



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 05:14 AM EST

PDB ID : 6DJU  
EMDB ID : EMD-7942  
Title : Mtb ClpB in complex with ATPgammaS and casein, Conformer 1  
Authors : Yu, H.J.; Li, H.L.  
Deposited on : 2018-05-26  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

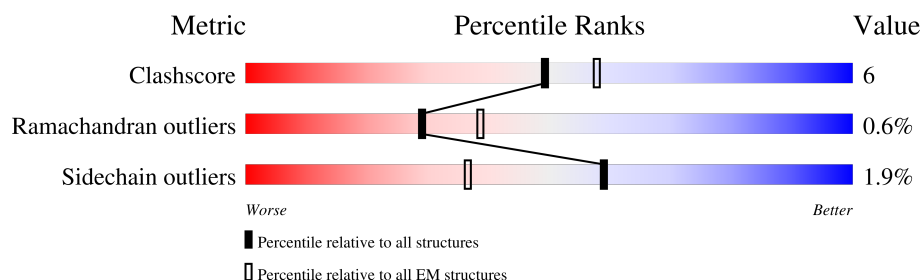
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	848	<div> <div>12%</div> <div>63%</div> <div>9%</div> <div>28%</div> </div>
1	B	848	<div> <div>9%</div> <div>63%</div> <div>8%</div> <div>28%</div> </div>
1	C	848	<div> <div>8%</div> <div>61%</div> <div>11%</div> <div>28%</div> </div>
1	D	848	<div> <div>5%</div> <div>58%</div> <div>8%</div> <div>34%</div> </div>
1	E	848	<div> <div>18%</div> <div>56%</div> <div>8%</div> <div>35%</div> </div>
1	F	848	<div> <div>38%</div> <div>49%</div> <div>12%</div> <div>37%</div> </div>
2	N	26	<div> <div>19%</div> <div>96%</div> <div>.</div> </div>

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	AGS	D	902	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27140 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.

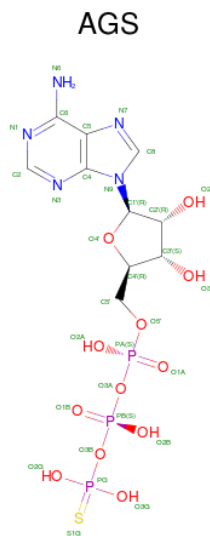
- Molecule 1 is a protein called Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	610	Total	C	N	O	S	0	0
			4649	2912	843	885	9		
1	B	611	Total	C	N	O	S	0	0
			4657	2916	844	888	9		
1	C	614	Total	C	N	O	S	0	0
			4674	2926	847	892	9		
1	D	562	Total	C	N	O	S	0	0
			4321	2701	790	821	9		
1	E	548	Total	C	N	O	S	0	0
			4230	2647	772	802	9		
1	F	531	Total	C	N	O	S	0	0
			4115	2575	752	779	9		

- Molecule 2 is a protein called casein polyAlanine model.

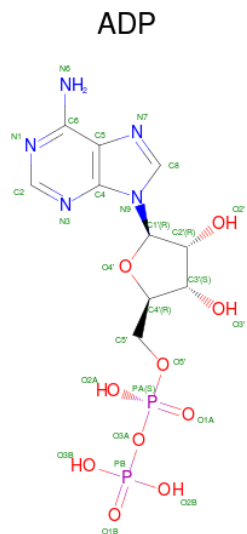
Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



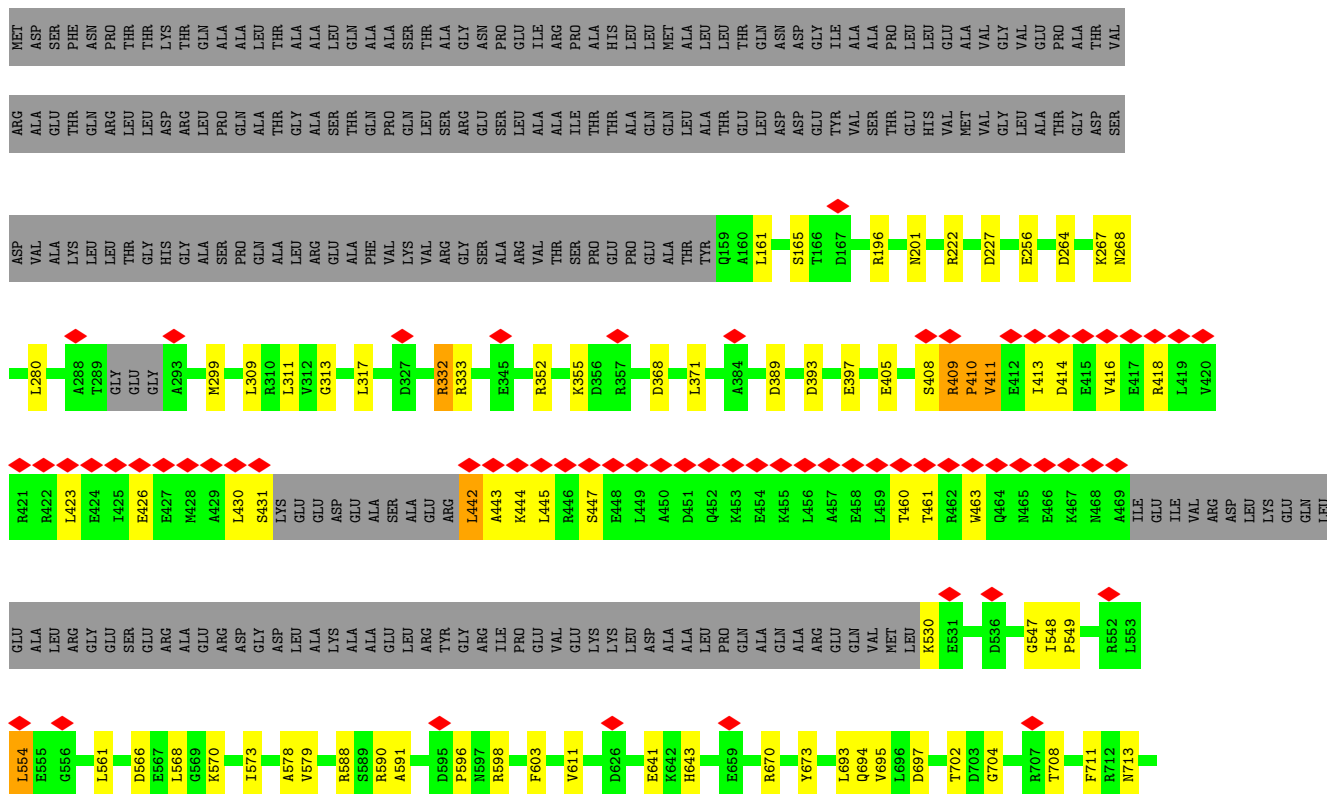
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	A	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	B	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	B	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	C	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	C	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	D	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	D	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
3	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

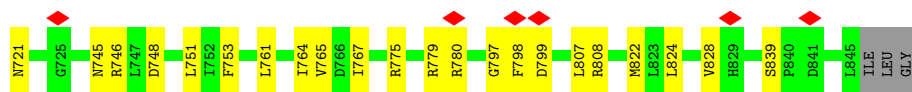
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



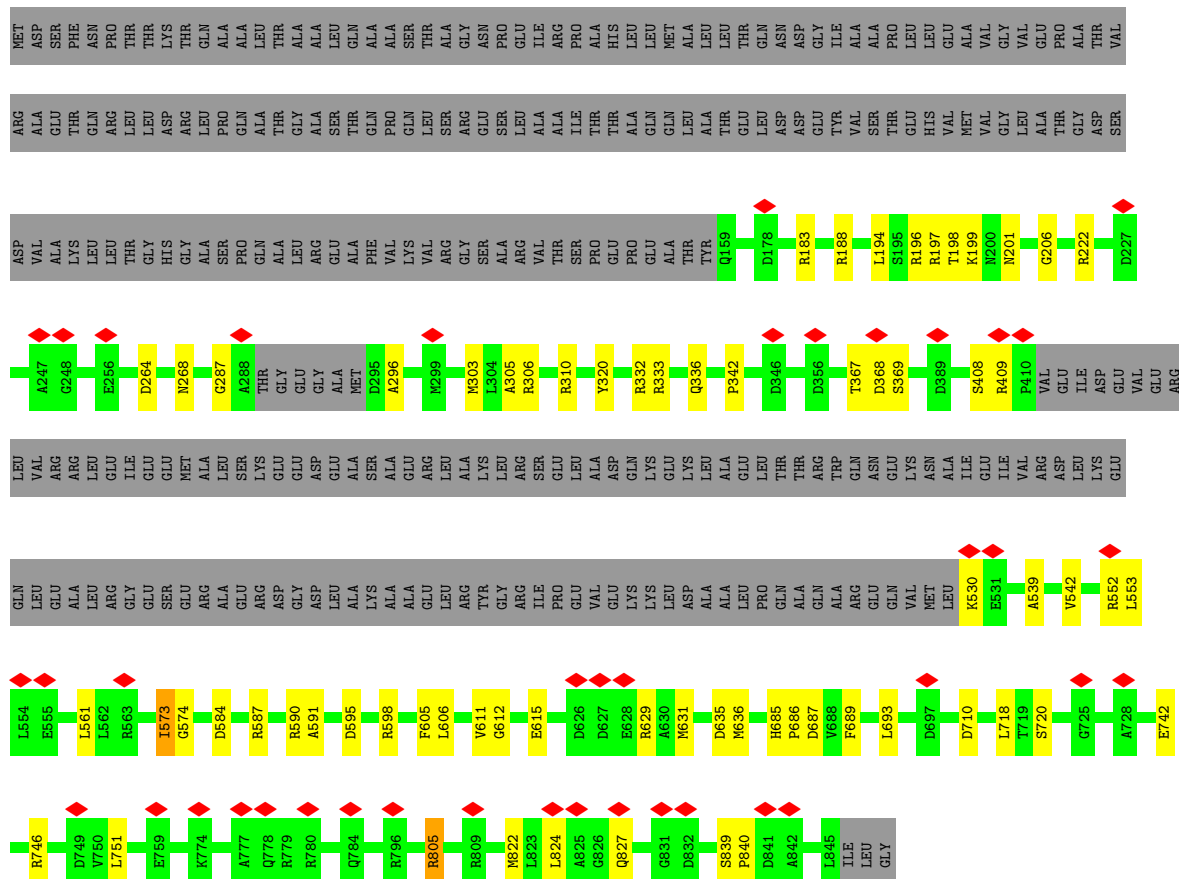
Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total 27	C 10	N 5	O 10	P 2	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0



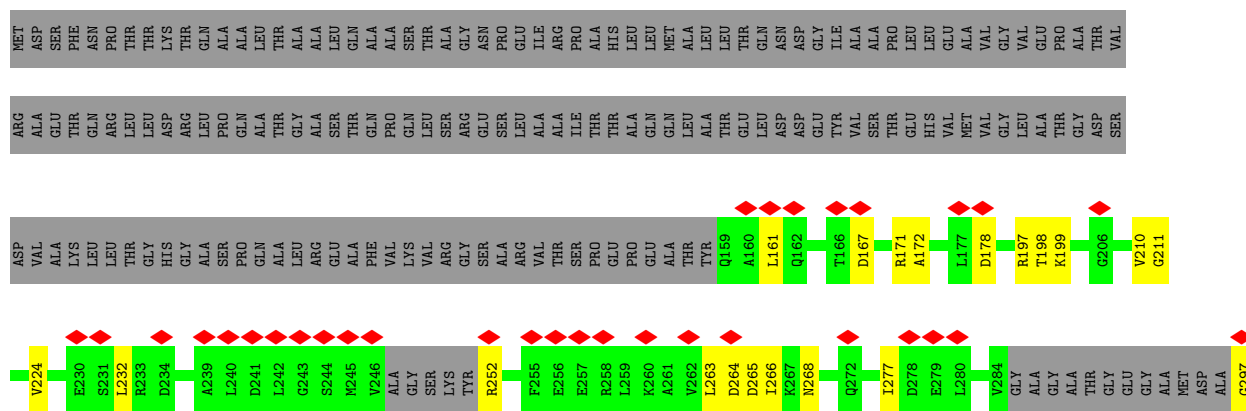


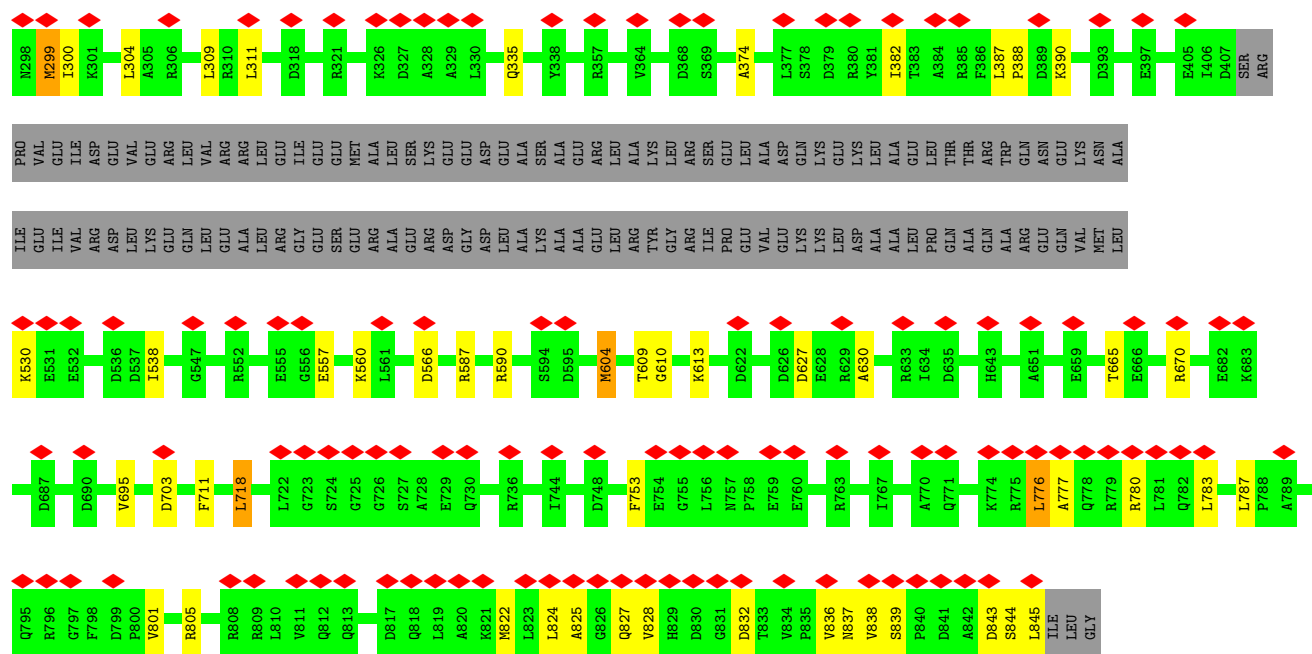


• Molecule 1: Chaperone protein ClpB

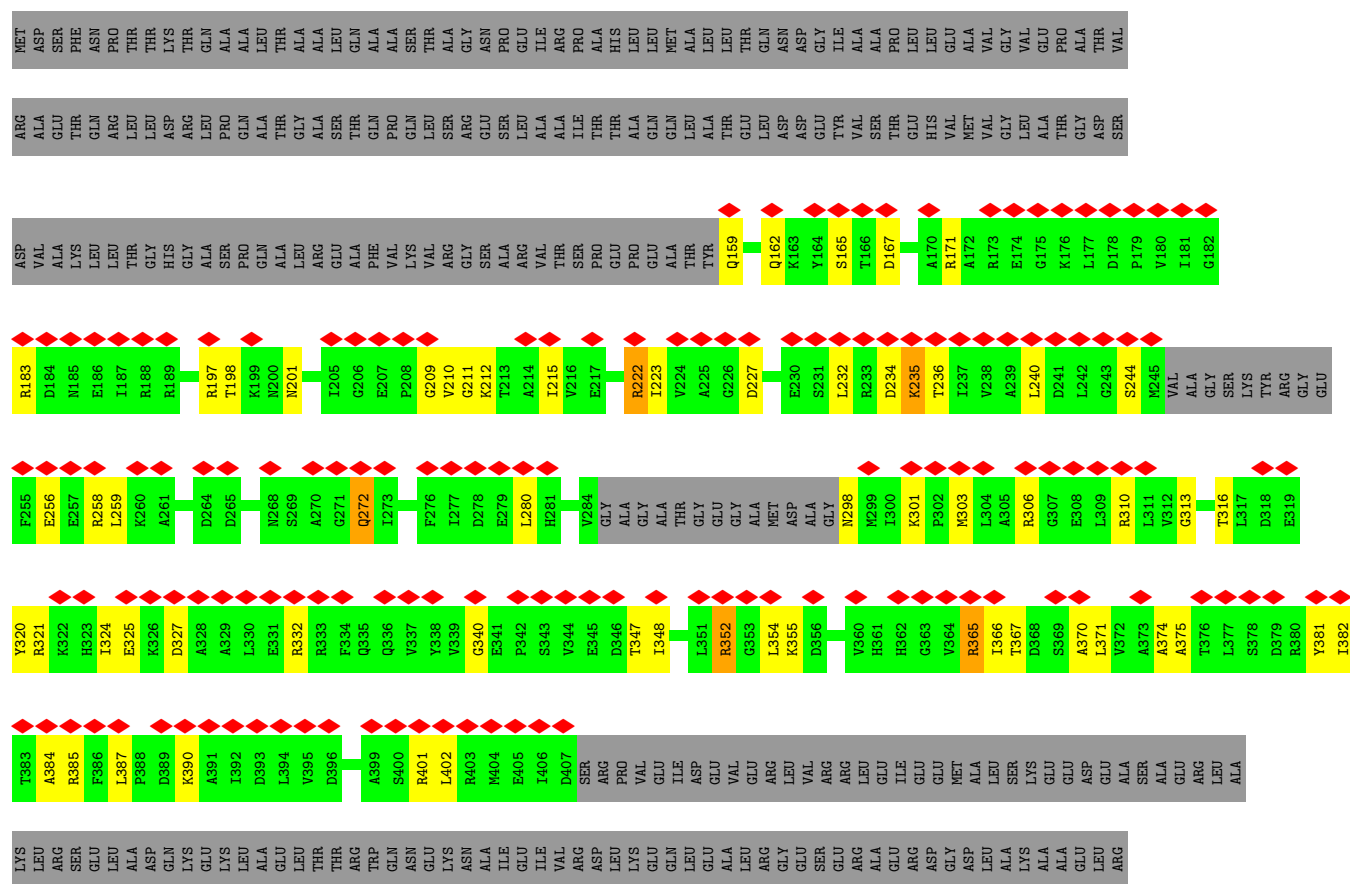
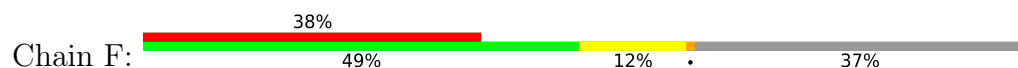


