



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:07 AM UTC

PDB ID : 9GI1 / pdb_00009gi1
EMDB ID : EMD-51367
Title : Structure of the S.aureus MecA/ClpC/ClpP degradation system
Authors : Azinas, S.; Wallden, K.; Katikaridis, P.; Schahl, A.; Mogk, A.; Carroni, M.
Deposited on : 2024-08-16
Resolution : 3.00 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

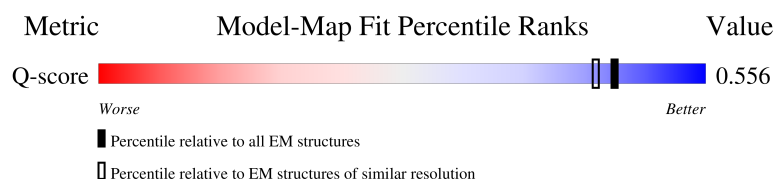
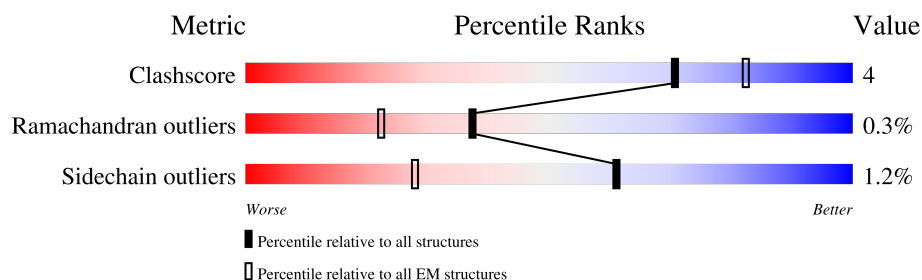
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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





The reported resolution of this entry is 3.00 Å.

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













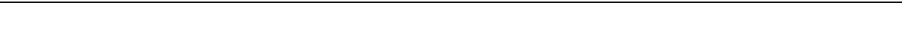

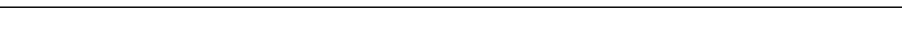
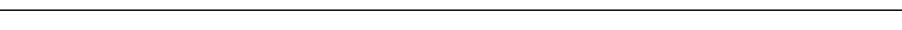
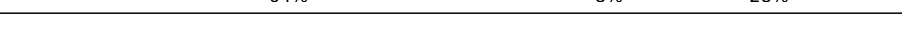


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	Pa	195	 92% 6% .
1	Pb	195	 92% 5% .
1	Pc	195	 88% 9% . .
1	Pd	195	 91% 6% . .

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Mol	Chain	Length	Quality of chain
1	Pe	195	 89% 7% . .
1	Pf	195	 91% 6% . .
1	Pg	195	 85% 7% . 7%
1	Ph	195	 89% 5% 6%
1	Pi	195	 86% 7% 7%
1	Pl	195	 83% 10% 7%
1	Pm	195	 88% 7% 6%
1	Pn	195	 89% 5% 6%
1	Po	195	 86% 5% . 8%
1	Pq	195	 85% 7% 8%
2	S	28	 57% 43%
3	a	818	 56% 8% 36%
3	b	818	 63% 8% . 29%
3	c	818	 64% 8% 28%
3	d	818	 61% 9% 30%
3	e	818	 63% 8% 29%
3	f	818	 55% 14% 31%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 47097 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Pa	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
1	Pb	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
1	Pc	189	Total	C	N	O	S	0	0
			1459	916	251	286	6		
1	Pd	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
1	Pe	188	Total	C	N	O	S	0	0
			1445	908	245	286	6		
1	Pf	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
1	Pg	182	Total	C	N	O	S	0	0
			1403	884	237	276	6		
1	Ph	183	Total	C	N	O	S	0	0
			1411	890	238	277	6		
1	Pi	182	Total	C	N	O	S	0	0
			1402	885	237	274	6		
1	Pl	182	Total	C	N	O	S	0	0
			1402	885	237	274	6		
1	Pm	184	Total	C	N	O	S	0	0
			1422	896	242	278	6		
1	Pn	183	Total	C	N	O	S	0	0
			1413	891	241	275	6		
1	Po	179	Total	C	N	O	S	0	0
			1377	867	234	270	6		
1	Pq	179	Total	C	N	O	S	0	0
			1377	867	234	270	6		

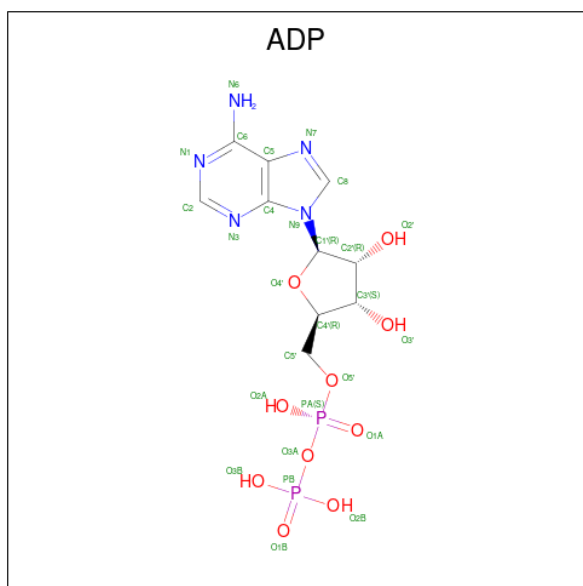
- Molecule 2 is a protein called Unidentified substrate of the MecA-ClpC-ClpP complex from *S.aureus*.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 3 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	524	Total	C	N	O	S	0	0
			4107	2579	719	797	12		
3	b	581	Total	C	N	O	S	0	0
			4536	2840	796	888	12		
3	c	588	Total	C	N	O	S	0	0
			4595	2874	806	902	13		
3	d	576	Total	C	N	O	S	0	0
			4504	2822	788	882	12		
3	e	582	Total	C	N	O	S	0	0
			4550	2848	797	893	12		
3	f	566	Total	C	N	O	S	0	0
			4441	2782	779	868	12		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



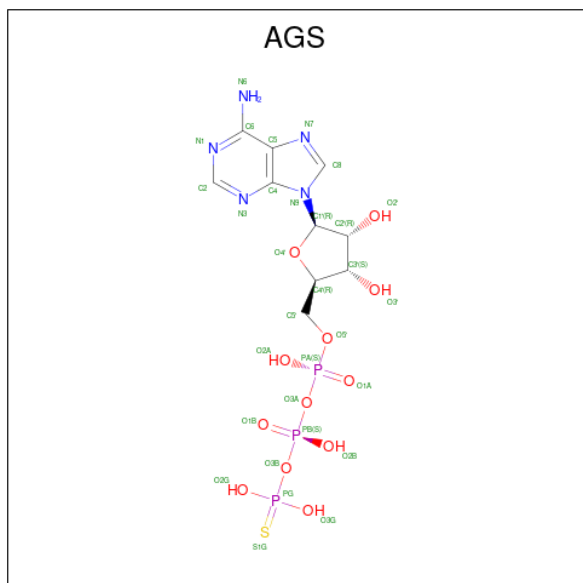
Mol	Chain	Residues	Atoms					AltConf
4	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	b	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	b	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	c	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	c	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	d	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	d	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	e	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	b	1	Total 1	Mg 1	0
6	c	2	Total 2	Mg 2	0
6	d	2	Total 2	Mg 2	0
6	e	2	Total 2	Mg 2	0

3 Residue-property plots [i](#)

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

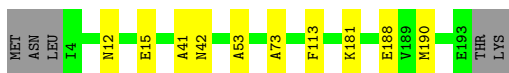
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pa: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pb: 



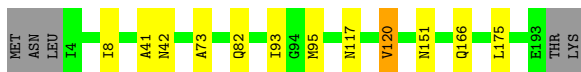
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pc: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pd: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pe: 




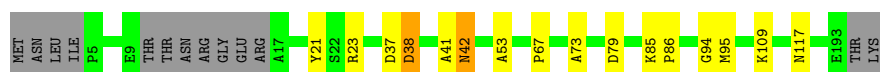
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pf:  91% 6% ..



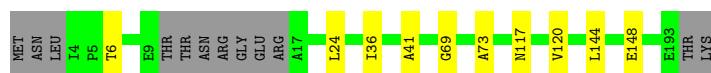
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pg:  85% 7% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Ph:  89% 5% 6%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pi:  86% 7% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pl:  83% 10% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pm:  88% 7% 6%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pn:  89% 5% 6%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Po:  86% 5% • 8%



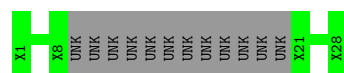
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Pq:  85% 7% 8%



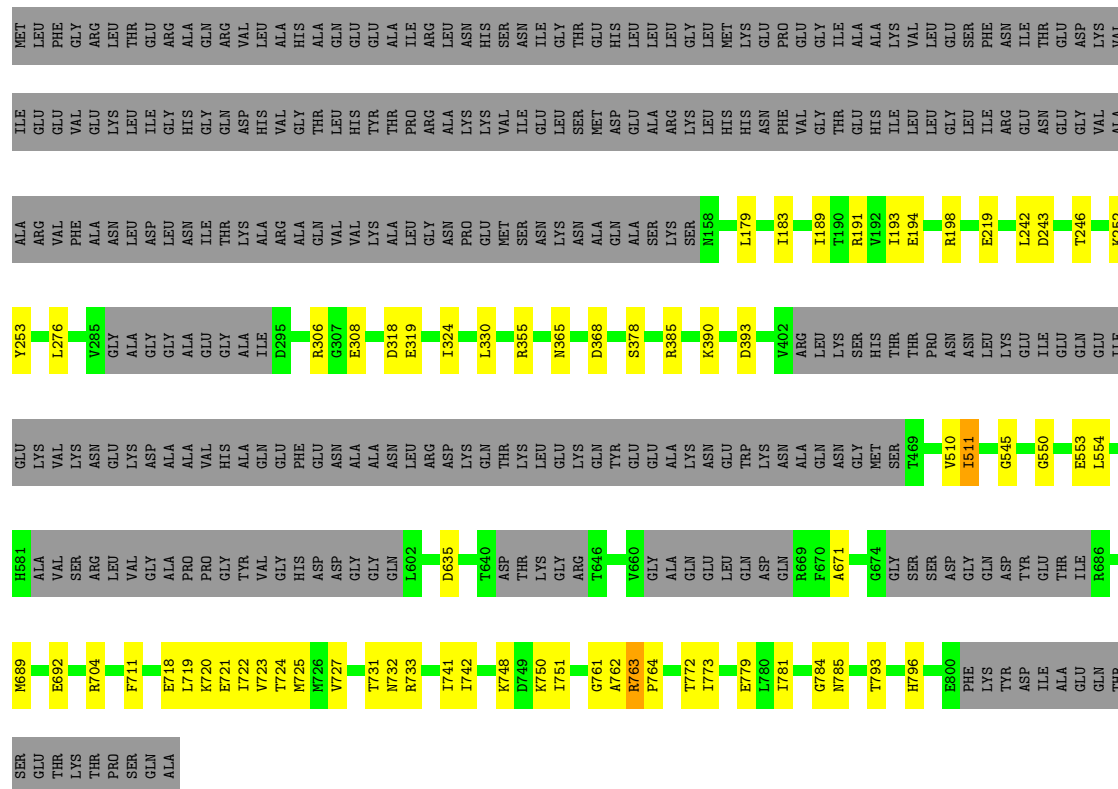
- Molecule 2: Unidentified substrate of the MecA-ClpC-ClpP complex from S.aureus

Chain S:  57% 43%



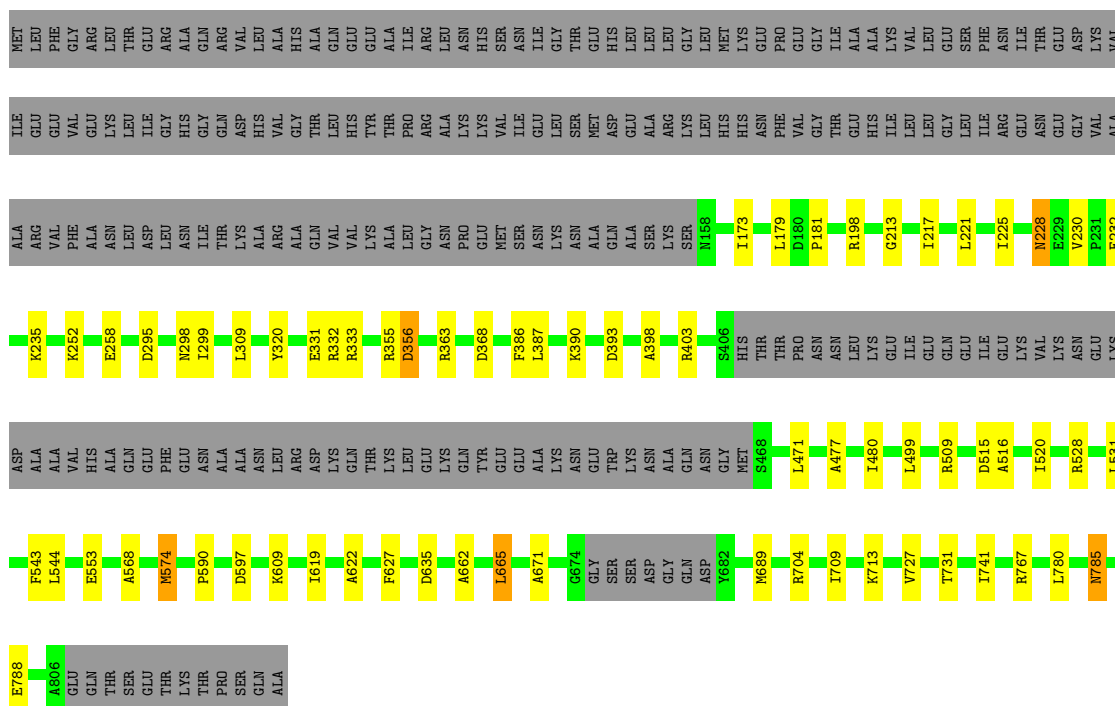
- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain a:  56% 8% 36%

