WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Jun 26, 2025 – 07:27 PM JST

PDB ID	:	7FID / pdb_00007fid
EMDB ID	:	EMD-31589
Title	:	Processive cleavage of substrate at individual proteolytic active sites of the Lon proteasecomplex (conformation 1)
Authors	:	Li, S.; Hsieh, K.; Kuo, C.; Su, S.; Huang, K.; Zhang, K.; Chang, C.I.
Deposited on	:	2021-07-31
Resolution	:	2.44 Å(reported)

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

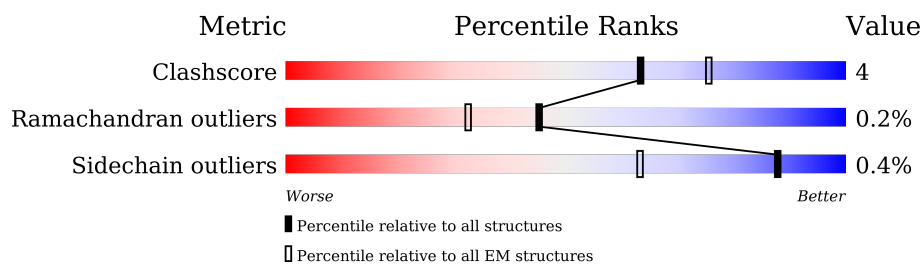|		
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.44 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		0.4%

Worse ... *Better*

∎ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	806	28% / 87% 9% ·
1	B	806	27% / 86% 10% ·
1	C	806	29% / 88% 9% ·
1	D	806	26% / 85% 11% ·
1	E	806	30% / 84% 12% ·
1	F	806	27% / 79% 17% ·
2	S	22	18% / 100%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 36992 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 Lon protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	C	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	D	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	E	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	F	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	A	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	794	LYS	-	expression tag	UNP A0A059VAZ3
B	795	LEU	-	expression tag	UNP A0A059VAZ3
B	796	ALA	-	expression tag	UNP A0A059VAZ3
B	797	ALA	-	expression tag	UNP A0A059VAZ3
B	798	ALA	-	expression tag	UNP A0A059VAZ3
B	799	LEU	-	expression tag	UNP A0A059VAZ3
B	800	GLU	-	expression tag	UNP A0A059VAZ3
B	801	HIS	-	expression tag	UNP A0A059VAZ3
B	802	HIS	-	expression tag	UNP A0A059VAZ3
B	803	HIS	-	expression tag	UNP A0A059VAZ3
B	804	HIS	-	expression tag	UNP A0A059VAZ3
B	805	HIS	-	expression tag	UNP A0A059VAZ3
B	806	HIS	-	expression tag	UNP A0A059VAZ3
C	794	LYS	-	expression tag	UNP A0A059VAZ3
C	795	LEU	-	expression tag	UNP A0A059VAZ3
C	796	ALA	-	expression tag	UNP A0A059VAZ3
C	797	ALA	-	expression tag	UNP A0A059VAZ3
C	798	ALA	-	expression tag	UNP A0A059VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	799	LEU	-	expression tag	UNP A0A059VAZ3
C	800	GLU	-	expression tag	UNP A0A059VAZ3
C	801	HIS	-	expression tag	UNP A0A059VAZ3
C	802	HIS	-	expression tag	UNP A0A059VAZ3
C	803	HIS	-	expression tag	UNP A0A059VAZ3
C	804	HIS	-	expression tag	UNP A0A059VAZ3
C	805	HIS	-	expression tag	UNP A0A059VAZ3
C	806	HIS	-	expression tag	UNP A0A059VAZ3
D	794	LYS	-	expression tag	UNP A0A059VAZ3
D	795	LEU	-	expression tag	UNP A0A059VAZ3
D	796	ALA	-	expression tag	UNP A0A059VAZ3
D	797	ALA	-	expression tag	UNP A0A059VAZ3
D	798	ALA	-	expression tag	UNP A0A059VAZ3
D	799	LEU	-	expression tag	UNP A0A059VAZ3
D	800	GLU	-	expression tag	UNP A0A059VAZ3
D	801	HIS	-	expression tag	UNP A0A059VAZ3
D	802	HIS	-	expression tag	UNP A0A059VAZ3
D	803	HIS	-	expression tag	UNP A0A059VAZ3
D	804	HIS	-	expression tag	UNP A0A059VAZ3
D	805	HIS	-	expression tag	UNP A0A059VAZ3
D	806	HIS	-	expression tag	UNP A0A059VAZ3
E	794	LYS	-	expression tag	UNP A0A059VAZ3
E	795	LEU	-	expression tag	UNP A0A059VAZ3
E	796	ALA	-	expression tag	UNP A0A059VAZ3
E	797	ALA	-	expression tag	UNP A0A059VAZ3
E	798	ALA	-	expression tag	UNP A0A059VAZ3
E	799	LEU	-	expression tag	UNP A0A059VAZ3
E	800	GLU	-	expression tag	UNP A0A059VAZ3
E	801	HIS	-	expression tag	UNP A0A059VAZ3
E	802	HIS	-	expression tag	UNP A0A059VAZ3
E	803	HIS	-	expression tag	UNP A0A059VAZ3
E	804	HIS	-	expression tag	UNP A0A059VAZ3
E	805	HIS	-	expression tag	UNP A0A059VAZ3
E	806	HIS	-	expression tag	UNP A0A059VAZ3
F	794	LYS	-	expression tag	UNP A0A059VAZ3
F	795	LEU	-	expression tag	UNP A0A059VAZ3
F	796	ALA	-	expression tag	UNP A0A059VAZ3
F	797	ALA	-	expression tag	UNP A0A059VAZ3
F	798	ALA	-	expression tag	UNP A0A059VAZ3
F	799	LEU	-	expression tag	UNP A0A059VAZ3
F	800	GLU	-	expression tag	UNP A0A059VAZ3
F	801	HIS	-	expression tag	UNP A0A059VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	802	HIS	-	expression tag	UNP A0A059VAZ3
F	803	HIS	-	expression tag	UNP A0A059VAZ3
F	804	HIS	-	expression tag	UNP A0A059VAZ3
F	805	HIS	-	expression tag	UNP A0A059VAZ3
F	806	HIS	-	expression tag	UNP A0A059VAZ3
A	794	LYS	-	expression tag	UNP A0A059VAZ3
A	795	LEU	-	expression tag	UNP A0A059VAZ3
A	796	ALA	-	expression tag	UNP A0A059VAZ3
A	797	ALA	-	expression tag	UNP A0A059VAZ3
A	798	ALA	-	expression tag	UNP A0A059VAZ3
A	799	LEU	-	expression tag	UNP A0A059VAZ3
A	800	GLU	-	expression tag	UNP A0A059VAZ3
A	801	HIS	-	expression tag	UNP A0A059VAZ3
A	802	HIS	-	expression tag	UNP A0A059VAZ3
A	803	HIS	-	expression tag	UNP A0A059VAZ3
A	804	HIS	-	expression tag	UNP A0A059VAZ3
A	805	HIS	-	expression tag	UNP A0A059VAZ3
A	806	HIS	-	expression tag	UNP A0A059VAZ3

- Molecule 2 is a protein called unknown endogenous substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	22	110	66	22	22	0	0

- Molecule 3 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).
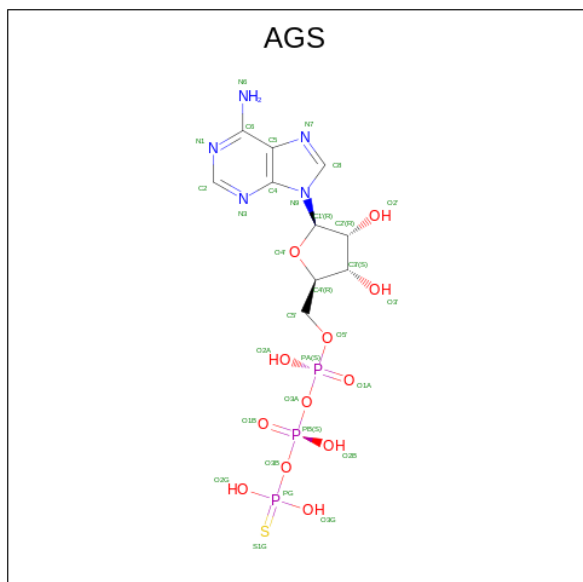
Mol	Chain	Residues	Atoms							AltConf
3	B	1	Total	C	N	O	P	S		0
			31	10	5	12	3	1		
3	C	1	Total	C	N	O	P	S		0
			31	10	5	12	3	1		
3	A	1	Total	C	N	O	P	S		0
			31	10	5	12	3	1		

