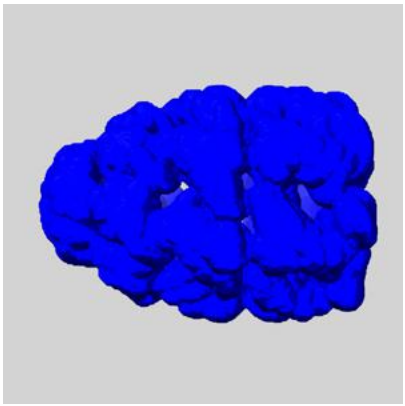
A mask typically either:

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

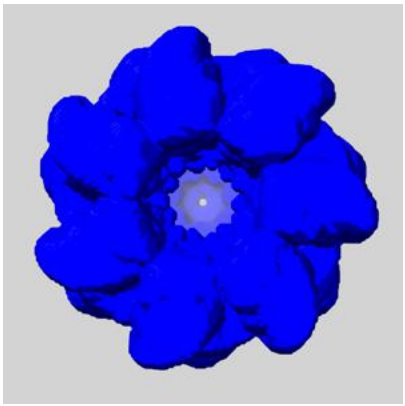
6.5.1 emd_13308_msk_1.map (i)



X



Y

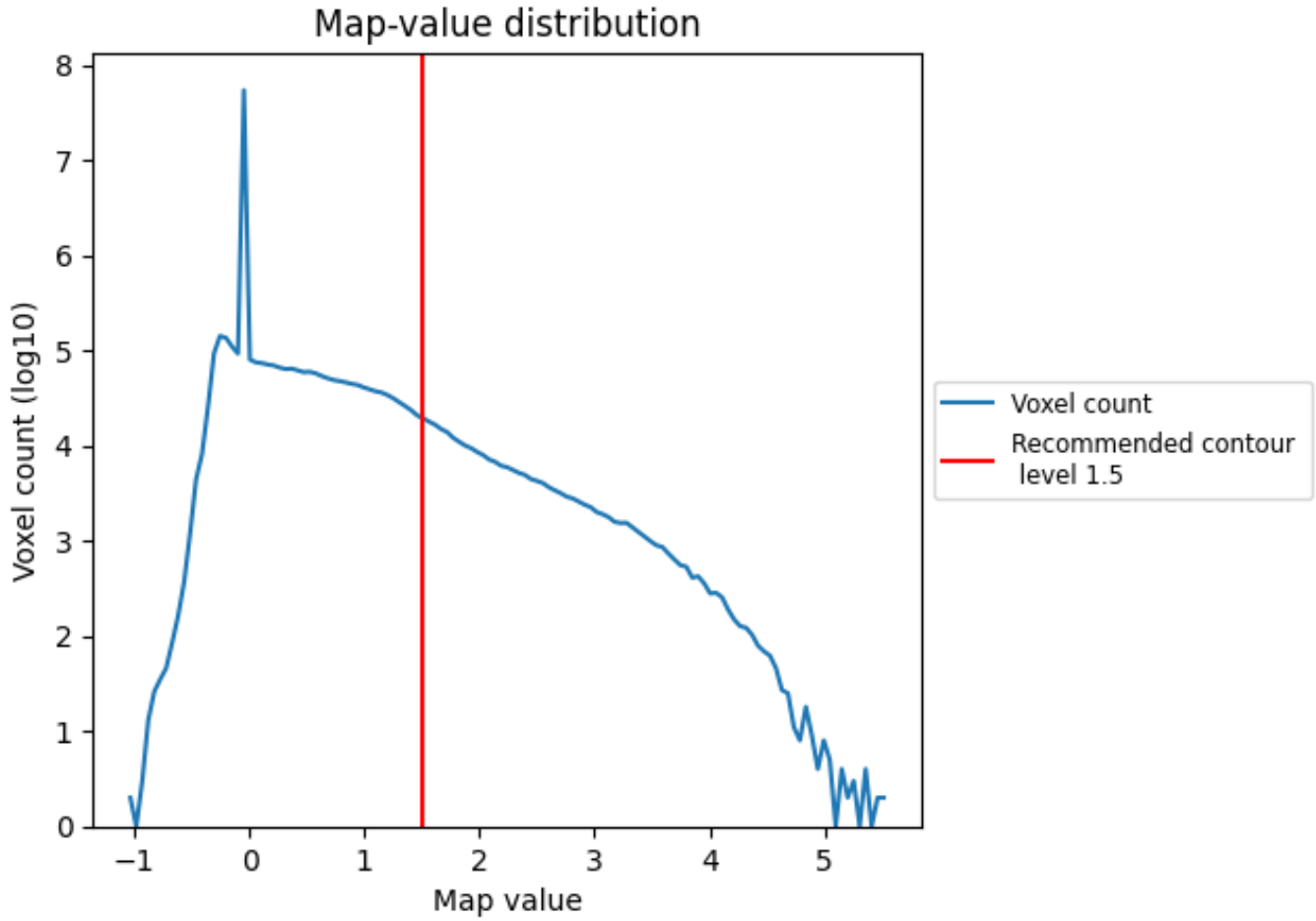


Z

7 Map analysis

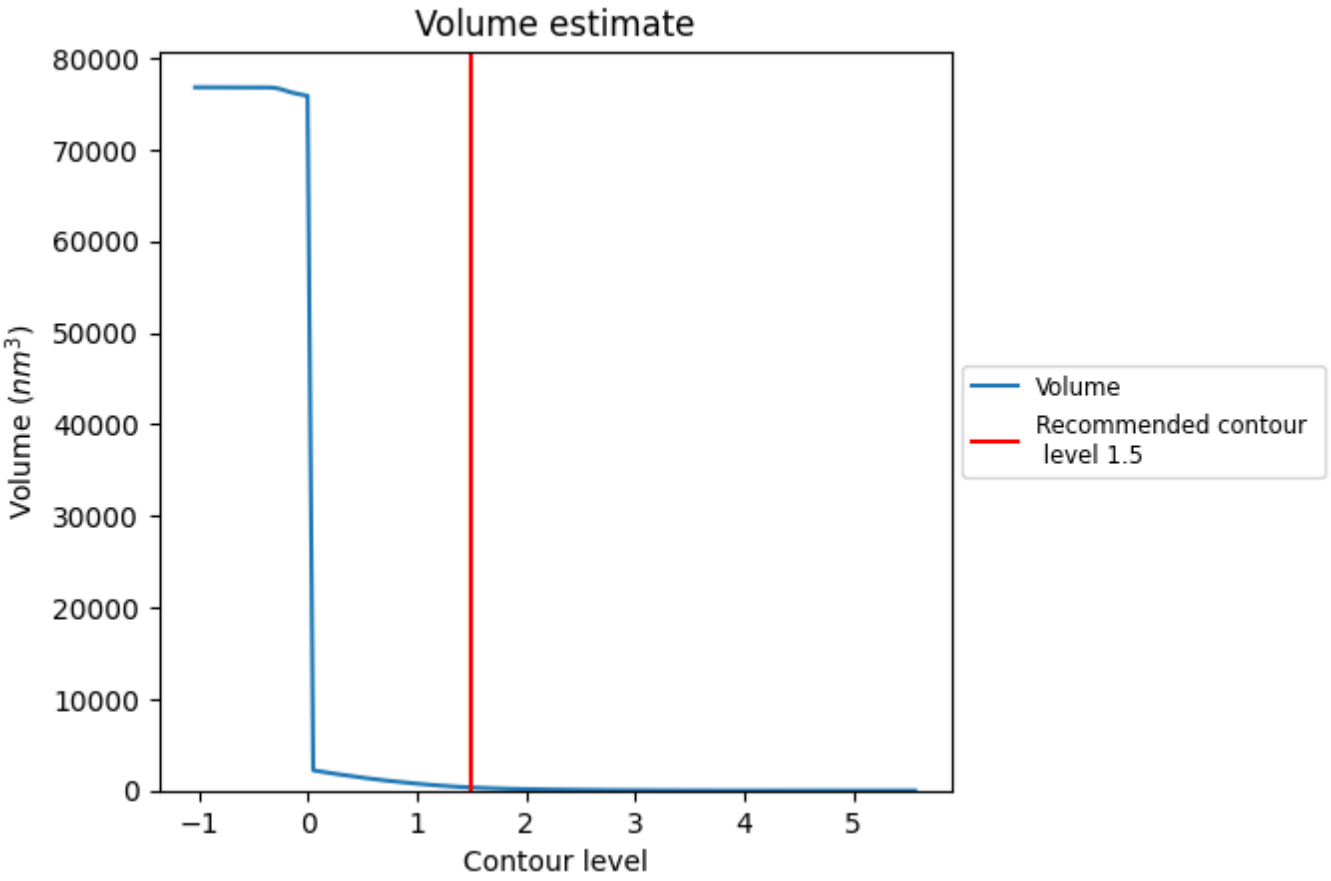
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