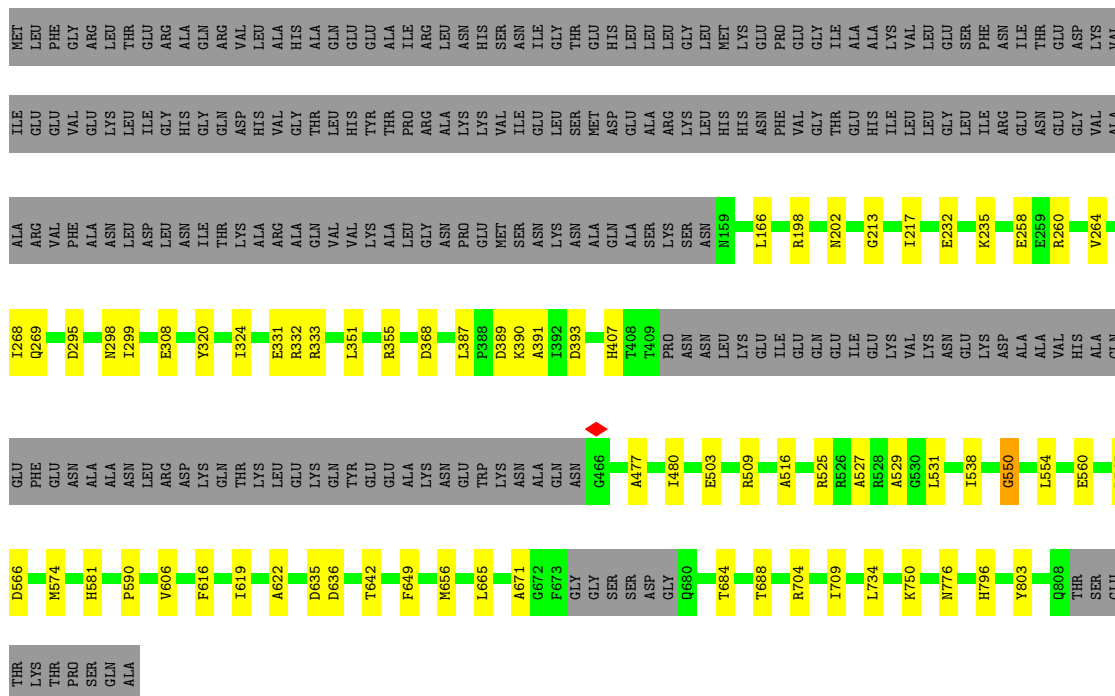


- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain b:  63% 8% • 29%

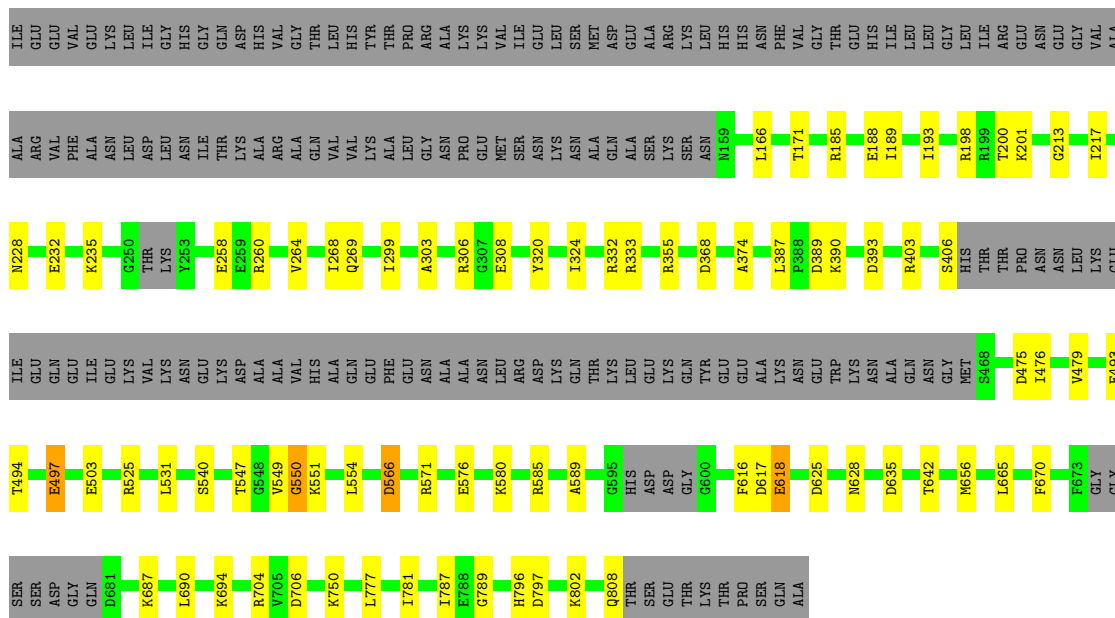


- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC

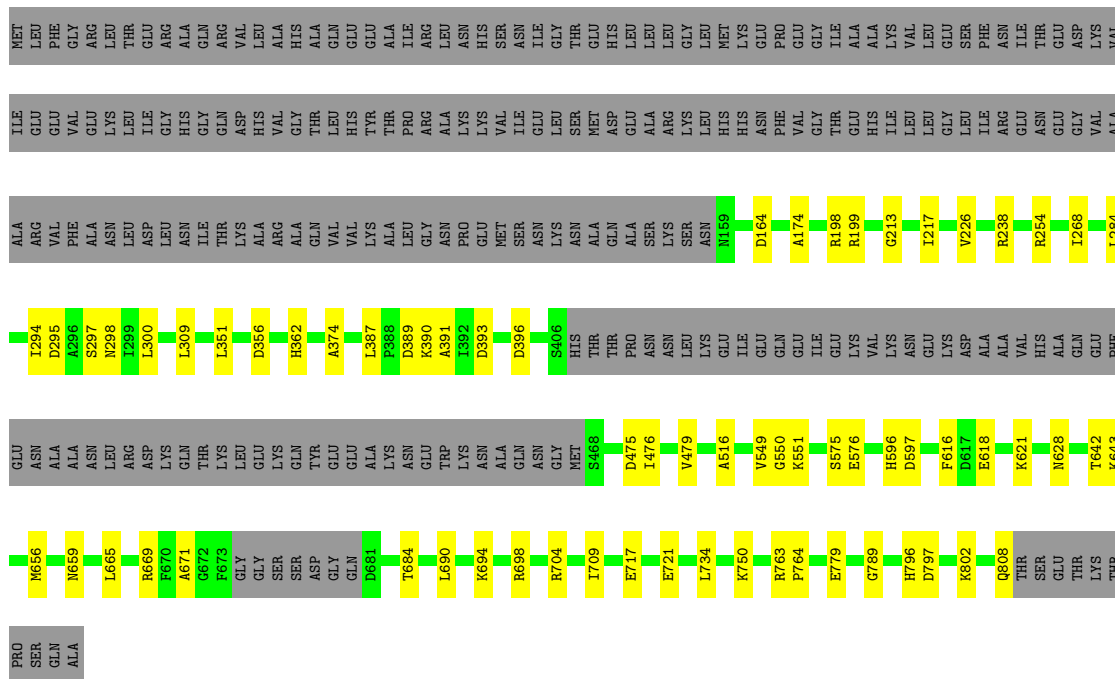


- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC

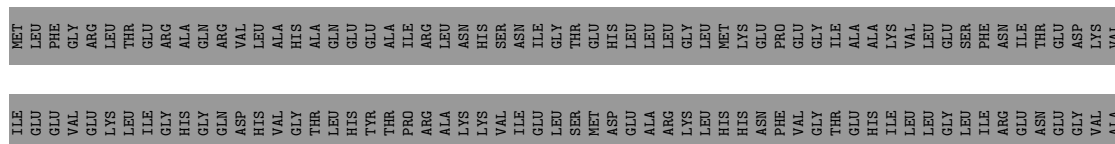




- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC



- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	19.734	Depositor
Minimum map value	-0.503	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.557	Depositor
Recommended contour level	0.744	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	Pa	0.12	0/1487	0.31	0/2008
1	Pb	0.13	0/1487	0.35	0/2008
1	Pc	0.14	0/1478	0.36	0/1996
1	Pd	0.13	0/1487	0.33	0/2008
1	Pe	0.13	0/1464	0.35	0/1979
1	Pf	0.13	0/1487	0.34	0/2008
1	Pg	0.12	0/1421	0.33	0/1917
1	Ph	0.11	0/1429	0.31	0/1929
1	Pi	0.12	0/1420	0.29	0/1917
1	Pl	0.12	0/1420	0.30	0/1917
1	Pm	0.12	0/1440	0.30	0/1943
1	Pn	0.11	0/1431	0.32	0/1931
1	Po	0.11	0/1394	0.31	0/1880
1	Pq	0.12	0/1394	0.32	0/1880
3	a	0.11	0/4152	0.36	0/5593
3	b	0.14	0/4592	0.36	0/6191
3	c	0.14	0/4652	0.37	0/6272
3	d	0.14	0/4557	0.38	0/6141
3	e	0.13	0/4606	0.35	0/6210
3	f	0.12	0/4495	0.38	0/6061
All	All	0.13	0/47293	0.35	0/63789

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	Pc	0	2
3	b	0	1
3	e	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Pc	130	GLN	Peptide
1	Pc	131	GLY	Peptide
3	b	386	PHE	Peptide
3	e	704	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Pa	1468	0	1480	6	0
1	Pb	1468	0	1480	7	0
1	Pc	1459	0	1474	10	0
1	Pd	1468	0	1480	9	0
1	Pe	1445	0	1450	8	0
1	Pf	1468	0	1480	8	0
1	Pg	1403	0	1414	10	0
1	Ph	1411	0	1424	5	0
1	Pi	1402	0	1418	9	0
1	Pl	1402	0	1418	11	0
1	Pm	1422	0	1437	8	0
1	Pn	1413	0	1431	5	0
1	Po	1377	0	1394	6	0
1	Pq	1377	0	1394	5	0
2	S	80	0	22	0	0
3	a	4107	0	4201	42	0
3	b	4536	0	4617	46	0
3	c	4595	0	4666	41	0
3	d	4504	0	4586	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	e	4550	0	4625	38	0
3	f	4441	0	4523	69	0
4	a	27	0	12	1	0
4	b	27	0	12	0	0
4	e	27	0	12	0	0
4	f	27	0	12	0	0
5	b	31	0	12	1	0
5	c	62	0	24	2	0
5	d	62	0	24	2	0
5	e	31	0	12	0	0
6	b	1	0	0	0	0
6	c	2	0	0	0	0
6	d	2	0	0	0	0
6	e	2	0	0	0	0
All	All	47097	0	47534	335	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 4.

