



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:12 PM UTC

PDB ID : 7FIE / pdb_00007fie
EMDB ID : EMD-31590
Title : Processive cleavage of substrate at individual proteolytic active sites of the Lon protease complex (conformation 2)
Authors : Li, S.; Hsieh, K.; Kuo, C.; Su, S.; Huang, K.; Zhang, K.; Chang, C.I.
Deposited on : 2021-07-31
Resolution : 2.36 Å(reported)

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

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

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:

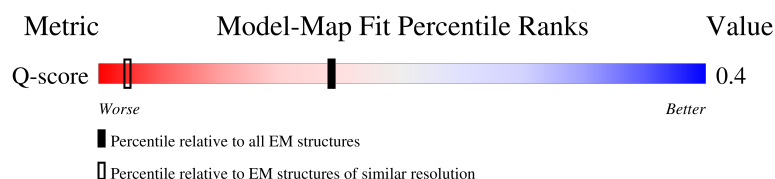
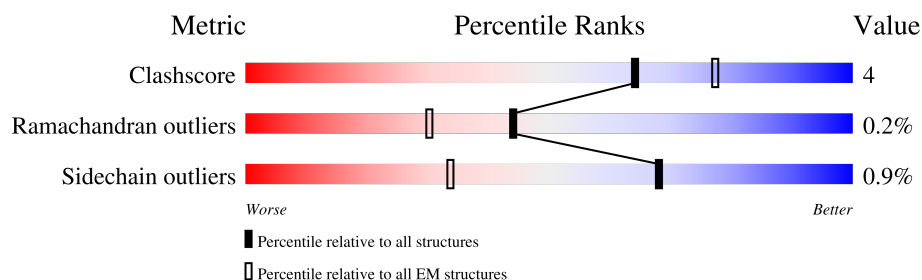
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.36 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	4686 (1.86 - 2.86)

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	A	806	
1	B	806	
1	C	806	
1	D	806	

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Mol	Chain	Length	Quality of chain
1	E	806	27% 83% 14%
1	F	806	28% 84% 11%
2	S	22	23% 95% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36997 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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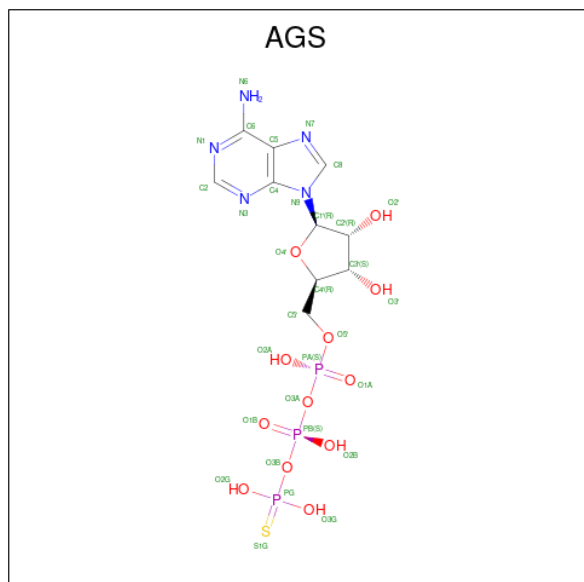
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Chain	Residue	Modelled	Actual	Comment	Reference
F	802	HIS	-	expression tag	UNP A0A059VAZ3
F	803	HIS	-	expression tag	UNP A0A059VAZ3
F	804	HIS	-	expression tag	UNP A0A059VAZ3
F	805	HIS	-	expression tag	UNP A0A059VAZ3
F	806	HIS	-	expression tag	UNP A0A059VAZ3
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.

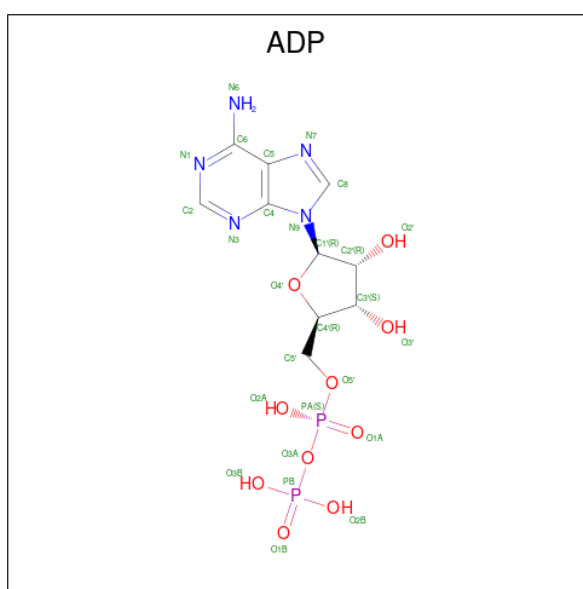
Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	22	Total	C	N	O	0	0
			111	66	22	23		

- 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).