- 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).
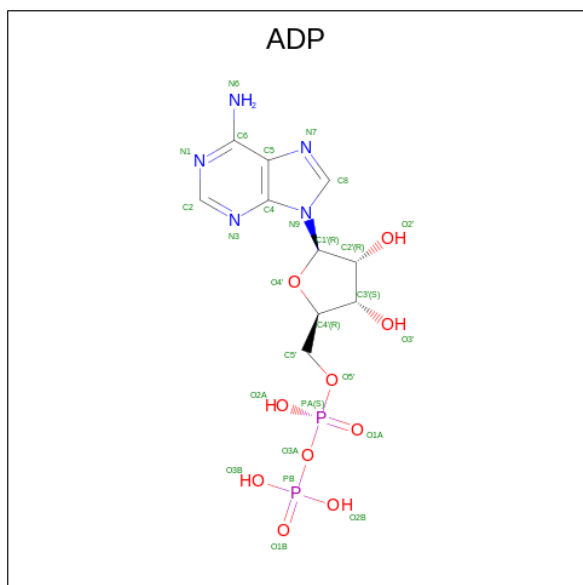
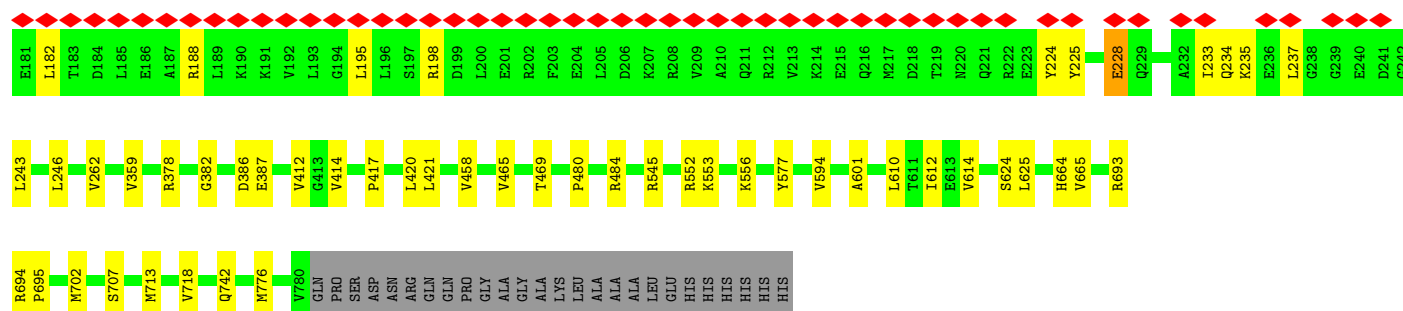| Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots ⓘ

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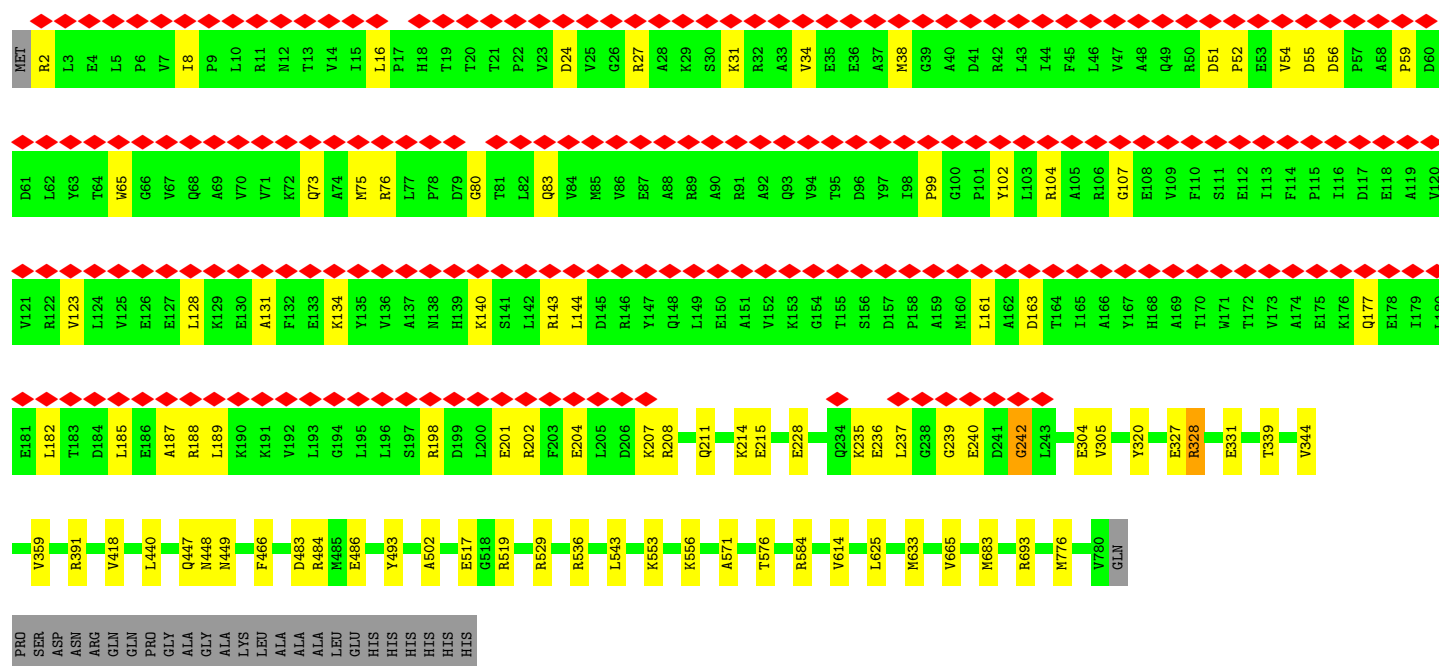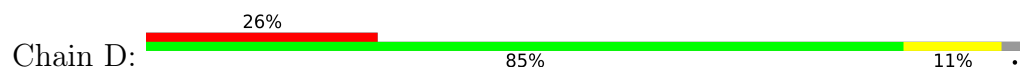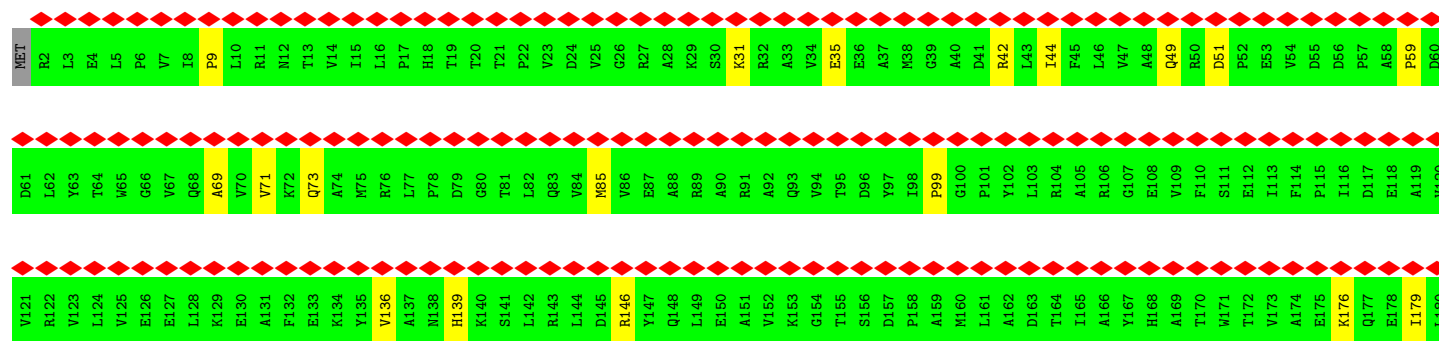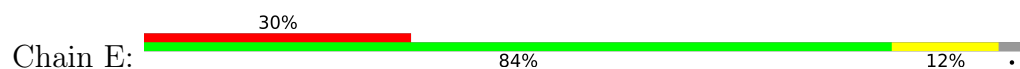
- Molecule 1: Lon protease

- Molecule 1: Lon protease

E181 L182 T183 D184 L185 E186 A187 R188 L189 K190 K191 V192 L193 G194 L195 L196 S197 R198 D199 L200 E201 R202 F203 E204 L205 D206 K207 R208 V209 A210 Q211 R212 V213 K214 E215 Q216 M217 D218 T219 N220 Q221 R222 E223 Y224 Y225 E228 Q229 A232 I233 Q234 K235 E236 L237 G238 E239 E240 D241 G242

L243 L246 V262 V359 R378 G382 D386 E387 V412 G413 V414 P417 L420 L421 V458 V465 T469 P480 R484 R545 R552 K553 K556 Y577 V594 A601 L610 T611 I612 E613 V614 S624 L625 H664 V665 R693

R694 P695 M702 S707 M713 V718 Q742 M776 V780 GLN PRO SER ASP ASN ARG GLN GLN PRO GLY ALA GLY ALA LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Lon protease

26%

Chain D:　　85%　　11%

MET R2 L3 E4 L5 P6 V7 I8 P9 L10 R11 N12 T13 V14 I15 L16 P17 H18 T19 T20 T21 P22 V23 D24 V25 G26 R27 A28 K29 S30 K31 R32 A33 V34 E35 E36 A37 M38 G39 A40 D41 R42 L43 I44 F45 L46 V47 A48 Q49 R50 D51 P52 E53 V54 D55 D56 P57 A58 P59 D60

D61 L62 Y63 T64 W65 G66 V67 Q68 A69 V70 V71 K72 Q73 A74 M75 R76 L77 P78 D79 G80 T81 L82 Q83 V84 M85 V86 E87 A88 R89 A90 R91 A92 Q93 V94 T95 D96 Y97 I98 P99 G100 P101 Y102 L103 R104 A105 R106 G107 E108 V109 F110 S111 E112 I113 F114 P115 I116 D117 E118 A119 V120

V121 R122 V123 L124 V125 E126 E127 L128 K129 E130 A131 F132 E133 K134 Y135 V136 A137 N138 H139 K140 S141 L142 R143 L144 D145 R146 Y147 Q148 L149 E150 A151 V152 K153 G154 T155 S156 D157 P158 A159 M160 L161 A162 D163 T164 I165 A166 Y167 H168 A169 T170 W171 T172 V173 A174 E175 K176 Q177 E178 I179 L180

E181 L182 T183 D184 L185 E186 A187 R188 L189 K190 K191 V192 L193 G194 L195 L196 S197 R198 D199 L200 E201 R202 F203 E204 L205 D206 K207 R208 Q211 K214 E215 E228 Q234 K235 L237 G238 E239 E240 D241 G242 L243 E304 V305 Y320 E327 R328 E331 T339 V344

V359 R391 V418 L440 Q447 N448 N449 F466 D483 R484 M485 E486 Y493 A502 E517 G518 R519 R529 R536 L543 K553 K556 A571 T576 R584 V614 L625 M633 V665 M683 R693 M776 V780 GLN

PRO SER ASP ASN ARG GLN GLN PRO GLY ALA GLY ALA LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Lon protease