All (335) 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)
3:b:704:ARG:NH2	5:c:902:AGS:S1G	2.56	0.78
3:a:198:ARG:NH2	3:b:393:ASP:OD1	2.17	0.77
3:d:198:ARG:NH2	3:e:393:ASP:OD1	2.17	0.74
3:c:198:ARG:NH2	3:d:393:ASP:OD1	2.18	0.74
3:a:355:ARG:NH1	3:a:368:ASP:OD1	2.20	0.73
3:f:746:LYS:NZ	3:f:796:HIS:O	2.21	0.73
3:f:230:VAL:O	3:f:235:LYS:NZ	2.21	0.73
3:a:733:ARG:HH22	3:f:533:ASP:HB3	1.55	0.71
3:b:198:ARG:NH2	3:c:393:ASP:OD1	2.19	0.71
3:d:616:PHE:HB2	3:d:656:MET:HG2	1.72	0.70
3:b:387:LEU:HA	3:b:390:LYS:HE2	1.74	0.70
3:c:332:ARG:NH1	3:d:389:ASP:OD1	2.25	0.70
3:f:511:ILE:HG12	3:f:721:GLU:HG2	1.75	0.69
3:a:243:ASP:O	3:f:298:ASN:ND2	2.25	0.68
3:c:529:ALA:HB1	3:d:781:ILE:HD11	1.72	0.68
3:c:333:ARG:NH1	5:d:901:AGS:S1G	2.61	0.68
3:b:780:LEU:O	3:b:785:ASN:ND2	2.26	0.68
1:Pa:41:ALA:HB2	1:Pa:73:ALA:HB1	1.76	0.67
3:b:574:MET:HB3	3:b:622:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:306:ARG:NH2	3:d:308:GLU:OE1	2.25	0.66
3:e:549:VAL:O	3:e:551:LYS:N	2.28	0.66
3:f:397:GLU:OE2	3:f:483:TRP:NE1	2.22	0.66
3:a:378:SER:HB3	3:a:390:LYS:HB3	1.79	0.65
3:b:332:ARG:NH1	3:c:389:ASP:OD1	2.30	0.65
3:f:634:LEU:HD11	3:f:704:ARG:HG3	1.77	0.65
1:Pc:41:ALA:HB2	1:Pc:73:ALA:HB1	1.79	0.65
3:d:355:ARG:NH1	3:d:368:ASP:OD1	2.27	0.64
3:a:779:GLU:OE2	3:f:525:ARG:NH1	2.30	0.64
3:e:797:ASP:OD2	3:e:802:LYS:NZ	2.30	0.64
3:f:180:ASP:OD1	3:f:357:ARG:NH1	2.30	0.63
3:a:733:ARG:NH1	3:f:533:ASP:OD2	2.29	0.63
3:e:789:GLY:O	3:e:808:GLN:NE2	2.28	0.63
3:e:387:LEU:HA	3:e:390:LYS:HE2	1.80	0.63
3:f:387:LEU:HA	3:f:390:LYS:HE2	1.81	0.63
1:Pq:41:ALA:HB2	1:Pq:73:ALA:HB1	1.81	0.63
1:Pm:6:THR:N	1:Pn:22:SER:OG	2.30	0.62
3:f:355:ARG:NH2	3:f:368:ASP:OD1	2.28	0.61
1:Pf:9:GLU:OE1	3:e:669:ARG:NH2	2.32	0.60
1:Pn:193:GLU:OE1	1:Po:85:LYS:NZ	2.30	0.60
3:f:522:LYS:O	3:f:526:ARG:NH1	2.35	0.60
3:b:727:VAL:O	3:b:731:THR:HG23	2.02	0.60
3:d:503:GLU:CD	3:d:525:ARG:HH12	2.09	0.60
3:d:549:VAL:O	3:d:551:LYS:N	2.32	0.60
1:Po:41:ALA:HB2	1:Po:73:ALA:HB1	1.84	0.59
1:Pf:37:ASP:OD1	1:Pf:38:ASP:N	2.32	0.59
1:Pq:36:ILE:HB	1:Pq:69:GLY:HA3	1.85	0.59
3:e:659:ASN:O	3:e:659:ASN:ND2	2.36	0.58
3:f:777:LEU:O	3:f:781:ILE:HG12	2.03	0.58
3:f:200:THR:HG23	3:f:201:LYS:H	1.67	0.58
3:e:618:GLU:OE1	3:e:621:LYS:NZ	2.29	0.58
1:Pl:41:ALA:HB2	1:Pl:73:ALA:HB1	1.84	0.58
3:a:183:ILE:H	4:a:901:ADP:HN62	1.52	0.57
3:a:781:ILE:HA	3:a:785:ASN:HB2	1.86	0.57
1:Ph:36:ILE:HB	1:Ph:69:GLY:HA3	1.86	0.57
3:d:403:ARG:NH2	3:d:406:SER:OG	2.36	0.57
3:e:597:ASP:HA	3:e:643:LYS:HD3	1.85	0.57
3:a:742:ILE:HB	3:a:793:THR:HA	1.87	0.57
3:c:166:LEU:HD21	3:c:260:ARG:HD3	1.87	0.57
1:Pb:181:LYS:HD3	1:Pb:188:GLU:HA	1.86	0.57
3:b:213:GLY:O	3:b:217:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Pc:16:ARG:HG2	1:Pd:8:ILE:HG21	1.87	0.57
1:Pm:41:ALA:HB2	1:Pm:73:ALA:HB1	1.86	0.56
3:a:545:GLY:HA3	3:a:711:PHE:HB2	1.87	0.56
3:a:731:THR:HG23	3:a:741:ILE:HB	1.87	0.56
3:f:542:ILE:HG12	3:f:705:VAL:HG11	1.86	0.56
1:Pb:41:ALA:HB2	1:Pb:73:ALA:HB1	1.87	0.56
3:e:374:ALA:HB2	3:e:476:ILE:HD13	1.87	0.55
3:b:355:ARG:NH1	3:b:368:ASP:OD1	2.30	0.55
3:d:618:GLU:OE1	5:d:902:AGS:O2G	2.23	0.55
1:Pg:41:ALA:HB2	1:Pg:73:ALA:HB1	1.88	0.55
3:a:720:LYS:O	3:a:724:THR:HG23	2.06	0.55
3:d:576:GLU:OE1	3:d:585:ARG:NH1	2.34	0.55
3:e:698:ARG:NH2	3:f:618:GLU:OE2	2.39	0.55
3:e:268:ILE:HG21	3:e:309:LEU:HD23	1.89	0.55
3:b:333:ARG:NH2	5:c:901:AGS:S1G	2.59	0.55
3:a:252:LYS:HE3	3:a:253:TYR:CZ	2.42	0.54
3:d:797:ASP:OD2	3:d:802:LYS:NZ	2.31	0.54
1:Pg:37:ASP:OD1	1:Pg:38:ASP:N	2.34	0.54
3:d:580:LYS:NZ	3:d:625:ASP:OD2	2.39	0.54
1:Pe:53:ALA:HB2	3:e:671:ALA:HA	1.90	0.54
3:c:619:ILE:HG21	3:c:656:MET:HB3	1.90	0.54
3:d:201:LYS:HD2	3:d:333:ARG:HA	1.88	0.54
3:f:183:ILE:HB	3:f:350:ILE:HG22	1.89	0.54
1:Pi:41:ALA:HB2	1:Pi:73:ALA:HB1	1.89	0.54
3:b:221:LEU:O	3:b:225:ILE:HG12	2.08	0.54
3:c:355:ARG:NH1	3:c:368:ASP:OD1	2.25	0.54
3:a:179:LEU:HD21	3:a:219:GLU:HB3	1.88	0.54
3:b:520:ILE:HD11	3:b:543:PHE:HZ	1.72	0.54
3:f:727:VAL:O	3:f:731:THR:HG23	2.07	0.54
3:a:689:MET:HA	3:a:692:GLU:HG2	1.88	0.53
3:f:301:LYS:O	3:f:305:ALA:N	2.41	0.53
3:f:509:ARG:HD2	3:f:557:ALA:HB2	1.91	0.53
3:e:295:ASP:OD1	3:e:298:ASN:ND2	2.39	0.53
1:Pf:41:ALA:HB2	1:Pf:73:ALA:HB1	1.89	0.53
1:Ph:41:ALA:HB2	1:Ph:73:ALA:HB1	1.88	0.53
3:c:503:GLU:CD	3:c:525:ARG:HH12	2.17	0.53
3:c:387:LEU:HA	3:c:390:LYS:HE2	1.91	0.53
1:Pi:8:ILE:HG12	1:Pi:17:ALA:HA	1.90	0.53
1:Pn:41:ALA:HB2	1:Pn:73:ALA:HB1	1.91	0.53
1:Pl:193:GLU:OE1	1:Pm:85:LYS:NZ	2.36	0.53
3:a:718:GLU:O	3:a:722:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:351:LEU:HD11	3:f:391:ALA:HB1	1.90	0.52
3:f:537:PRO:HA	3:f:650:ARG:HA	1.91	0.52
3:f:635:ASP:OD1	3:f:704:ARG:NH2	2.42	0.52
3:f:720:LYS:O	3:f:724:THR:HG23	2.10	0.52
1:Po:120:VAL:HG22	1:Po:175:LEU:HB2	1.90	0.52
3:d:387:LEU:HA	3:d:390:LYS:HE2	1.92	0.51
3:a:242:LEU:HB2	3:a:276:LEU:HD11	1.91	0.51
3:e:198:ARG:NH2	3:f:393:ASP:OD1	2.35	0.51
3:d:781:ILE:HG22	3:d:787:ILE:HB	1.92	0.51
3:a:635:ASP:OD1	3:a:704:ARG:NE	2.43	0.51
3:c:320:TYR:OH	3:c:331:GLU:OE2	2.24	0.51
1:Pf:79:ASP:OD1	1:Pg:117:ASN:ND2	2.44	0.51
3:c:232:GLU:HG3	3:c:235:LYS:HE2	1.93	0.51
3:f:575:SER:HA	3:f:578:MET:HE2	1.93	0.51
3:f:757:ASP:HB3	3:f:764:PRO:HG2	1.93	0.51
3:f:699:PRO:O	3:f:703:ASN:ND2	2.34	0.50
1:Pe:9:GLU:OE2	1:Pe:23:ARG:NH1	2.44	0.50
1:Pq:28:ARG:NH2	1:Pq:58:LYS:O	2.43	0.50
1:Pa:139:ALA:O	1:Pa:143:ILE:HG12	2.12	0.50
3:a:246:THR:OG1	3:f:298:ASN:HB2	2.11	0.50
3:b:731:THR:HG22	3:b:741:ILE:HG23	1.92	0.50
3:d:320:TYR:CE1	3:d:324:ILE:HD11	2.46	0.50
3:e:213:GLY:O	3:e:217:ILE:HG12	2.11	0.50
1:Pd:120:VAL:HG22	1:Pd:175:LEU:HB2	1.94	0.50
3:f:521:SER:C	3:f:523:ALA:H	2.19	0.50
3:f:562:MET:HB3	3:f:611:TYR:CE2	2.46	0.50
3:c:295:ASP:OD1	3:c:298:ASN:ND2	2.45	0.50
3:a:318:ASP:OD1	3:a:319:GLU:N	2.44	0.49
3:a:750:LYS:HD2	3:a:796:HIS:CE1	2.47	0.49
1:Pa:151:ASN:ND2	1:Pa:166:GLN:OE1	2.45	0.49
1:Pd:41:ALA:HB2	1:Pd:73:ALA:HB1	1.94	0.49
3:a:393:ASP:OD2	3:f:201:LYS:NZ	2.39	0.49
3:d:777:LEU:O	3:d:781:ILE:HG23	2.12	0.49
3:a:189:ILE:O	3:a:193:ILE:HG12	2.13	0.49
1:Pe:54:GLN:HE22	1:Pf:11:THR:HG21	1.77	0.49
3:d:232:GLU:HA	3:d:235:LYS:HB2	1.94	0.49
1:Pd:151:ASN:ND2	1:Pd:166:GLN:OE1	2.45	0.49
3:c:213:GLY:O	3:c:217:ILE:HG12	2.13	0.49
3:b:320:TYR:OH	3:b:331:GLU:OE2	2.26	0.49
3:c:684:THR:O	3:c:688:THR:HG22	2.12	0.49
3:f:507:HIS:HA	3:f:510:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Pa:9:GLU:OE2	1:Pa:26:LYS:NZ	2.44	0.49
3:c:636:ASP:OD2	3:d:571:ARG:NH1	2.45	0.49
3:e:616:PHE:HB2	3:e:656:MET:HG2	1.94	0.49
3:f:268:ILE:HG23	3:f:274:VAL:HG21	1.95	0.49
1:Pe:72:THR:HG21	1:Pd:95:MET:HB2	1.95	0.49
1:Pe:57:GLU:OE1	3:d:687:LYS:NZ	2.27	0.49
1:Pe:41:ALA:HB2	1:Pe:73:ALA:HB1	1.95	0.48
3:a:511:ILE:HD12	3:a:722:ILE:HD13	1.95	0.48
3:f:232:GLU:HA	3:f:235:LYS:HE2	1.96	0.48
3:d:258:GLU:HG3	3:d:299:ILE:HD11	1.95	0.48
1:Pl:6:THR:N	1:Pm:22:SER:OG	2.42	0.48
3:b:295:ASP:OD1	3:b:298:ASN:ND2	2.45	0.48
3:e:750:LYS:HG3	3:e:796:HIS:CG	2.48	0.48
1:Pi:28:ARG:NH2	1:Pi:58:LYS:O	2.45	0.48
3:a:727:VAL:HG11	3:a:748:LYS:HD3	1.96	0.48
3:b:520:ILE:HD11	3:b:543:PHE:CZ	2.49	0.48
3:c:550:GLY:O	3:c:554:LEU:N	2.45	0.48
3:c:776:ASN:ND2	3:c:803:TYR:OH	2.46	0.48
3:d:589:ALA:O	3:d:642:THR:HG21	2.14	0.48
3:d:789:GLY:O	3:d:808:GLN:NE2	2.34	0.48
1:Pi:115:LEU:HD13	1:Pl:79:ASP:HB3	1.96	0.48
3:d:635:ASP:HB2	3:d:704:ARG:HH11	1.78	0.48
3:a:689:MET:SD	3:a:689:MET:N	2.83	0.48
3:e:254:ARG:HH12	3:f:253:TYR:HD1	1.60	0.48
3:e:174:ALA:HB3	3:e:226:VAL:HG21	1.94	0.48
3:f:574:MET:HE1	3:f:616:PHE:HB3	1.96	0.47
1:Pa:16:ARG:NH2	1:Pb:15:GLU:OE2	2.41	0.47
1:Pf:42:ASN:ND2	1:Pg:21:TYR:OH	2.47	0.47
3:c:635:ASP:HB2	3:c:704:ARG:HH11	1.79	0.47
3:f:517:VAL:HA	3:f:520:ILE:HG22	1.97	0.47
3:b:516:ALA:HB2	3:b:709:ILE:HG21	1.96	0.47
3:b:635:ASP:HB2	3:b:704:ARG:HH11	1.80	0.47
1:Pi:193:GLU:OE1	1:Pl:85:LYS:NZ	2.35	0.47
3:b:619:ILE:HB	3:b:627:PHE:CZ	2.50	0.47
1:Ph:144:LEU:O	1:Ph:148:GLU:HG2	2.15	0.47
3:b:398:ALA:HB1	3:b:471:LEU:HD11	1.96	0.47
3:f:473:GLU:H	3:f:473:GLU:CD	2.22	0.47
3:a:763:ARG:HB2	3:a:764:PRO:HD3	1.97	0.46
1:Pl:8:ILE:HD13	1:Pl:17:ALA:HA	1.95	0.46
3:e:690:LEU:O	3:e:694:LYS:HG2	2.16	0.46
3:f:626:VAL:HA	3:f:629:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Po:63:TYR:HE1	1:Po:91:ILE:HD12	1.81	0.46
3:f:260:ARG:HA	3:f:263:LYS:HG2	1.97	0.46
3:b:515:ASP:OD1	3:b:515:ASP:N	2.47	0.46
3:e:351:LEU:HD11	3:e:391:ALA:HB1	1.96	0.46
1:Pc:120:VAL:HG22	1:Pc:175:LEU:HB2	1.98	0.46
3:a:393:ASP:OD1	3:f:198:ARG:NH2	2.42	0.46
3:c:527:ALA:HB2	3:c:538:ILE:HG23	1.96	0.46
3:d:374:ALA:HB2	3:d:476:ILE:HD13	1.97	0.46
3:d:628:ASN:HB3	3:e:575:SER:HB2	1.96	0.46
3:f:620:GLU:HA	3:f:697:PHE:CZ	2.51	0.46
3:a:772:THR:HG23	3:a:773:ILE:HG13	1.96	0.46
3:f:298:ASN:HA	3:f:301:LYS:HB2	1.98	0.46
3:c:750:LYS:HG3	3:c:796:HIS:CG	2.51	0.46
3:f:641:ASP:OD1	3:f:644:GLY:N	2.48	0.46
1:Pm:93:ILE:HG22	1:Pn:76:ALA:HB1	1.98	0.45
3:b:225:ILE:HD13	3:b:230:VAL:HG11	1.97	0.45
3:d:750:LYS:HG3	3:d:796:HIS:CG	2.51	0.45
3:e:717:GLU:O	3:e:721:GLU:HG3	2.16	0.45
3:c:269:GLN:NE2	3:c:308:GLU:OE1	2.47	0.45
3:f:623:HIS:ND1	3:f:625:ASP:OD1	2.34	0.45
1:Pc:53:ALA:HB2	3:c:671:ALA:HA	1.97	0.45
1:Pc:76:ALA:HB1	1:Pd:93:ILE:HG22	1.98	0.45
3:b:597:ASP:OD1	3:b:597:ASP:N	2.49	0.45
3:d:566:ASP:N	3:d:566:ASP:OD1	2.49	0.45
3:a:784:GLY:C	3:a:785:ASN:HD22	2.25	0.45
3:b:356:ASP:OD1	3:b:356:ASP:N	2.47	0.45
3:c:477:ALA:HA	3:c:480:ILE:HG22	1.99	0.45
3:d:269:GLN:HB2	3:d:308:GLU:OE2	2.16	0.45
3:c:202:ASN:OD1	3:c:202:ASN:N	2.48	0.45
3:f:606:VAL:HA	3:f:610:PRO:HA	1.98	0.45
1:Pb:42:ASN:HD21	1:Pc:31:MET:HG2	1.82	0.45
3:f:574:MET:SD	3:f:616:PHE:HD2	2.40	0.45
3:f:631:LEU:HD13	3:f:700:GLU:HG2	1.99	0.45
1:Pb:41:ALA:CB	1:Pb:73:ALA:HB1	2.47	0.44
1:Pg:53:ALA:HB2	3:a:671:ALA:HA	1.99	0.44
3:b:181:PRO:O	5:b:901:AGS:H2	2.17	0.44
3:c:258:GLU:HG3	3:c:299:ILE:HD11	1.99	0.44
3:e:516:ALA:HB2	3:e:709:ILE:HG21	1.99	0.44
3:f:612:SER:O	3:f:652:THR:HG23	2.18	0.44
3:d:185:ARG:NH1	3:d:188:GLU:OE2	2.50	0.44
1:Pm:113:PHE:HB3	1:Pm:190:MET:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:306:ARG:HE	3:a:308:GLU:CD	2.26	0.44
3:b:232:GLU:HA	3:b:235:LYS:HE2	1.99	0.44
3:b:258:GLU:HG3	3:b:299:ILE:HD11	2.00	0.44
3:b:499:LEU:HD11	3:b:528:ARG:HD3	1.99	0.44
3:c:616:PHE:HB2	3:c:656:MET:HG2	1.99	0.44
1:Pi:19:ASP:OD1	1:Pi:22:SER:N	2.41	0.44
3:b:173:ILE:HG22	3:b:179:LEU:HG	2.00	0.43
3:d:531:LEU:HD23	3:e:734:LEU:HD21	2.00	0.43
1:Pl:23:ARG:HH12	1:Pl:27:ASP:CG	2.26	0.43
3:d:550:GLY:O	3:d:554:LEU:N	2.45	0.43
3:b:713:LYS:HE2	3:b:713:LYS:HB3	1.87	0.43
3:d:166:LEU:HD21	3:d:260:ARG:HD3	2.00	0.43
1:Pe:152:ARG:NH1	1:Pe:156:GLU:OE2	2.50	0.43
3:b:232:GLU:OE1	3:c:407:HIS:NE2	2.50	0.43
3:b:590:PRO:HG2	3:c:581:HIS:ND1	2.33	0.43
3:d:189:ILE:O	3:d:193:ILE:HG12	2.18	0.43
1:Pb:113:PHE:HB3	1:Pb:190:MET:HG3	2.01	0.43
3:a:324:ILE:HG23	3:a:330:LEU:HB3	1.99	0.43
3:c:665:LEU:HD21	3:c:688:THR:HG23	1.99	0.43
3:d:332:ARG:NH1	3:e:389:ASP:OD1	2.49	0.43
3:d:475:ASP:O	3:d:479:VAL:HG23	2.19	0.43
1:Pi:144:LEU:O	1:Pi:148:GLU:HG2	2.19	0.43
3:d:303:ALA:HB1	3:d:308:GLU:HB3	2.01	0.43
3:e:356:ASP:OD1	3:e:356:ASP:N	2.52	0.43
3:f:776:ASN:O	3:f:780:LEU:HG	2.19	0.43
1:Ph:117:ASN:ND2	1:Pi:79:ASP:OD1	2.52	0.43
1:Po:115:LEU:HD13	1:Pq:79:ASP:HB3	1.99	0.43
3:f:584:SER:O	3:f:588:GLY:N	2.40	0.43
3:d:540:SER:N	3:d:706:ASP:OD2	2.45	0.43
1:Pe:110:GLY:N	1:Pe:187:ASP:OD2	2.50	0.43
1:Pq:109:LYS:NZ	1:Pq:157:ARG:O	2.49	0.43
3:b:477:ALA:HA	3:b:480:ILE:HG22	2.01	0.43
3:b:509:ARG:NH2	3:b:553:GLU:OE2	2.44	0.43
3:c:320:TYR:CD1	3:c:324:ILE:HD11	2.53	0.43
3:d:213:GLY:O	3:d:217:ILE:HG12	2.18	0.43
3:d:494:THR:O	3:d:497:GLU:HG3	2.19	0.43
3:f:576:GLU:HG3	3:f:577:PHE:CD1	2.54	0.43
1:Pa:117:ASN:ND2	1:Pg:79:ASP:OD1	2.52	0.42
1:Pl:113:PHE:HB3	1:Pl:190:MET:HG3	2.01	0.42
1:Ph:6:THR:O	1:Pi:22:SER:HB3	2.19	0.42
3:b:568:ALA:HB1	3:b:609:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:284:LEU:HD21	3:e:300:LEU:HD12	2.01	0.42
3:f:775:ASP:OD1	3:f:776:ASN:N	2.53	0.42
1:Pl:93:ILE:HG22	1:Pm:76:ALA:HB1	2.01	0.42
3:a:719:LEU:O	3:a:723:VAL:HG23	2.19	0.42
3:a:732:ASN:OD1	3:a:733:ARG:N	2.52	0.42
3:c:509:ARG:NH1	3:c:560:GLU:OE1	2.37	0.42
3:b:363:ARG:O	3:b:403:ARG:NH2	2.52	0.42
1:Pf:154:LEU:HB3	1:Pf:165:ILE:HD13	2.01	0.42
3:b:574:MET:HE2	3:b:574:MET:HA	2.02	0.42
3:f:535:LYS:NZ	3:f:635:ASP:O	2.51	0.42
1:Pc:41:ALA:CB	1:Pc:73:ALA:HB1	2.48	0.42
1:Po:151:ASN:ND2	1:Po:166:GLN:OE1	2.53	0.42
3:d:525:ARG:NH2	3:e:779:GLU:OE2	2.53	0.42
3:e:362:HIS:NE2	3:e:396:ASP:OD1	2.40	0.42
3:f:544:LEU:HB2	3:f:710:VAL:HG22	2.01	0.42
1:Pg:42:ASN:OD1	1:Pg:42:ASN:C	2.62	0.42
3:a:191:ARG:NH1	3:a:194:GLU:OE2	2.41	0.42
3:a:253:TYR:CE1	3:b:252:LYS:HE3	2.55	0.42
3:d:264:VAL:O	3:d:268:ILE:HG12	2.19	0.42
3:c:590:PRO:HA	3:c:642:THR:HG21	2.00	0.42
1:Pc:132:GLN:O	1:Pc:135:GLU:N	2.51	0.42
3:a:721:GLU:O	3:a:725:MET:HG3	2.19	0.42
1:Pe:41:ALA:CB	1:Pe:73:ALA:HB1	2.50	0.42
3:f:191:ARG:O	3:f:195:VAL:HG23	2.20	0.42
3:f:228:ASN:O	3:f:235:LYS:NZ	2.41	0.42
1:Pc:79:ASP:OD1	1:Pd:117:ASN:ND2	2.53	0.41
3:c:565:ASP:OD1	3:c:566:ASP:N	2.53	0.41
3:d:617:ASP:OD2	3:d:618:GLU:OE1	2.37	0.41
3:e:596:HIS:HE1	3:e:642:THR:HG22	1.85	0.41
1:Pg:41:ALA:CB	1:Pg:73:ALA:HB1	2.50	0.41
3:d:690:LEU:O	3:d:694:LYS:HG2	2.20	0.41
3:e:295:ASP:OD2	3:e:297:SER:OG	2.22	0.41
3:f:209:GLU:HG3	3:f:386:PHE:CZ	2.55	0.41
3:a:510:VAL:HG11	3:a:554:LEU:HD13	2.01	0.41
3:c:516:ALA:HB2	3:c:709:ILE:HG21	2.03	0.41
3:f:683:GLU:OE1	3:f:686:ARG:HD3	2.21	0.41
3:b:788:GLU:OE1	3:b:788:GLU:N	2.46	0.41
3:b:228:ASN:O	3:b:228:ASN:ND2	2.46	0.41
3:e:199:ARG:HG3	3:f:361:HIS:CD2	2.55	0.41
3:b:544:LEU:HD21	3:b:689:MET:HG2	2.02	0.41
1:Pg:67:PRO:HA	1:Pg:95:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:763:ARG:N	3:e:764:PRO:HD2	2.36	0.41
1:Pb:53:ALA:HB2	3:b:671:ALA:HA	2.03	0.41
1:Pf:9:GLU:O	1:Pf:10:THR:OG1	2.30	0.41
1:Pl:144:LEU:O	1:Pl:148:GLU:HG2	2.21	0.41
3:a:385:ARG:HG2	3:a:385:ARG:HH11	1.86	0.41
3:a:704:ARG:HA	3:b:767:ARG:HH21	1.86	0.41
3:c:606:VAL:HG21	3:c:649:PHE:CE2	2.56	0.41
3:d:200:THR:OG1	3:d:201:LYS:N	2.53	0.41
3:e:628:ASN:OD1	3:e:698:ARG:NH1	2.54	0.41
3:f:185:ARG:NH1	3:f:188:GLU:OE2	2.43	0.41
3:f:493:GLU:HA	3:f:496:SER:HB3	2.02	0.41
3:f:518:ASN:O	3:f:522:LYS:HD3	2.21	0.41
3:f:521:SER:HA	3:f:524:VAL:HG12	2.02	0.41
3:f:562:MET:HB3	3:f:611:TYR:CZ	2.56	0.41
3:f:591:PRO:HA	3:f:596:HIS:CD2	2.56	0.41
3:f:620:GLU:HA	3:f:697:PHE:HZ	1.86	0.41
3:c:264:VAL:O	3:c:268:ILE:HG12	2.20	0.40
3:e:164:ASP:CG	3:e:238:ARG:HH22	2.29	0.40
1:Pd:41:ALA:CB	1:Pd:73:ALA:HB1	2.50	0.40
1:Pd:42:ASN:OD1	1:Pd:42:ASN:C	2.64	0.40
1:Pm:67:PRO:HA	1:Pm:95:MET:HE3	2.03	0.40
3:c:351:LEU:HD11	3:c:391:ALA:HB1	2.03	0.40
3:c:574:MET:HB3	3:c:622:ALA:HB2	2.03	0.40
1:Pl:18:TYR:HB3	1:Pl:22:SER:HB2	2.04	0.40
3:b:531:LEU:HD23	3:c:734:LEU:HD21	2.03	0.40
1:Pg:85:LYS:HB2	1:Pg:86:PRO:HD3	2.03	0.40
1:Pn:67:PRO:HA	1:Pn:95:MET:HE3	2.04	0.40
3:b:662:ALA:O	3:b:665:LEU:HD23	2.21	0.40
3:e:475:ASP:O	3:e:479:VAL:HG23	2.22	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	Pa	188/195 (96%)	184 (98%)	3 (2%)	1 (0%)	24	60
1	Pb	188/195 (96%)	185 (98%)	2 (1%)	1 (0%)	24	60
1	Pc	187/195 (96%)	184 (98%)	2 (1%)	1 (0%)	24	60
1	Pd	188/195 (96%)	183 (97%)	5 (3%)	0	100	100
1	Pe	186/195 (95%)	183 (98%)	2 (1%)	1 (0%)	24	60
1	Pf	188/195 (96%)	181 (96%)	6 (3%)	1 (0%)	24	60
1	Pg	178/195 (91%)	171 (96%)	5 (3%)	2 (1%)	11	43
1	Ph	179/195 (92%)	174 (97%)	5 (3%)	0	100	100
1	Pi	178/195 (91%)	175 (98%)	3 (2%)	0	100	100
1	Pl	178/195 (91%)	175 (98%)	3 (2%)	0	100	100
1	Pm	180/195 (92%)	175 (97%)	5 (3%)	0	100	100
1	Pn	179/195 (92%)	175 (98%)	3 (2%)	1 (1%)	21	56
1	Po	175/195 (90%)	172 (98%)	3 (2%)	0	100	100
1	Pq	175/195 (90%)	171 (98%)	3 (2%)	1 (1%)	21	56
3	a	510/818 (62%)	481 (94%)	24 (5%)	5 (1%)	12	45
3	b	575/818 (70%)	556 (97%)	19 (3%)	0	100	100
3	c	582/818 (71%)	566 (97%)	15 (3%)	1 (0%)	43	76
3	d	566/818 (69%)	546 (96%)	19 (3%)	1 (0%)	43	76
3	e	576/818 (70%)	558 (97%)	17 (3%)	1 (0%)	43	76
3	f	558/818 (68%)	527 (94%)	28 (5%)	3 (0%)	24	60
All	All	5914/7638 (77%)	5722 (97%)	172 (3%)	20 (0%)	37	70