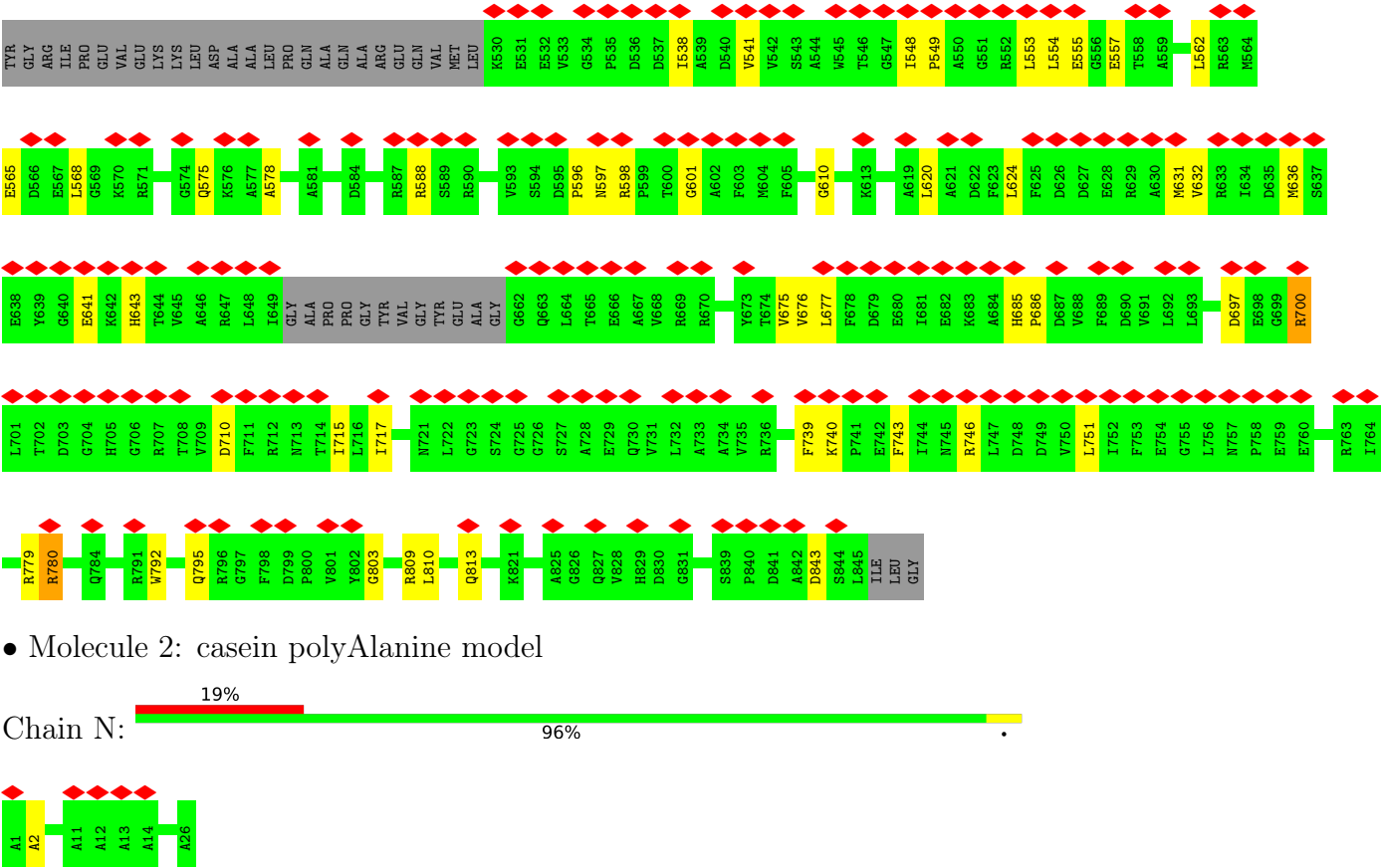
• Molecule 1: Chaperone protein ClpB





• Molecule 1: Chaperone protein ClpB





• Molecule 2: casein polyAlanine model

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size ( $\text{\AA}$ )	313.608, 313.608, 313.608	wwPDB
Map dimensions	292, 292, 292	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.074, 1.074, 1.074	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.39	3/4709 (0.1%)	0.58	0/6356
1	B	0.42	3/4717 (0.1%)	0.62	1/6367 (0.0%)
1	C	0.43	3/4734 (0.1%)	0.62	2/6391 (0.0%)
1	D	0.37	1/4380 (0.0%)	0.65	4/5914 (0.1%)
1	E	0.31	0/4286	0.64	4/5786 (0.1%)
1	F	0.31	0/4166	0.66	3/5621 (0.1%)
2	N	0.28	0/129	0.59	0/179
All	All	0.38	10/27121 (0.0%)	0.63	14/36614 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	5
All	All	0	11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	SER	CB-OG	8.84	1.53	1.42
1	C	447	SER	CB-OG	8.79	1.53	1.42
1	A	447	SER	CB-OG	8.77	1.53	1.42
1	C	431	SER	CB-OG	7.97	1.52	1.42
1	B	431	SER	CB-OG	7.96	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	SER	CB-OG	7.90	1.52	1.42
1	D	206	GLY	C-N	-5.69	1.21	1.34
1	C	460	THR	CB-OG1	5.18	1.53	1.43
1	A	460	THR	CB-OG1	5.14	1.53	1.43
1	B	460	THR	CB-OG1	5.14	1.53	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	573	ILE	CB-CA-C	-9.45	92.71	111.60
1	D	574	GLY	N-CA-C	-9.06	90.44	113.10
1	D	718	LEU	CA-CB-CG	6.51	130.28	115.30
1	F	354	LEU	CA-CB-CG	6.10	129.32	115.30
1	D	573	ILE	N-CA-C	6.07	127.39	111.00
1	C	799	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	787	LEU	CA-CB-CG	5.91	128.89	115.30
1	C	798	PHE	C-N-CA	5.81	136.22	121.70
1	E	776	LEU	CA-CB-CG	5.80	128.65	115.30
1	E	718	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	799	ASP	CB-CG-OD1	5.49	123.24	118.30
1	F	562	LEU	CA-CB-CG	5.23	127.33	115.30
1	F	780	ARG	CA-CB-CG	5.08	124.57	113.40
1	E	232	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	PRO	Peptide
1	A	798	PHE	Peptide
1	B	387	LEU	Peptide
1	C	839	SER	Peptide
1	D	839	SER	Peptide
1	E	839	SER	Peptide
1	F	548	ILE	Peptide
1	F	553	LEU	Peptide
1	F	555	GLU	Peptide
1	F	596	PRO	Peptide
1	F	740	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4649	0	4654	54	0
1	B	4657	0	4658	67	0
1	C	4674	0	4672	69	0
1	D	4321	0	4377	63	0
1	E	4230	0	4292	39	0
1	F	4115	0	4188	61	0
2	N	130	0	132	1	0
3	A	62	0	24	10	0
3	B	62	0	24	5	0
3	C	62	0	24	9	0
3	D	62	0	24	10	0
3	E	31	0	12	3	0
3	F	31	0	12	3	0
4	E	27	0	12	2	0
4	F	27	0	12	8	0
All	All	27140	0	27117	330	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:GLY:HA2	3:D:902:AGS:O2A	1.32	1.27
1:F:211:GLY:HA2	4:F:902:ADP:O2A	1.52	1.08
1:D:573:ILE:O	1:D:573:ILE:CG2	1.96	0.99
1:D:573:ILE:O	1:D:573:ILE:HG22	1.18	0.98
3:C:902:AGS:S1G	1:D:333:ARG:NH1	2.37	0.97
3:C:902:AGS:S1G	1:D:333:ARG:CZ	2.56	0.93
1:B:430:LEU:CD2	1:C:368:ASP:OD2	2.19	0.90
1:B:412:GLU:O	1:B:415:GLU:N	2.03	0.90
1:A:426:GLU:HG2	1:A:445:LEU:HD21	1.55	0.88
3:A:902:AGS:S1G	1:B:746:ARG:NH2	2.47	0.88
1:F:211:GLY:CA	4:F:902:ADP:O2A	2.22	0.85
1:B:430:LEU:HD22	1:C:368:ASP:OD2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:O	1:A:415:GLU:N	2.09	0.84
1:D:612:GLY:CA	3:D:902:AGS:O2A	2.23	0.83
1:D:805:ARG:NH2	3:D:902:AGS:S1G	2.52	0.82
3:A:901:AGS:S1G	1:B:333:ARG:NH2	2.53	0.81
1:F:211:GLY:HA2	4:F:902:ADP:PA	2.20	0.81
1:C:430:LEU:HD21	1:D:368:ASP:OD2	1.80	0.80
3:A:902:AGS:S1G	1:B:746:ARG:NE	2.56	0.79
1:B:412:GLU:O	1:B:414:ASP:N	2.17	0.78
1:A:430:LEU:CD2	1:B:368:ASP:OD2	2.33	0.77
1:C:430:LEU:CD2	1:D:368:ASP:OD2	2.35	0.75
1:D:805:ARG:HG3	1:D:805:ARG:HH11	1.50	0.75
3:A:901:AGS:S1G	1:B:333:ARG:CZ	2.75	0.75
1:D:612:GLY:HA2	3:D:902:AGS:PA	2.28	0.73
3:A:902:AGS:S1G	1:B:746:ARG:CZ	2.79	0.70
4:F:902:ADP:H2'	4:F:902:ADP:N3	2.05	0.70
1:B:808:ARG:HH12	1:C:598:ARG:HH22	1.40	0.69
1:C:549:PRO:HG2	1:C:590:ARG:HH12	1.58	0.68
1:D:264:ASP:O	1:D:268:ASN:HB2	1.94	0.68
1:A:430:LEU:HD21	1:B:368:ASP:OD2	1.93	0.67
1:F:610:GLY:HA3	1:F:803:GLY:HA3	1.74	0.67
1:F:210:VAL:N	4:F:902:ADP:O2B	2.27	0.67
3:B:901:AGS:S1G	1:C:333:ARG:NH1	2.67	0.66
1:D:805:ARG:CZ	3:D:902:AGS:S1G	2.84	0.66
1:A:426:GLU:CG	1:A:445:LEU:HD21	2.26	0.64
3:C:902:AGS:S1G	1:D:333:ARG:NH2	2.71	0.64
1:A:426:GLU:CG	1:A:445:LEU:CD2	2.76	0.64
1:D:822:MET:SD	1:D:827:GLN:NE2	2.71	0.63
1:E:557:GLU:HG3	1:E:590:ARG:HD3	1.81	0.63
1:A:426:GLU:HG2	1:A:445:LEU:CD2	2.27	0.63
3:A:901:AGS:S1G	1:B:332:ARG:NH2	2.72	0.63
1:F:381:TYR:HB3	1:F:385:ARG:HH12	1.64	0.62
1:D:595:ASP:H	1:D:598:ARG:HH21	1.47	0.62
1:B:822:MET:SD	1:B:827:GLN:NE2	2.72	0.62
1:A:412:GLU:O	1:A:414:ASP:N	2.33	0.62
1:B:605:PHE:HB3	1:B:751:LEU:HB2	1.82	0.62
3:C:902:AGS:S1G	1:D:332:ARG:NH1	2.73	0.62
1:E:560:LYS:HB2	1:E:590:ARG:HH12	1.64	0.62
1:F:641:GLU:HG2	1:F:643:HIS:H	1.65	0.62
1:D:605:PHE:HB3	1:D:751:LEU:HB2	1.81	0.61
1:A:426:GLU:CD	1:A:445:LEU:HD22	2.22	0.60
1:B:306:ARG:HH21	1:B:308:GLU:HG3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG21	1:A:283:ILE:HD11	1.84	0.60
1:B:377:LEU:HD21	1:B:542:VAL:HG11	1.83	0.60
1:E:828:VAL:HG23	1:E:832:ASP:HB3	1.82	0.60
1:F:183:ARG:NH2	1:F:340:GLY:O	2.35	0.60
1:B:333:ARG:HH21	1:B:333:ARG:CG	2.14	0.59
1:D:693:LEU:O	1:D:746:ARG:NH1	2.35	0.59
1:E:777:ALA:O	1:E:780:ARG:NH1	2.33	0.59
1:A:252:ARG:HD2	2:N:2:ALA:HB3	1.83	0.59
1:B:412:GLU:O	1:B:413:ILE:C	2.40	0.59
1:E:627:ASP:HB2	1:E:630:ALA:HB2	1.85	0.58
1:D:805:ARG:HH11	1:D:805:ARG:CG	2.14	0.58
1:C:409:ARG:HD3	1:C:414:ASP:CG	2.23	0.58
1:E:776:LEU:HD21	1:E:783:LEU:HD11	1.85	0.57
1:B:693:LEU:HD21	1:B:746:ARG:HH22	1.68	0.57
1:E:805:ARG:NH2	4:E:902:ADP:O1B	2.37	0.57
1:C:408:SER:O	1:C:463:TRP:CZ2	2.58	0.57
1:B:367:THR:HG22	1:B:369:SER:H	1.69	0.57
1:F:675:VAL:HG23	1:F:715:ILE:HB	1.86	0.57
1:A:745:ASN:O	1:F:809:ARG:NH1	2.38	0.56
1:A:817:ASP:OD1	1:B:588:ARG:NH2	2.36	0.56
1:C:414:ASP:CB	1:D:188:ARG:HH12	2.18	0.56
1:A:603:PHE:HB3	1:A:748:ASP:HB2	1.87	0.56
3:B:902:AGS:O1B	3:B:902:AGS:O2G	2.23	0.56
1:D:303:MET:SD	1:D:306:ARG:NH2	2.79	0.56
1:C:590:ARG:NH2	1:C:673:TYR:OH	2.39	0.56
1:D:320:TYR:OH	1:D:336:GLN:NE2	2.39	0.56
1:B:393:ASP:OD1	1:C:196:ARG:NH2	2.35	0.56
1:B:178:ASP:OD1	1:B:357:ARG:NH2	2.39	0.55
3:A:901:AGS:S1G	1:B:333:ARG:NH1	2.79	0.55
1:E:822:MET:HA	1:E:825:ALA:HB3	1.89	0.55
1:F:159:GLN:O	1:F:162:GLN:NE2	2.39	0.55
1:A:412:GLU:O	1:A:413:ILE:C	2.45	0.55
1:C:721:ASN:ND2	1:D:742:GLU:OE1	2.40	0.55
1:D:305:ALA:CB	1:D:333:ARG:HH21	2.19	0.55
3:A:902:AGS:O1B	3:A:902:AGS:O2G	2.25	0.55
1:A:408:SER:OG	1:A:409:ARG:NH1	2.40	0.55
1:A:573:ILE:HD11	1:A:767:ILE:HD12	1.89	0.54
1:A:638:GLU:OE2	1:B:694:GLN:NE2	2.40	0.54
3:C:902:AGS:O2G	3:C:902:AGS:O1B	2.25	0.54
1:E:665:THR:HG21	1:E:703:ASP:HB3	1.89	0.54
1:F:209:GLY:N	4:F:902:ADP:O2B	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD23	1:C:313:GLY:HA3	1.89	0.54
1:F:385:ARG:HD3	1:F:390:LYS:HB3	1.90	0.54
1:E:264:ASP:OD1	1:E:268:ASN:ND2	2.41	0.54
1:B:426:GLU:OE2	1:C:352:ARG:NH1	2.41	0.54
1:B:647:ARG:HH12	1:C:704:GLY:HA2	1.72	0.54
1:C:775:ARG:NH2	1:D:595:ASP:OD1	2.40	0.54
1:E:263:LEU:HA	1:E:266:ILE:HD12	1.90	0.53
1:F:256:GLU:HG2	1:F:259:LEU:HD22	1.91	0.53
1:E:557:GLU:O	1:E:590:ARG:NH1	2.41	0.53
1:A:351:LEU:HB3	1:A:371:LEU:HD22	1.91	0.53
1:C:693:LEU:O	1:C:746:ARG:NH1	2.42	0.53
1:D:595:ASP:HB2	1:D:598:ARG:HE	1.73	0.53
1:C:702:THR:HG22	1:C:708:THR:HG22	1.91	0.53
1:F:402:LEU:HD11	1:F:538:ILE:HG22	1.91	0.52
1:A:702:THR:HG22	1:A:708:THR:HG22	1.92	0.52
1:B:695:VAL:HG13	1:B:711:PHE:HD2	1.75	0.52
3:C:901:AGS:O1B	3:C:901:AGS:O2G	2.26	0.52
1:F:232:LEU:HD12	1:F:235:LYS:HG3	1.91	0.52
1:F:316:THR:O	1:F:320:TYR:N	2.42	0.52
1:A:397:GLU:OE2	1:B:196:ARG:NH1	2.42	0.52
1:F:575:GLN:HB3	1:F:578:ALA:HB3	1.92	0.52
1:B:547:GLY:HA3	1:B:671:ARG:HH21	1.75	0.52
1:E:838:VAL:HA	1:E:843:ASP:HA	1.92	0.52
1:A:571:ARG:NH1	1:A:618:LYS:O	2.43	0.52
1:C:561:LEU:HD21	1:C:590:ARG:HG3	1.92	0.52
1:C:611:VAL:HG11	1:C:753:PHE:HB3	1.92	0.51
1:D:805:ARG:CG	1:D:805:ARG:NH1	2.73	0.51
1:C:414:ASP:HB3	1:D:188:ARG:HH12	1.76	0.51
1:C:548:ILE:HD13	1:C:713:ASN:HD21	1.75	0.51
1:D:805:ARG:NH1	3:D:902:AGS:S1G	2.84	0.51
1:A:308:GLU:O	1:A:310:ARG:NH1	2.43	0.51
1:A:660:ALA:O	1:B:321:ARG:NH2	2.43	0.51
1:B:646:ALA:HA	1:B:649:ILE:HG22	1.92	0.51
1:B:779:ARG:HH12	1:B:823:LEU:HD21	1.74	0.51
1:C:389:ASP:OD2	1:D:332:ARG:NE	2.38	0.51
1:D:584:ASP:OD1	1:D:587:ARG:NH2	2.44	0.51
1:B:333:ARG:HH21	1:B:333:ARG:HG3	1.76	0.51
1:F:244:SER:O	1:F:258:ARG:NH2	2.43	0.51
1:C:409:ARG:HD3	1:C:414:ASP:OD1	2.10	0.51
1:F:601:GLY:HA3	1:F:715:ILE:HG12	1.91	0.51
1:F:236:THR:OG1	1:F:272:GLN:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:901:AGS:O2G	3:B:901:AGS:O1B	2.29	0.51
1:B:333:ARG:NH2	1:B:333:ARG:CG	2.73	0.50
1:D:824:LEU:HD21	1:E:587:ARG:HG2	1.93	0.50
1:B:799:ASP:O	1:B:801:VAL:N	2.39	0.50
1:D:287:GLY:HA2	1:D:296:ALA:HB3	1.93	0.50
1:F:324:ILE:HD12	1:F:327:ASP:HB3	1.93	0.50