30%

Chain E:　　84%　　12%

MET R2 L3 E4 L5 P6 V7 I8 P9 L10 R11 N12 T13 V14 I15 L16 P17 H18 T19 T20 T21 P22 V23 D24 V25 G26 R27 A28 K29 S30 K31 R32 A33 V34 E35 E36 A37 M38 G39 A40 D41 R42 L43 I44 F45 L46 V47 A48 Q49 R50 D51 P52 E53 V54 D55 D56 P57 A58 P59 D60

D61 L62 Y63 T64 W65 G66 V67 Q68 A69 V70 V71 K72 Q73 A74 M75 R76 L77 P78 D79 G80 T81 L82 Q83 V84 M85 V86 E87 A88 R89 A90 R91 A92 Q93 V94 T95 D96 Y97 I98 P99 G100 P101 Y102 L103 R104 A105 R106 G107 E108 V109 F110 S111 E112 I113 F114 P115 I116 D117 E118 A119 V120

V121 R122 V123 L124 V125 E126 E127 L128 K129 E130 A131 F132 E133 K134 Y135 V136 A137 N138 H139 K140 S141 L142 R143 L144 D145 R146 Y147 Q148 L149 E150 A151 V152 K153 G154 T155 S156 D157 P158 A159 M160 L161 A162 D163 T164 I165 A166 Y167 H168 A169 T170 W171 T172 V173 A174 E175 K176 Q177 E178 I179 L180

- Molecule 1: Lon protease

Chain F:

- Molecule 1: Lon protease

Chain A:

D61 L62 Y63 T64 W65 G66 V67 Q68 A69 V70 V71 K72 Q73 A74 M75 R76 L77 P78 D79 G80 T81 L82 Q83 V84 M85 V86 E87 A88 R89 A90 R91 A92 Q93 V94 T95 D96 Y97 I98 P99 G100 P101 Y102 L103 R104 A105 R106 G107 E108 V109 F110 S111 E112 I113 F114 P115 I116 D117 E118 A119 V120

V121 R122 V123 L124 V125 E126 E127 L128 K129 E130 A131 F132 E133 K134 Y135 V136 A137 N138 H139 K140 S141 L142 R143 L144 D145 R146 Y147 Q148 L149 E150 A151 V152 K153 G154 T155 S156 D157 P158 A159 M160 L161 A162 D163 T164 I165 A166 Y167 H168 A169 T170 W171 T172 V173 A174 E175 K176 Q177 E178 I179 L180

E181 L182 T183 D184 L185 E186 A187 R188 L189 K190 K191 V192 L193 G194 L195 L196 S197 R198 D199 L200 E201 R202 F203 E204 L205 D206 K207 R208 V209 A210 Q211 R212 V213 K214 E215 Q216 M217 D218 T219 N220 Q221 R222 E223 R227 K231 Q234 G238 D241 D245 L246 E247 A248 L249 R250

K251 K252 I253 E254 E255 M258 D271 M276 Q277 Q278 G279 S280 A283 T288 V305 E327 R328 E331 Y332 L333 R336 T339 Q340 G341 L342 D343 V344 R345 G358 V359 R374 E389 V412 G413 V414 I415 N416 P417 L421 D422 D425 N448

L462 V465 T469 T470 T476 E486 R529 G539 A571 T603 G606 L625 V665 T672 P673 K674 R693 S707 L708 R709 M713 M776 V780 GLN PRO SER ASP ASN ARG GLN GLN PRO GLY ALA GLY ALA LYS LEU ALA ALA ALA LEU GLU

HIS HIS HIS HIS HIS

• Molecule 2: unknown endogenous substrate

Chain S:

18%

100%

X1 X4 X5 X6 X7 X22

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	324693	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.848	Depositor
Minimum map value	-1.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	275.52, 275.52, 275.52	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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, 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	0.42	0/6229	0.60	0/8444
1	B	0.45	0/6229	0.67	3/8444 (0.0%)
1	C	0.42	0/6229	0.59	1/8444 (0.0%)
1	D	0.39	0/6229	0.65	5/8444 (0.1%)
1	E	0.32	0/6229	0.58	2/8444 (0.0%)
1	F	0.38	0/6229	0.68	3/8444 (0.0%)
All	All	0.40	0/37374	0.63	14/50664 (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	3
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	5
1	F	0	3
All	All	0	16

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	161	LEU	CA-CB-CG	8.55	146.21	116.30
1	D	328	ARG	CB-CG-CD	6.58	126.45	111.30
1	D	242	GLY	N-CA-C	-5.57	108.03	115.32
1	F	52	PRO	N-CA-C	5.25	119.44	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	395	ARG	CA-CB-CG	5.23	124.57	114.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLU	Peptide
1	B	51	ASP	Peptide
1	C	51	ASP	Peptide
1	D	304	GLU	Peptide
1	D	51	ASP	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	6118	0	6236	45	0
1	B	6118	0	6236	49	0
1	C	6118	0	6236	42	0
1	D	6118	0	6236	48	0
1	E	6118	0	6236	56	0
1	F	6118	0	6236	82	0
2	S	110	0	34	0	0
3	A	31	0	12	2	0
3	B	31	0	12	2	0
3	C	31	0	12	2	0
4	D	27	0	12	1	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
All	All	36992	0	37522	297	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.

The worst 5 of 297 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:208:ARG:HE	1:D:211:GLN:HE21	1.32	0.77
1:F:439:MET:O	1:F:443:LEU:HB2	1.87	0.74
1:B:385:ARG:HH22	1:C:387:GLU:H	1.36	0.72
1:B:272:ARG:HE	1:A:288:THR:HG21	1.56	0.70
1:C:234:GLN:HB3	1:C:235:LYS:HZ3	1.56	0.70

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	777/806 (96%)	736 (95%)	41 (5%)	0	100	100
1	B	777/806 (96%)	735 (95%)	40 (5%)	2 (0%)	37	44
1	C	777/806 (96%)	744 (96%)	32 (4%)	1 (0%)	48	60
1	D	777/806 (96%)	733 (94%)	41 (5%)	3 (0%)	30	36
1	E	777/806 (96%)	716 (92%)	60 (8%)	1 (0%)	48	60
1	F	777/806 (96%)	724 (93%)	52 (7%)	1 (0%)	48	60
All	All	4662/4836 (96%)	4388 (94%)	266 (6%)	8 (0%)	45	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	448	ASN
1	B	304	GLU
1	B	305	VAL
1	D	305	VAL
1	E	491	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	655/675 (97%)	655 (100%)	0	100	100
1	B	655/675 (97%)	652 (100%)	3 (0%)	86	92
1	C	655/675 (97%)	652 (100%)	3 (0%)	86	92
1	D	655/675 (97%)	652 (100%)	3 (0%)	86	92
1	E	655/675 (97%)	652 (100%)	3 (0%)	86	92
1	F	655/675 (97%)	653 (100%)	2 (0%)	91	95
All	All	3930/4050 (97%)	3916 (100%)	14 (0%)	88	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	215	GLU
1	D	237	LEU
1	F	342	LEU
1	E	715	ILE
1	F	235	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	168	HIS
1	F	49	GLN
1	E	177	GLN
1	E	277	GLN
1	F	454	HIS

5.3.3   RNA   ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

6 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	#$|Z| > 2$
3	AGS	A	901	-	26,33,33	0.84	0	26,52,52	1.31	2 (7%)
3	AGS	C	901	-	26,33,33	0.86	1 (3%)	26,52,52	1.01	2 (7%)
4	ADP	F	901	-	24,29,29	0.92	1 (4%)	29,45,45	1.30	4 (13%)
4	ADP	D	901	-	24,29,29	1.00	1 (4%)	29,45,45	1.37	3 (10%)
3	AGS	B	901	-	26,33,33	0.92	2 (7%)	26,52,52	1.09	2 (7%)
4	ADP	E	901	-	24,29,29	0.91	1 (4%)	29,45,45	1.47	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
3	AGS	A	901	-	-	0/17/38/38	0/3/3/3
3	AGS	C	901	-	-	3/17/38/38	0/3/3/3
4	ADP	F	901	-	-	2/12/32/32	0/3/3/3
4	ADP	D	901	-	-	1/12/32/32	0/3/3/3
3	AGS	B	901	-	-	1/17/38/38	0/3/3/3
4	ADP	E	901	-	-	1/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	901	ADP	C5-C4	2.28	1.47	1.40
4	E	901	ADP	C5-C4	2.10	1.46	1.40
3	C	901	AGS	C8-N7	-2.07	1.31	1.34
3	B	901	AGS	C8-N7	-2.07	1.31	1.34
3	B	901	AGS	PG-S1G	2.07	1.95	1.90

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	AGS	PA-O3A-PB	-5.23	114.89	132.83
3	B	901	AGS	PA-O3A-PB	-4.02	119.04	132.83
4	D	901	ADP	PA-O3A-PB	-3.70	120.12	132.83
4	E	901	ADP	PA-O3A-PB	-3.54	120.69	132.83
4	E	901	ADP	C3'-C2'-C1'	3.37	106.05	100.98

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	AGS	2	0
3	C	901	AGS	2	0
4	D	901	ADP	1	0
3	B	901	AGS	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AGS A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand AGS C 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 901