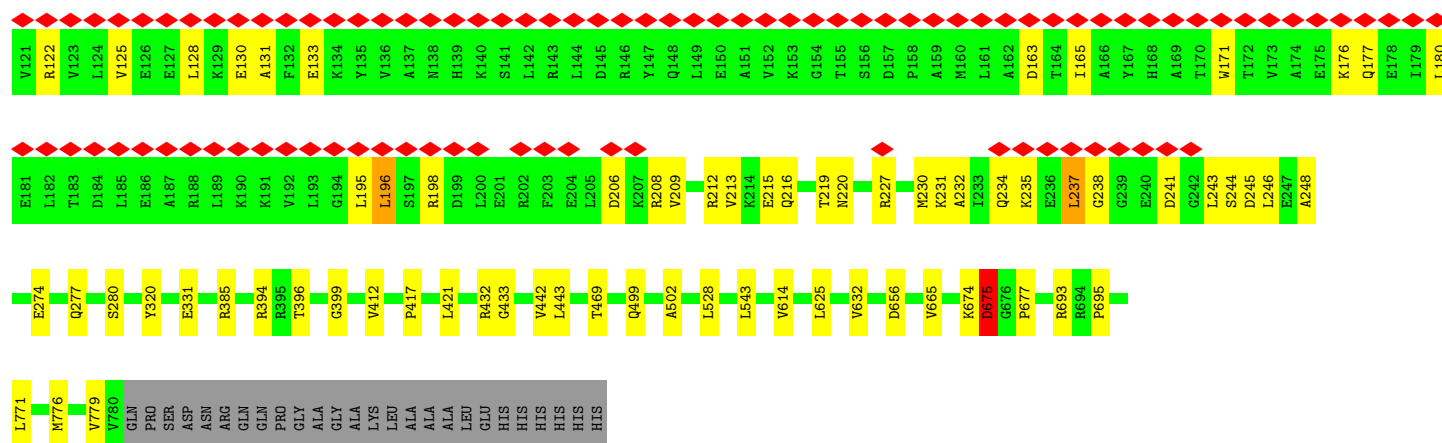


Mol	Chain	Residues	Atoms					AltConf	
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

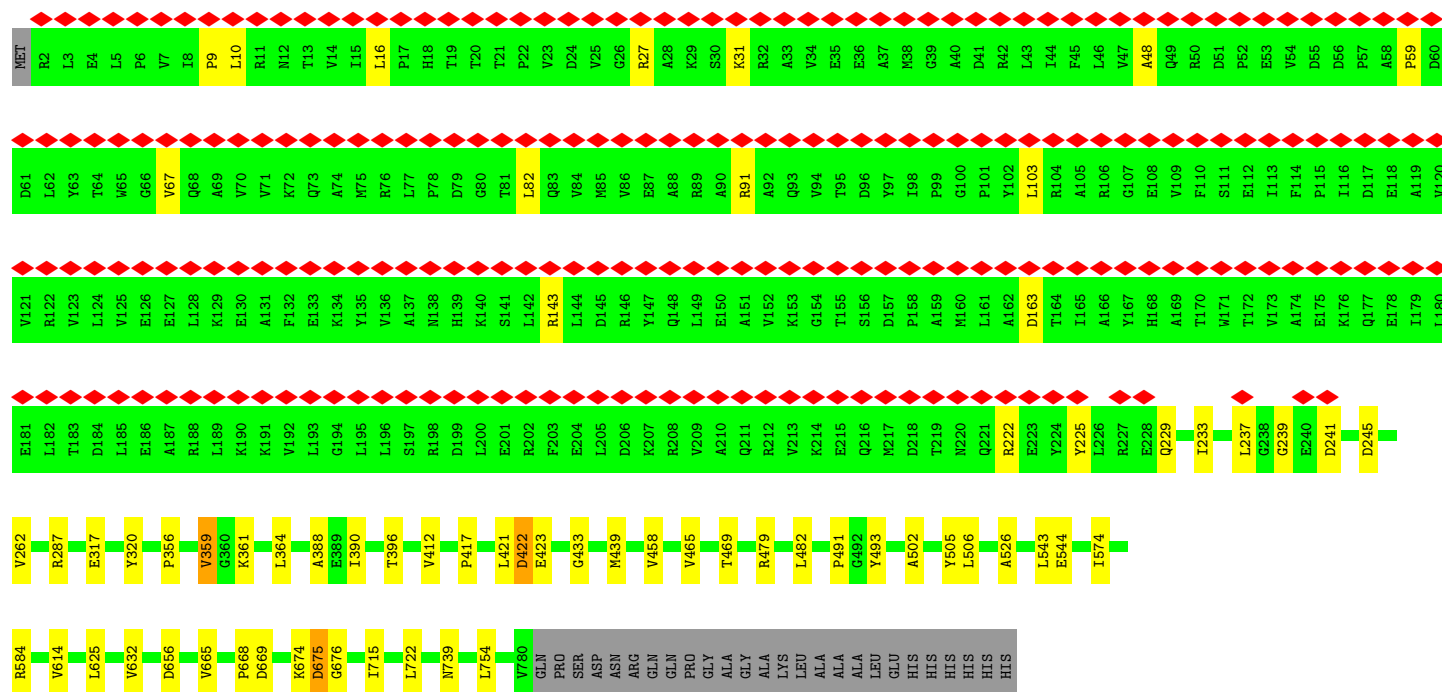
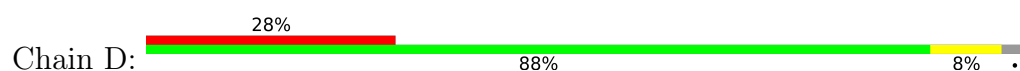
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



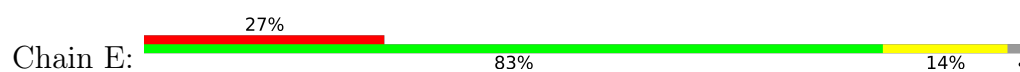
Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