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	550	GLY
1	Pg	94	GLY
3	a	511	ILE
3	e	550	GLY
1	Pb	12	ASN
1	Pc	94	GLY
1	Pf	38	ASP
1	Pg	38	ASP
3	a	761	GLY
3	a	762	ALA
3	f	577	PHE

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Mol	Chain	Res	Type
1	Pa	94	GLY
1	Pe	94	GLY
3	a	763	ARG
3	a	550	GLY
3	c	550	GLY
3	f	610	PRO
3	f	668	GLN
1	Pn	94	GLY
1	Pq	94	GLY

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	Pa	158/163 (97%)	158 (100%)	0	100	100
1	Pb	158/163 (97%)	158 (100%)	0	100	100
1	Pc	157/163 (96%)	153 (98%)	4 (2%)	42	72
1	Pd	158/163 (97%)	156 (99%)	2 (1%)	61	81
1	Pe	155/163 (95%)	152 (98%)	3 (2%)	50	76
1	Pf	158/163 (97%)	155 (98%)	3 (2%)	50	76
1	Pg	151/163 (93%)	148 (98%)	3 (2%)	48	76
1	Ph	152/163 (93%)	150 (99%)	2 (1%)	61	81
1	Pi	151/163 (93%)	150 (99%)	1 (1%)	76	86
1	Pl	151/163 (93%)	148 (98%)	3 (2%)	48	76
1	Pm	153/163 (94%)	151 (99%)	2 (1%)	61	81
1	Pn	152/163 (93%)	150 (99%)	2 (1%)	61	81
1	Po	149/163 (91%)	147 (99%)	2 (1%)	61	81
1	Pq	149/163 (91%)	146 (98%)	3 (2%)	48	76
3	a	453/695 (65%)	450 (99%)	3 (1%)	76	86
3	b	496/695 (71%)	490 (99%)	6 (1%)	63	82
3	c	503/695 (72%)	502 (100%)	1 (0%)	87	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	d	493/695 (71%)	484 (98%)	9 (2%)	51	77
3	e	498/695 (72%)	494 (99%)	4 (1%)	73	86
3	f	489/695 (70%)	481 (98%)	8 (2%)	55	79
All	All	5084/6452 (79%)	5023 (99%)	61 (1%)	61	82

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Pc	82	GLN
1	Pc	85	LYS
1	Pc	120	VAL
1	Pc	182	GLU
1	Pd	82	GLN
1	Pd	120	VAL
1	Pe	23	ARG
1	Pe	120	VAL
1	Pe	178	GLU
1	Pf	7	VAL
1	Pf	38	ASP
1	Pf	120	VAL
1	Pg	23	ARG
1	Pg	42	ASN
1	Pg	109	LYS
1	Ph	24	LEU
1	Ph	120	VAL
1	Pi	120	VAL
1	Pl	72	THR
1	Pl	120	VAL
1	Pl	121	MET
1	Pm	16	ARG
1	Pm	120	VAL
1	Pn	82	GLN
1	Pn	119	GLU
1	Po	120	VAL
1	Po	182	GLU
1	Pq	23	ARG
1	Pq	120	VAL
1	Pq	121	MET
3	a	365	ASN
3	a	553	GLU
3	a	751	ILE

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Mol	Chain	Res	Type
3	b	228	ASN
3	b	309	LEU
3	b	356	ASP
3	b	574	MET
3	b	665	LEU
3	b	785	ASN
3	c	531	LEU
3	d	171	THR
3	d	228	ASN
3	d	493	GLU
3	d	497	GLU
3	d	547	THR
3	d	566	ASP
3	d	618	GLU
3	d	665	LEU
3	d	670	PHE
3	e	294	ILE
3	e	576	GLU
3	e	665	LEU
3	e	684	THR
3	f	275	ILE
3	f	339	VAL
3	f	473	GLU
3	f	476	ILE
3	f	607	ARG
3	f	630	LEU
3	f	653	ILE
3	f	737	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	Pa	47	GLN
1	Pa	142	HIS
1	Pb	42	ASN
1	Pb	47	GLN
1	Pb	151	ASN
1	Pc	12	ASN
1	Pc	47	GLN
1	Pc	132	GLN
1	Pc	151	ASN
1	Pc	160	GLN

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Mol	Chain	Res	Type
1	Pd	47	GLN
1	Pd	82	GLN
1	Pd	83	HIS
1	Pe	47	GLN
1	Pe	151	ASN
1	Pf	42	ASN
1	Pf	47	GLN
1	Pf	52	GLN
1	Pf	117	ASN
1	Pf	151	ASN
1	Pf	160	GLN
1	Ph	47	GLN
1	Ph	54	GLN
1	Ph	117	ASN
1	Pi	47	GLN
1	Pi	117	ASN
1	Pl	117	ASN
1	Pm	47	GLN
1	Pm	160	GLN
1	Pn	117	ASN
1	Pn	160	GLN
1	Po	47	GLN
1	Po	83	HIS
1	Po	142	HIS
1	Pq	47	GLN
1	Pq	142	HIS
1	Pq	151	ASN
3	a	298	ASN
3	a	365	ASN
3	a	507	HIS
3	a	623	HIS
3	b	379	ASN
3	b	776	ASN
3	c	159	ASN
3	c	668	GLN
3	c	738	ASN
3	c	776	ASN
3	d	159	ASN
3	d	269	GLN
3	d	738	ASN
3	d	740	ASN
3	d	776	ASN

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Mol	Chain	Res	Type
3	d	786	GLN
3	e	310	GLN
3	e	581	HIS
3	e	668	GLN
3	e	776	ASN
3	e	786	GLN
3	f	228	ASN
3	f	361	HIS
3	f	728	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	e	901	6	28,29,29	1.40	4 (14%)	43,45,45	1.84	7 (16%)
5	AGS	c	901	-	32,33,33	0.52	1 (3%)	45,52,52	0.68	1 (2%)
4	ADP	b	902	-	28,29,29	1.39	5 (17%)	43,45,45	1.83	7 (16%)
5	AGS	c	902	6	32,33,33	0.54	0	45,52,52	0.71	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AGS	d	901	6	32,33,33	0.54	1 (3%)	45,52,52	0.69	1 (2%)
5	AGS	e	902	6	32,33,33	0.53	1 (3%)	45,52,52	0.69	1 (2%)
4	ADP	f	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.77	7 (16%)
4	ADP	a	901	-	28,29,29	1.39	5 (17%)	43,45,45	1.77	8 (18%)
5	AGS	d	902	6	32,33,33	0.54	1 (3%)	45,52,52	0.63	1 (2%)
5	AGS	b	901	6	32,33,33	0.58	1 (3%)	45,52,52	0.65	1 (2%)

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	901	6	-	2/16/32/32	0/3/3/3
5	AGS	c	901	-	-	1/21/38/38	0/3/3/3
4	ADP	b	902	-	-	5/16/32/32	0/3/3/3
5	AGS	c	902	6	-	1/21/38/38	0/3/3/3
5	AGS	d	901	6	-	2/21/38/38	0/3/3/3
5	AGS	e	902	6	-	0/21/38/38	0/3/3/3
4	ADP	f	901	-	-	5/16/32/32	0/3/3/3
4	ADP	a	901	-	-	1/16/32/32	0/3/3/3
5	AGS	d	902	6	-	0/21/38/38	0/3/3/3
5	AGS	b	901	6	-	1/21/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	901	ADP	C5-C4	4.73	1.47	1.39
4	f	901	ADP	C5-C4	4.72	1.47	1.39
4	a	901	ADP	C5-C4	4.60	1.47	1.39
4	b	902	ADP	C5-C4	4.47	1.47	1.39
4	f	901	ADP	C5-C6	2.67	1.48	1.41
4	b	902	ADP	C5-N7	-2.64	1.34	1.39
4	a	901	ADP	C5-C6	2.60	1.48	1.41
4	e	901	ADP	C5-C6	2.58	1.48	1.41
4	e	901	ADP	C5-N7	-2.47	1.34	1.39
4	b	902	ADP	C5-C6	2.46	1.47	1.41
4	a	901	ADP	C5-N7	-2.36	1.34	1.39
4	f	901	ADP	C8-N7	2.31	1.36	1.31
4	f	901	ADP	C5-N7	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	901	ADP	C8-N7	2.31	1.36	1.31
5	d	902	AGS	PG-S1G	2.25	1.95	1.90
4	b	902	ADP	C8-N7	2.21	1.35	1.31
4	e	901	ADP	C8-N7	2.21	1.35	1.31
5	b	901	AGS	PG-S1G	2.13	1.95	1.90
5	e	902	AGS	PG-S1G	2.09	1.95	1.90
5	c	901	AGS	PG-S1G	2.06	1.95	1.90
5	d	901	AGS	PG-S1G	2.05	1.95	1.90
4	a	901	ADP	C4-N9	-2.02	1.33	1.37
4	b	902	ADP	C4-N9	-2.02	1.33	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	901	ADP	C5-C4-N3	-6.42	117.88	126.72
4	b	902	ADP	C5-C4-N3	-6.04	118.40	126.72
4	f	901	ADP	C5-C4-N3	-5.94	118.53	126.72
4	a	901	ADP	C5-C4-N3	-5.69	118.88	126.72
4	e	901	ADP	N3-C4-N9	5.10	135.84	127.17
4	f	901	ADP	N3-C4-N9	4.64	135.05	127.17
4	b	902	ADP	N3-C4-N9	4.43	134.70	127.17
4	a	901	ADP	N3-C4-N9	4.40	134.65	127.17
4	e	901	ADP	C2-N3-C4	3.81	121.12	111.83
4	f	901	ADP	C2-N3-C4	3.70	120.86	111.83
4	b	902	ADP	C2-N3-C4	3.59	120.59	111.83
5	d	901	AGS	PB-O3B-PG	-3.58	120.07	133.17
4	a	901	ADP	C2-N3-C4	3.57	120.54	111.83
5	c	902	AGS	PB-O3B-PG	-3.55	120.18	133.17
4	b	902	ADP	C4-C5-N7	-3.51	106.56	110.58
5	e	902	AGS	PB-O3B-PG	-3.50	120.36	133.17
4	a	901	ADP	C4-C5-N7	-3.46	106.62	110.58
4	f	901	ADP	C4-C5-N7	-3.45	106.63	110.58
5	b	901	AGS	PB-O3B-PG	-3.41	120.67	133.17
5	c	901	AGS	PB-O3B-PG	-3.41	120.71	133.17
4	e	901	ADP	C4-C5-N7	-3.27	106.84	110.58
5	d	902	AGS	PB-O3B-PG	-3.15	121.62	133.17
4	f	901	ADP	N3-C2-N1	-3.14	123.83	128.58
4	b	902	ADP	O4'-C1'-N9	3.09	114.02	108.09
4	a	901	ADP	N3-C2-N1	-3.03	123.99	128.58
4	e	901	ADP	N3-C2-N1	-3.02	124.00	128.58
4	b	902	ADP	N3-C2-N1	-2.83	124.30	128.58
4	a	901	ADP	C4-N9-C8	2.51	108.37	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	901	ADP	C5-N7-C8	2.47	107.33	103.45
4	a	901	ADP	C5-N7-C8	2.44	107.29	103.45
4	e	901	ADP	C5-N7-C8	2.40	107.22	103.45
4	b	902	ADP	C5-N7-C8	2.39	107.21	103.45
4	f	901	ADP	C4-N9-C8	2.38	108.24	105.74
4	e	901	ADP	C4-N9-C8	2.21	108.06	105.74
4	a	901	ADP	C6-C5-N7	2.06	136.06	132.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

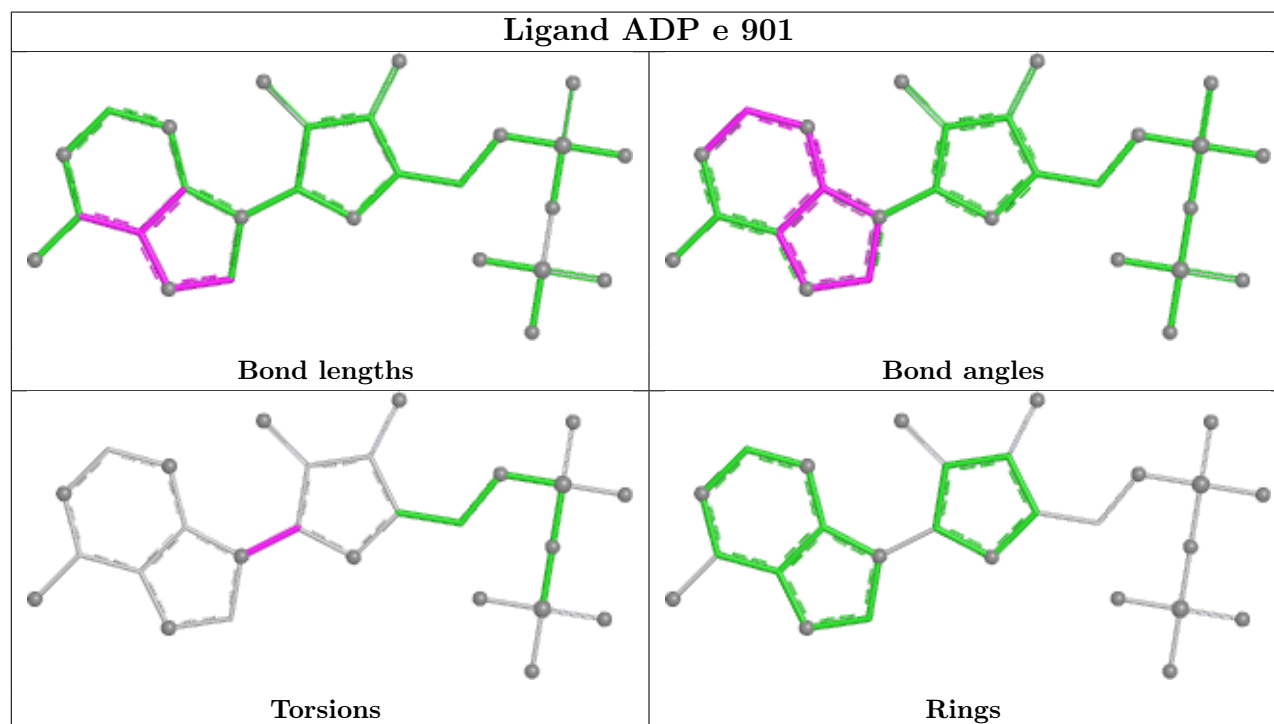
Mol	Chain	Res	Type	Atoms
4	b	902	ADP	C5'-O5'-PA-O2A
4	b	902	ADP	C5'-O5'-PA-O3A
4	f	901	ADP	C5'-O5'-PA-O1A
4	f	901	ADP	O4'-C4'-C5'-O5'
5	d	901	AGS	PA-O3A-PB-O1B
4	b	902	ADP	PA-O3A-PB-O1B
4	a	901	ADP	PA-O3A-PB-O3B
4	f	901	ADP	C3'-C4'-C5'-O5'
4	f	901	ADP	C5'-O5'-PA-O2A
4	f	901	ADP	C5'-O5'-PA-O3A
5	c	902	AGS	PA-O3A-PB-O2B
4	e	901	ADP	C2'-C1'-N9-C4
5	d	901	AGS	PA-O3A-PB-O2B
4	b	902	ADP	PA-O3A-PB-O2B
4	b	902	ADP	PA-O3A-PB-O3B
4	e	901	ADP	C2'-C1'-N9-C8
5	c	901	AGS	PG-O3B-PB-O1B
5	b	901	AGS	O4'-C4'-C5'-O5'

There are no ring outliers.