Bond lengths

Bond angles

Torsions

Rings

Ligand AGS B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 901

Bond lengths

Bond angles

Torsions

Rings
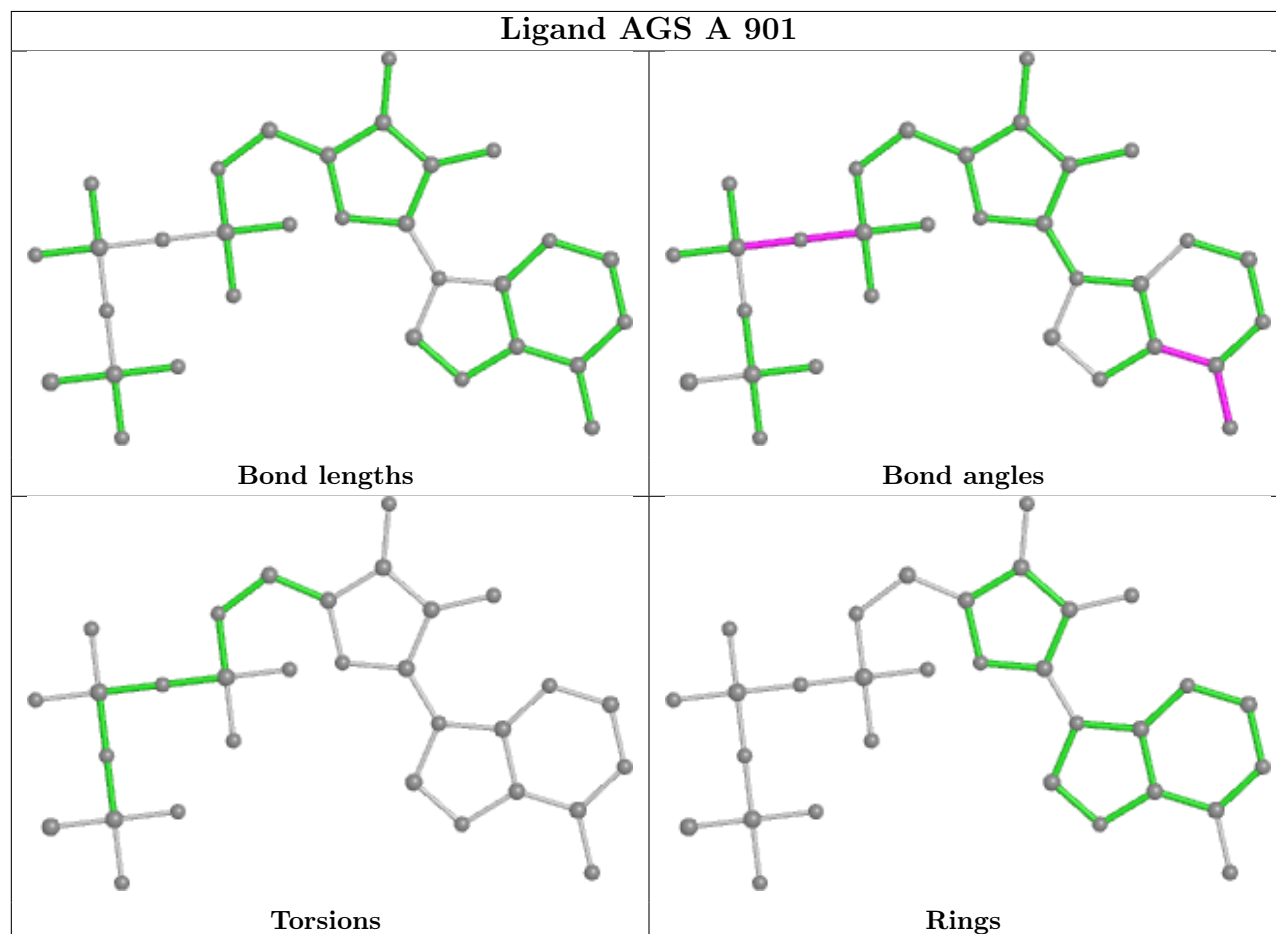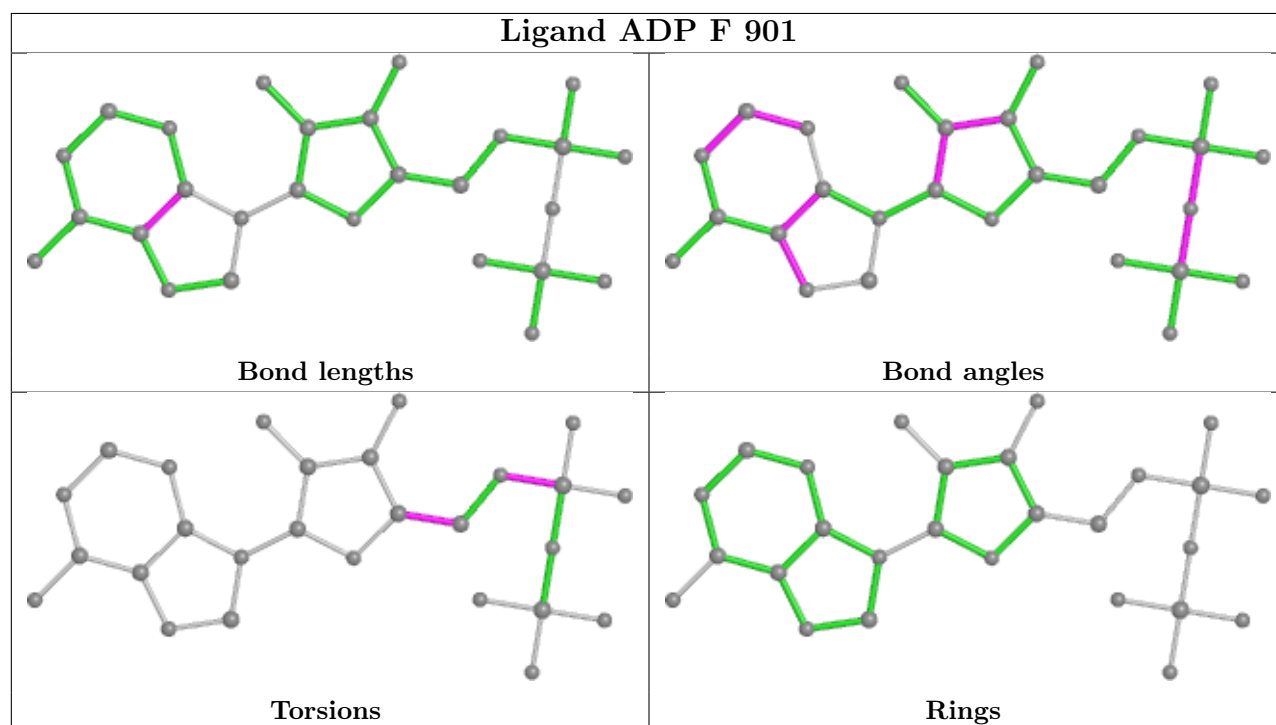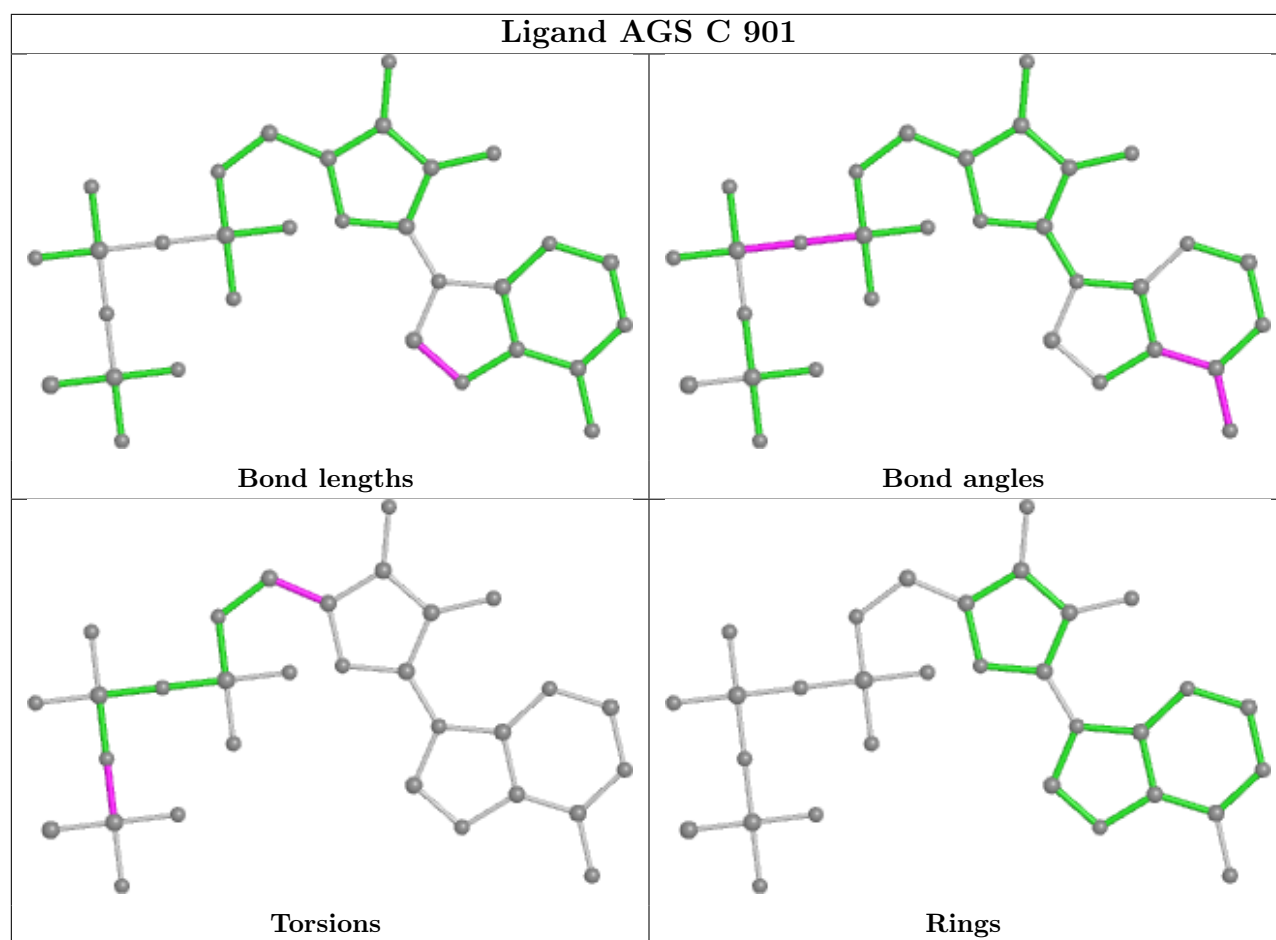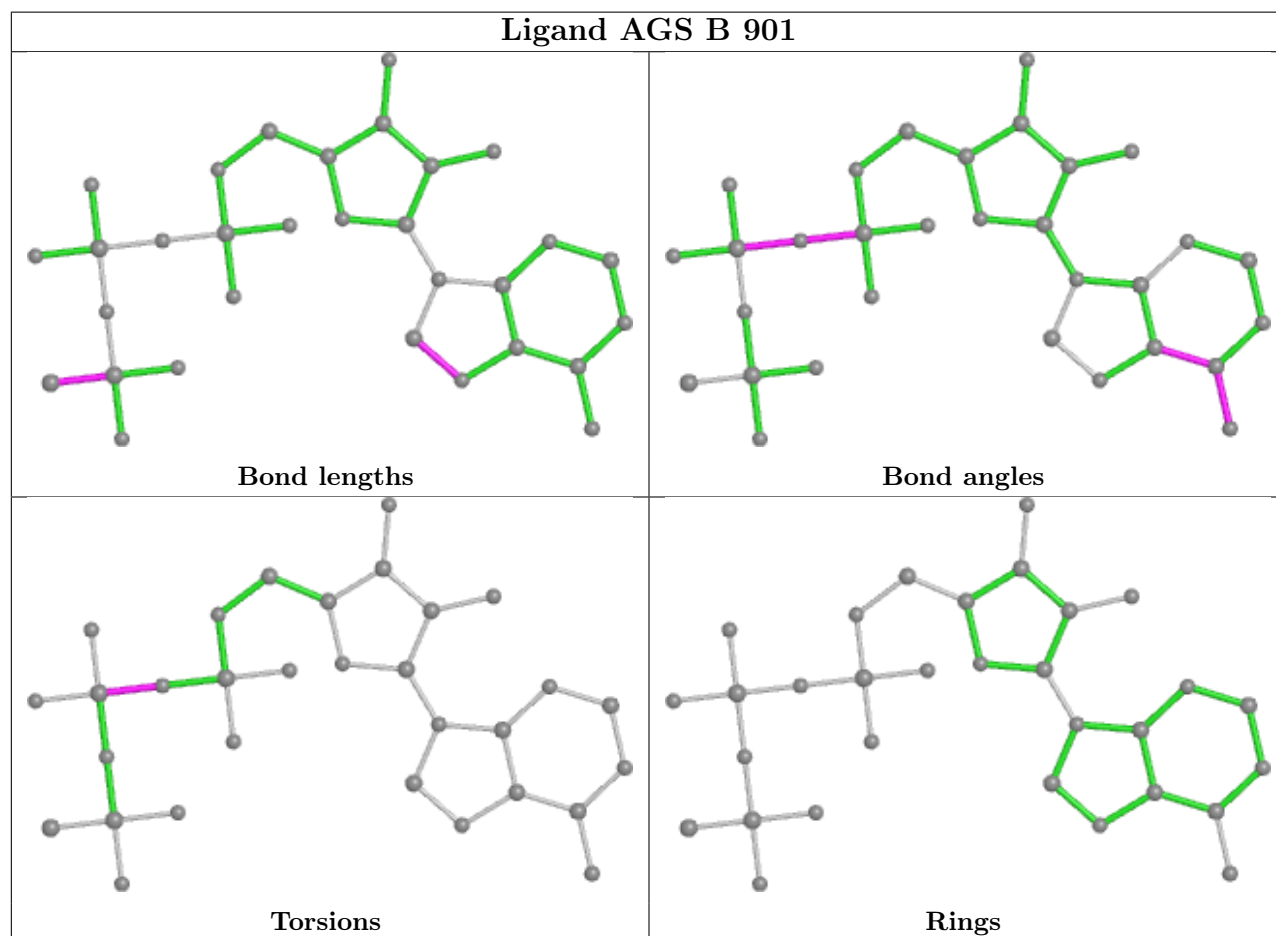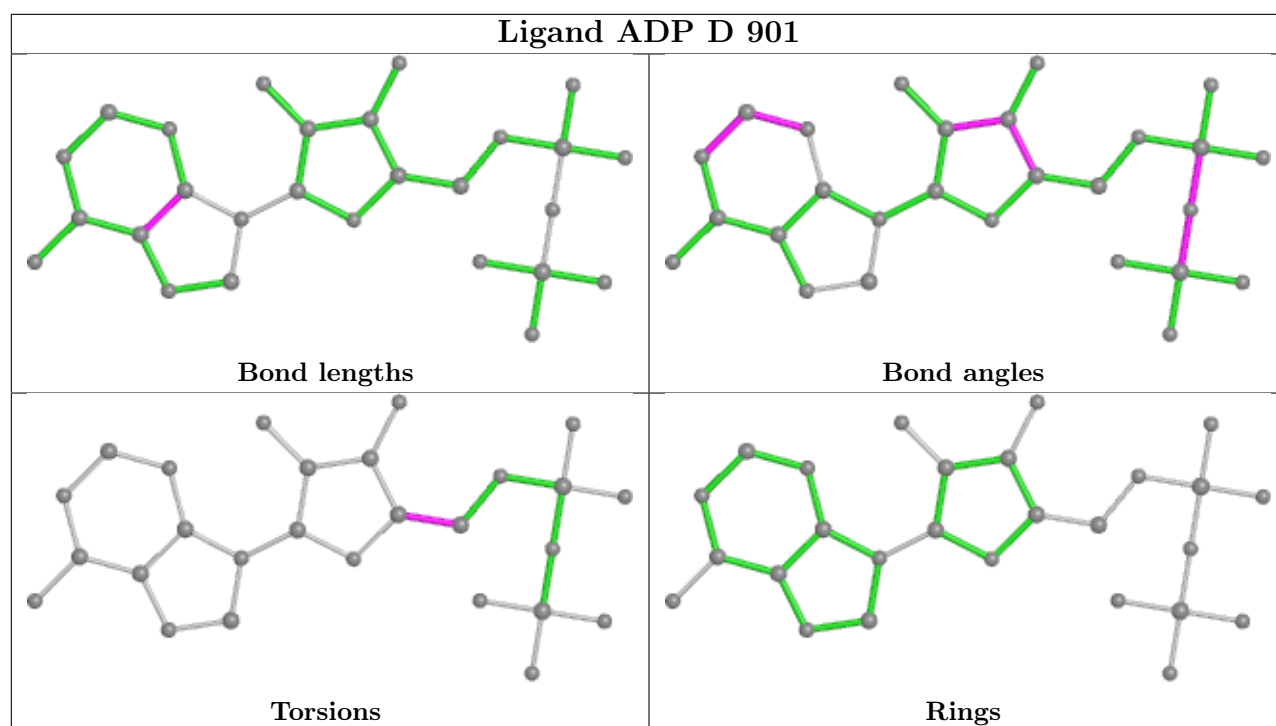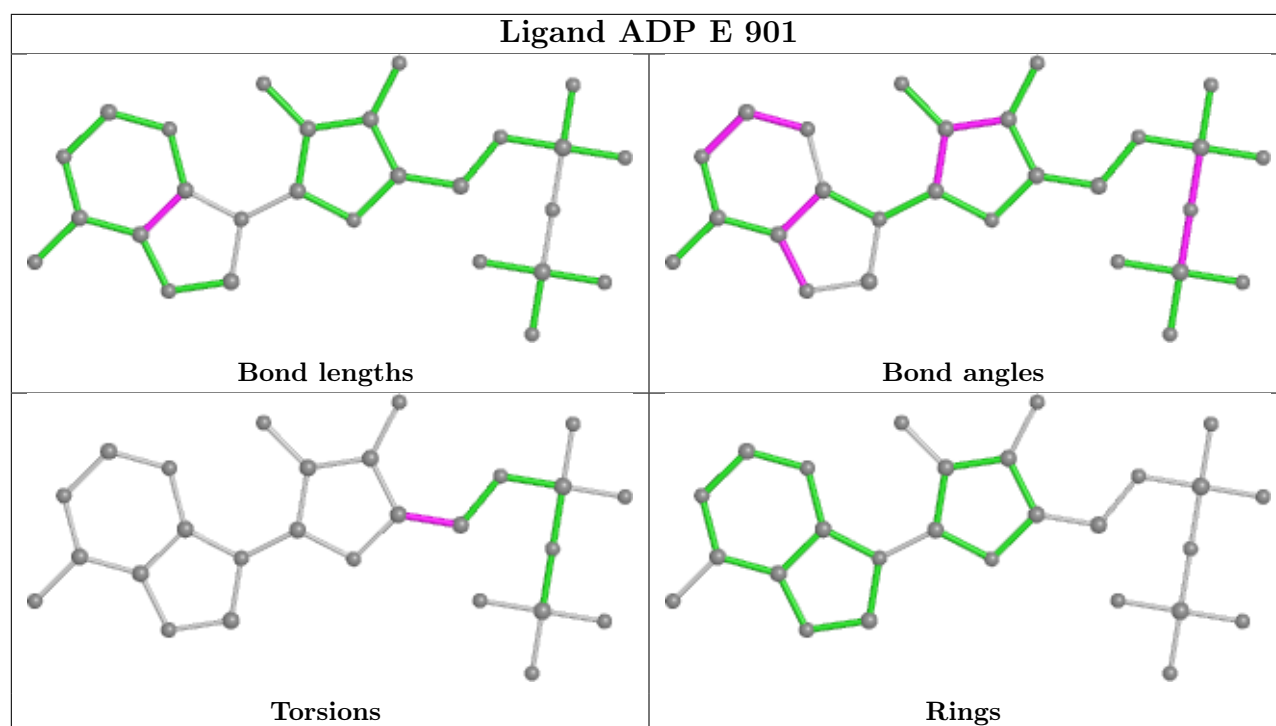
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-31589. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
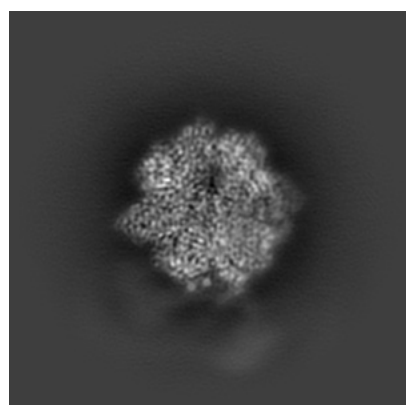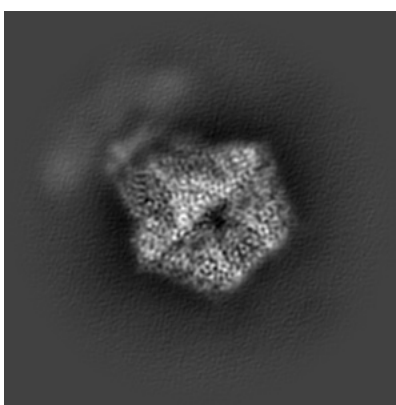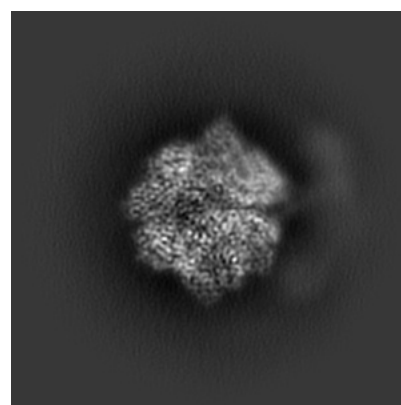