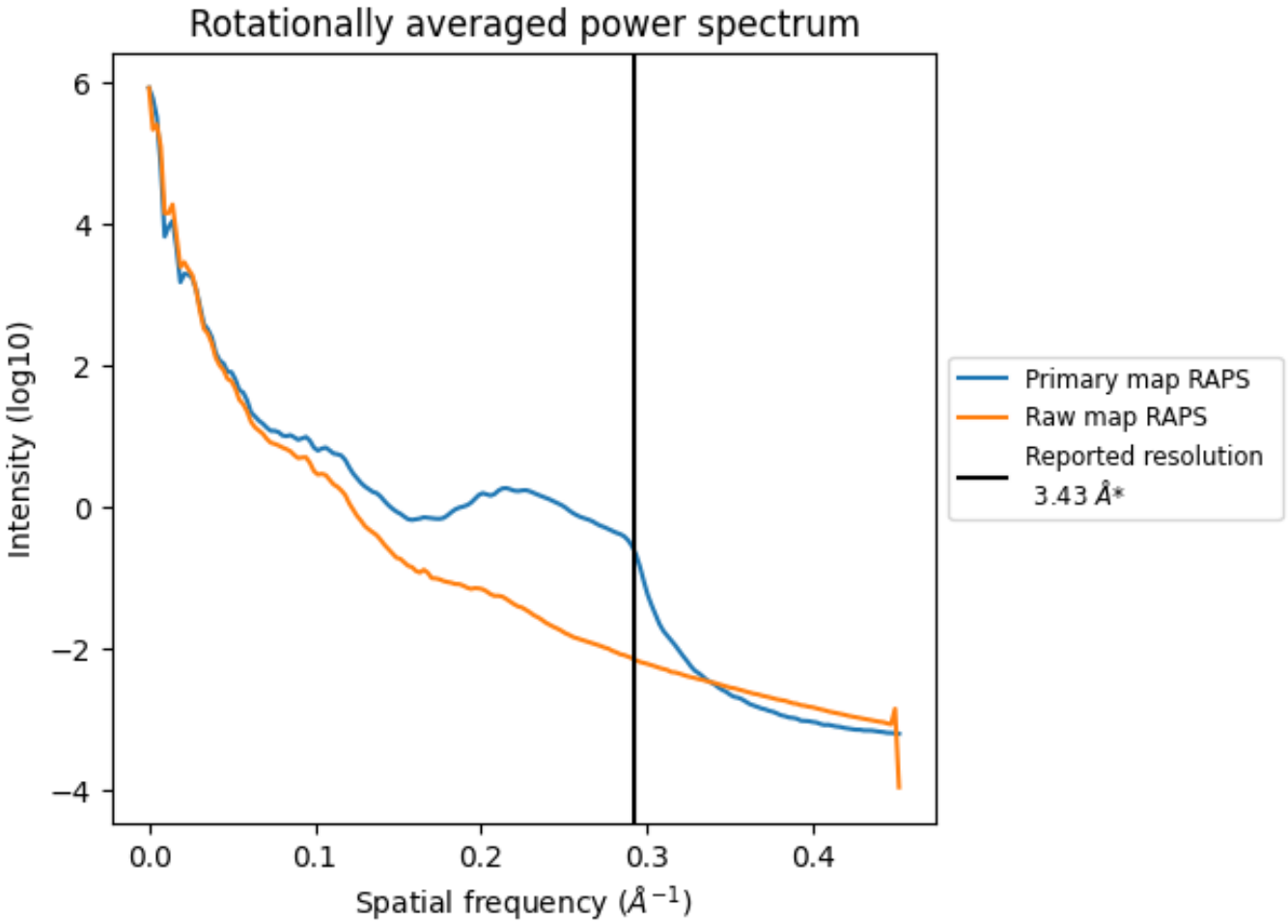
7.2 Volume estimate



The volume at the recommended contour level is 334 nm^3; this corresponds to an approximate mass of 302 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)