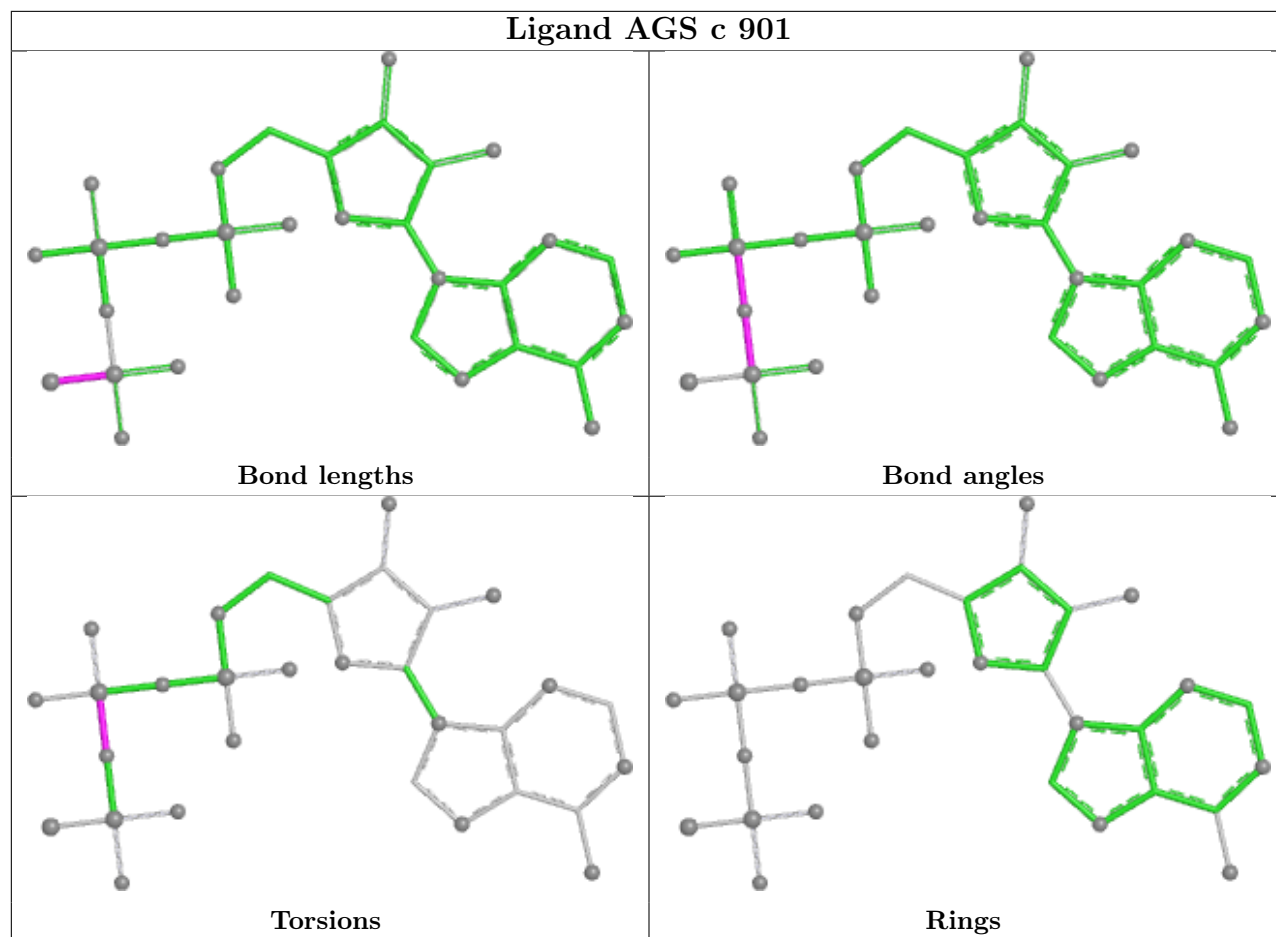
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	c	901	AGS	1	0
5	c	902	AGS	1	0
5	d	901	AGS	1	0
4	a	901	ADP	1	0
5	d	902	AGS	1	0
5	b	901	AGS	1	0

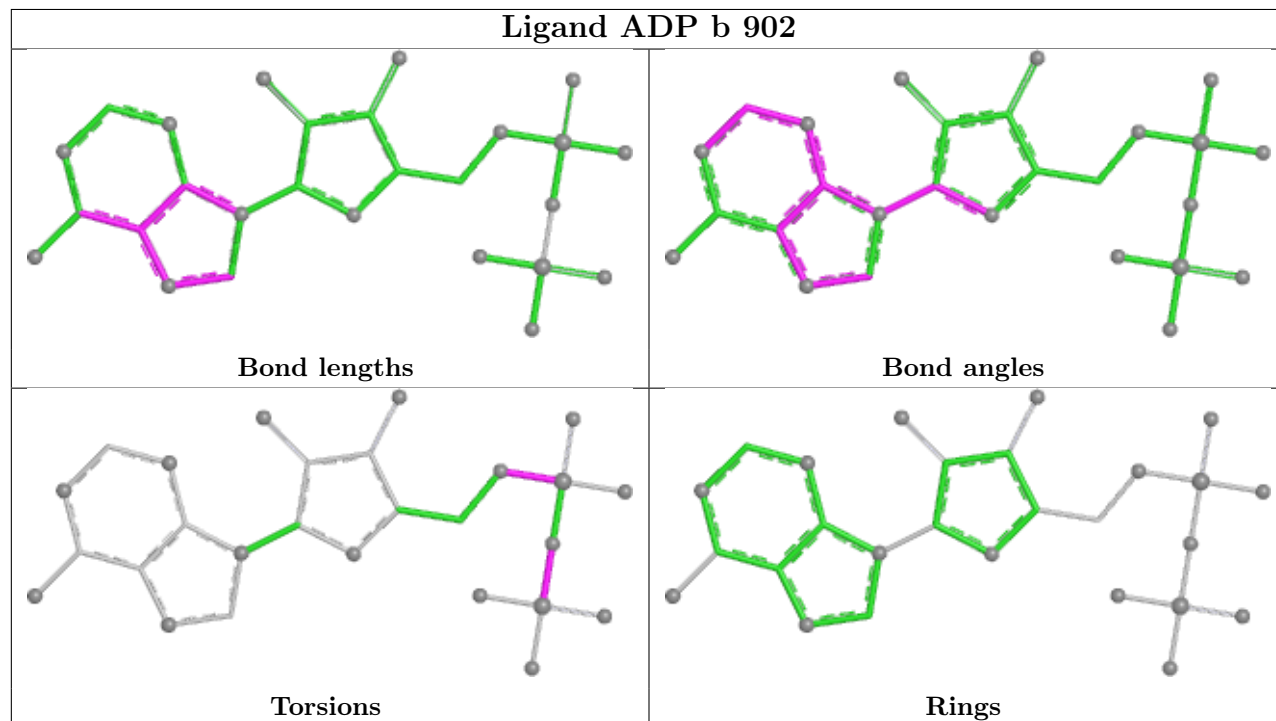
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