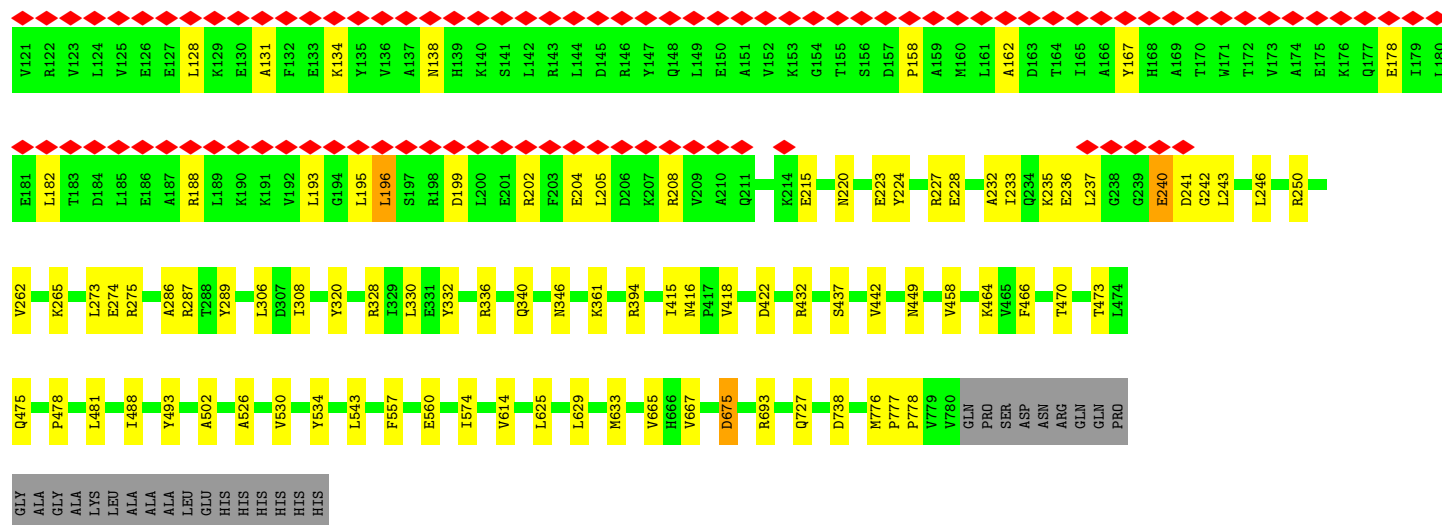


• Molecule 1: Lon protease

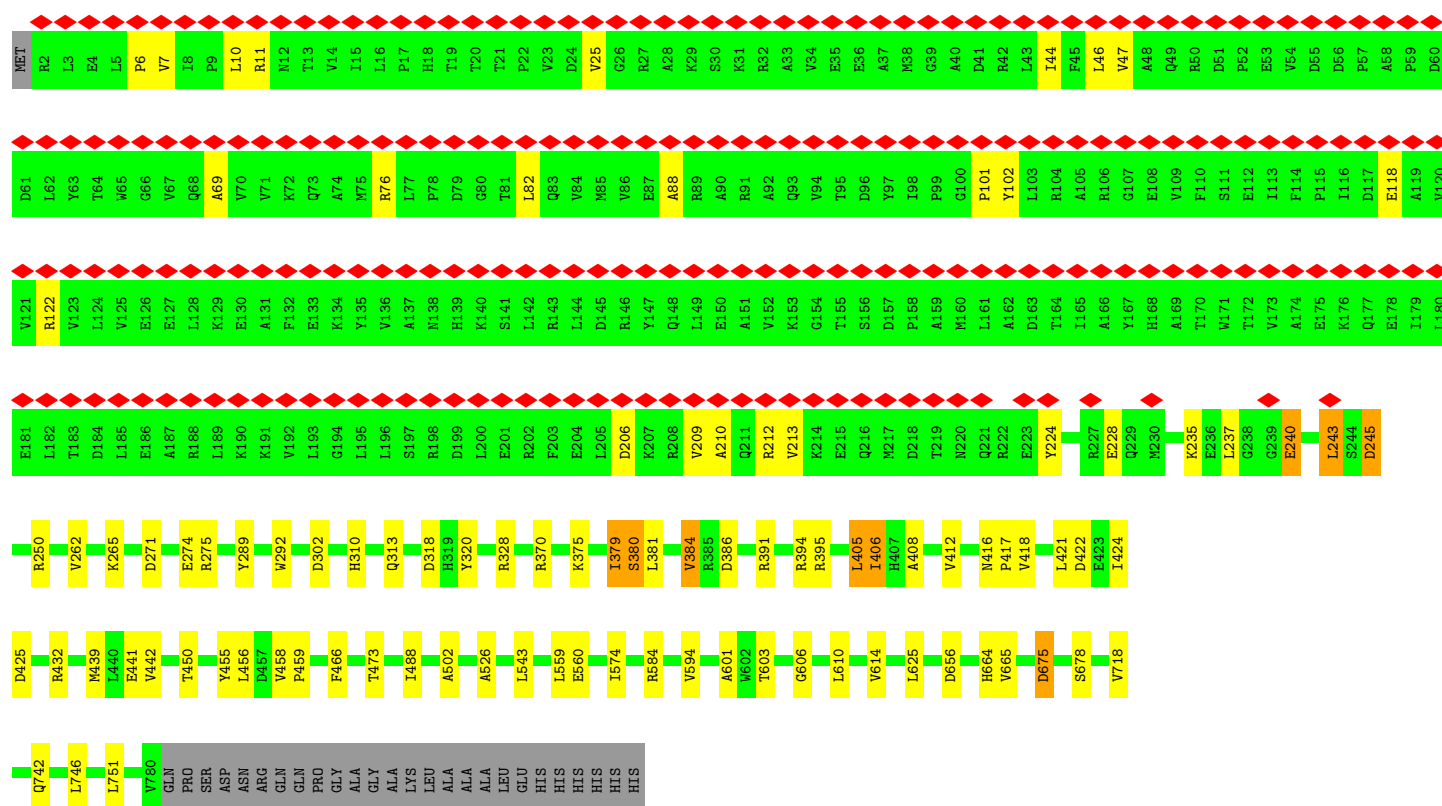
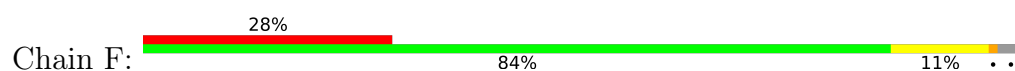


• Molecule 1: Lon protease

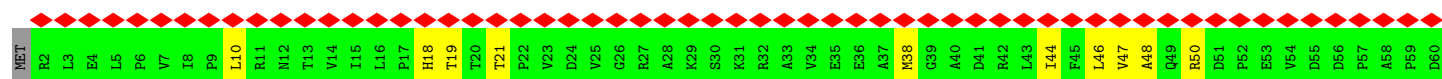
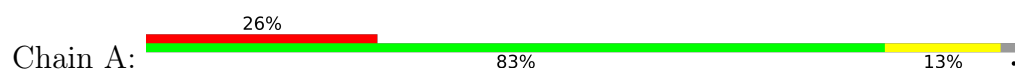