1:A:192:GLN:HE22	1:F:401:ARG:HD2	1.77	0.50
3:A:901:AGS:O2G	3:A:901:AGS:O1B	2.28	0.50
1:C:264:ASP:OD1	1:C:267:LYS:NZ	2.44	0.50
1:C:410:PRO:HD2	1:C:413:ILE:HD12	1.92	0.50
1:C:697:ASP:HB2	1:C:746:ARG:HD2	1.93	0.50
3:B:901:AGS:O2A	3:B:901:AGS:O2B	2.30	0.50
1:F:167:ASP:O	1:F:171:ARG:NH1	2.45	0.50
1:E:304:LEU:HD12	1:E:309:LEU:HD21	1.93	0.50
1:F:165:SER:HB3	1:F:240:LEU:HD13	1.93	0.50
1:D:553:LEU:HD21	1:D:590:ARG:HG2	1.94	0.50
1:F:280:LEU:HD23	1:F:313:GLY:HA3	1.92	0.50
1:A:426:GLU:CD	1:A:445:LEU:CD2	2.81	0.49
1:E:210:VAL:HA	1:E:388:PRO:HG2	1.95	0.49
1:F:347:THR:HG21	1:F:387:LEU:HG	1.93	0.49
1:B:332:ARG:NH2	1:B:333:ARG:HH22	2.09	0.49
1:B:423:LEU:HB3	1:B:445:LEU:HD11	1.95	0.49
3:C:901:AGS:S1G	1:D:746:ARG:NH2	2.79	0.49
1:F:370:ALA:O	1:F:374:ALA:HB2	2.11	0.49
1:C:423:LEU:HB3	1:C:445:LEU:HD11	1.94	0.49
1:E:613:LYS:HA	1:E:753:PHE:HE2	1.78	0.49
1:B:761:LEU:HD12	1:B:764:ILE:HD12	1.94	0.49
1:C:309:LEU:HD12	1:C:311:LEU:HB2	1.95	0.49
1:E:167:ASP:H	1:E:171:ARG:HH12	1.60	0.49
1:E:297:GLY:N	1:E:299:MET:SD	2.86	0.49
1:F:352:ARG:HA	1:F:355:LYS:HE3	1.95	0.49
1:A:426:GLU:CG	1:A:427:GLU:N	2.75	0.48
1:F:365:ARG:NH1	1:F:366:ILE:O	2.46	0.48
1:A:566:ASP:O	1:A:570:LYS:NZ	2.37	0.48
1:B:681:ILE:HG12	1:B:689:PHE:HE1	1.77	0.48
1:A:625:PHE:HZ	1:A:674:THR:HA	1.79	0.48
1:D:201:ASN:OD1	1:D:201:ASN:N	2.43	0.48
1:E:836:VAL:HA	1:E:845:LEU:HA	1.95	0.48
1:C:566:ASP:O	1:C:570:LYS:NZ	2.45	0.48
1:F:598:ARG:NH2	1:F:746:ARG:O	2.45	0.48
1:F:197:ARG:HD3	1:F:198:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:MET:HG2	1:F:306:ARG:HH12	1.79	0.48
1:C:201:ASN:N	1:C:201:ASN:OD1	2.47	0.48
1:C:695:VAL:HG13	1:C:711:PHE:HD2	1.79	0.47
1:E:387:LEU:HA	1:E:390:LYS:HE2	1.96	0.47
3:F:901:AGS:O2G	3:F:901:AGS:O2A	2.32	0.47
1:C:603:PHE:HB3	1:C:748:ASP:HB2	1.96	0.47
1:B:383:THR:OG1	1:B:710:ASP:OD2	2.32	0.47
1:E:695:VAL:HG13	1:E:711:PHE:HD2	1.78	0.47
1:F:256:GLU:HA	1:F:259:LEU:HD13	1.97	0.47
1:A:263:LEU:HD23	1:A:266:ILE:HD12	1.97	0.47
1:A:410:PRO:O	1:A:414:ASP:OD2	2.33	0.47
1:B:412:GLU:C	1:B:414:ASP:N	2.67	0.47
3:C:902:AGS:O2A	3:C:902:AGS:O2B	2.32	0.47
1:A:423:LEU:HB3	1:A:445:LEU:HD11	1.94	0.47
1:F:697:ASP:HB2	1:F:746:ARG:HH21	1.78	0.47
1:C:765:VAL:HG22	1:C:807:LEU:HD21	1.97	0.47
3:A:902:AGS:O2A	3:A:902:AGS:O2B	2.33	0.47
1:B:670:ARG:HG2	1:C:317:LEU:HD21	1.97	0.47
1:D:183:ARG:HH22	1:D:342:PRO:HD3	1.80	0.47
1:D:685:HIS:O	1:D:687:ASP:N	2.46	0.47
1:E:300:ILE:O	1:E:304:LEU:N	2.48	0.47
3:B:902:AGS:O2B	3:B:902:AGS:O2A	2.33	0.47
1:C:808:ARG:HH22	1:D:598:ARG:HD3	1.80	0.47
1:E:161:LEU:HB2	1:E:265:ASP:HB2	1.96	0.47
1:B:389:ASP:OD2	1:C:332:ARG:NH2	2.48	0.46
1:B:817:ASP:OD1	1:C:588:ARG:NH2	2.48	0.46
1:C:393:ASP:OD1	1:D:199:LYS:NZ	2.42	0.46
1:D:408:SER:O	1:D:409:ARG:NE	2.42	0.46
1:F:402:LEU:HG	1:F:541:VAL:HG11	1.97	0.46
1:A:280:LEU:HD23	1:A:313:GLY:HA3	1.98	0.46
1:D:561:LEU:HG	1:D:587:ARG:HG2	1.97	0.46
1:A:796:ARG:HE	1:A:810:LEU:HD11	1.81	0.46
1:F:212:LYS:HA	1:F:215:ILE:HD12	1.97	0.46
1:A:646:ALA:HA	1:A:649:ILE:HG22	1.96	0.46
1:D:805:ARG:HA	1:D:805:ARG:HD3	1.51	0.46
1:E:197:ARG:HG3	1:E:198:THR:HG23	1.97	0.46
1:F:620:LEU:HB2	1:F:624:LEU:HD23	1.98	0.46
1:A:713:ASN:OD1	1:A:713:ASN:N	2.47	0.46
1:E:199:LYS:HG2	1:E:335:GLN:HE21	1.81	0.46
1:E:382:ILE:HB	1:E:390:LYS:HD2	1.98	0.46
1:F:321:ARG:O	1:F:325:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:NH1	1:B:184:ASP:OD1	2.48	0.46
1:B:823:LEU:HD23	1:C:591:ALA:HB1	1.98	0.46
1:C:761:LEU:HD12	1:C:764:ILE:HD12	1.97	0.46
1:E:604:MET:HB2	1:E:718:LEU:HB2	1.98	0.46
1:C:418:ARG:CZ	1:D:222:ARG:HH12	2.27	0.46
3:C:901:AGS:O2B	3:C:901:AGS:O2A	2.34	0.46
1:F:385:ARG:HB2	1:F:390:LYS:HG3	1.98	0.46
1:C:824:LEU:HD23	1:D:591:ALA:HB2	1.97	0.45
1:A:549:PRO:HB2	1:A:590:ARG:HH12	1.80	0.45
1:D:197:ARG:HG2	1:D:198:THR:HG23	1.98	0.45
1:F:382:ILE:HG13	1:F:384:ALA:H	1.81	0.45
1:B:638:GLU:OE2	1:C:694:GLN:NE2	2.50	0.45
1:C:222:ARG:HG3	1:C:227:ASP:HB2	1.98	0.45
1:F:223:ILE:HG23	1:F:234:ASP:HA	1.98	0.45
1:C:822:MET:HG3	1:C:828:VAL:HG21	1.98	0.45
1:E:609:THR:OG1	1:E:801:VAL:O	2.35	0.45
1:F:843:ASP:N	1:F:843:ASP:OD1	2.49	0.45
3:F:901:AGS:O2G	3:F:901:AGS:O1B	2.35	0.45
1:F:792:TRP:HA	1:F:795:GLN:HE22	1.82	0.45
1:A:605:PHE:HB3	1:A:751:LEU:HB2	1.98	0.45
1:F:201:ASN:ND2	1:F:310:ARG:O	2.50	0.45
1:E:374:ALA:HB2	1:E:538:ILE:HD13	1.98	0.44
1:F:565:GLU:HA	1:F:568:LEU:HB3	1.99	0.44
1:C:405:GLU:OE2	1:C:411:VAL:CG1	2.66	0.44
1:A:412:GLU:C	1:A:414:ASP:N	2.70	0.44
1:C:256:GLU:HG3	1:C:299:MET:HE1	1.99	0.44
1:C:554:LEU:H	1:C:554:LEU:HG	1.68	0.44
1:B:426:GLU:O	1:B:430:LEU:HG	2.18	0.44
1:D:305:ALA:HB3	1:D:333:ARG:NH2	2.33	0.44
1:D:367:THR:HG22	1:D:369:SER:H	1.83	0.44
1:D:573:ILE:N	3:D:902:AGS:N1	2.66	0.43
1:E:837:ASN:O	1:E:844:SER:N	2.51	0.43
1:A:409:ARG:HG3	1:A:463:TRP:HH2	1.82	0.43
1:E:172:ALA:HB1	1:E:224:VAL:HG21	1.98	0.43
1:E:277:ILE:HD12	1:E:311:LEU:HD21	2.00	0.43
1:F:211:GLY:HA2	4:F:902:ADP:O5'	2.18	0.43
3:D:901:AGS:O2G	3:D:901:AGS:O1B	2.36	0.43
1:F:677:LEU:HD23	1:F:717:ILE:HB	1.99	0.43
1:A:426:GLU:O	1:A:430:LEU:HG	2.18	0.43
1:C:161:LEU:O	1:C:165:SER:OG	2.25	0.43
1:B:201:ASN:OD1	1:B:201:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:GLU:HG3	1:C:643:HIS:CE1	2.53	0.43
1:F:810:LEU:HA	1:F:813:GLN:HB2	2.00	0.43
1:C:426:GLU:O	1:C:430:LEU:HG	2.18	0.43
1:E:610:GLY:N	4:E:902:ADP:O2B	2.45	0.43
1:F:211:GLY:CA	4:F:902:ADP:PA	2.99	0.43
1:C:264:ASP:O	1:C:268:ASN:HB2	2.18	0.43
1:D:686:PRO:HA	1:D:689:PHE:HD2	1.84	0.43
1:B:443:ALA:O	1:B:445:LEU:N	2.52	0.42
1:B:713:ASN:OD1	1:B:713:ASN:N	2.52	0.42
1:C:393:ASP:HA	1:D:196:ARG:HH22	1.84	0.42
1:E:304:LEU:HA	1:E:309:LEU:HD21	1.99	0.42
1:A:351:LEU:HD11	1:A:391:ALA:HB1	2.01	0.42
1:C:409:ARG:HD3	1:C:414:ASP:OD2	2.20	0.42
1:D:305:ALA:HB3	1:D:333:ARG:HH21	1.84	0.42
1:D:606:LEU:HB3	1:D:720:SER:HB3	2.01	0.42
1:B:430:LEU:HD13	1:B:442:LEU:HD12	2.02	0.42
1:C:761:LEU:HD21	1:C:797:GLY:HA3	2.00	0.42
1:D:611:VAL:O	3:D:902:AGS:N7	2.52	0.42
1:F:632:VAL:HG13	1:F:676:VAL:HG23	2.02	0.42
1:A:426:GLU:HG2	1:A:427:GLU:N	2.34	0.42
1:A:843:ASP:OD1	1:A:843:ASP:N	2.53	0.42
1:C:408:SER:O	1:C:463:TRP:HZ2	2.00	0.42
1:C:443:ALA:O	1:C:445:LEU:N	2.52	0.42
1:D:710:ASP:OD1	1:D:710:ASP:N	2.53	0.42
1:A:423:LEU:HD22	1:A:445:LEU:HD11	2.02	0.42
1:A:443:ALA:O	1:A:445:LEU:N	2.52	0.42
1:F:578:ALA:HA	1:F:751:LEU:HD13	2.00	0.42
1:A:430:LEU:HD13	1:A:442:LEU:HD12	2.02	0.42
1:B:426:GLU:CD	1:B:445:LEU:HD22	2.40	0.42
1:C:355:LYS:HD3	1:C:371:LEU:HD11	2.01	0.42
1:C:423:LEU:HD22	1:C:445:LEU:HD11	2.02	0.42
1:F:348:ILE:HG12	1:F:375:ALA:HB3	2.02	0.42
1:D:635:ASP:OD1	1:D:636:MET:N	2.53	0.42
1:F:401:ARG:HB3	1:F:541:VAL:HG13	2.01	0.42
1:B:426:GLU:HG2	1:B:427:GLU:N	2.34	0.42
1:D:615:GLU:HG3	3:D:902:AGS:H2'	2.01	0.42
1:D:539:ALA:HA	1:D:542:VAL:HG12	2.01	0.41
1:A:201:ASN:HD21	1:A:304:LEU:HD22	1.85	0.41
1:A:685:HIS:HA	1:A:686:PRO:HD3	1.92	0.41
1:B:805:ARG:HD3	1:C:745:ASN:ND2	2.35	0.41
1:E:178:ASP:OD2	3:E:901:AGS:O2'	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:VAL:N	3:E:901:AGS:O2B	2.53	0.41
1:E:824:LEU:HD22	1:F:557:GLU:HB3	2.02	0.41
1:C:397:GLU:OE2	1:D:196:ARG:NH1	2.53	0.41
1:F:700:ARG:HB2	1:F:710:ASP:HA	2.02	0.41
1:F:739:PHE:HB3	1:F:743:PHE:HB2	2.02	0.41
1:C:568:LEU:HD23	1:C:579:VAL:HG13	2.03	0.41
1:F:367:THR:O	1:F:371:LEU:N	2.52	0.41
1:B:551:GLY:H	1:B:590:ARG:HH12	1.68	0.41
1:B:693:LEU:HD23	1:B:746:ARG:HH12	1.86	0.41
1:D:305:ALA:HB2	1:D:333:ARG:HH21	1.85	0.41
1:A:611:VAL:HG11	1:A:753:PHE:HB3	2.03	0.41
1:A:710:ASP:HB2	1:A:712:ARG:HG3	2.02	0.41
1:F:222:ARG:HE	1:F:227:ASP:HB3	1.86	0.41
1:B:332:ARG:NH2	1:B:333:ARG:NH2	2.69	0.41
1:B:423:LEU:HD22	1:B:445:LEU:HD11	2.02	0.41
1:B:582:VAL:HG11	1:B:620:LEU:HD22	2.03	0.41
1:C:418:ARG:NH1	1:D:222:ARG:HH12	2.19	0.41
1:C:578:ALA:HB1	1:C:751:LEU:HD13	2.02	0.41
1:D:194:LEU:HD11	1:D:310:ARG:HB3	2.01	0.41
1:C:430:LEU:HD13	1:C:442:LEU:HD12	2.02	0.41
1:A:549:PRO:HB2	1:A:590:ARG:NH1	2.36	0.40
1:B:775:ARG:HE	1:C:596:PRO:HD3	1.86	0.40
1:C:573:ILE:HD11	1:C:767:ILE:HD12	2.04	0.40
1:E:211:GLY:N	3:E:901:AGS:O2B	2.54	0.40
1:F:298:ASN:HA	1:F:301:LYS:HE3	2.04	0.40
1:B:553:LEU:HG	1:B:590:ARG:HH21	1.86	0.40
1:F:685:HIS:HA	1:F:686:PRO:HD3	1.90	0.40
1:B:693:LEU:HD21	1:B:746:ARG:NH2	2.36	0.40
1:B:693:LEU:CD2	1:B:746:ARG:HH12	2.35	0.40
1:A:746:ARG:NH2	3:F:901:AGS:S1G	2.95	0.40
1:B:678:PHE:HE2	1:B:716:LEU:HD22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	602/848 (71%)	524 (87%)	74 (12%)	4 (1%)	22	60
1	B	603/848 (71%)	527 (87%)	70 (12%)	6 (1%)	15	52
1	C	606/848 (72%)	523 (86%)	80 (13%)	3 (0%)	29	66
1	D	556/848 (66%)	480 (86%)	75 (14%)	1 (0%)	47	79
1	E	540/848 (64%)	460 (85%)	79 (15%)	1 (0%)	47	79
1	F	521/848 (61%)	448 (86%)	69 (13%)	4 (1%)	19	57
2	N	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
All	All	3452/5114 (68%)	2983 (86%)	450 (13%)	19 (1%)	29	62