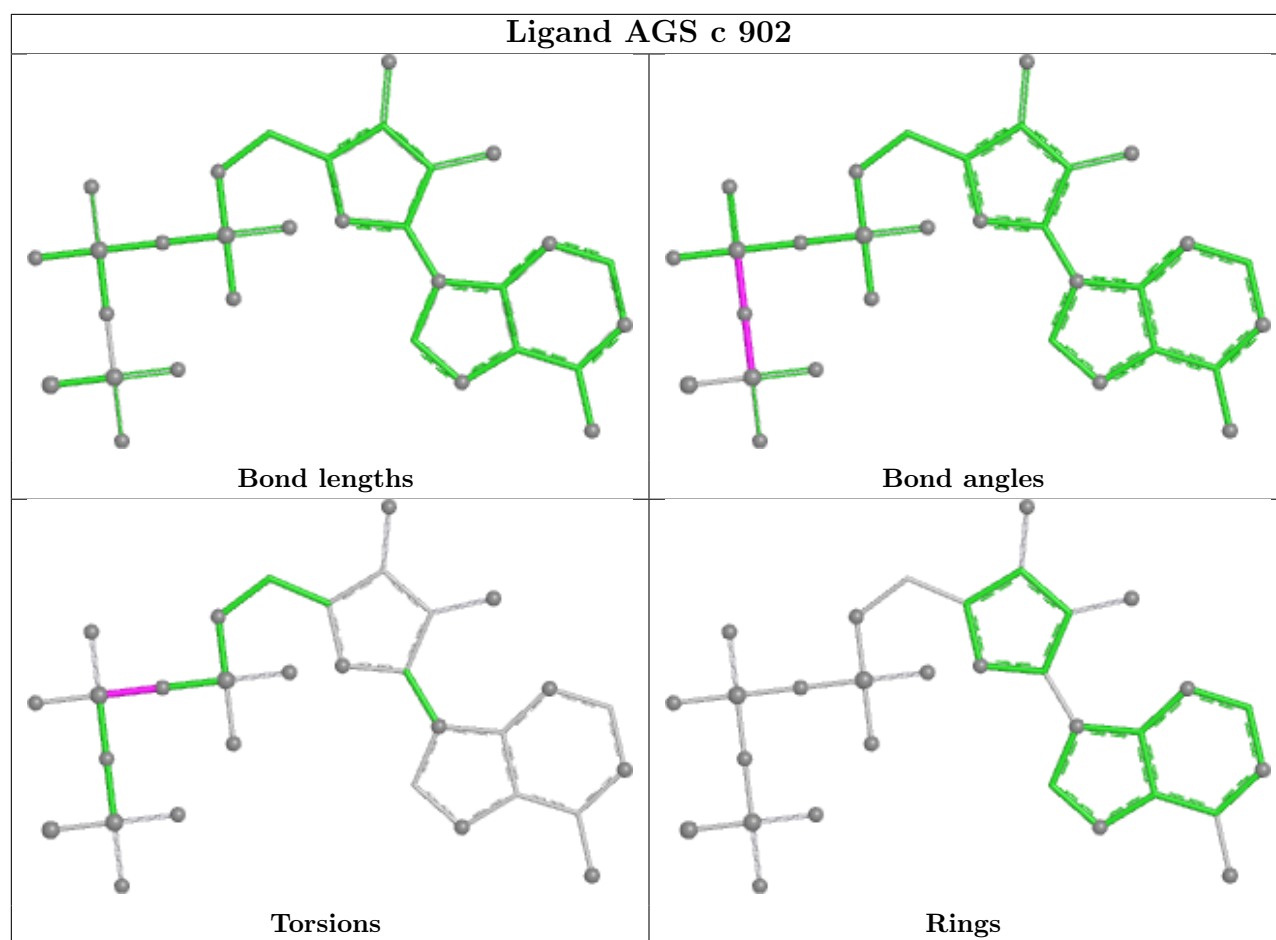


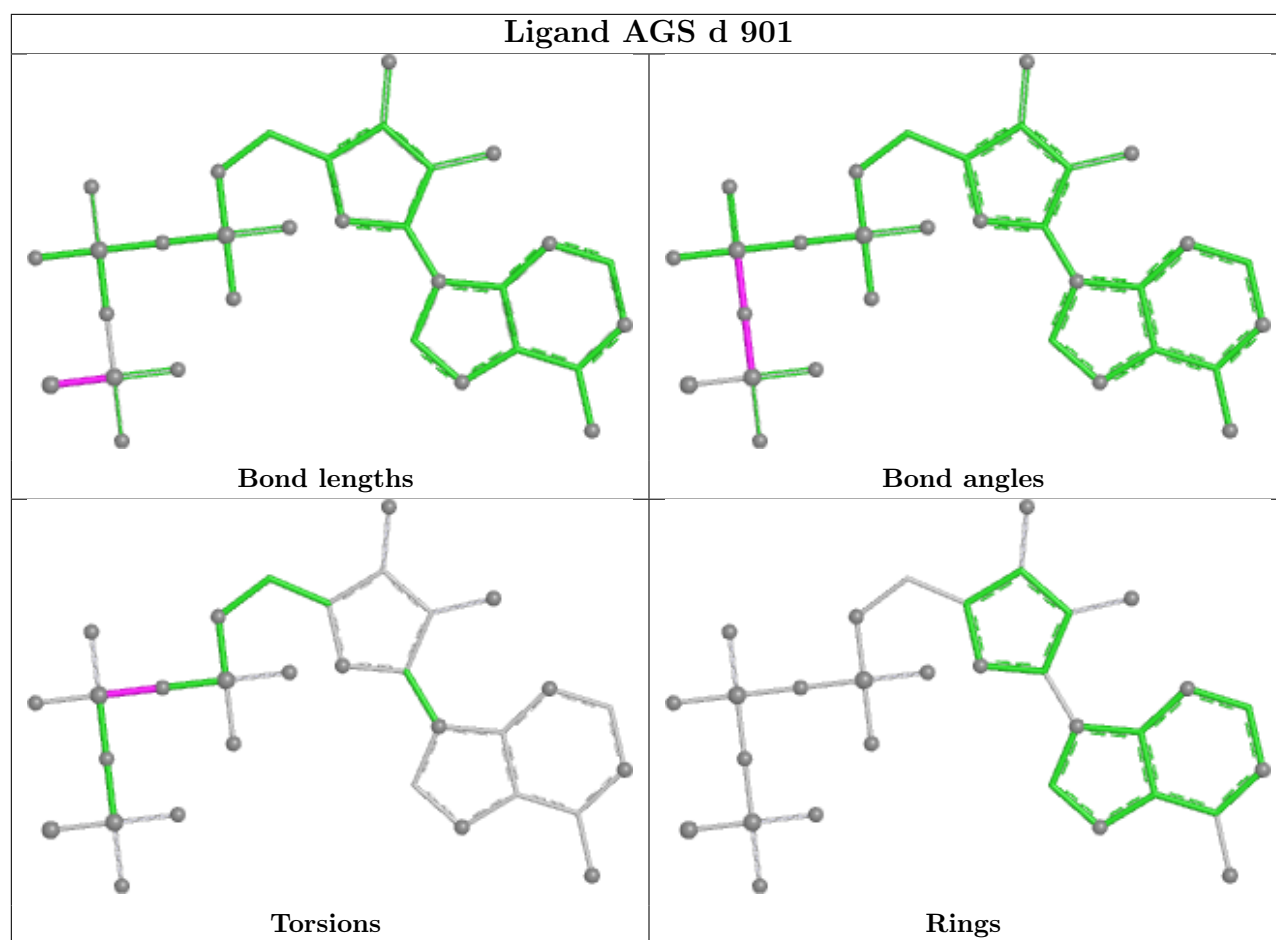
Ligand AGS c 901

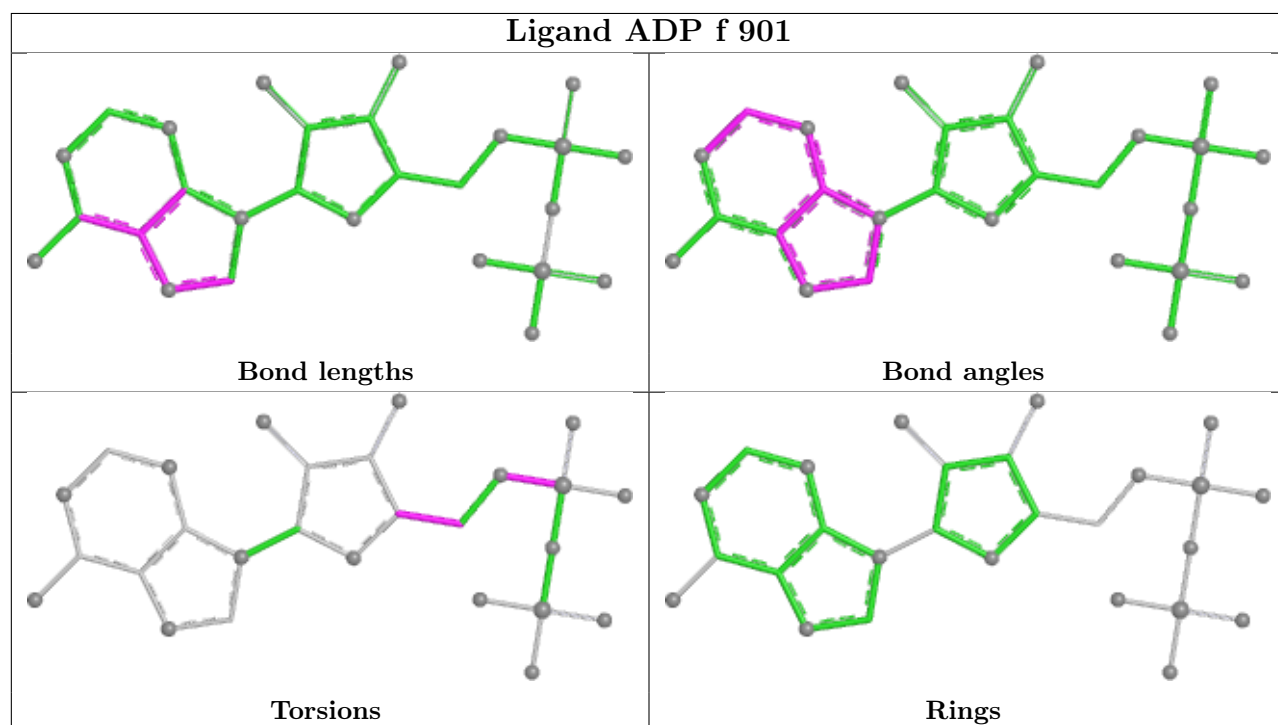
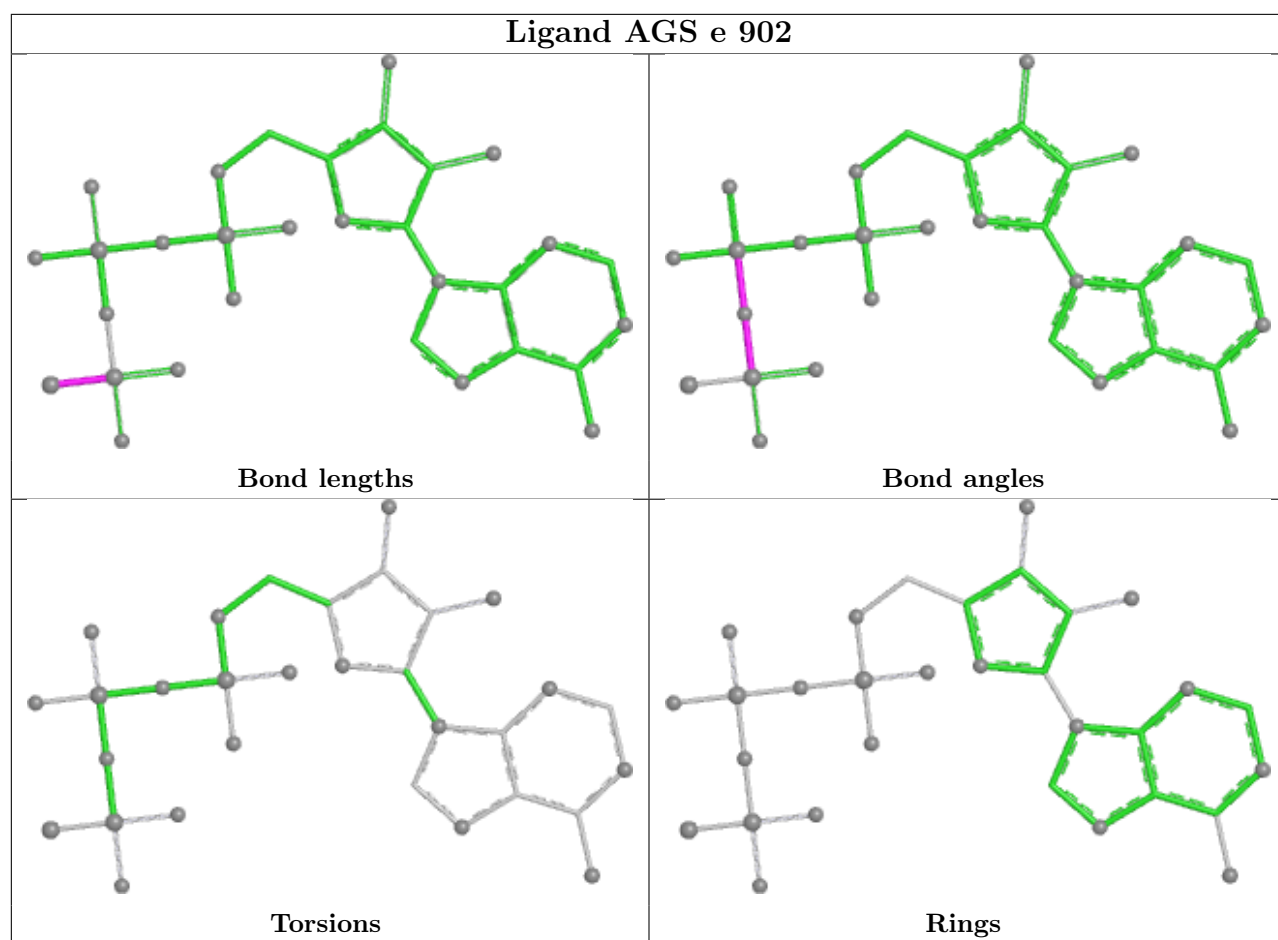


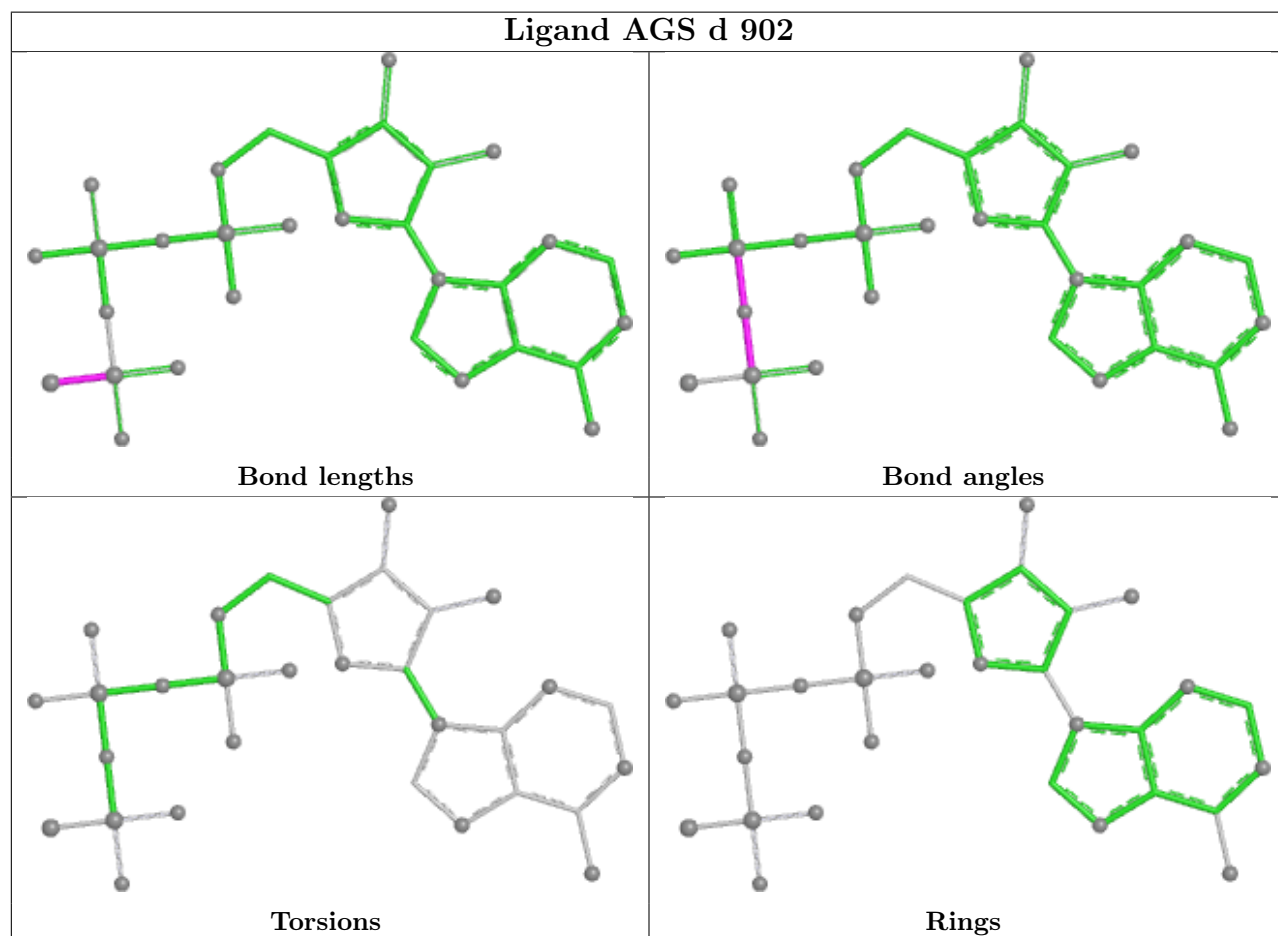
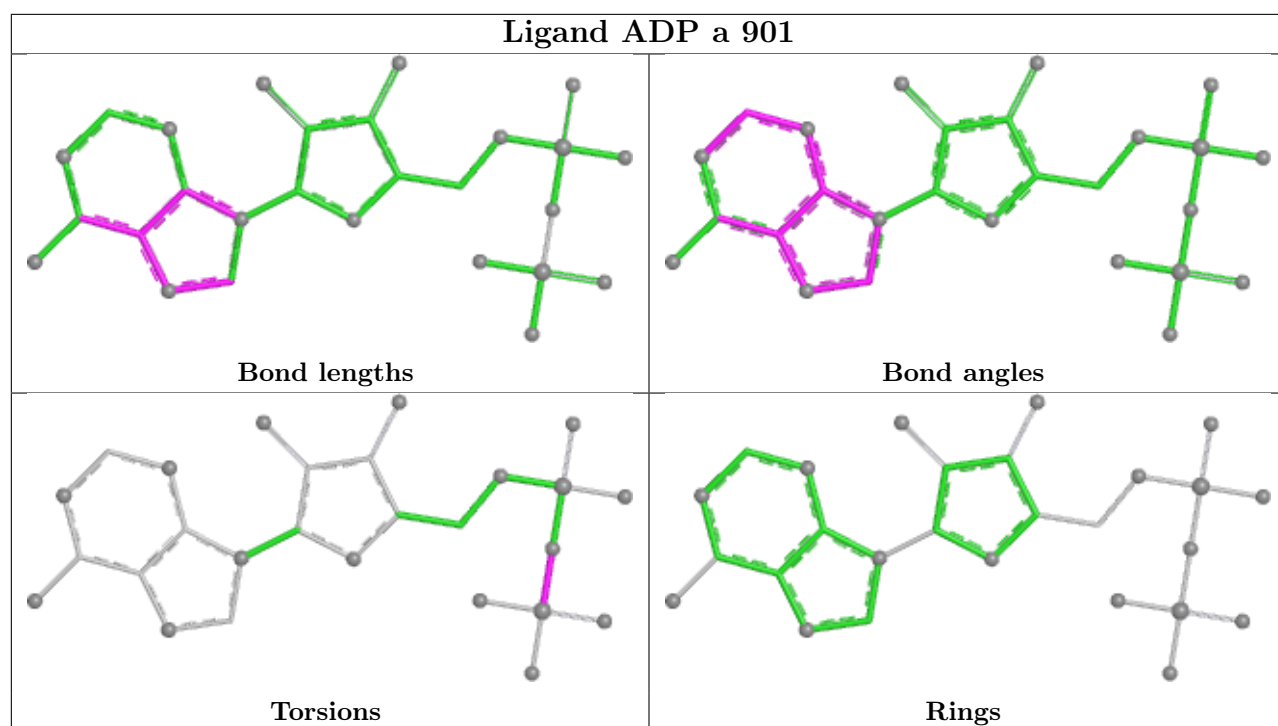
Ligand ADP b 902

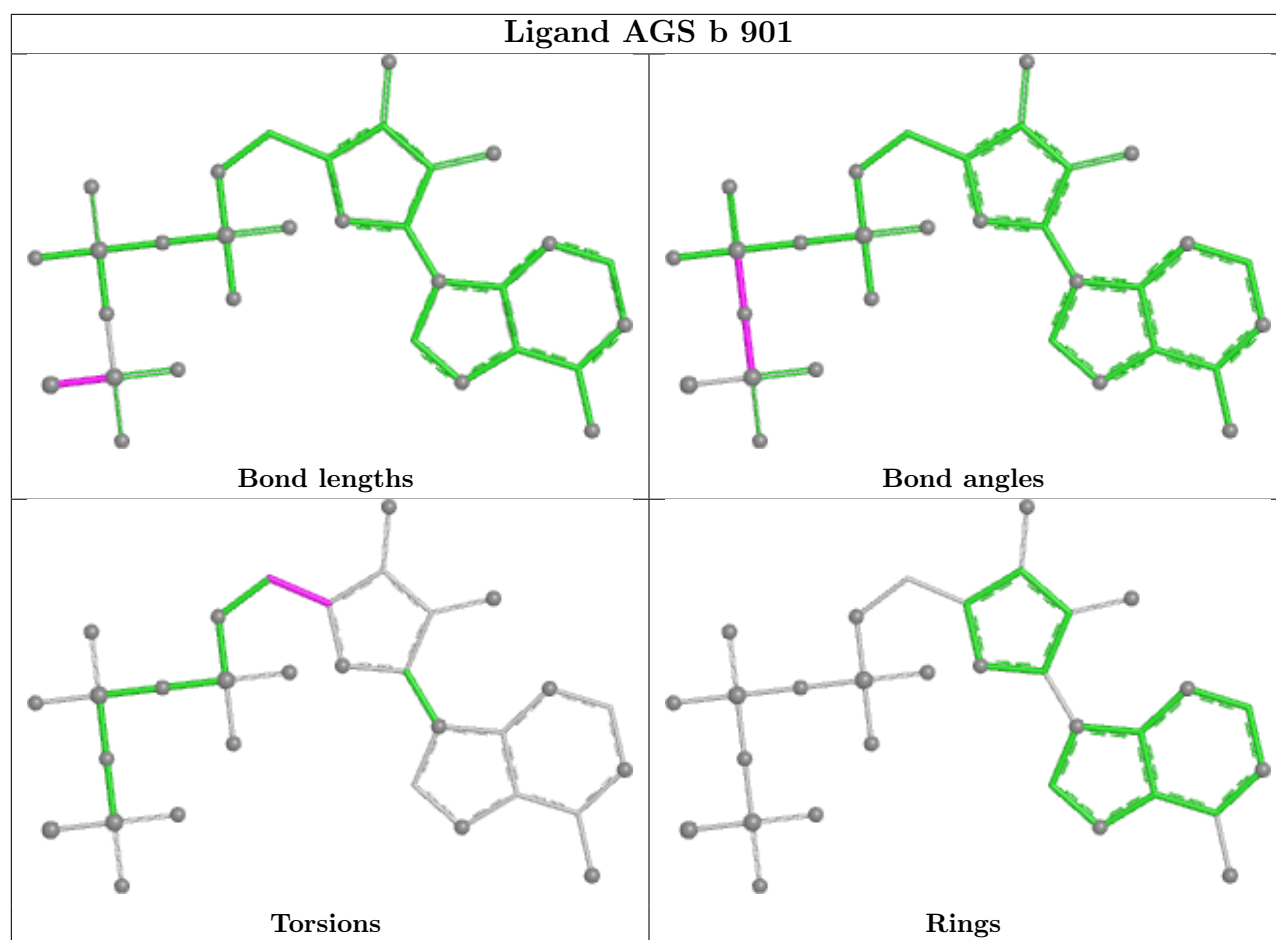












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

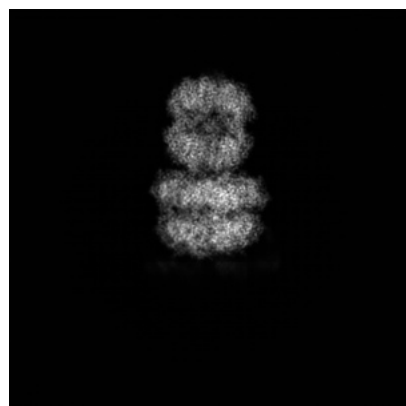
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51367. These allow visual inspection of the internal detail of the map and identification of artifacts.