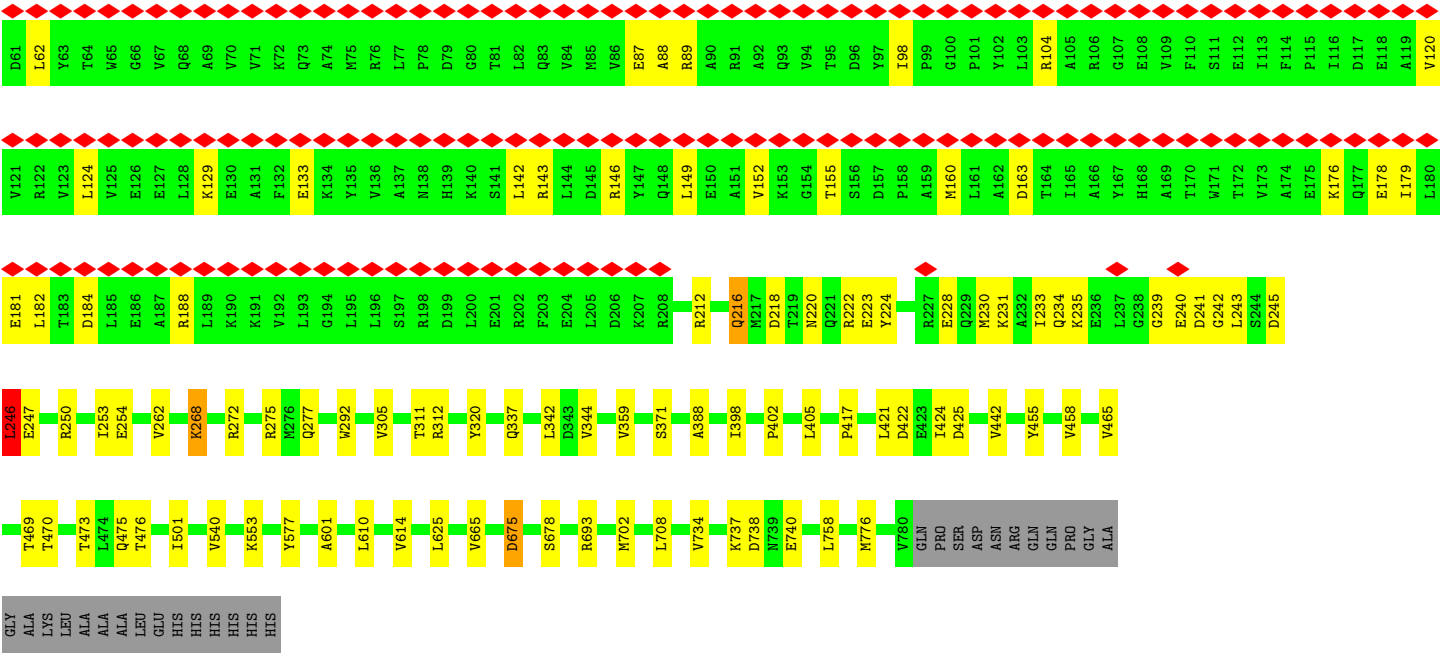


• Molecule 1: Lon protease

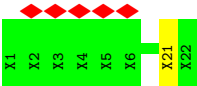
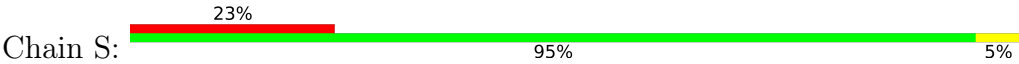


• Molecule 1: Lon protease





● Molecule 2: Unknown endogenous substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	361692	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 ($e^-/\text{\AA}^2$)	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	4.052	Depositor
Minimum map value	-1.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.204	Depositor
Map size ($\text{\AA}$)	275.52, 275.52, 275.52	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	1/6229 (0.0%)	0.72	3/8444 (0.0%)
1	B	0.42	2/6229 (0.0%)	0.67	10/8444 (0.1%)
1	C	0.40	1/6229 (0.0%)	0.68	6/8444 (0.1%)
1	D	0.44	2/6229 (0.0%)	0.66	6/8444 (0.1%)
1	E	0.34	1/6229 (0.0%)	0.67	5/8444 (0.1%)
1	F	0.36	1/6229 (0.0%)	0.65	1/8444 (0.0%)
All	All	0.39	8/37374 (0.0%)	0.68	31/50664 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	3
All	All	0	11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	675	ASP	C-O	-9.30	1.12	1.23
1	E	675	ASP	C-O	-9.07	1.13	1.23
1	F	675	ASP	C-O	-8.97	1.13	1.23
1	A	675	ASP	C-O	-8.93	1.13	1.23
1	C	675	ASP	C-O	-8.91	1.13	1.23
1	B	675	ASP	C-O	-8.71	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	356	PRO	C-O	-5.70	1.18	1.24
1	B	677	PRO	C-O	-5.13	1.18	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	675	ASP	O-C-N	-16.10	106.19	123.42
1	A	675	ASP	O-C-N	-15.00	107.51	123.26
1	E	675	ASP	O-C-N	-14.85	107.67	123.26
1	F	675	ASP	O-C-N	-14.77	107.75	123.26
1	C	675	ASP	O-C-N	-14.72	107.67	123.42
1	B	675	ASP	O-C-N	-13.70	107.64	123.25
1	A	239	GLY	N-CA-C	-7.22	106.10	114.69
1	C	109	VAL	CA-C-N	7.12	131.91	121.31
1	C	109	VAL	C-N-CA	7.12	131.91	121.31
1	D	359	VAL	N-CA-C	-6.68	102.66	110.21
1	B	279	GLY	N-CA-C	-6.53	97.70	113.18
1	D	317	GLU	N-CA-C	-6.43	105.36	113.72
1	B	279	GLY	CA-C-N	6.37	130.61	122.64
1	B	279	GLY	C-N-CA	6.37	130.61	122.64
1	D	543	LEU	N-CA-C	-5.74	105.02	111.28
1	B	440	LEU	CA-C-N	5.68	132.38	121.54
1	B	440	LEU	C-N-CA	5.68	132.38	121.54
1	E	449	ASN	N-CA-C	-5.63	107.42	114.56
1	C	677	PRO	N-CA-CB	-5.61	97.36	103.25
1	B	240	GLU	N-CA-C	-5.51	106.51	113.23
1	E	442	VAL	N-CA-C	-5.49	107.45	113.43
1	E	237	LEU	N-CA-C	-5.37	105.80	112.93
1	C	108	GLU	CA-C-N	5.36	127.80	120.35
1	C	108	GLU	C-N-CA	5.36	127.80	120.35
1	D	237	LEU	N-CA-C	-5.36	104.96	112.25
1	A	246	LEU	N-CA-C	-5.33	105.87	112.38
1	D	239	GLY	CA-C-O	-5.25	117.68	122.24
1	B	237	LEU	N-CA-C	-5.18	105.25	112.30
1	E	437	SER	N-CA-C	-5.11	107.70	114.04
1	B	273	LEU	CA-C-N	5.04	127.74	120.38
1	B	273	LEU	C-N-CA	5.04	127.74	120.38