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ILE
1	B	387	LEU
1	B	413	ILE
1	F	554	LEU
1	B	388	PRO
1	C	410	PRO
1	C	547	GLY
1	F	597	ASN
1	A	412	GLU
1	B	410	PRO
1	E	566	ASP
1	F	235	LYS
1	A	444	LYS
1	B	412	GLU
1	B	444	LYS
1	C	444	LYS
1	F	549	PRO
1	A	411	VAL
1	D	840	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	478/682 (70%)	467 (98%)	11 (2%)	50	72
1	B	478/682 (70%)	470 (98%)	8 (2%)	60	78
1	C	479/682 (70%)	468 (98%)	11 (2%)	50	72
1	D	455/682 (67%)	450 (99%)	5 (1%)	73	85
1	E	448/682 (66%)	442 (99%)	6 (1%)	69	82
1	F	439/682 (64%)	428 (98%)	11 (2%)	47	70
All	All	2777/4092 (68%)	2725 (98%)	52 (2%)	59	76

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	LYS
1	A	416	VAL
1	A	418	ARG
1	A	426	GLU
1	A	442	LEU
1	A	461	THR
1	A	530	LYS
1	A	700	ARG
1	A	779	ARG
1	A	780	ARG
1	A	796	ARG
1	B	321	ARG
1	B	333	ARG
1	B	387	LEU
1	B	411	VAL
1	B	416	VAL
1	B	442	LEU
1	B	461	THR
1	B	530	LYS
1	C	332	ARG
1	C	409	ARG
1	C	411	VAL
1	C	416	VAL
1	C	442	LEU
1	C	461	THR
1	C	530	LYS
1	C	554	LEU

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Mol	Chain	Res	Type
1	C	670	ARG
1	C	779	ARG
1	C	780	ARG
1	D	530	LYS
1	D	552	ARG
1	D	629	ARG
1	D	631	MET
1	D	805	ARG
1	E	252	ARG
1	E	299	MET
1	E	530	LYS
1	E	604	MET
1	E	670	ARG
1	E	827	GLN
1	F	222	ARG
1	F	272	GLN
1	F	332	ARG
1	F	352	ARG
1	F	365	ARG
1	F	588	ARG
1	F	631	MET
1	F	636	MET
1	F	700	ARG
1	F	779	ARG
1	F	780	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	201	ASN
1	A	336	GLN
1	A	575	GLN
1	A	705	HIS
1	B	643	HIS
1	B	685	HIS
1	C	336	GLN
1	C	721	ASN
1	C	812	GLN
1	D	336	GLN
1	D	361	HIS
1	E	335	GLN

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Mol	Chain	Res	Type
1	E	575	GLN
1	F	162	GLN
1	F	201	ASN
1	F	575	GLN
1	F	705	HIS
1	F	795	GLN
1	F	818	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 ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ADP	E	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.66	6 (20%)
3	AGS	B	902	-	26,33,33	0.76	0	26,52,52	1.35	2 (7%)
3	AGS	B	901	-	26,33,33	0.71	0	26,52,52	1.37	2 (7%)
3	AGS	E	901	-	26,33,33	0.74	1 (3%)	26,52,52	1.27	2 (7%)
3	AGS	C	902	-	26,33,33	0.80	1 (3%)	26,52,52	1.33	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AGS	D	902	-	26,33,33	1.89	3 (11%)	26,52,52	1.59	4 (15%)
3	AGS	C	901	-	26,33,33	0.75	0	26,52,52	1.47	2 (7%)
3	AGS	A	901	-	26,33,33	0.75	0	26,52,52	1.29	2 (7%)
3	AGS	F	901	-	26,33,33	0.77	0	26,52,52	1.04	2 (7%)
3	AGS	A	902	-	26,33,33	0.78	0	26,52,52	1.46	2 (7%)
3	AGS	D	901	-	26,33,33	0.75	0	26,52,52	1.28	2 (7%)
4	ADP	F	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

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
4	ADP	E	902	-	-	2/12/32/32	0/3/3/3
3	AGS	B	902	-	-	3/17/38/38	0/3/3/3
3	AGS	B	901	-	-	4/17/38/38	0/3/3/3
3	AGS	E	901	-	-	2/17/38/38	0/3/3/3
3	AGS	C	902	-	-	7/17/38/38	0/3/3/3
3	AGS	D	902	-	-	2/17/38/38	0/3/3/3
3	AGS	C	901	-	-	4/17/38/38	0/3/3/3
3	AGS	A	901	-	-	8/17/38/38	0/3/3/3
3	AGS	F	901	-	-	8/17/38/38	0/3/3/3
3	AGS	A	902	-	-	2/17/38/38	0/3/3/3
3	AGS	D	901	-	-	7/17/38/38	0/3/3/3
4	ADP	F	902	-	-	1/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	AGS	PG-S1G	7.97	2.08	1.90
4	E	902	ADP	C5-C4	2.57	1.47	1.40
4	F	902	ADP	C5-C4	2.52	1.47	1.40
3	D	902	AGS	C5-C4	2.50	1.47	1.40
3	C	902	AGS	PG-S1G	2.17	1.95	1.90
3	E	901	AGS	PG-S1G	2.09	1.95	1.90
3	D	902	AGS	PG-O3G	-2.00	1.48	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	AGS	PA-O3A-PB	-6.38	110.93	132.83
3	A	902	AGS	PA-O3A-PB	-6.24	111.40	132.83
3	C	902	AGS	PA-O3A-PB	-5.73	113.16	132.83
3	B	901	AGS	PA-O3A-PB	-5.64	113.48	132.83
3	A	901	AGS	PA-O3A-PB	-5.46	114.11	132.83
3	D	901	AGS	PA-O3A-PB	-5.44	114.14	132.83
3	B	902	AGS	PA-O3A-PB	-5.35	114.46	132.83
3	E	901	AGS	PA-O3A-PB	-5.15	115.16	132.83
4	E	902	ADP	C3'-C2'-C1'	4.01	107.02	100.98
4	E	902	ADP	PA-O3A-PB	-3.87	119.56	132.83
3	F	901	AGS	PA-O3A-PB	-3.82	119.71	132.83
3	D	902	AGS	PA-O3A-PB	-3.60	120.48	132.83
4	F	902	ADP	PA-O3A-PB	-3.59	120.50	132.83
4	E	902	ADP	C1'-N9-C4	3.45	132.71	126.64
4	F	902	ADP	C3'-C2'-C1'	3.40	106.09	100.98
3	D	902	AGS	C3'-C2'-C1'	3.39	106.08	100.98
3	D	902	AGS	N3-C2-N1	-3.20	123.67	128.68
4	F	902	ADP	N3-C2-N1	-3.16	123.74	128.68
4	E	902	ADP	N3-C2-N1	-2.93	124.11	128.68
4	F	902	ADP	C4-C5-N7	-2.71	106.58	109.40
3	D	902	AGS	C4-C5-N7	-2.70	106.58	109.40
3	C	902	AGS	C5-C6-N6	2.32	123.88	120.35
3	C	901	AGS	C5-C6-N6	2.29	123.83	120.35
3	E	901	AGS	C5-C6-N6	2.29	123.83	120.35
4	E	902	ADP	C4-C5-N7	-2.29	107.02	109.40
3	B	902	AGS	C5-C6-N6	2.29	123.83	120.35
3	A	902	AGS	C5-C6-N6	2.28	123.82	120.35
3	F	901	AGS	C5-C6-N6	2.27	123.81	120.35
3	B	901	AGS	C5-C6-N6	2.24	123.76	120.35
3	D	901	AGS	C5-C6-N6	2.23	123.75	120.35
3	A	901	AGS	C5-C6-N6	2.21	123.70	120.35
4	E	902	ADP	O2A-PA-O1A	2.02	122.23	112.24

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	AGS	PB-O3B-PG-O2G
3	A	901	AGS	PB-O3B-PG-O3G
3	A	901	AGS	C5'-O5'-PA-O2A
3	A	902	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	B	901	AGS	C5'-O5'-PA-O1A
3	B	901	AGS	C5'-O5'-PA-O2A
3	B	902	AGS	PB-O3B-PG-O2G
3	B	902	AGS	PB-O3B-PG-O3G
3	C	902	AGS	PB-O3B-PG-O2G
3	C	902	AGS	PB-O3B-PG-O3G
3	C	902	AGS	C5'-O5'-PA-O1A
3	C	902	AGS	C5'-O5'-PA-O2A
3	D	901	AGS	PB-O3B-PG-O2G
3	D	901	AGS	PB-O3B-PG-O3G
3	D	901	AGS	C5'-O5'-PA-O2A
3	D	902	AGS	PB-O3B-PG-O2G
3	D	902	AGS	PB-O3B-PG-O3G
3	F	901	AGS	PB-O3B-PG-O2G
3	F	901	AGS	PB-O3B-PG-O3G
3	F	901	AGS	C5'-O5'-PA-O3A
3	E	901	AGS	O4'-C4'-C5'-O5'
3	F	901	AGS	O4'-C4'-C5'-O5'
3	E	901	AGS	C3'-C4'-C5'-O5'
3	C	901	AGS	O4'-C4'-C5'-O5'
3	C	901	AGS	C3'-C4'-C5'-O5'
3	F	901	AGS	C3'-C4'-C5'-O5'
3	C	901	AGS	PG-O3B-PB-O1B
3	A	901	AGS	C5'-O5'-PA-O3A
3	B	901	AGS	C5'-O5'-PA-O3A
3	C	902	AGS	C5'-O5'-PA-O3A
3	D	901	AGS	C5'-O5'-PA-O3A
3	D	901	AGS	PB-O3A-PA-O2A
3	A	901	AGS	C5'-O5'-PA-O1A
3	A	902	AGS	C5'-O5'-PA-O2A
3	D	901	AGS	C5'-O5'-PA-O1A
3	F	901	AGS	C5'-O5'-PA-O1A
3	F	901	AGS	C5'-O5'-PA-O2A
4	E	902	ADP	C3'-C4'-C5'-O5'
3	A	901	AGS	PB-O3A-PA-O2A
3	A	901	AGS	O4'-C4'-C5'-O5'
4	E	902	ADP	O4'-C4'-C5'-O5'
3	C	901	AGS	PG-O3B-PB-O2B
3	C	902	AGS	O4'-C4'-C5'-O5'
3	A	901	AGS	PB-O3A-PA-O1A
3	B	902	AGS	PB-O3A-PA-O2A
3	C	902	AGS	PB-O3A-PA-O2A

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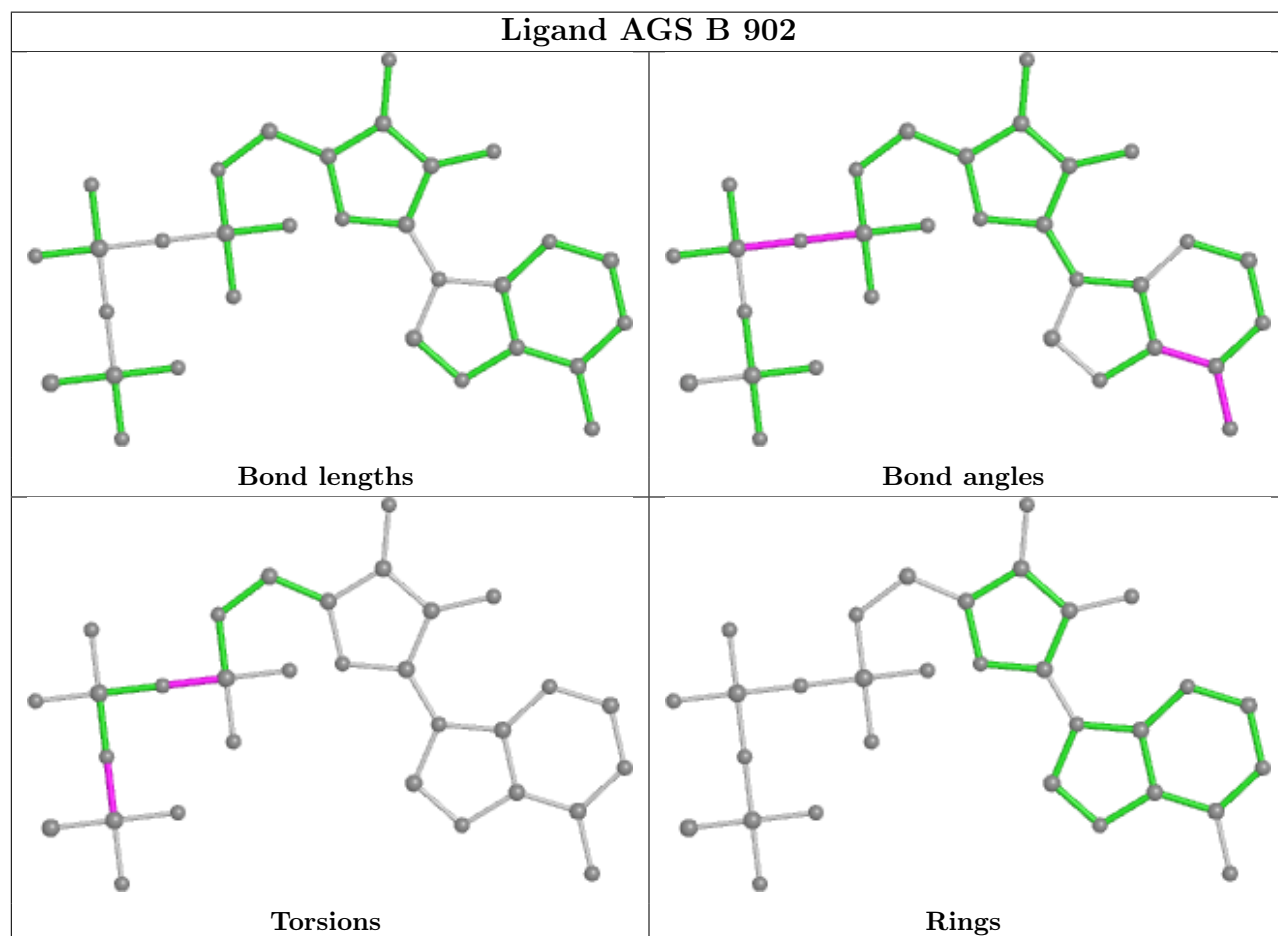
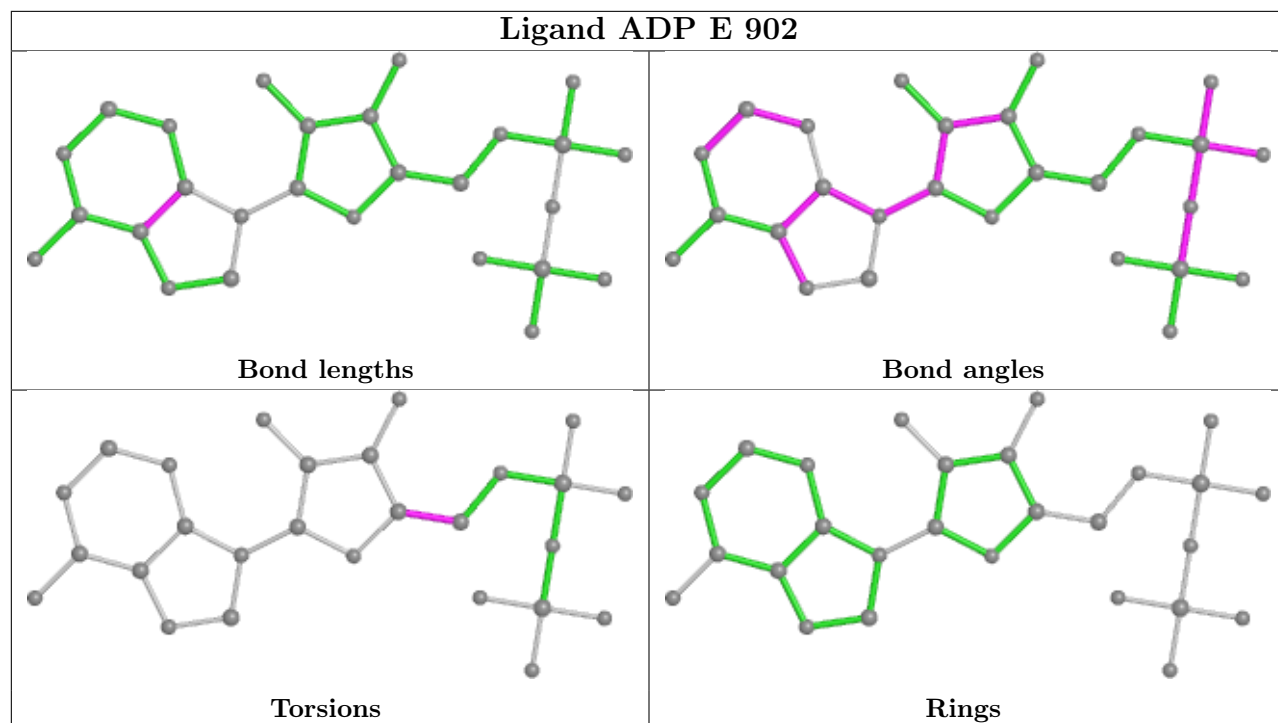
Mol	Chain	Res	Type	Atoms
3	F	901	AGS	PA-O3A-PB-O2B
4	F	902	ADP	C5'-O5'-PA-O1A
3	B	901	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	O4'-C4'-C5'-O5'