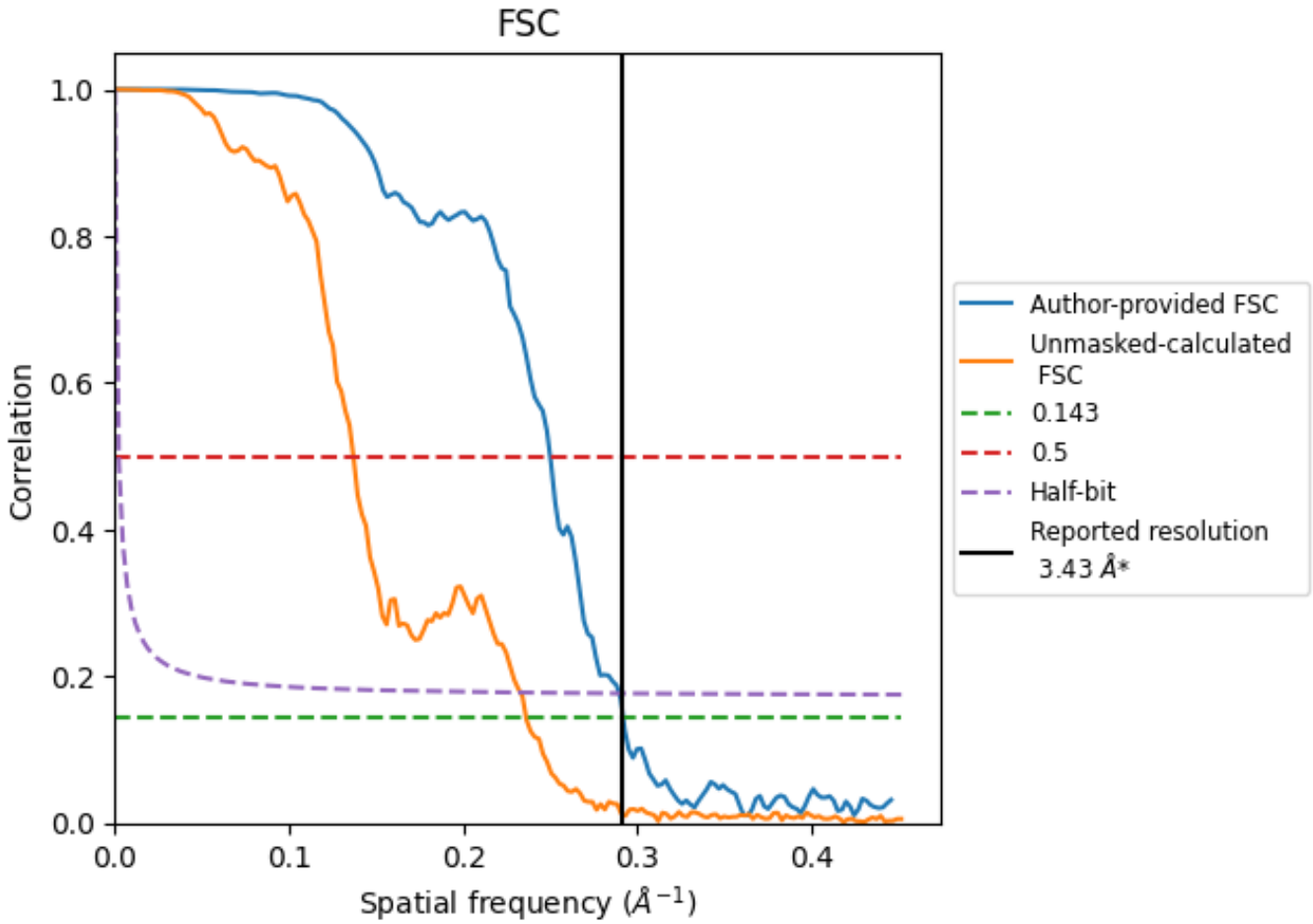


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

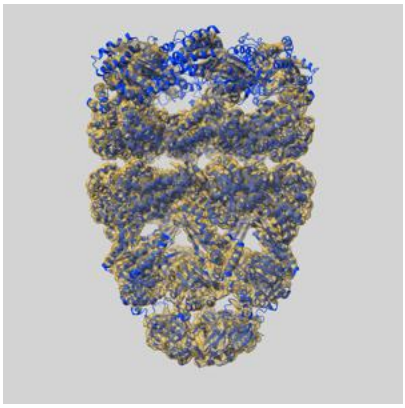
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.43	4.00	3.45
Unmasked-calculated*	4.23	7.30	4.29

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

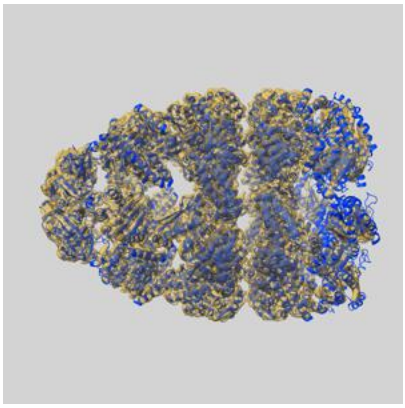
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13308 and PDB model 7PBX. Per-residue inclusion information can be found in section 3 on page 8.