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
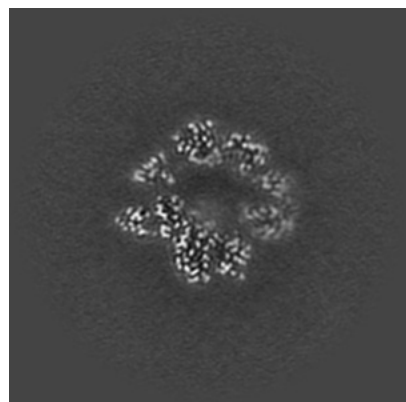
6.2.1 Primary map
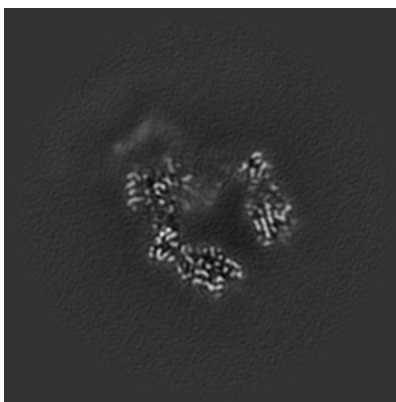
| X Index: 168 | Y Index: 168 | Z Index: 168 |
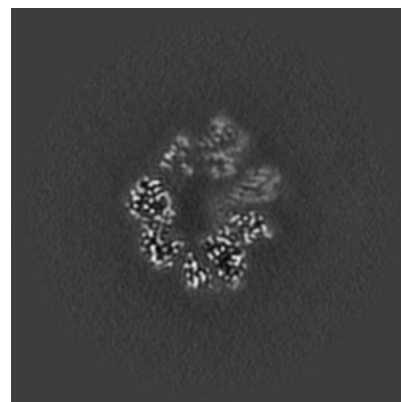
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
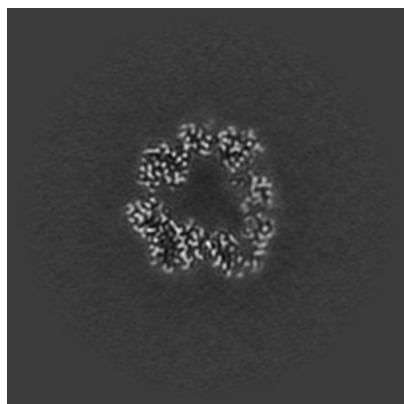
6.3.1   Primary map
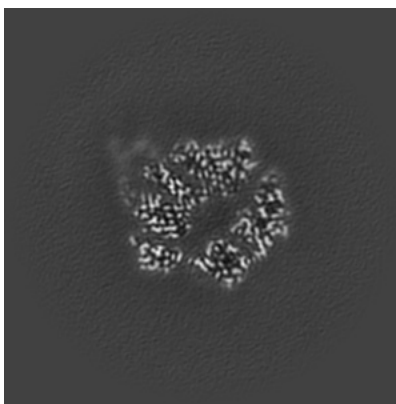
| X Index: 149 | Y Index: 148 | Z Index: 189 |
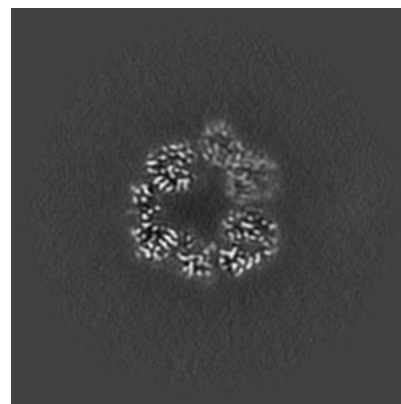
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1   Primary map