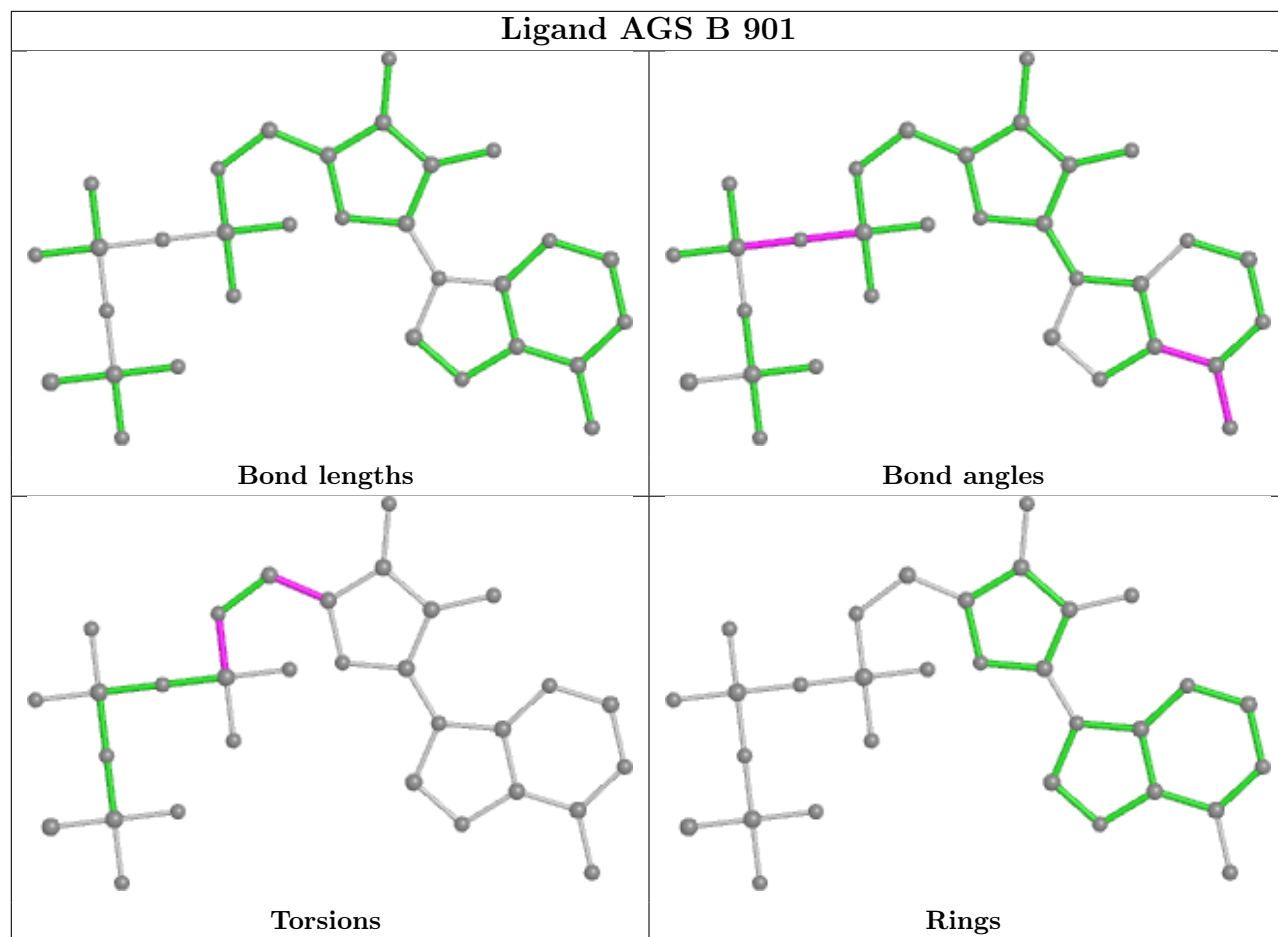
There are no ring outliers.

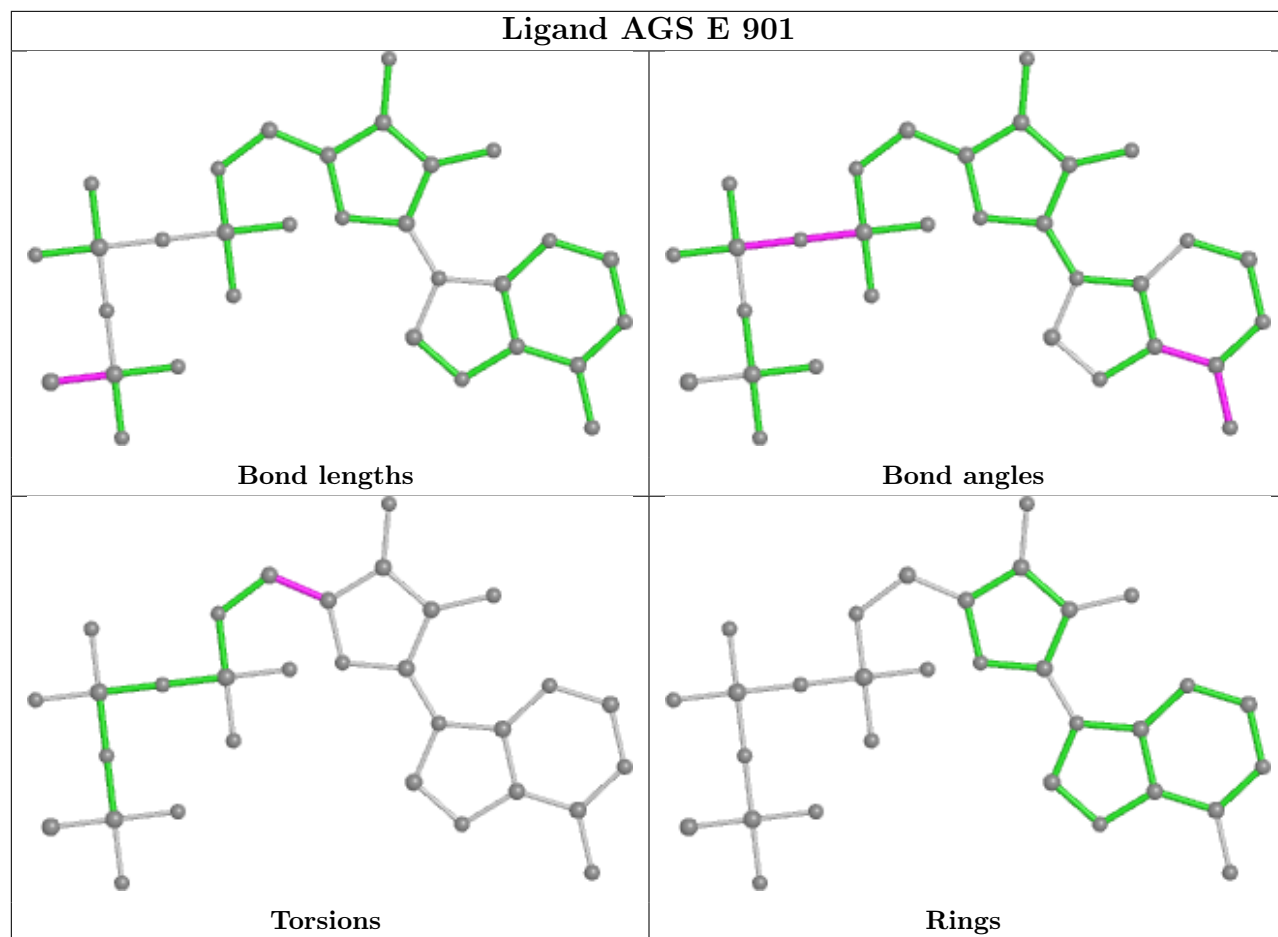
12 monomers are involved in 50 short contacts:

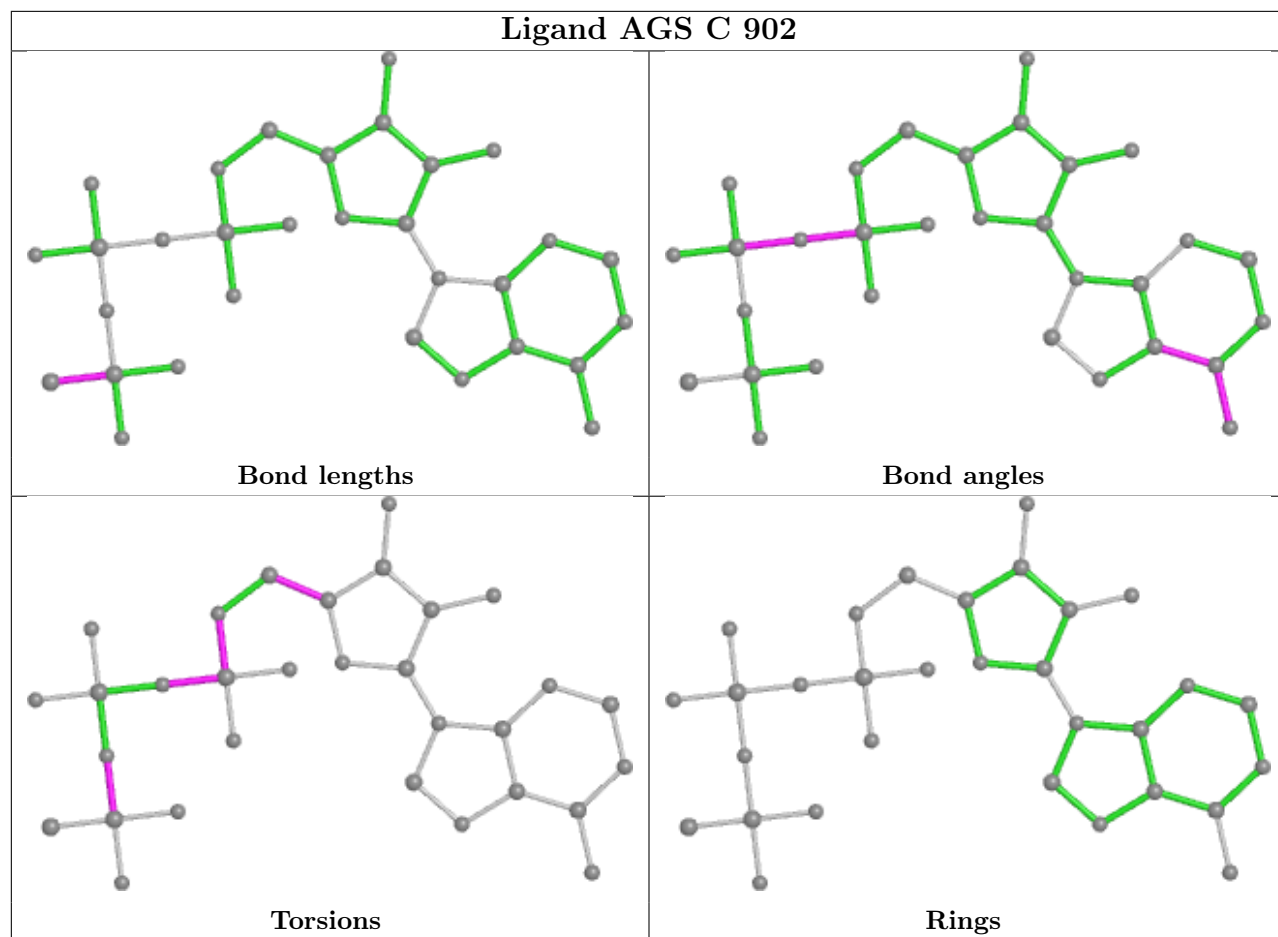
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	902	ADP	2	0
3	B	902	AGS	2	0
3	B	901	AGS	3	0
3	E	901	AGS	3	0
3	C	902	AGS	6	0
3	D	902	AGS	9	0
3	C	901	AGS	3	0
3	A	901	AGS	5	0
3	F	901	AGS	3	0
3	A	902	AGS	5	0
3	D	901	AGS	1	0
4	F	902	ADP	8	0

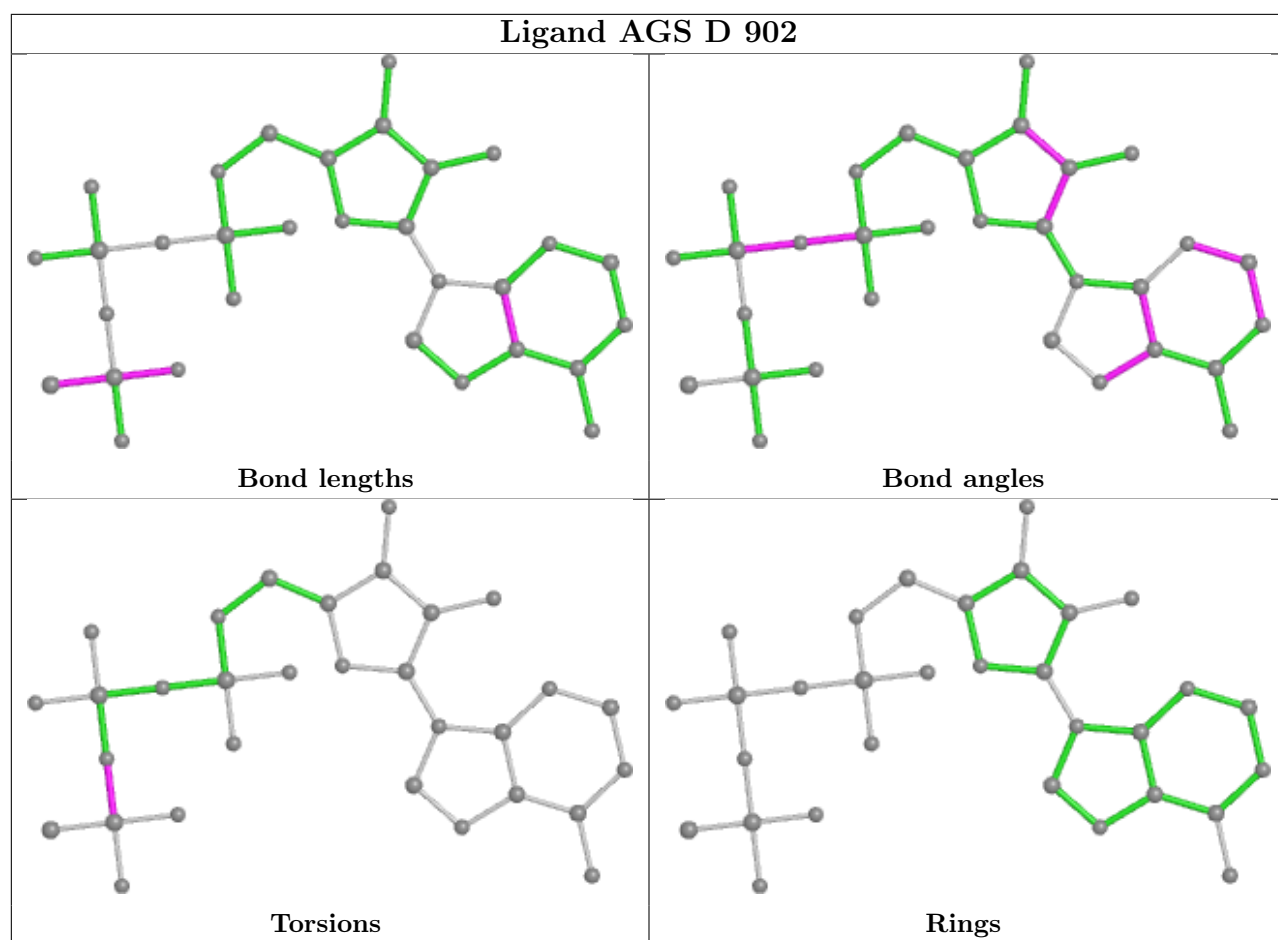
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