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	LYS	Peptide
1	A	675	ASP	Mainchain
1	B	278	GLN	Peptide
1	B	675	ASP	Mainchain
1	C	108	GLU	Peptide
1	C	675	ASP	Mainchain
1	D	675	ASP	Mainchain
1	E	675	ASP	Mainchain
1	F	245	ASP	Peptide
1	F	416	ASN	Peptide
1	F	675	ASP	Mainchain

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	69	0
1	B	6118	0	6236	34	0
1	C	6118	0	6236	67	0
1	D	6118	0	6236	38	0
1	E	6118	0	6236	71	0
1	F	6118	0	6236	61	0
2	S	111	0	24	2	0
3	A	31	0	12	2	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	2	0
All	All	36997	0	37512	306	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 (306) 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:C:216:GLN:HB3	1:E:228:GLU:OE2	1.76	0.86
1:F:379:ILE:HD11	1:F:408:ALA:HB2	1.58	0.85
1:C:238:GLY:HA2	1:D:222:ARG:HH12	1.42	0.84
1:C:216:GLN:CB	1:E:228:GLU:OE2	2.36	0.73
1:B:275:ARG:HH21	1:A:234:GLN:HE22	1.34	0.73
1:C:131:ALA:HB1	1:C:196:LEU:HD11	1.75	0.69
1:A:501:ILE:HD11	1:A:540:VAL:HG11	1.73	0.69
1:D:715:ILE:H	1:D:739:ASN:HD21	1.41	0.69
1:A:268:LYS:O	1:A:272:ARG:NH1	2.27	0.67
1:F:381:LEU:HD11	1:F:421:LEU:HD12	1.77	0.66
1:B:412:VAL:HG11	1:B:417:PRO:HB3	1.75	0.66
1:A:143:ARG:HG2	1:A:146:ARG:HH22	1.61	0.65
1:E:629:LEU:HD22	1:E:633:MET:HG2	1.78	0.65
1:E:416:ASN:HB3	1:E:464:LYS:HG2	1.80	0.64
1:D:417:PRO:HD2	1:D:465:VAL:HG12	1.79	0.64
1:C:245:ASP:N	1:C:245:ASP:OD1	2.28	0.64
1:A:243:LEU:HA	1:A:247:GLU:HB2	1.80	0.63
1:B:218:ASP:OD2	1:B:222:ARG:NH1	2.33	0.62
1:C:171:TRP:H	1:C:176:LYS:HE3	1.64	0.62
1:E:98:ILE:HB	1:E:104:ARG:HB2	1.81	0.61
1:E:12:ASN:HD22	1:E:23:VAL:HA	1.65	0.61
1:A:182:LEU:O	1:A:188:ARG:NH2	2.33	0.61
1:C:208:ARG:NH1	1:E:236:GLU:OE2	2.35	0.60
1:C:212:ARG:NH2	1:E:232:ALA:O	2.31	0.60
1:E:328:ARG:O	1:E:328:ARG:NH1	2.32	0.59
1:A:98:ILE:HD11	1:A:104:ARG:H	1.67	0.59
1:C:412:VAL:HG11	1:C:417:PRO:HB3	1.84	0.59
1:B:394:ARG:NH1	1:A:388:ALA:O	2.36	0.59
1:A:305:VAL:O	1:A:337:GLN:NE2	2.36	0.58
1:C:432:ARG:HE	1:C:433:GLY:H	1.49	0.58
1:C:421:LEU:HB2	1:C:469:THR:HG22	1.85	0.58
1:A:737:LYS:HA	1:A:758:LEU:HD23	1.85	0.58
1:C:65:TRP:HD1	1:C:180:LEU:HD23	1.69	0.57
1:F:381:LEU:HD12	1:F:424:ILE:HG13	1.84	0.57
1:C:232:ALA:HB2	1:A:216:GLN:HE22	1.69	0.57
1:E:693:ARG:NH2	1:E:776:MET:SD	2.77	0.57
1:C:220:ASN:ND2	1:E:224:TYR:OH	2.37	0.57
1:D:225:TYR:O	1:D:229:GLN:NE2	2.38	0.56
1:D:320:TYR:H	3:D:901:AGS:HN61	1.53	0.56
1:A:417:PRO:HD2	1:A:465:VAL:HG22	1.86	0.56
1:F:271:ASP:O	1:F:275:ARG:NH1	2.39	0.56
1:A:38:MET:HG3	1:A:44:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:MET:HB3	1:D:233:ILE:HG21	1.87	0.56
1:B:242:GLY:HA2	1:B:246:LEU:HD23	1.87	0.56
1:F:265:LYS:NZ	1:F:289:TYR:OH	2.38	0.56
1:D:10:LEU:HD21	1:D:48:ALA:HA	1.88	0.56
1:E:204:GLU:OE1	1:E:208:ARG:NH1	2.38	0.55
1:F:302:ASP:OD2	1:F:375:LYS:NZ	2.39	0.55
1:F:320:TYR:H	4:F:901:ADP:HN62	1.55	0.55
1:B:484:ARG:NH2	3:A:901:AGS:S1G	2.80	0.55