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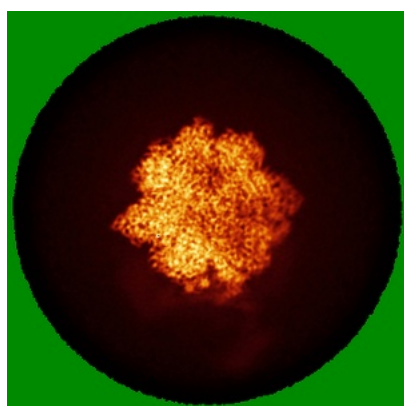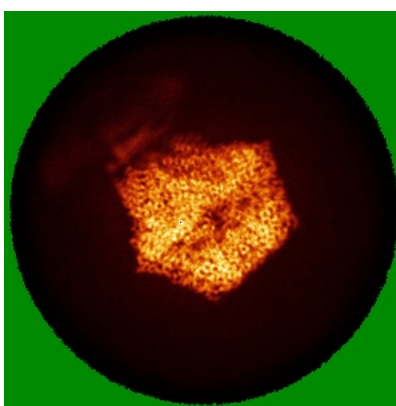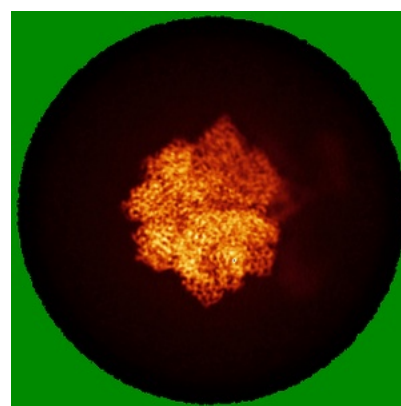
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
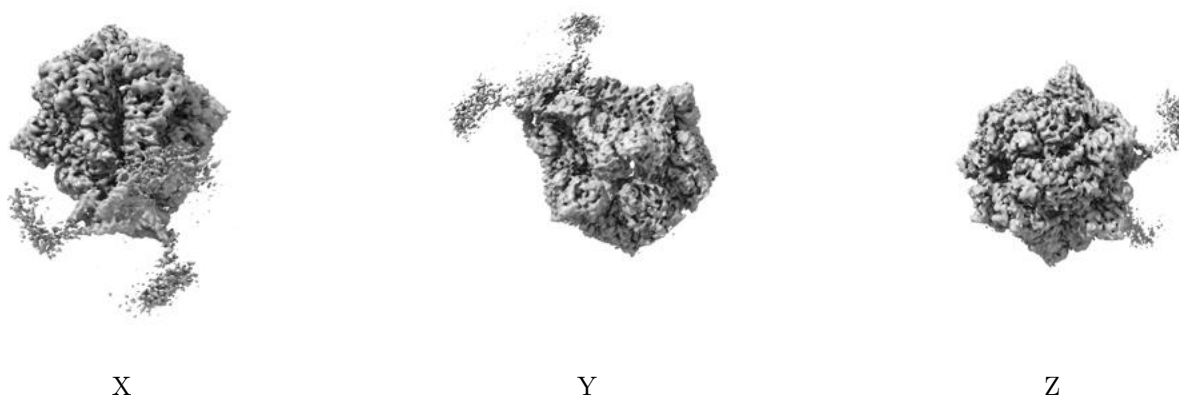
The images above show the 3D surface view of the map at the recommended contour level 0.204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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