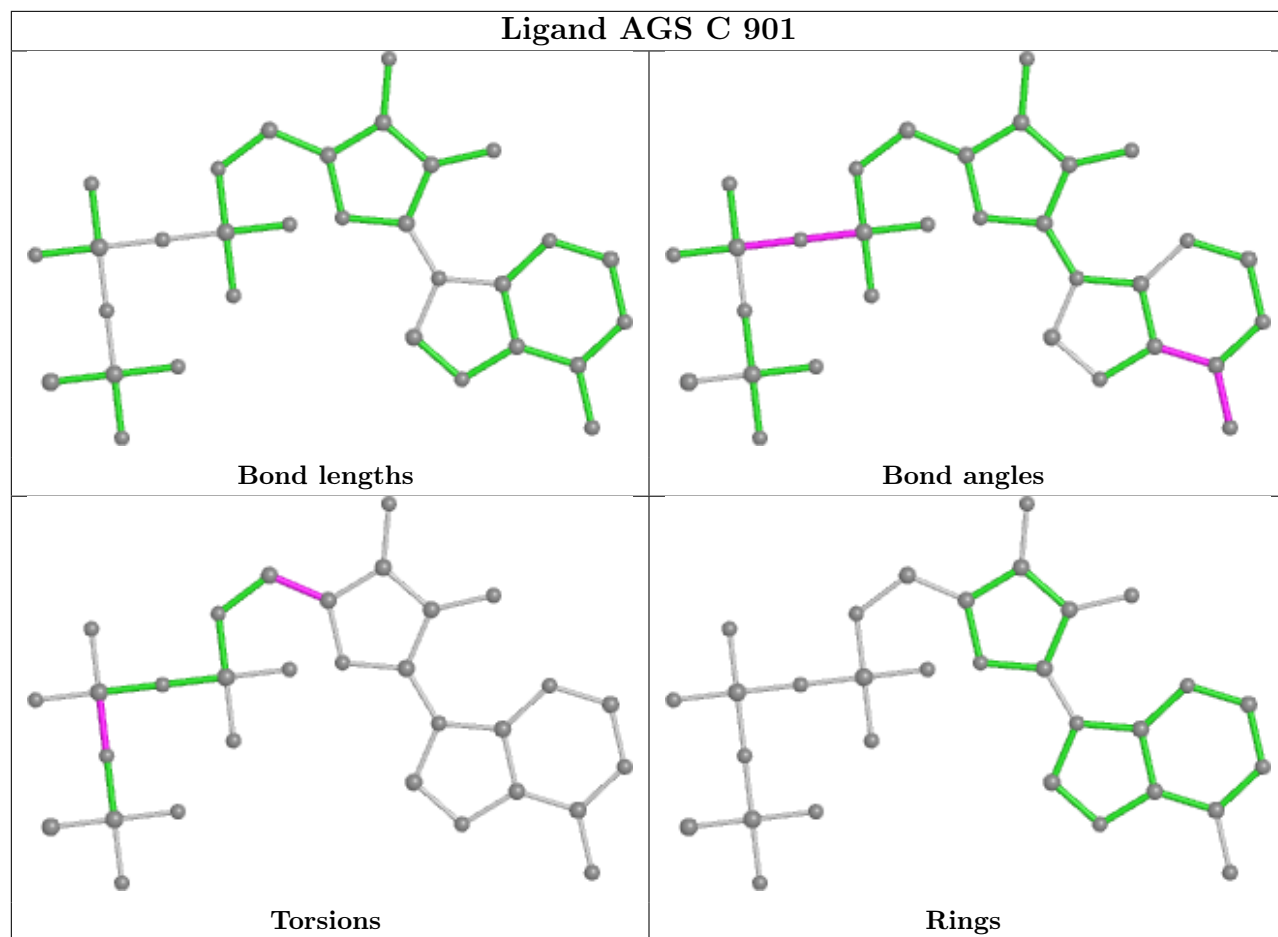


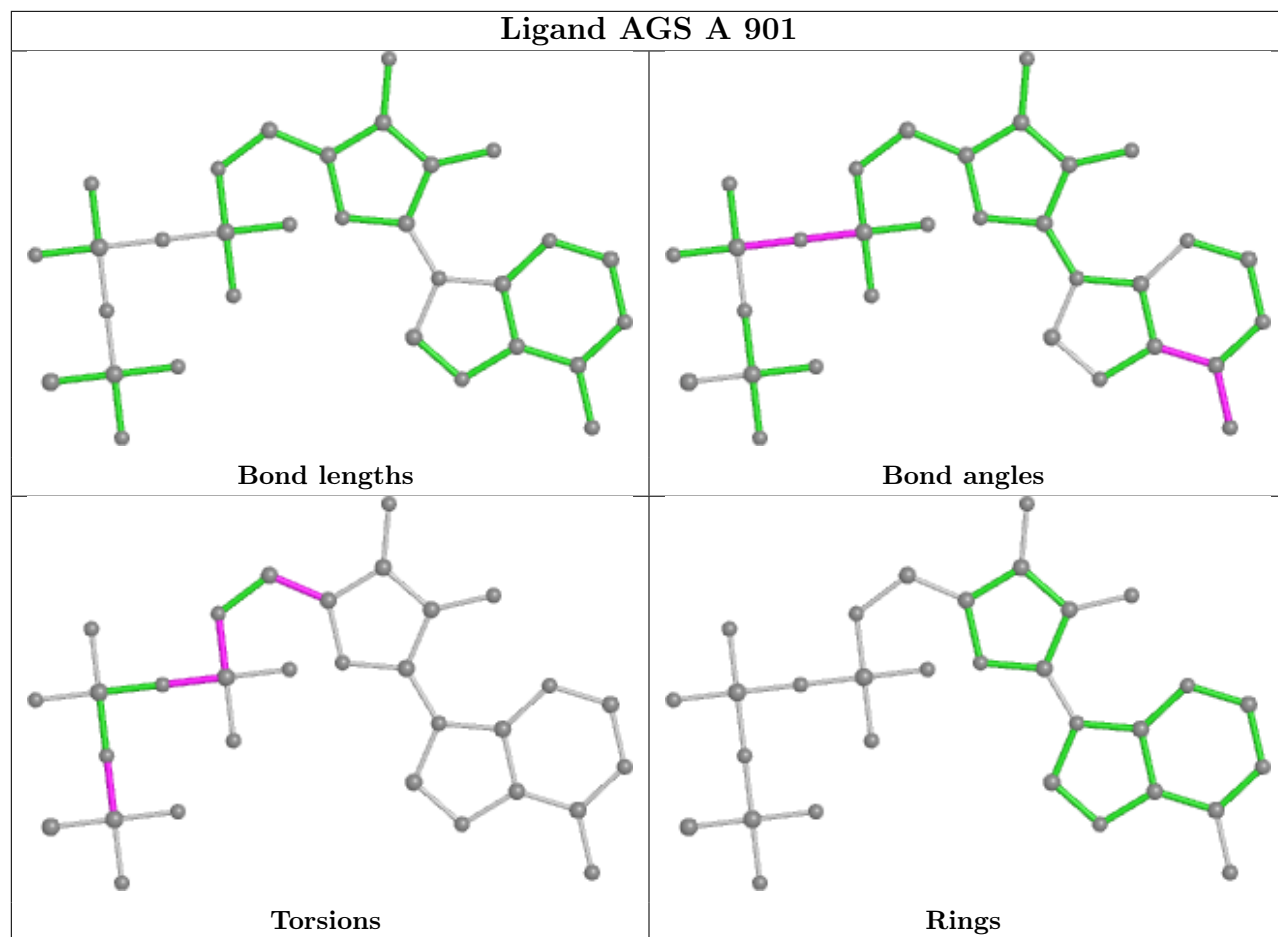


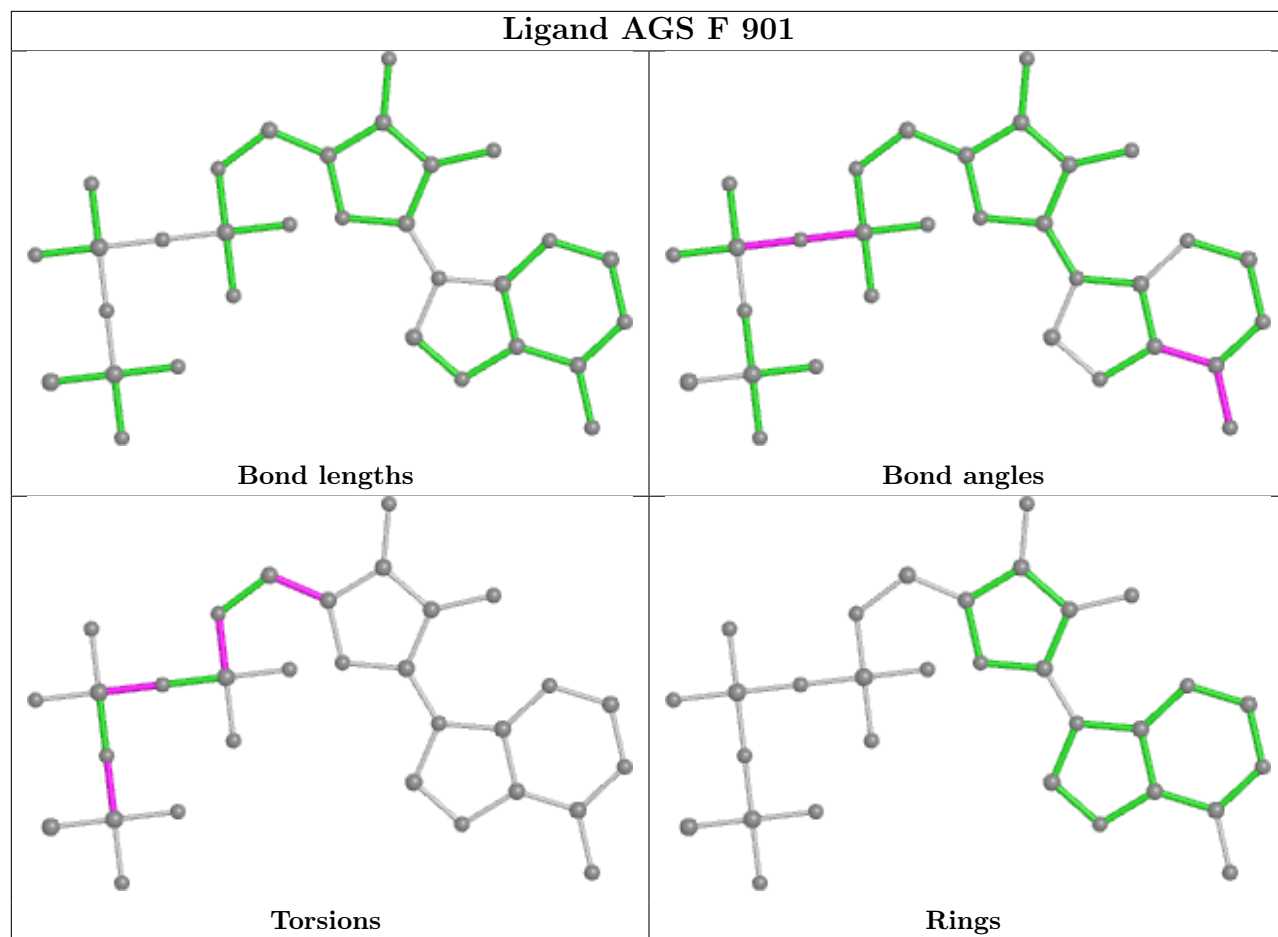


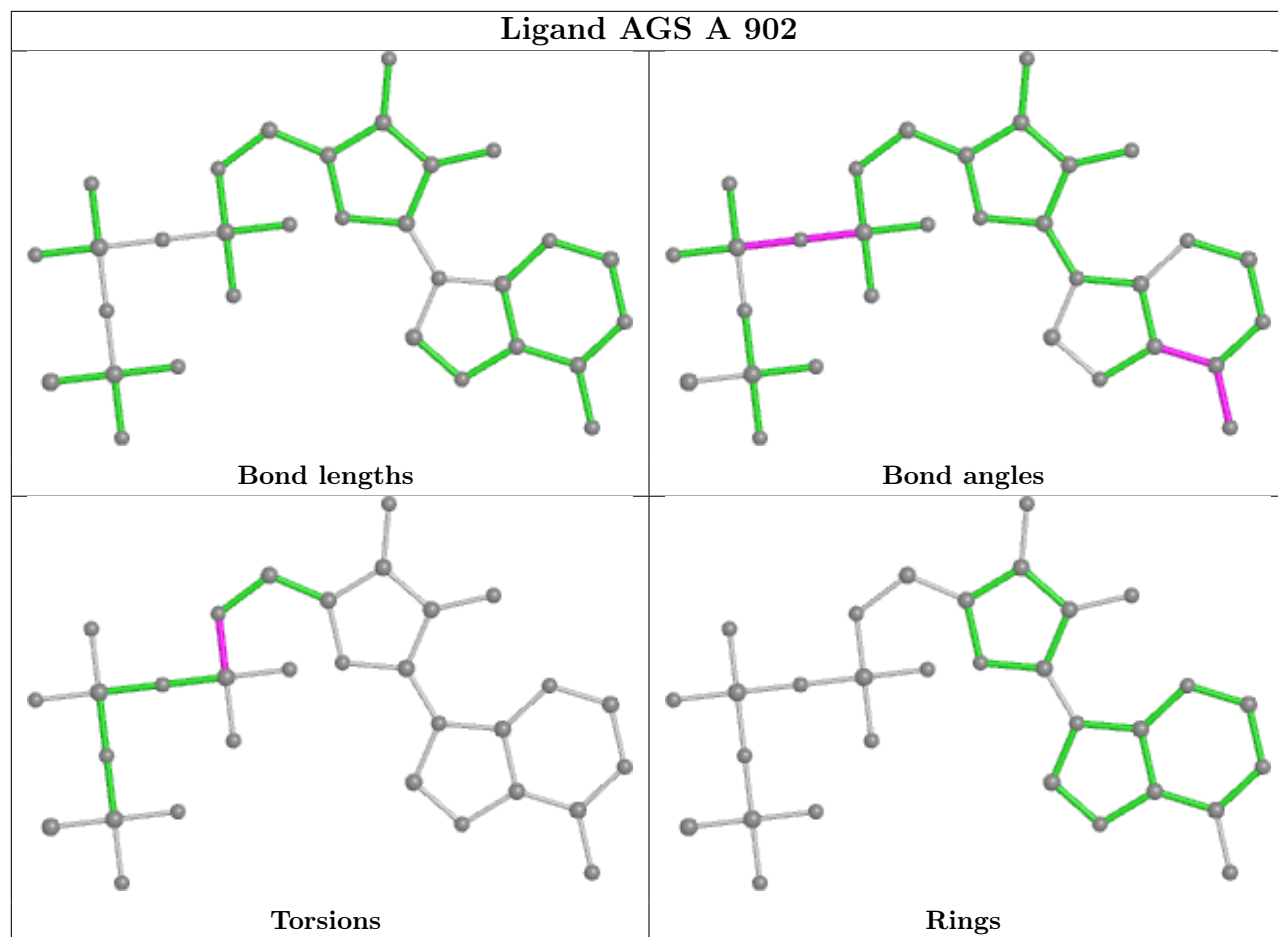




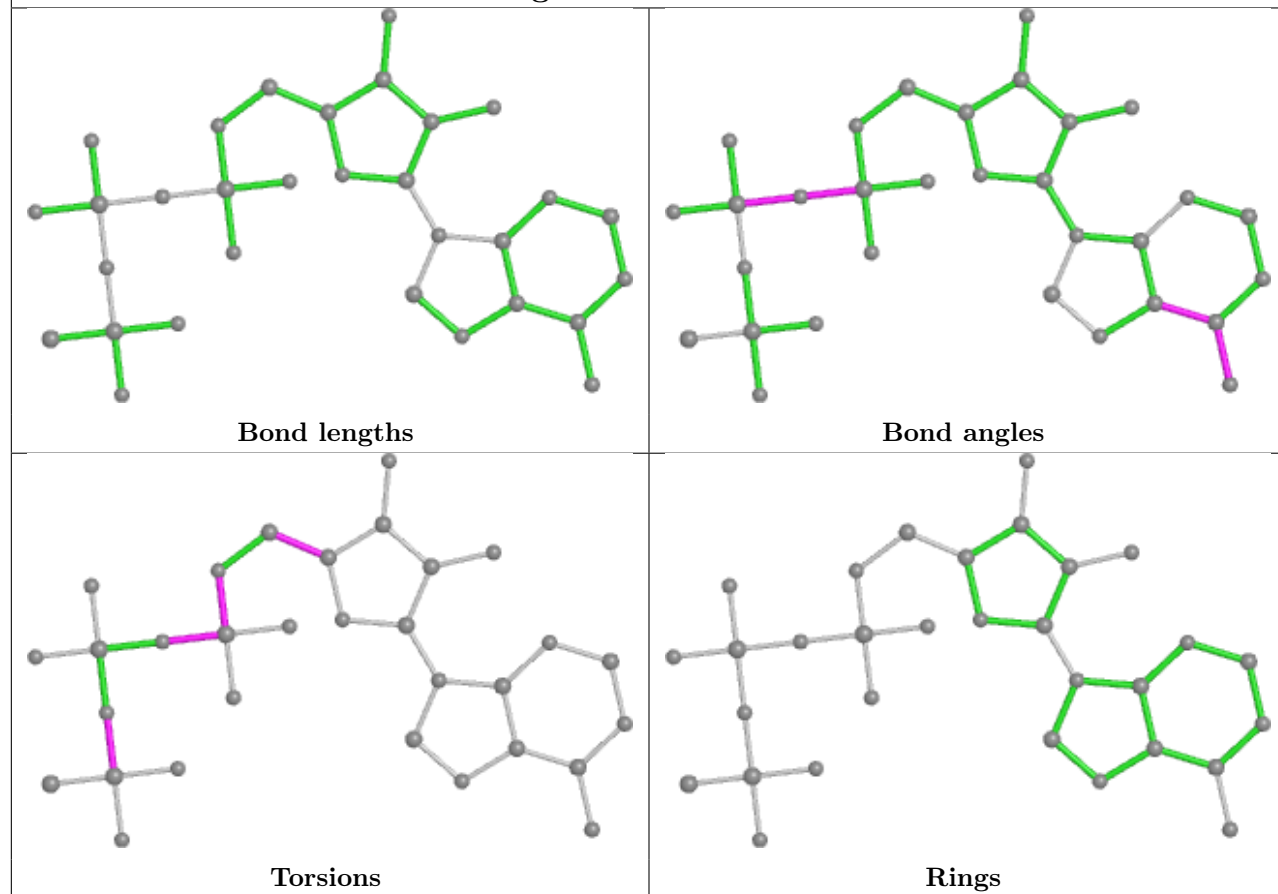




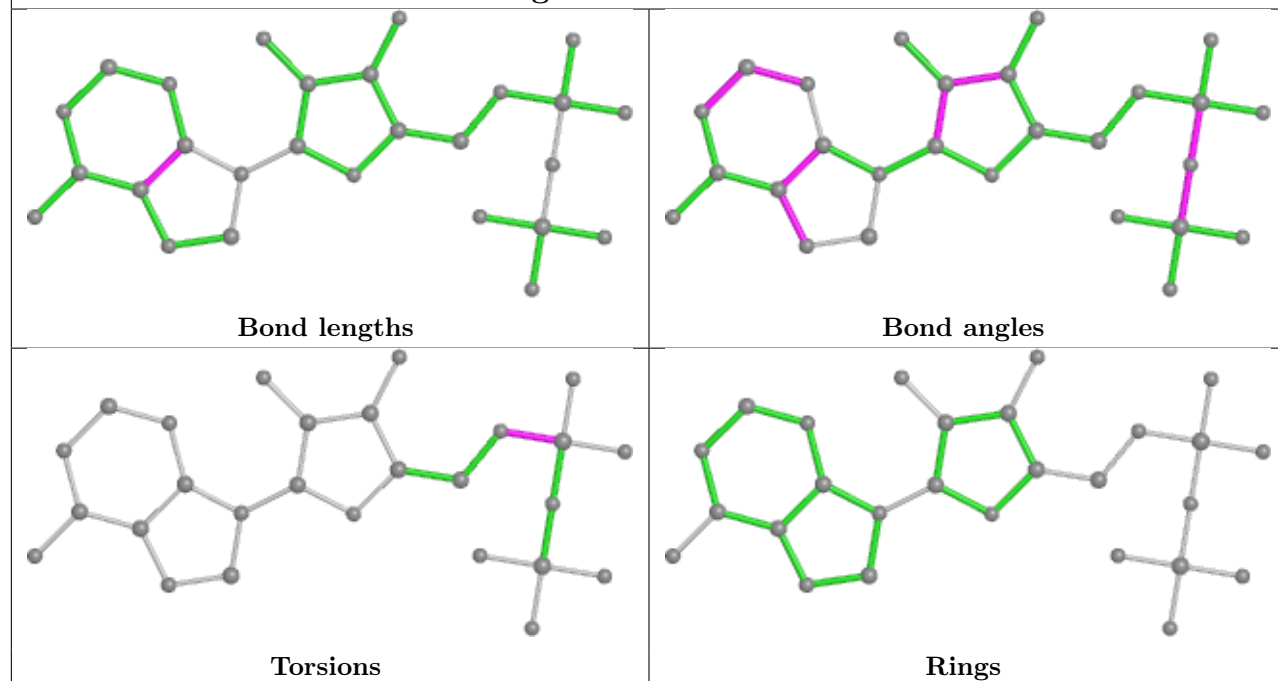




## Ligand AGS D 901



## Ligand ADP F 902



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

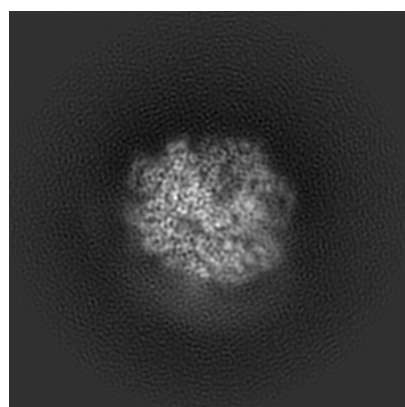
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7942. These allow visual inspection of the internal detail of the map and identification of artifacts.

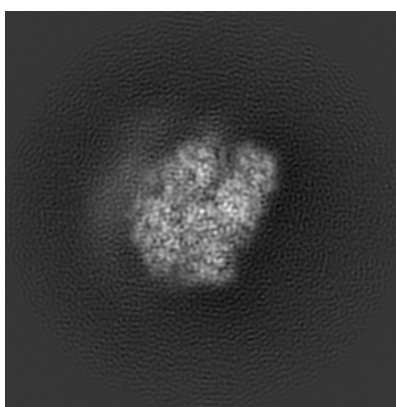
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

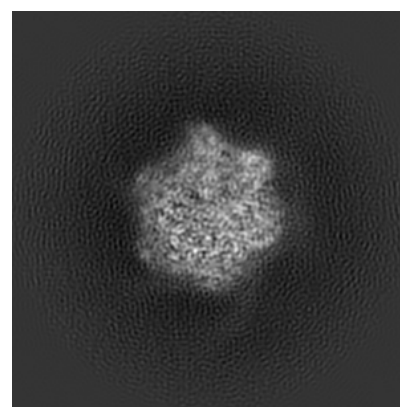
#### 6.1.1 Primary map



X



Y

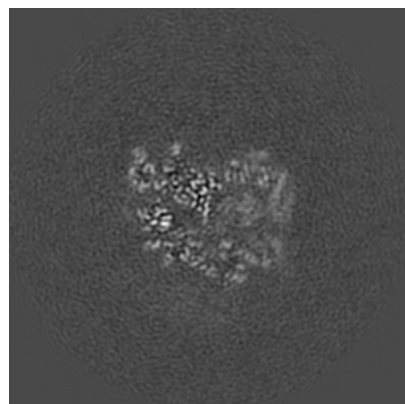


Z

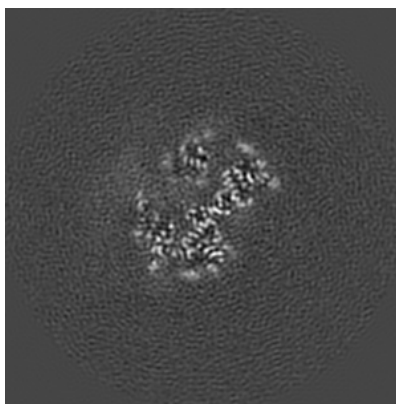