1:A:272:ARG:HG3	1:A:275:ARG:HE	1.71	0.55
1:F:235:LYS:HA	1:F:240:GLU:H	1.71	0.55
1:A:342:LEU:HD12	1:A:344:VAL:H	1.71	0.55
1:E:336:ARG:NH1	1:E:346:ASN:OD1	2.40	0.54
1:A:405:LEU:HD13	1:A:442:VAL:HG21	1.90	0.54
1:F:560:GLU:OE2	1:A:312:ARG:NH2	2.41	0.54
1:C:695:PRO:HG2	1:C:771:LEU:HD12	1.89	0.54
1:A:421:LEU:HB2	1:A:469:THR:HG22	1.89	0.54
1:F:664:HIS:HD2	1:A:708:LEU:HD11	1.72	0.54
1:F:76:ARG:HH11	1:F:82:LEU:HD22	1.73	0.54
1:E:473:THR:OG1	1:E:475:GLN:NE2	2.41	0.53
1:C:91:ARG:NH2	1:C:163:ASP:OD2	2.42	0.53
1:C:213:VAL:HG23	1:E:228:GLU:HG2	1.90	0.53
1:D:245:ASP:OD2	1:E:275:ARG:NH2	2.42	0.53
1:C:195:LEU:HA	1:C:198:ARG:HD3	1.89	0.53
1:E:182:LEU:O	1:E:188:ARG:NH1	2.41	0.53
1:F:584:ARG:HH12	1:A:738:ASP:HB3	1.72	0.53
1:A:235:LYS:O	1:A:240:GLU:HA	2.08	0.53
1:B:281:PRO:HB2	1:A:398:ILE:HD11	1.89	0.53
1:B:359:VAL:O	3:B:901:AGS:O2B	2.27	0.53
1:C:499:GLN:HE21	1:C:528:LEU:HD13	1.73	0.53
1:D:412:VAL:HG11	1:D:417:PRO:HB3	1.90	0.53
1:A:50:ARG:NH1	1:A:178:GLU:OE2	2.42	0.53
1:F:262:VAL:HG22	1:F:458:VAL:HG21	1.91	0.53
1:A:253:ILE:HD12	1:A:254:GLU:HG3	1.91	0.53
1:B:255:GLU:HG3	1:B:256:VAL:HG23	1.90	0.53
1:E:2:ARG:NH1	1:E:68:GLN:OE1	2.43	0.52
1:F:320:TYR:H	4:F:901:ADP:N6	2.06	0.52
1:D:9:PRO:HG2	1:D:27:ARG:HH21	1.74	0.52
1:E:246:LEU:HD13	1:E:274:GLU:HG2	1.90	0.52
1:A:320:TYR:HB3	1:A:501:ILE:HG22	1.91	0.52
1:C:237:LEU:HB2	1:C:241:ASP:HB3	1.90	0.52
1:F:250:ARG:NH2	1:F:274:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:ARG:HH21	1:C:779:VAL:HB	1.75	0.52
1:E:220:ASN:ND2	1:A:224:TYR:OH	2.41	0.52
1:B:129:LYS:NZ	1:B:133:GLU:OE2	2.42	0.52
1:E:250:ARG:NH2	1:E:274:GLU:OE2	2.43	0.52
1:E:629:LEU:HD21	1:E:667:VAL:HG21	1.92	0.52
1:A:625:LEU:HD23	1:A:665:VAL:HB	1.91	0.52
1:E:432:ARG:HH12	2:S:21:UNK:HA	1.76	0.51
1:F:46:LEU:HD13	1:F:69:ALA:HB3	1.91	0.51
1:B:242:GLY:CA	1:B:246:LEU:HD23	2.40	0.51
1:F:614:VAL:HG22	1:F:665:VAL:HG22	1.91	0.51
1:D:359:VAL:HG13	1:D:493:TYR:CE2	2.46	0.51
1:D:390:ILE:HD12	1:D:439:MET:HE2	1.92	0.51
1:E:493:TYR:O	1:E:727:GLN:NE2	2.44	0.51
1:D:526:ALA:HB1	1:D:574:ILE:HD11	1.92	0.51
1:A:44:ILE:HG23	1:A:46:LEU:HD23	1.92	0.51
1:C:632:VAL:HG22	1:C:675:ASP:OD1	2.11	0.51
1:C:232:ALA:O	1:A:212:ARG:NH2	2.44	0.51
1:A:129:LYS:NZ	1:A:152:VAL:O	2.44	0.50
1:F:386:ASP:HB3	1:F:432:ARG:HE	1.77	0.50
1:C:216:GLN:OE1	1:E:228:GLU:CG	2.59	0.50
1:E:16:LEU:HD13	1:E:167:TYR:HD1	1.77	0.50
1:C:47:VAL:HG23	1:C:49:GLN:HE21	1.77	0.50
1:B:226:LEU:HD11	1:A:233:ILE:HG23	1.93	0.49
1:D:421:LEU:HB2	1:D:469:THR:HG22	1.93	0.49
1:E:306:LEU:HD21	1:E:340:GLN:HE21	1.77	0.49
1:A:292:TRP:CE2	1:A:402:PRO:HG2	2.46	0.49
1:F:391:ARG:NH1	1:F:441:GLU:OE1	2.45	0.49
1:C:246:LEU:HD13	1:C:274:GLU:HG2	1.94	0.49
1:E:287:ARG:HB3	1:F:394:ARG:HH21	1.77	0.49
1:C:632:VAL:CG2	1:C:675:ASP:OD1	2.60	0.49
1:C:177:GLN:HA	1:C:180:LEU:HD13	1.95	0.49
1:C:399:GLY:HA3	1:D:396:THR:HA	1.94	0.49
1:C:206:ASP:HA	1:C:209:VAL:HG22	1.94	0.49