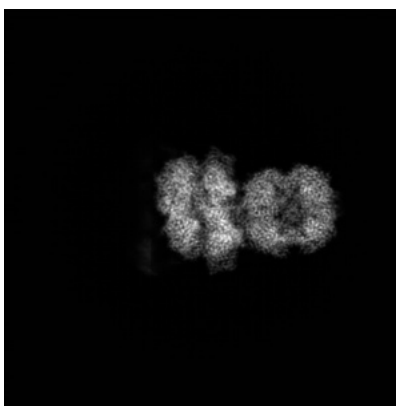
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

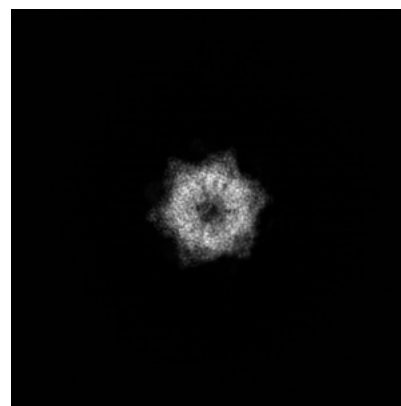
6.1.1 Primary map



X

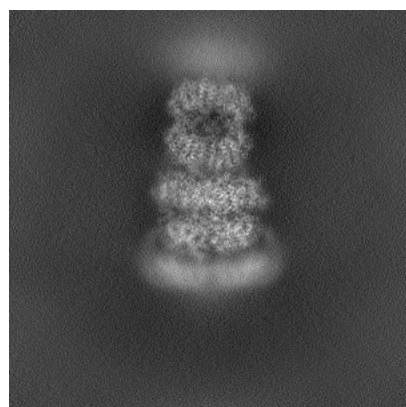


Y

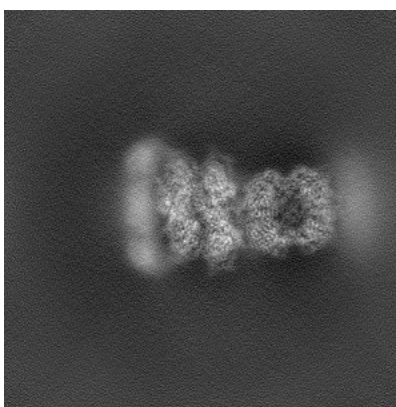


Z

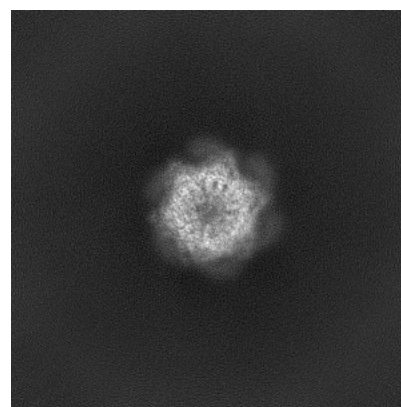
6.1.2 Raw map



X



Y

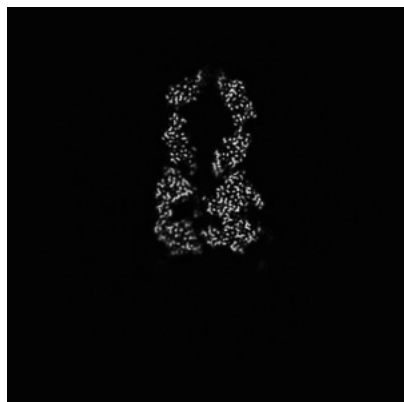


Z

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

6.2 Central slices [i](#)

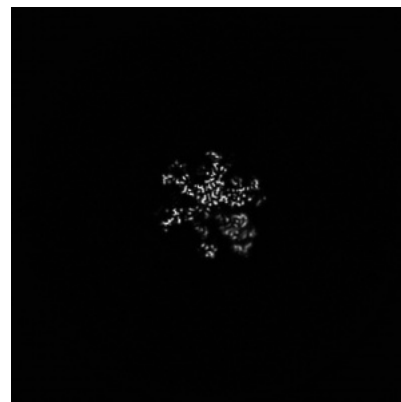
6.2.1 Primary map



X Index: 200

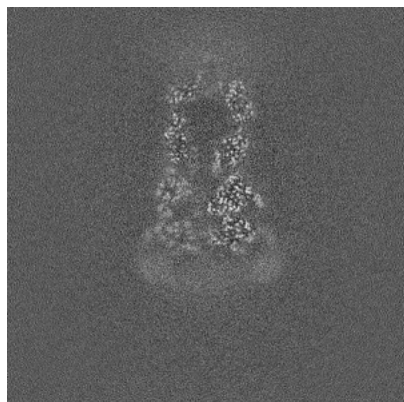


Y Index: 200

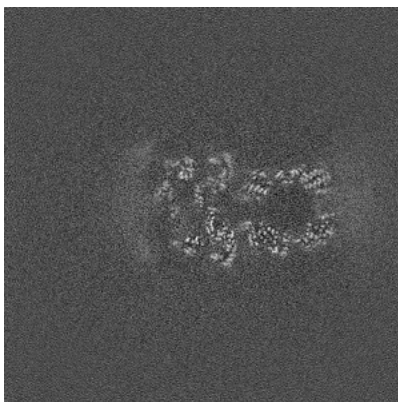


Z Index: 200

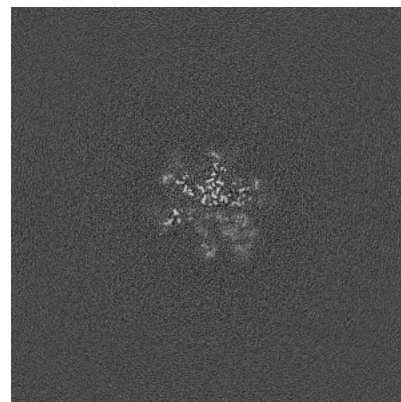
6.2.2 Raw map



X Index: 200



Y Index: 200

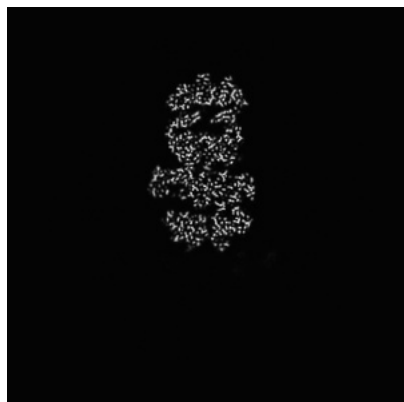


Z Index: 200

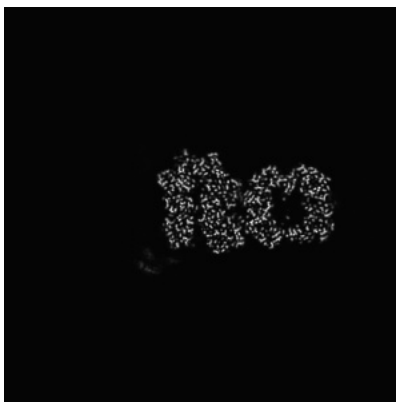
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

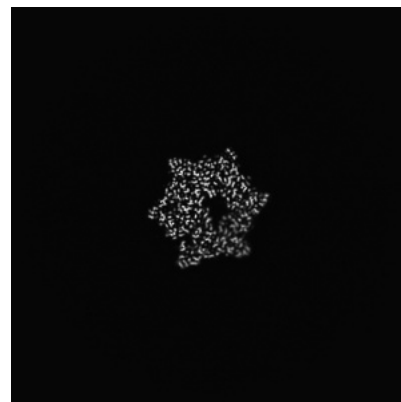
6.3.1 Primary map



X Index: 177

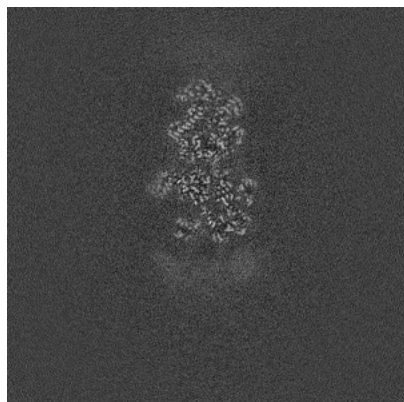


Y Index: 218

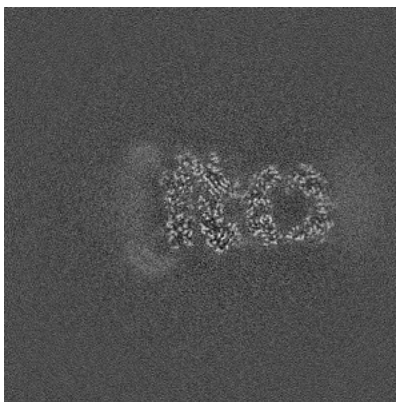


Z Index: 217

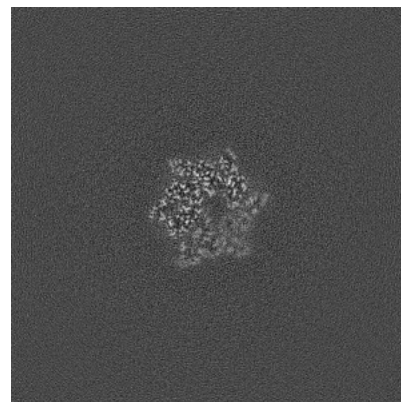
6.3.2 Raw map



X Index: 171



Y Index: 216

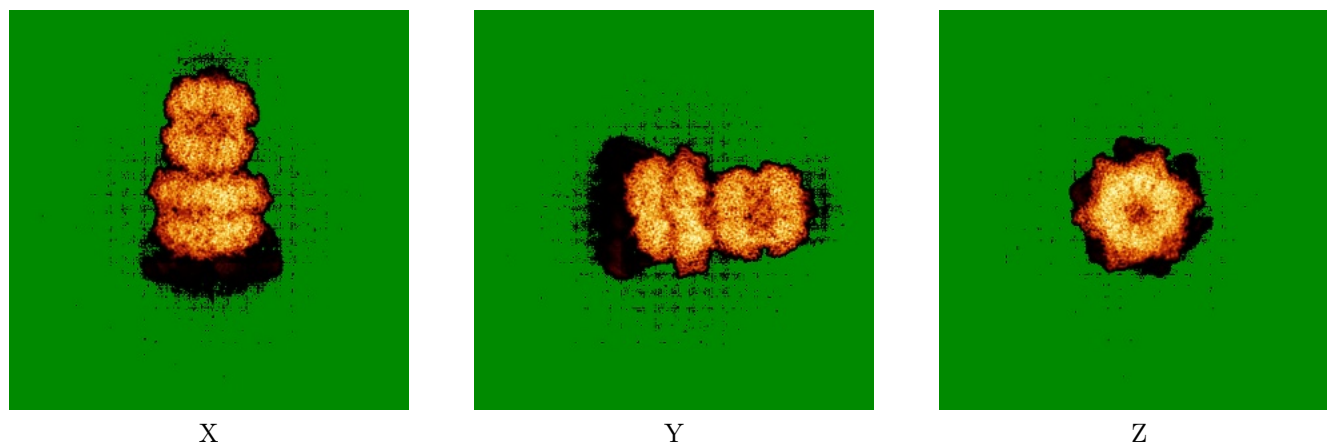


Z Index: 217

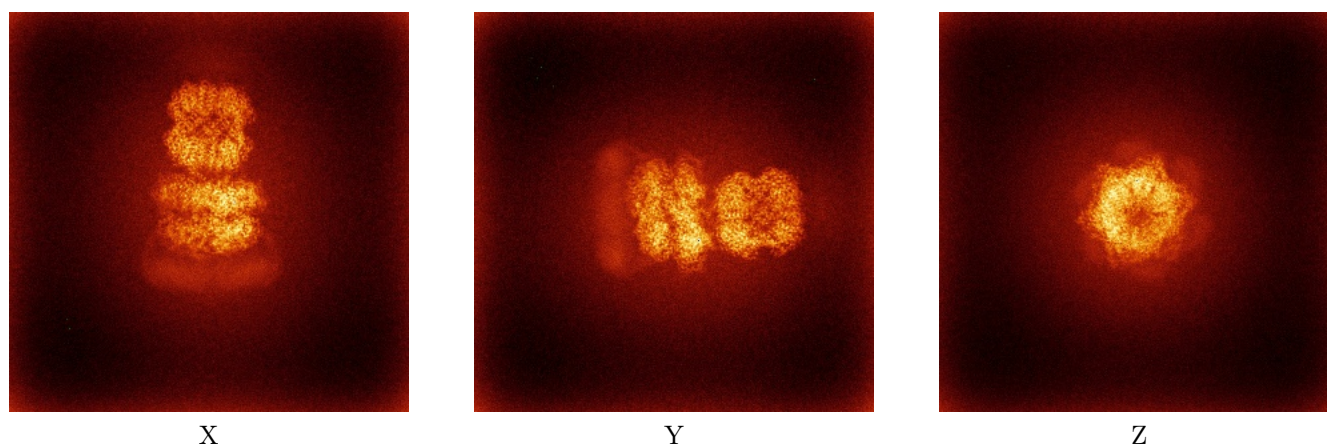
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

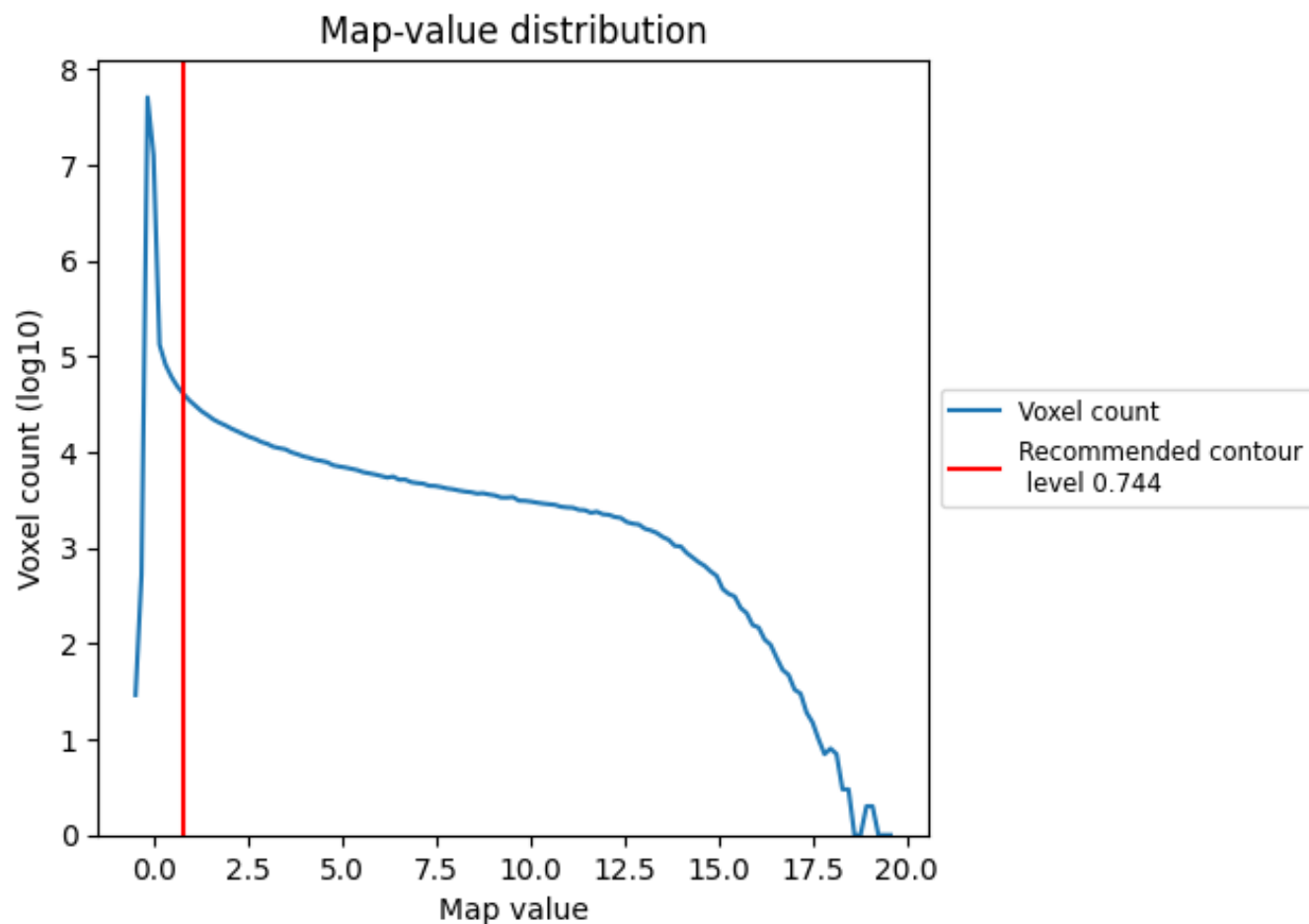
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

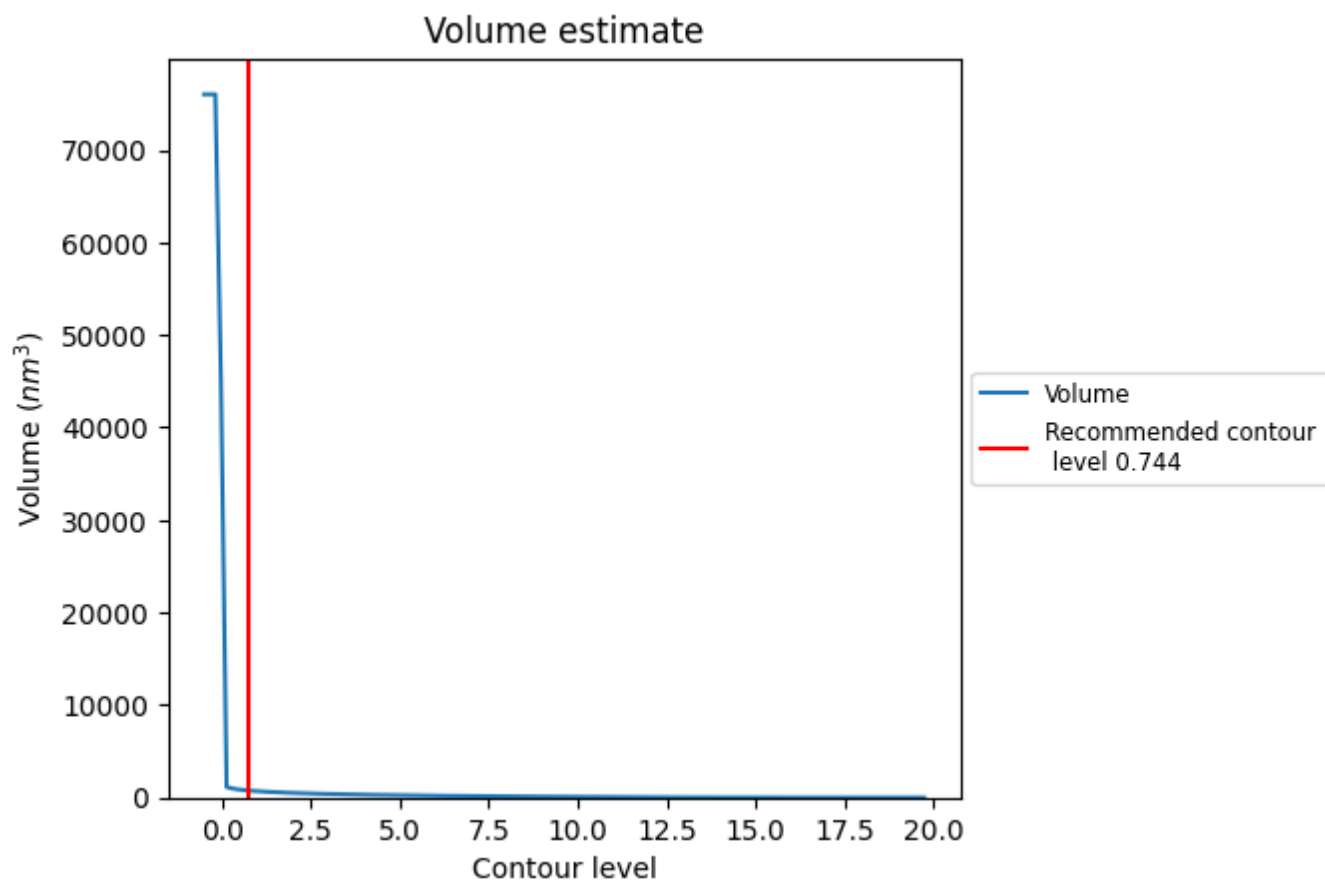
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