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

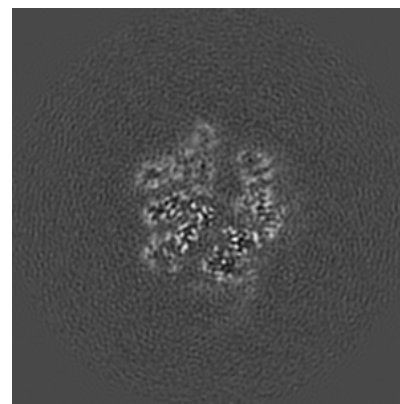
#### 6.2.1 Primary map



X Index: 146



Y Index: 146

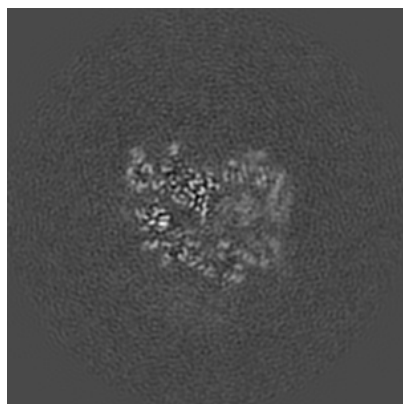


Z Index: 146

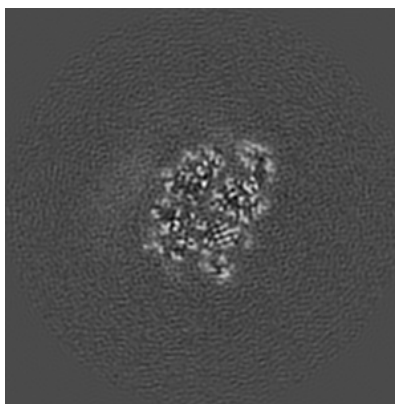
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

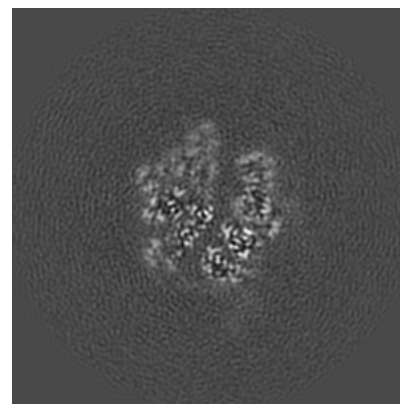
### 6.3.1 Primary map



X Index: 146



Y Index: 123

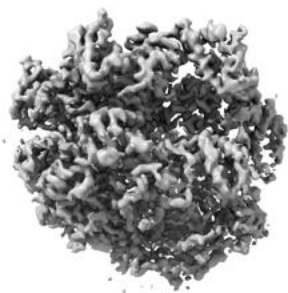


Z Index: 144

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

## 6.4 Orthogonal surface views [i](#)

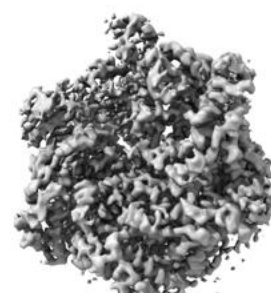
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

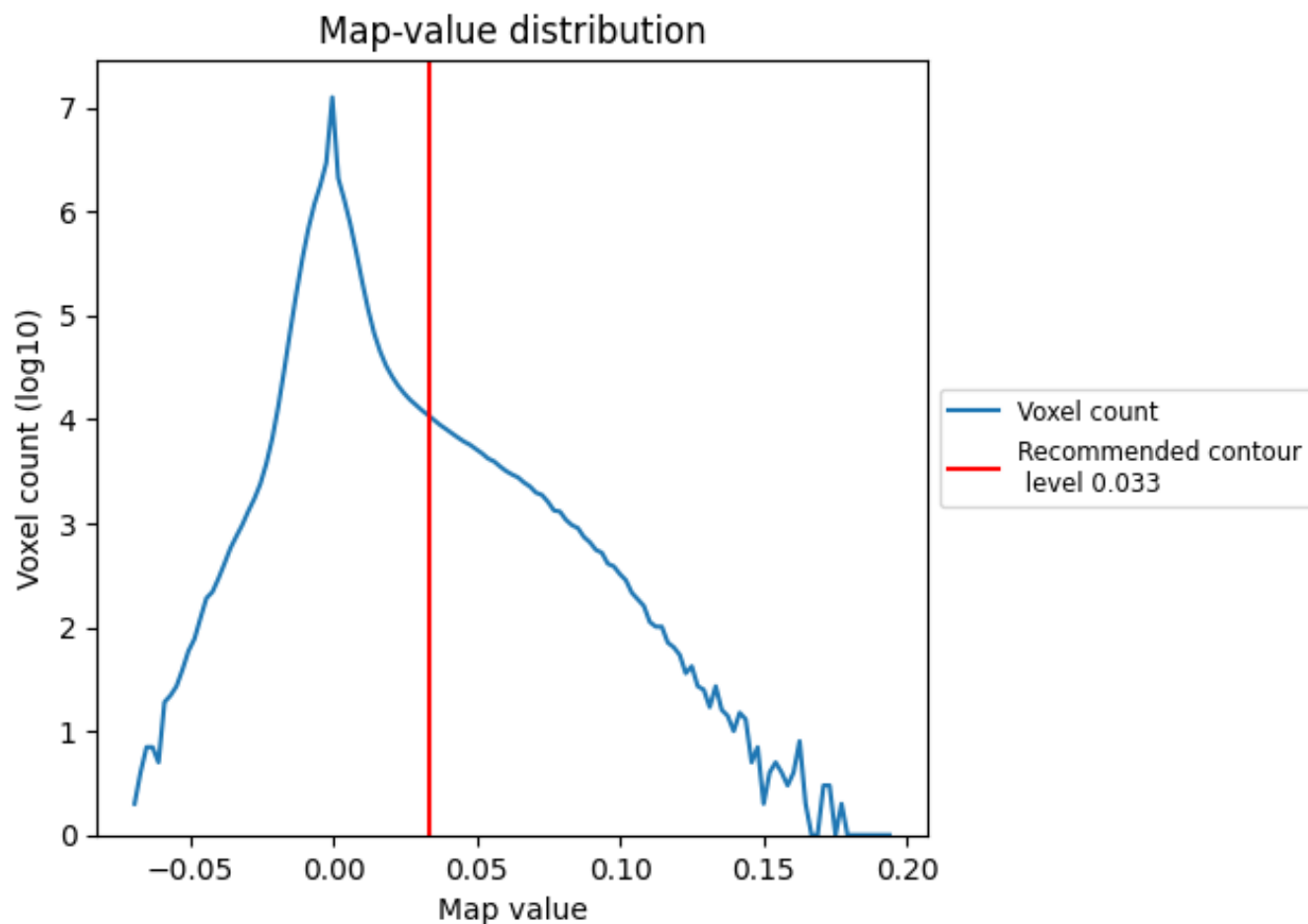
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

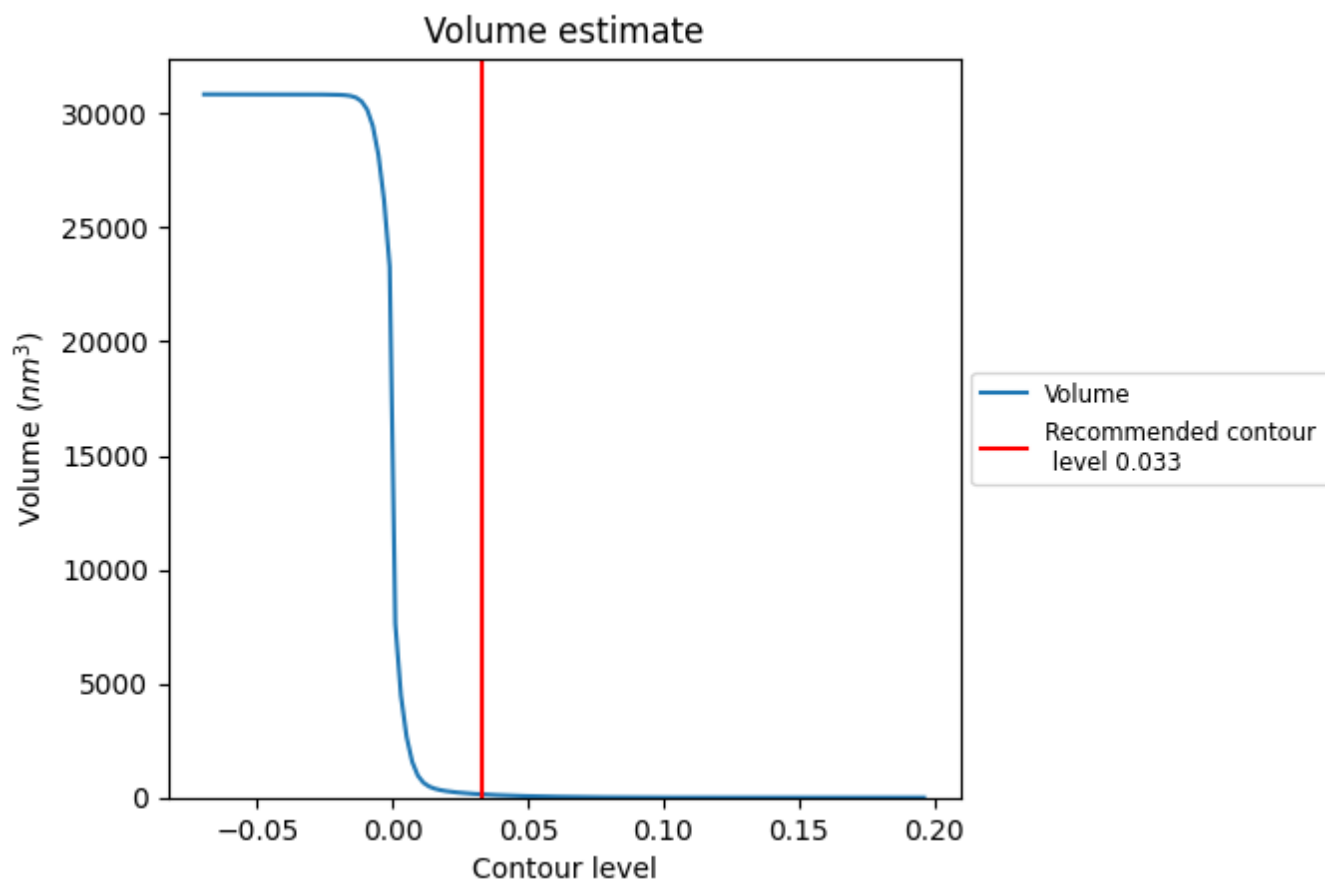
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