1:F:10:LEU:HD11	1:F:46:LEU:HD23	1.94	0.49
1:E:10:LEU:HD21	1:E:46:LEU:HD22	1.95	0.49
1:A:473:THR:OG1	1:A:475:GLN:OE1	2.31	0.49
1:B:233:ILE:HG21	1:A:230:MET:HB2	1.94	0.49
1:C:171:TRP:HB2	1:C:176:LYS:HG3	1.95	0.49
1:D:59:PRO:HB3	1:D:103:LEU:HD22	1.93	0.49
1:E:526:ALA:HB1	1:E:574:ILE:HD11	1.94	0.48
1:F:7:VAL:HG13	1:F:47:VAL:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:GLU:OE1	1:C:106:ARG:NH1	2.46	0.48
1:D:632:VAL:HG23	1:D:676:GLY:H	1.78	0.48
1:E:158:PRO:O	1:E:162:ALA:CB	2.62	0.48
1:F:418:VAL:HG12	1:F:466:PHE:HB3	1.95	0.48
1:A:18:HIS:ND1	1:A:163:ASP:OD2	2.41	0.48
1:A:178:GLU:HA	1:A:181:GLU:HB2	1.96	0.48
1:B:74:ALA:O	1:B:76:ARG:NH1	2.47	0.48
1:A:601:ALA:HB2	1:A:610:LEU:HG	1.96	0.48
1:B:25:VAL:HG13	1:B:27:ARG:HD3	1.96	0.48
1:C:209:VAL:HG11	1:E:233:ILE:HD13	1.96	0.48
1:E:328:ARG:HH12	1:E:332:TYR:HB2	1.77	0.48
1:C:320:TYR:H	3:C:901:AGS:HN61	1.62	0.47
1:D:287:ARG:HE	1:E:275:ARG:HH12	1.61	0.47
1:C:22:PRO:HB3	1:C:83:GLN:HG2	1.96	0.47
1:B:7:VAL:HG22	1:B:45:PHE:HB2	1.96	0.47
1:F:209:VAL:HG23	1:F:212:ARG:HE	1.79	0.47
1:C:14:VAL:HB	1:C:177:GLN:HE21	1.79	0.47
1:C:104:ARG:HD2	1:C:106:ARG:HH22	1.78	0.47
1:C:693:ARG:HD2	1:C:776:MET:HB2	1.97	0.47
1:E:240:GLU:O	1:E:242:GLY:N	2.48	0.47
1:F:318:ASP:OD2	1:F:370:ARG:NH1	2.47	0.47
1:F:379:ILE:HD11	1:F:408:ALA:CB	2.38	0.47
1:A:155:THR:HG21	1:A:160:MET:HE2	1.95	0.47
1:A:231:LYS:HD3	1:A:277:GLN:HB2	1.96	0.47
1:A:425:ASP:HB2	1:A:476:THR:HG23	1.96	0.47
1:C:442:VAL:HG23	1:C:443:LEU:HG	1.97	0.47
1:D:614:VAL:HG22	1:D:665:VAL:HG22	1.97	0.47
1:D:31:LYS:HG2	1:D:82:LEU:HD12	1.97	0.47
1:C:502:ALA:HB2	1:C:543:LEU:HD21	1.97	0.46
1:A:234:GLN:O	1:A:241:ASP:HB2	2.14	0.46
1:A:740:GLU:HB3	1:A:758:LEU:HD21	1.98	0.46
1:D:262:VAL:HG23	1:D:458:VAL:HG11	1.96	0.46
1:F:526:ALA:HB1	1:F:574:ILE:HD11	1.97	0.46
1:A:422:ASP:OD1	1:A:470:THR:OG1	2.33	0.46
1:F:292:TRP:HH2	1:F:406:ILE:HD13	1.80	0.46
1:F:395:ARG:NH1	1:F:455:TYR:O	2.49	0.46
1:A:553:LYS:NZ	1:A:577:TYR:O	2.47	0.46
1:D:67:VAL:HA	1:D:91:ARG:HA	1.98	0.46
1:D:502:ALA:HA	1:D:506:LEU:HB2	1.97	0.46
1:A:359:VAL:O	3:A:901:AGS:O2B	2.33	0.46
1:E:478:PRO:HD2	1:E:481:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:MET:HG2	1:A:734:VAL:HB	1.97	0.46
1:C:125:VAL:HA	1:C:128:LEU:HG	1.96	0.46
1:F:439:MET:HA	1:F:442:VAL:HG22	1.97	0.46
1:A:182:LEU:HD13	1:A:184:ASP:HB3	1.98	0.46
1:E:308:ILE:HG13	1:E:330:LEU:HD22	1.98	0.46
1:C:97:TYR:HA	1:C:105:ALA:HB1	1.96	0.45
1:C:5:LEU:HD23	1:C:40:ALA:HB1	1.98	0.45
1:F:406:ILE:H	1:F:406:ILE:HG13	1.48	0.45
1:E:47:VAL:HA	1:E:66:GLY:HA2	1.98	0.45
1:E:614:VAL:HG22	1:E:665:VAL:HG22	1.98	0.45
1:F:206:ASP:HA	1:F:209:VAL:HG12	1.98	0.45
1:F:381:LEU:O	1:F:384:VAL:HG22	2.17	0.45
1:B:625:LEU:HD23	1:B:665:VAL:HB	1.99	0.45
1:B:681:ILE:HD11	1:B:765:VAL:HG21	1.99	0.45
1:C:232:ALA:HA	1:C:235:LYS:HG2	1.99	0.45
1:B:273:LEU:HD13	1:B:286:ALA:HB3	1.98	0.45
1:C:8:ILE:HD13	1:C:44:ILE:HG23	1.97	0.45