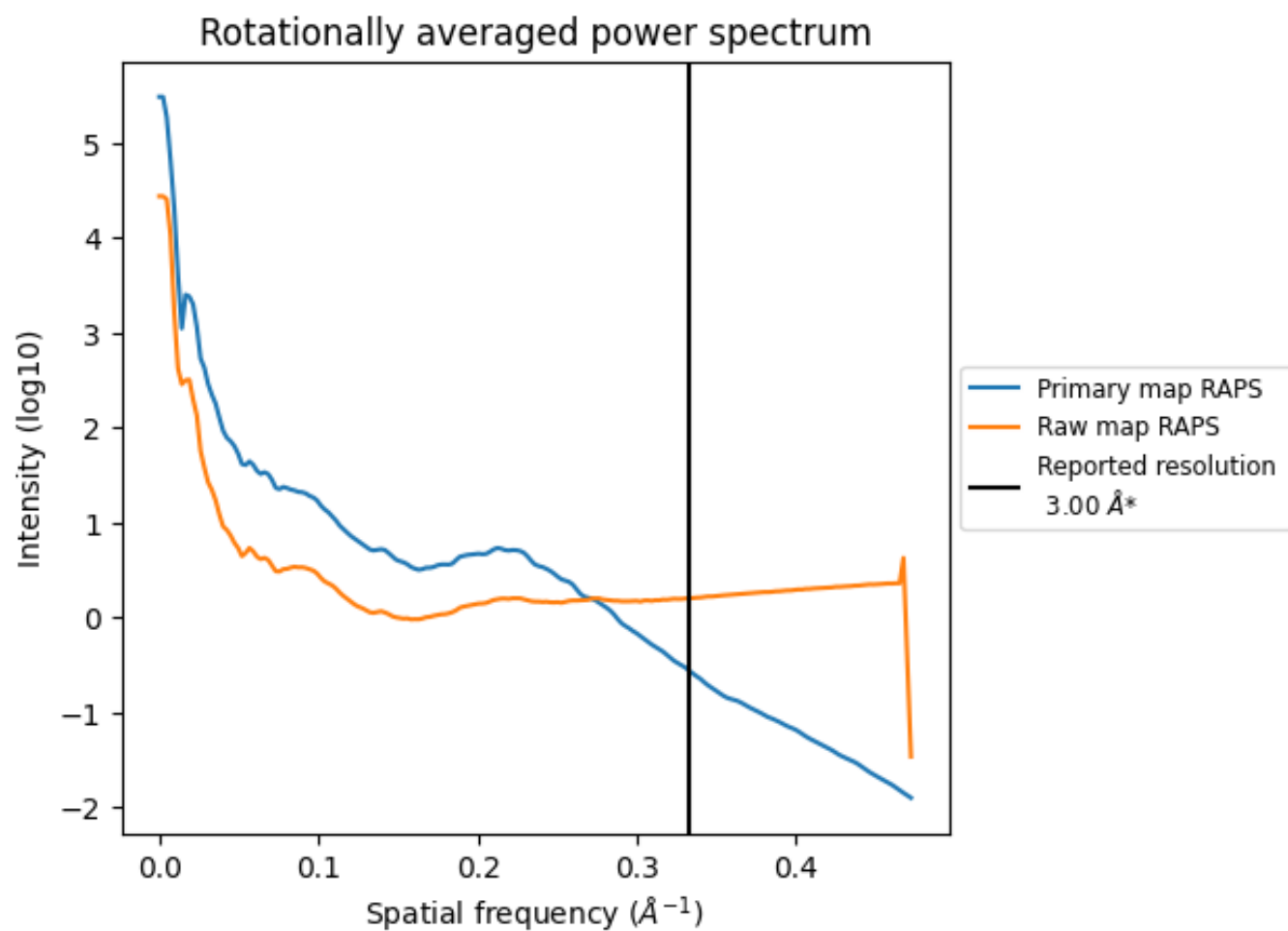
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 761 nm^3 ; this corresponds to an approximate mass of 687 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 ⓘ

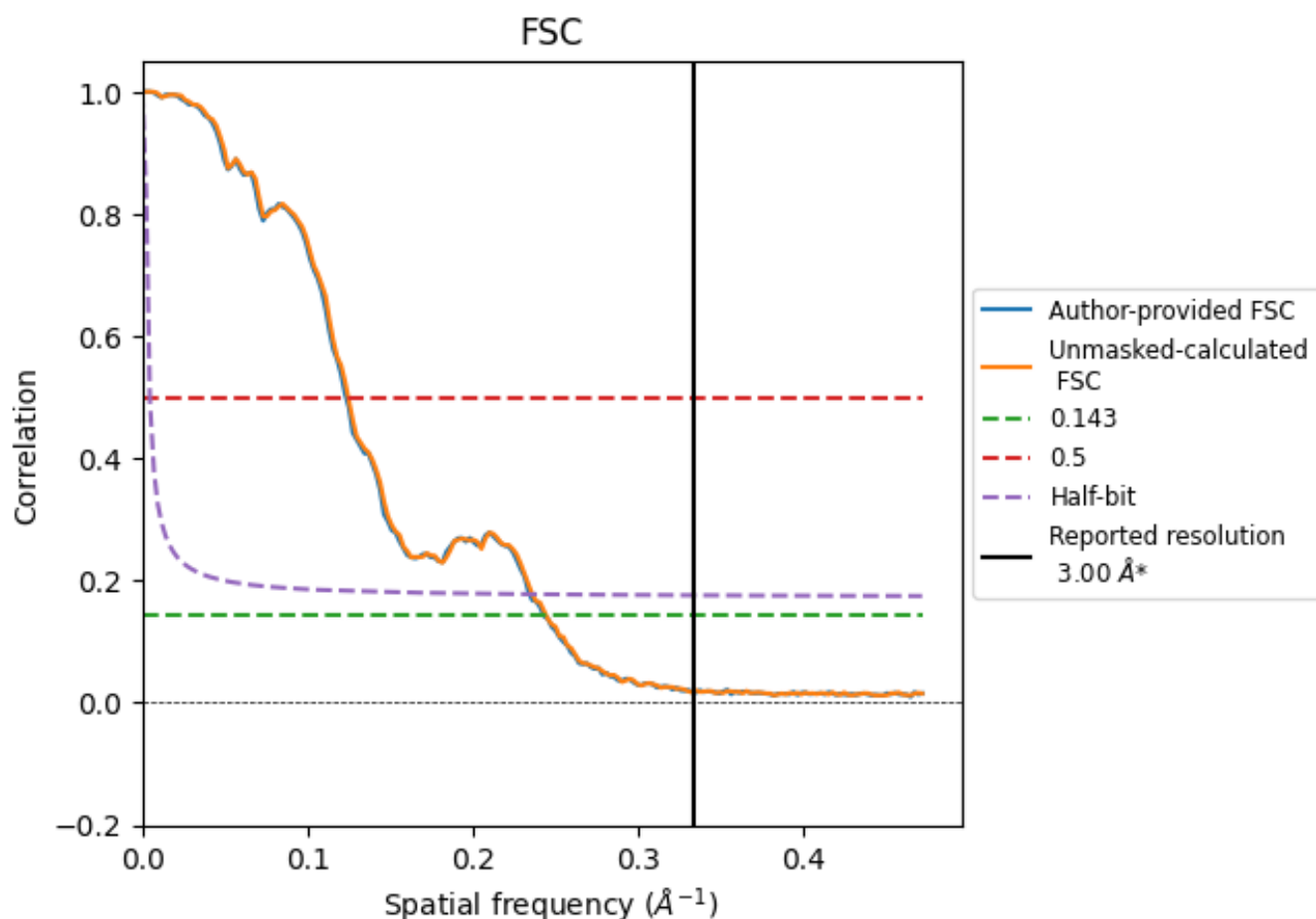


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	4.12	8.11	4.26
Unmasked-calculated*	4.09	8.02	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.0 by more than 10 %

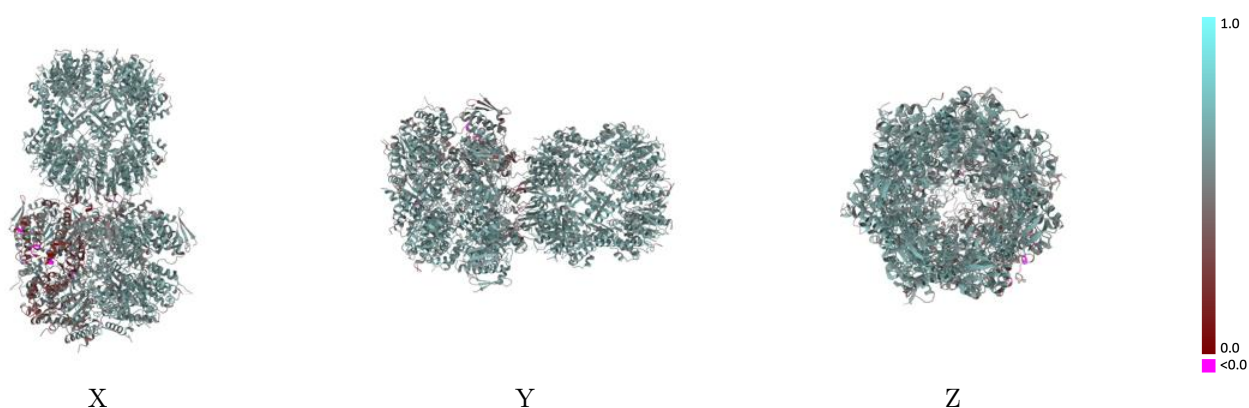
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-51367 and PDB model 9GI1. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

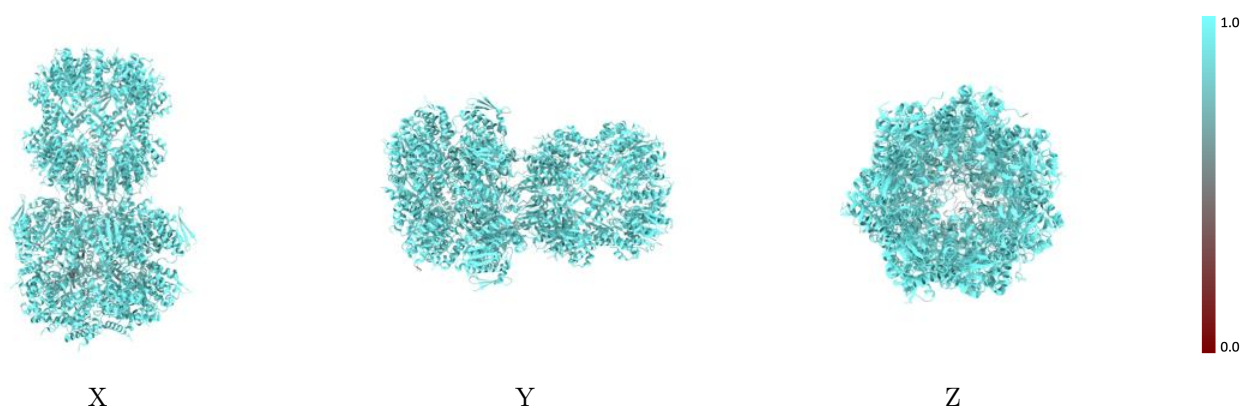
This section was not generated.

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



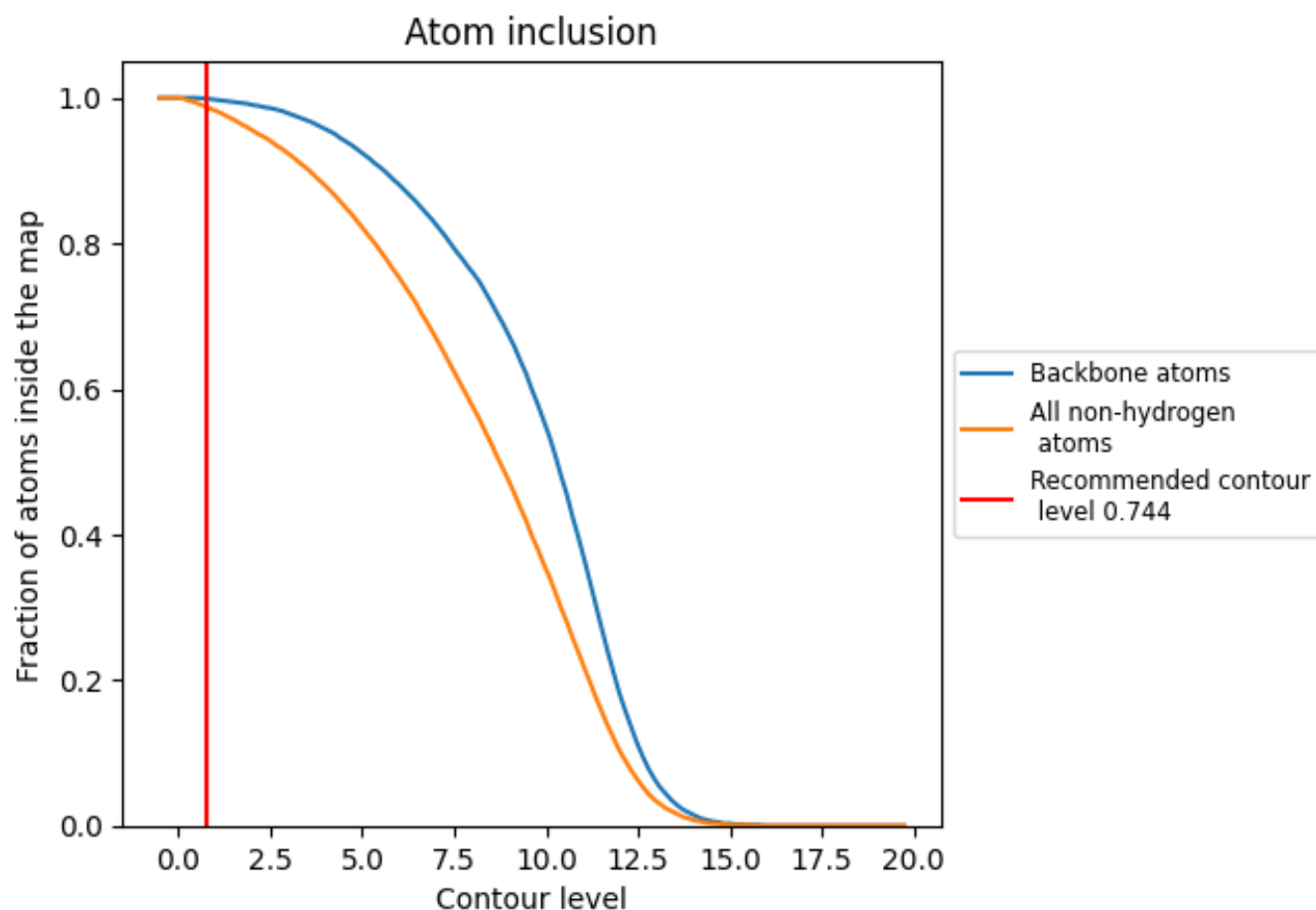
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.744).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.744) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.5560
Pa	 0.9900	 0.5860
Pb	 0.9870	 0.5860
Pc	 0.9990	 0.6110
Pd	 0.9900	 0.5960
Pe	 0.9920	 0.5870
Pf	 0.9890	 0.5660
Pg	 0.9940	 0.5850
Ph	 0.9910	 0.5790
Pi	 0.9910	 0.5880
Pl	 0.9890	 0.5830
Pm	 0.9910	 0.5780
Pn	 0.9880	 0.5750
Po	 0.9920	 0.5820
Pq	 0.9950	 0.5720
S	 0.9880	 0.4910
a	 0.9880	 0.4980
b	 0.9950	 0.5970
c	 0.9930	 0.5990
d	 0.9940	 0.5830
e	 0.9900	 0.5460
f	 0.9530	 0.3770