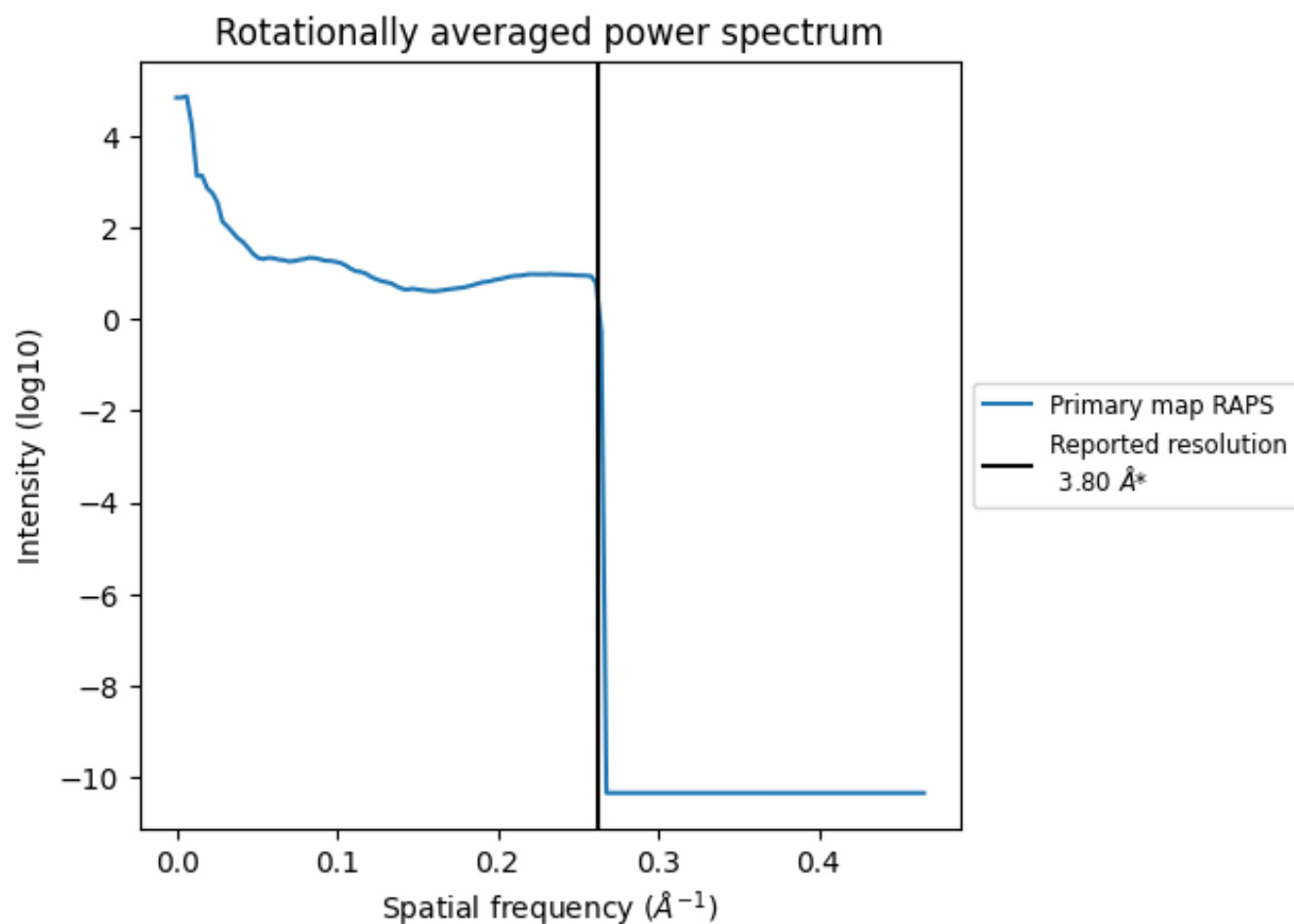
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm<sup>3</sup>; this corresponds to an approximate mass of 128 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

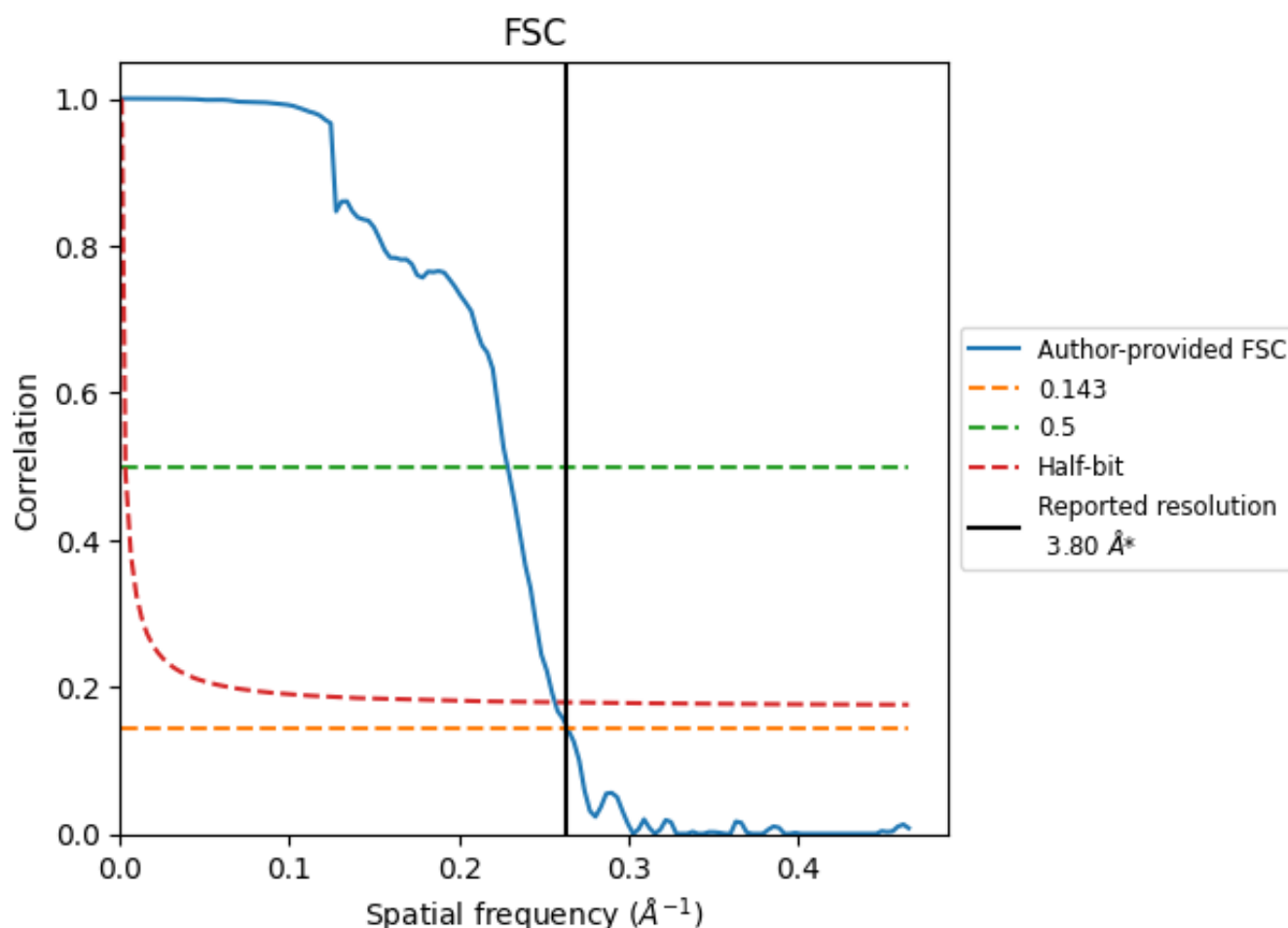


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

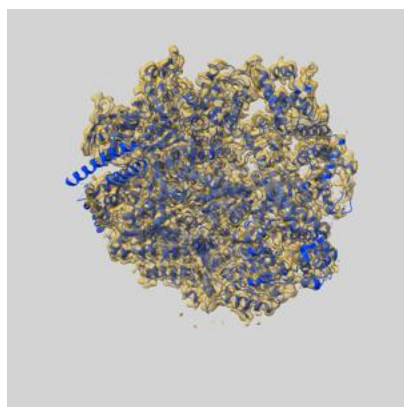
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.37	3.90
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

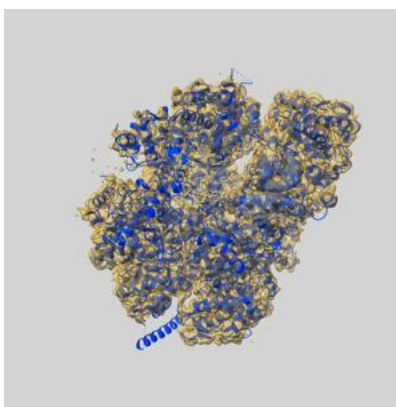
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7942 and PDB model 6DJU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

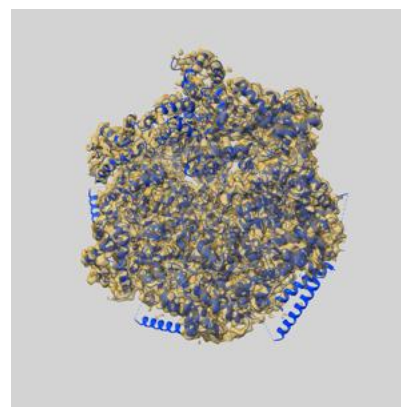
### 9.1 Map-model overlay [i](#)



X



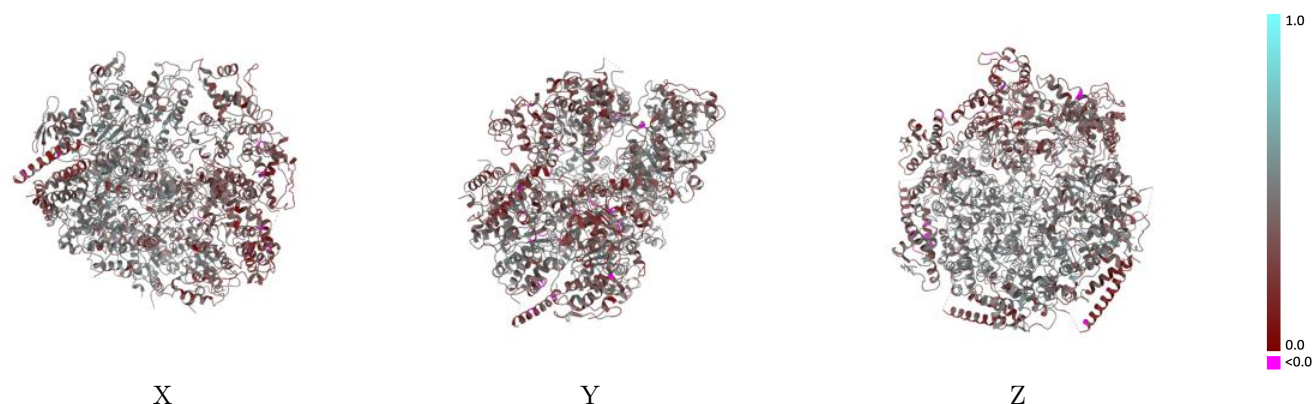
Y



Z

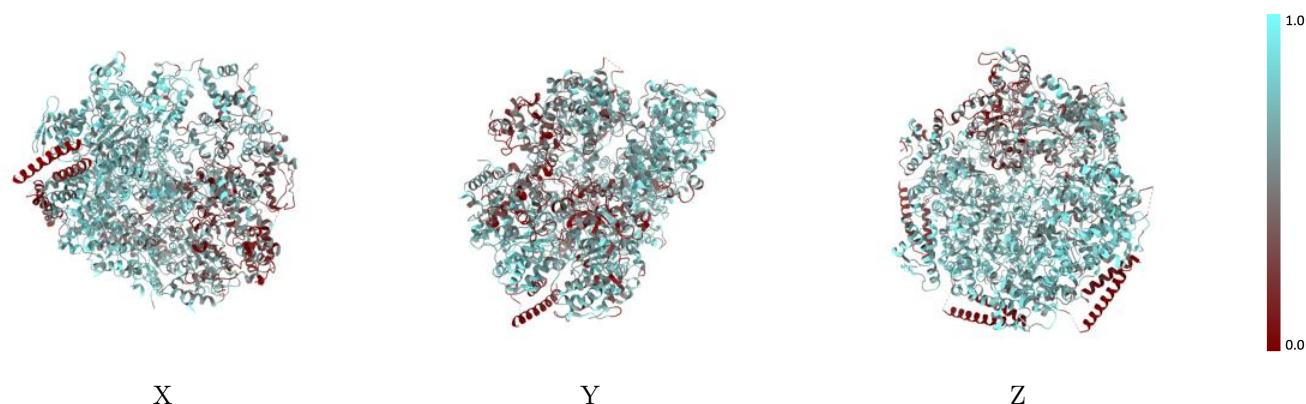
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



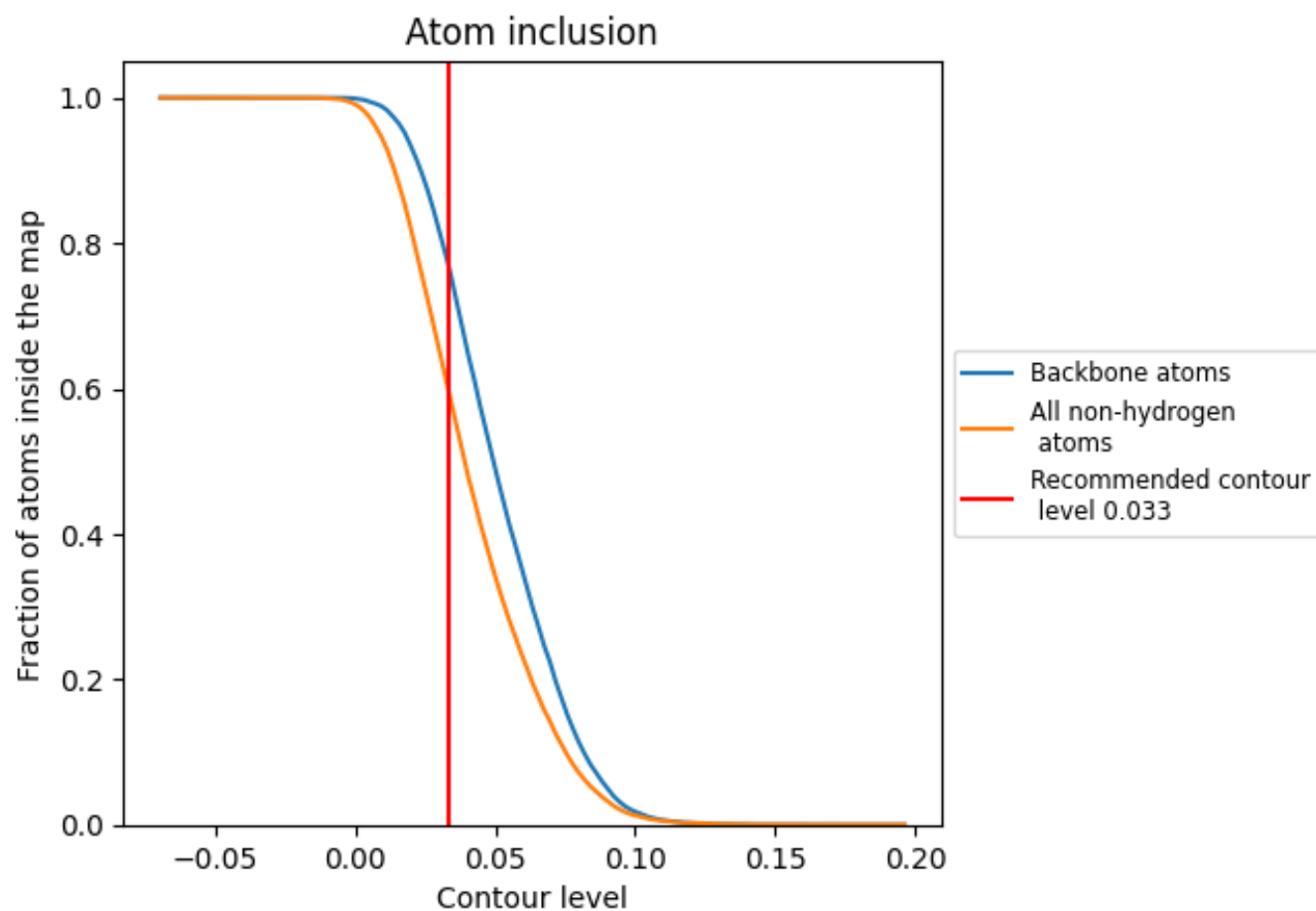
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6011	<div></div> 0.4010
A	<div></div> 0.6244	<div></div> 0.4080
B	<div></div> 0.6831	<div></div> 0.4430
C	<div></div> 0.6832	<div></div> 0.4420
D	<div></div> 0.6959	<div></div> 0.4400
E	<div></div> 0.5457	<div></div> 0.3600
F	<div></div> 0.3397	<div></div> 0.2980
N	<div></div> 0.7923	<div></div> 0.5070

1.0

0.0

<0.0