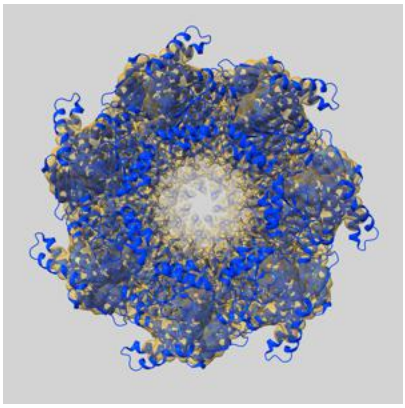
9.1 Map-model overlay



X



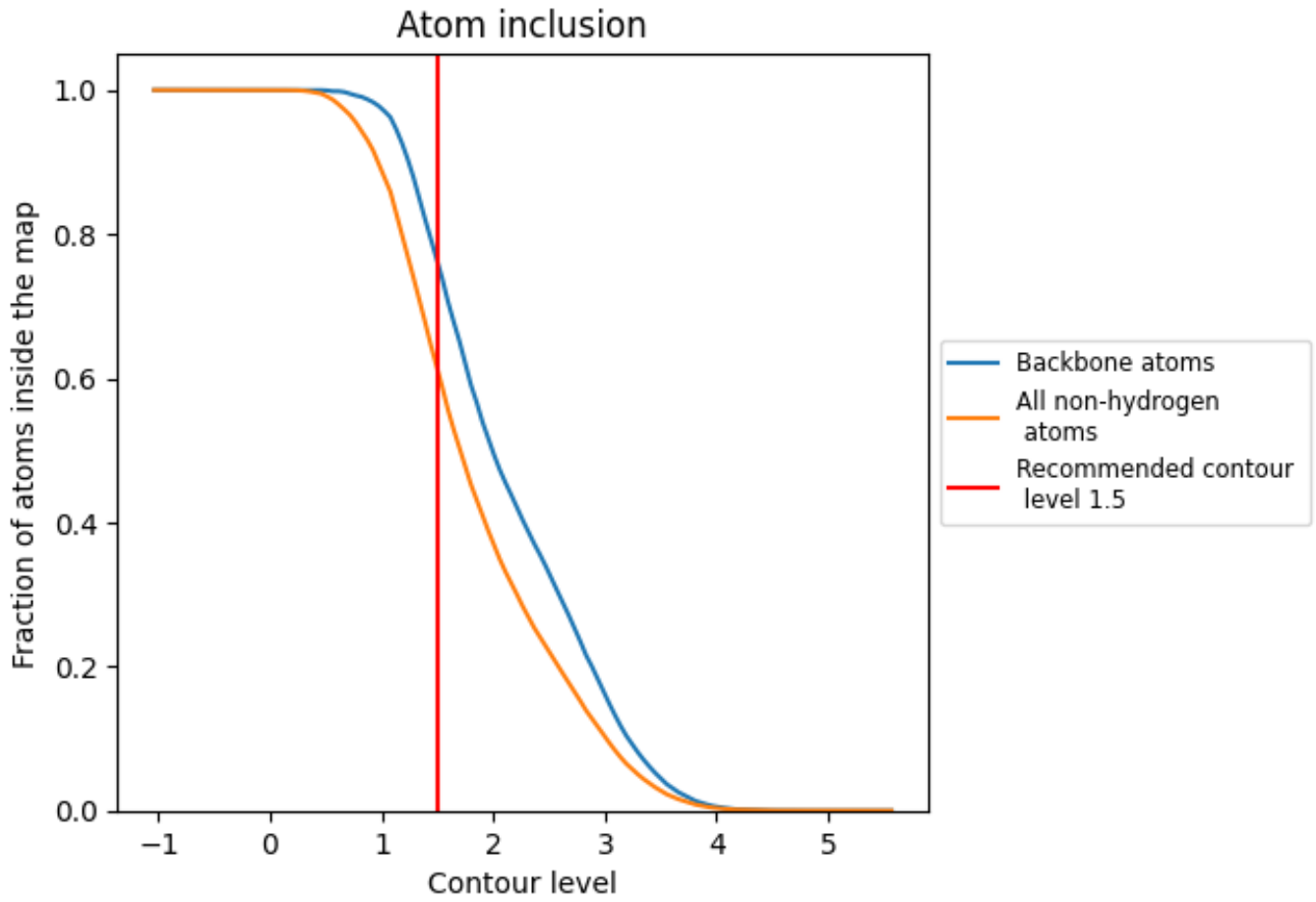
Y



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 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.