7   Map analysis ⓘ

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

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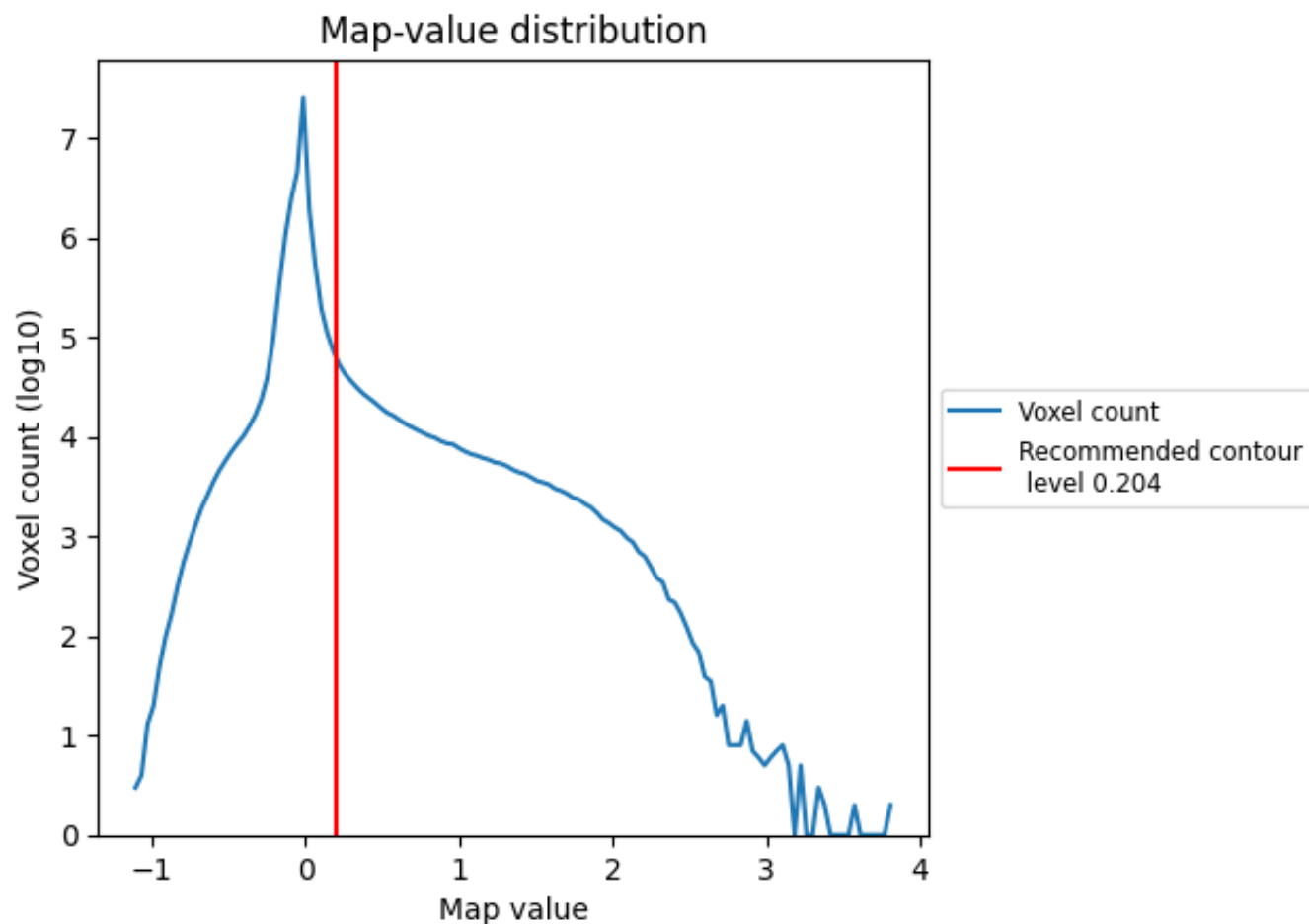
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
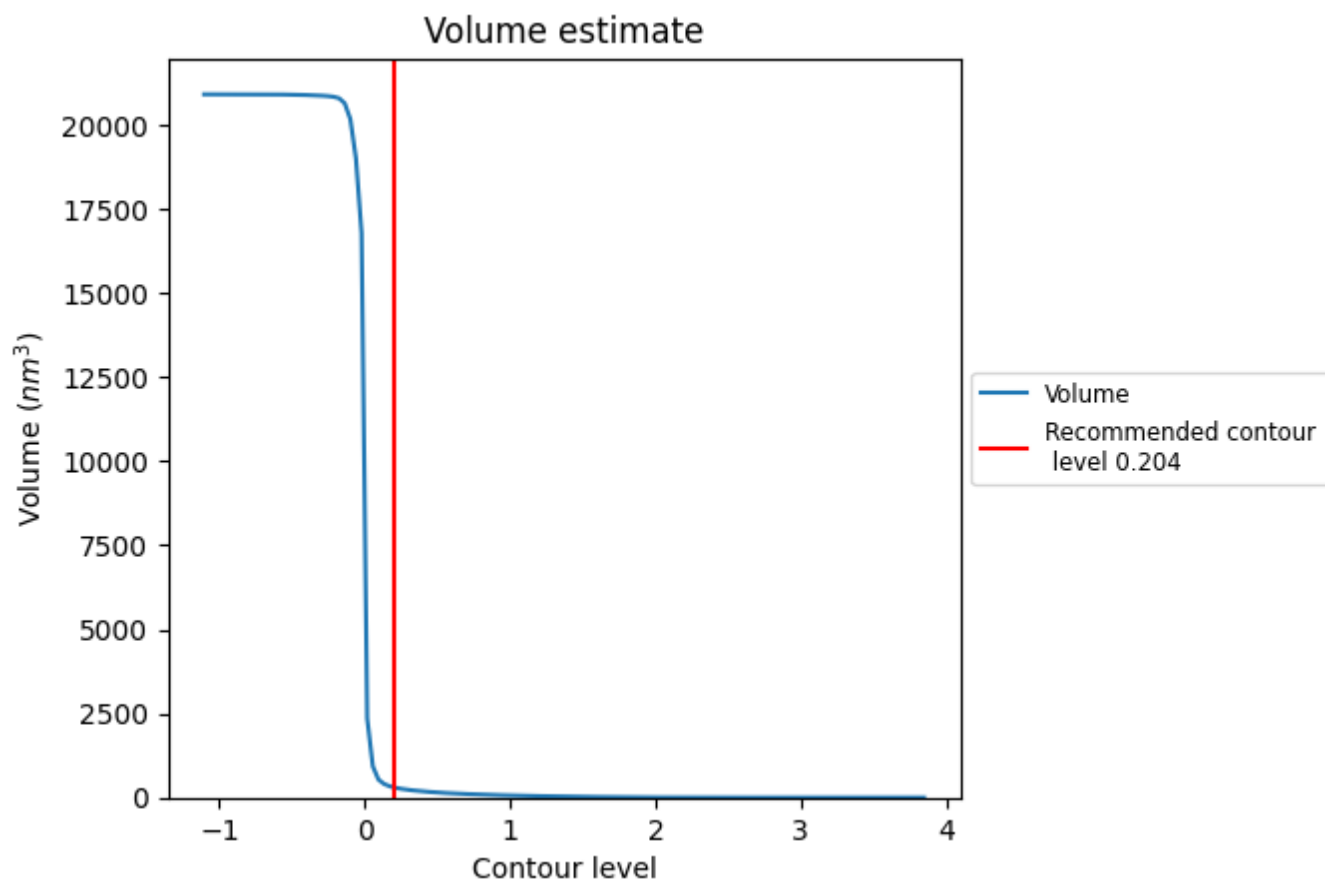
The volume at the recommended contour level is 300 nm^3; this corresponds to an approximate mass of 271 kDa.

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

7.3 Rotationally averaged power spectrum (i)
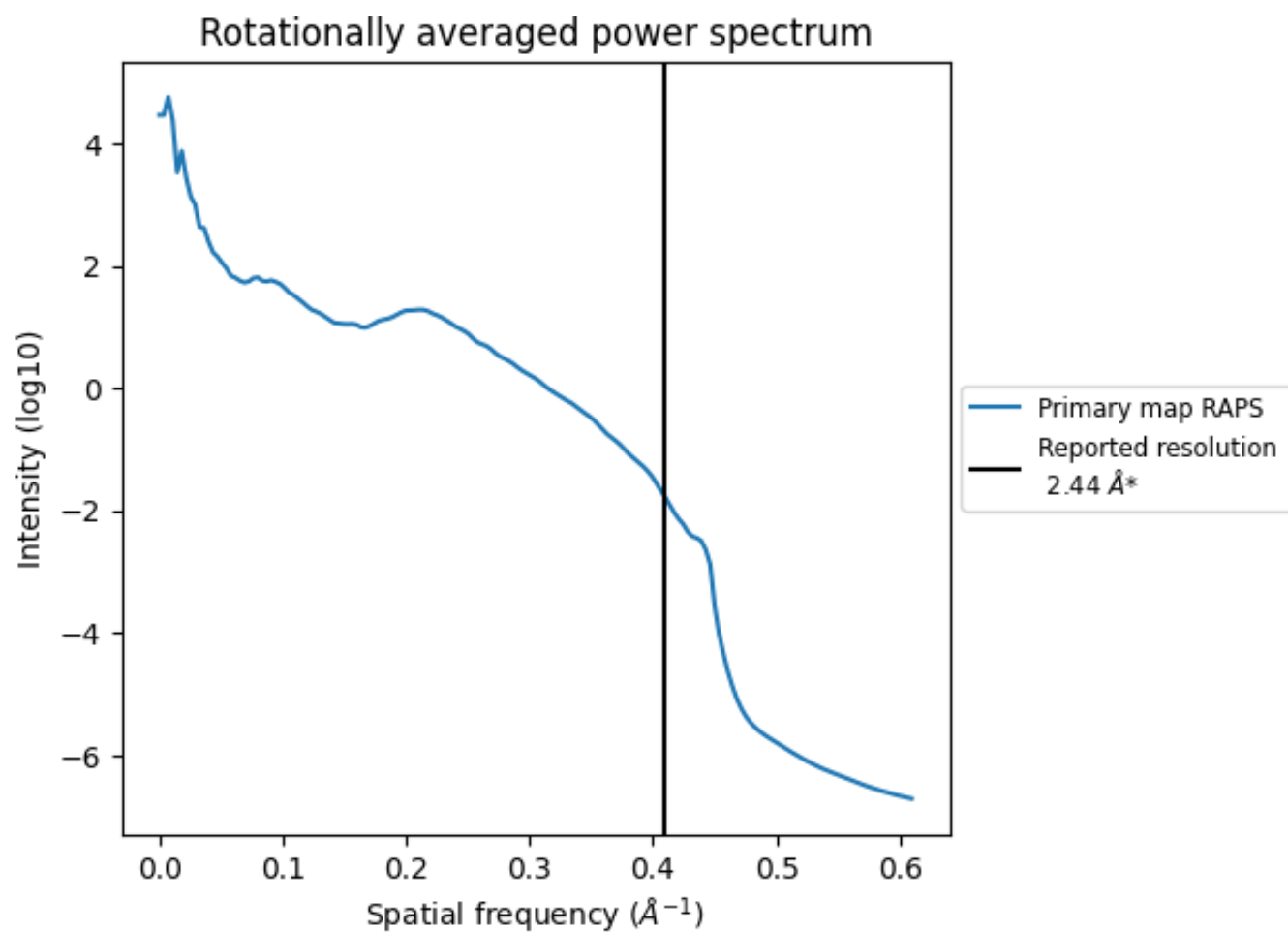
*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31589 and PDB model 7FID. Per-residue inclusion information can be found in section 3 on page 7.

9.1   Map-model overlay (i)
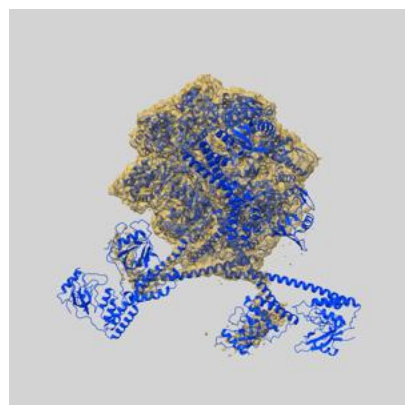
| X | Y | Z |
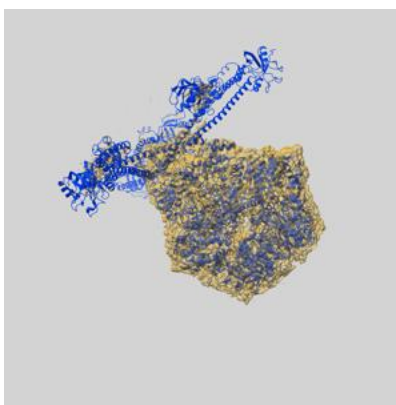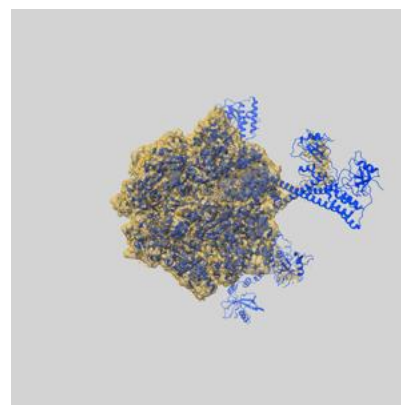
The images above show the 3D surface view of the map at the recommended contour level 0.204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ

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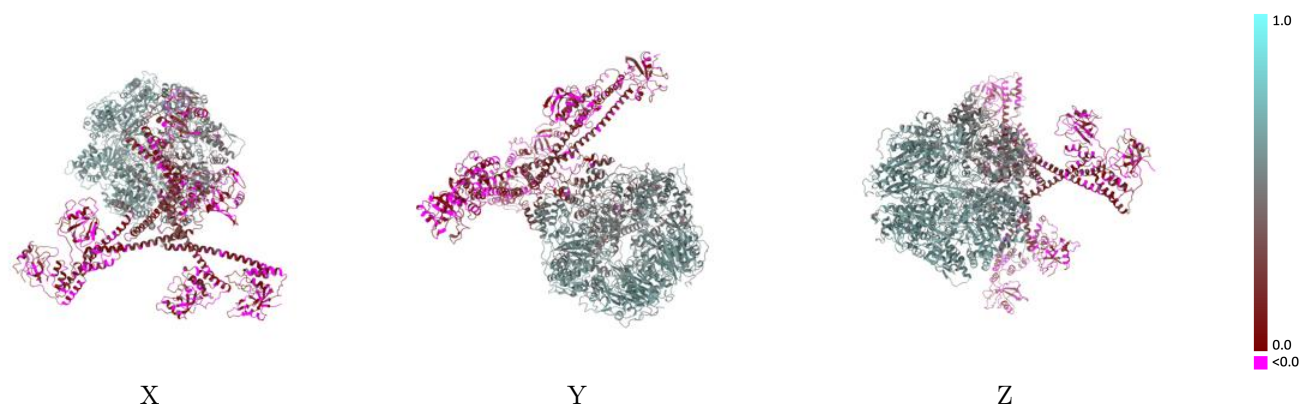
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model   ⓘ

X   Y   Z
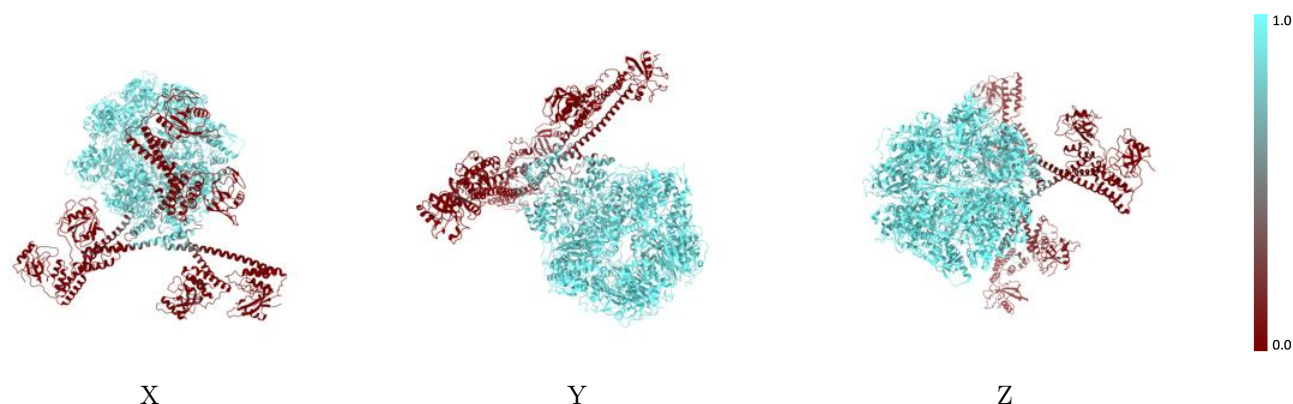
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.204).

9.4　Atom inclusion ⓘ
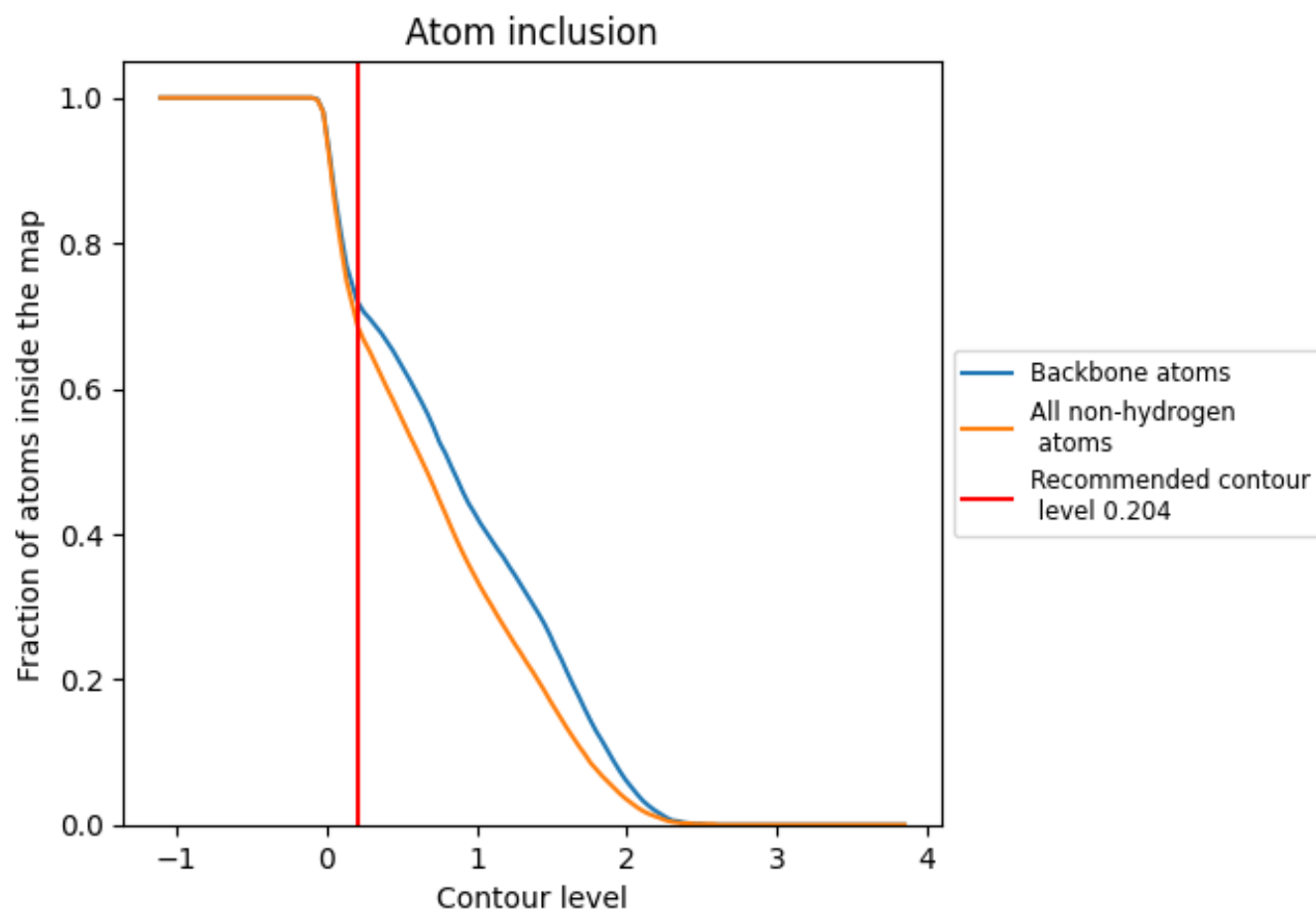
At the recommended contour level, 72% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.3990
A	0.6840	0.4110
B	0.7110	0.4370
C	0.6840	0.4310
D	0.7120	0.4140
E	0.6470	0.3530
F	0.6860	0.3490
S	0.8270	0.4590

1.0

0.0
<0.0