1:E:262:VAL:HG13	1:E:458:VAL:HG11	1.98	0.45
1:A:693:ARG:HD2	1:A:776:MET:HB2	1.99	0.45
1:D:422:ASP:C	1:D:423:GLU:HG2	2.42	0.45
1:F:625:LEU:HD23	1:F:665:VAL:HB	1.98	0.45
1:D:625:LEU:HD23	1:D:665:VAL:HB	1.98	0.45
1:A:176:LYS:HA	1:A:179:ILE:HG22	1.98	0.45
1:B:42:ARG:NH2	1:B:71:VAL:O	2.50	0.44
1:C:231:LYS:HG2	1:C:234:GLN:HE21	1.81	0.44
1:E:418:VAL:HG12	1:E:466:PHE:HB3	1.99	0.44
1:C:212:ARG:HH22	1:E:235:LYS:HB2	1.82	0.44
1:E:101:PRO:HA	1:E:102:TYR:HA	1.70	0.44
1:E:205:LEU:HA	1:E:208:ARG:HG2	1.98	0.44
1:F:380:SER:HA	1:F:422:ASP:HB2	2.00	0.44
1:A:262:VAL:HG12	1:A:458:VAL:HG11	2.00	0.44
1:B:388:ALA:O	1:C:394:ARG:NH1	2.50	0.44
1:D:9:PRO:O	1:D:27:ARG:NH2	2.50	0.44
1:E:361:LYS:HG2	1:E:470:THR:HG23	1.99	0.44
1:B:250:ARG:HH11	1:B:267:LEU:HD22	1.83	0.44
1:B:600:LEU:HD13	1:B:721:LYS:HB3	1.99	0.44
1:D:584:ARG:NH2	1:E:738:ASP:O	2.47	0.44
1:E:182:LEU:HD23	1:E:188:ARG:HB2	1.99	0.44
1:D:388:ALA:O	1:E:394:ARG:NH1	2.50	0.44
1:C:128:LEU:HA	1:C:131:ALA:HB3	2.00	0.44
1:F:456:LEU:HG	1:F:458:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:LEU:C	1:F:245:ASP:H	2.26	0.44
1:C:49:GLN:HE22	1:C:62:LEU:HG	1.83	0.44
1:C:216:GLN:HB2	1:E:228:GLU:OE2	2.15	0.44
1:E:193:LEU:HA	1:E:196:LEU:HD23	2.00	0.44
1:D:479:ARG:HH21	1:D:482:LEU:HD22	1.83	0.43
1:E:199:ASP:OD1	1:E:202:ARG:NH1	2.52	0.43
1:C:614:VAL:HG22	1:C:665:VAL:HG22	2.00	0.43
1:E:422:ASP:HA	1:E:470:THR:HB	1.99	0.43
1:A:242:GLY:HA2	1:A:246:LEU:HD21	2.01	0.43
1:E:22:PRO:HB3	1:E:83:GLN:HE21	1.82	0.43
1:E:557:PHE:HA	1:E:560:GLU:HG3	2.00	0.43
1:F:405:LEU:HD23	1:F:405:LEU:HA	1.74	0.43
1:F:601:ALA:HB2	1:F:610:LEU:HG	2.00	0.43
1:B:274:GLU:OE2	1:B:275:ARG:NH1	2.52	0.43
1:E:273:LEU:HD13	1:E:286:ALA:HB3	2.00	0.43
1:F:224:TYR:O	1:F:228:GLU:HB2	2.18	0.43
1:A:220:ASN:HA	1:A:223:GLU:HG2	2.00	0.43
1:B:96:ASP:OD2	1:B:106:ARG:NH2	2.50	0.43
1:D:320:TYR:HB2	1:D:505:TYR:CE2	2.53	0.43
1:F:450:THR:HA	1:F:459:PRO:HB3	2.00	0.43
1:A:19:THR:HG22	1:A:21:THR:HG23	2.01	0.43
1:A:87:GLU:OE2	1:A:89:ARG:NH2	2.52	0.43
1:F:328:ARG:HG3	1:F:488:ILE:HD12	2.01	0.43
1:D:143:ARG:HA	1:A:120:VAL:HG11	2.01	0.42
1:E:625:LEU:HD23	1:E:665:VAL:HB	2.01	0.42
1:E:131:ALA:HA	1:E:134:LYS:HE3	2.01	0.42
1:F:379:ILE:O	1:F:380:SER:HB3	2.19	0.42
1:F:746:LEU:HB2	1:F:751:LEU:HD23	1.99	0.42
1:A:18:HIS:HE1	1:A:88:ALA:HB2	1.83	0.42
1:C:37:ALA:HA	1:C:40:ALA:HB3	2.00	0.42
1:E:320:TYR:H	4:E:901:ADP:HN62	1.66	0.42
1:E:328:ARG:HD2	1:E:488:ILE:HG13	2.02	0.42
1:E:415:ILE:HG13	1:E:464:LYS:HD3	2.01	0.42
1:F:69:ALA:HA	1:F:88:ALA:HA	2.00	0.42
1:F:502:ALA:HB2	1:F:543:LEU:HD21	2.01	0.42
1:A:245:ASP:C	1:A:247:GLU:N	2.76	0.42
1:C:215:GLU:O	1:C:219:THR:OG1	2.29	0.42
1:F:6:PRO:HD2	1:F:44:ILE:HG22	2.00	0.42
1:E:777:PRO:HA	1:E:778:PRO:HD3	1.83	0.42
1:F:209:VAL:HA	1:F:212:ARG:HG2	2.00	0.42
1:C:277:GLN:HB2	1:C:280:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:HD13	1:D:163:ASP:HB3	2.00	0.42
1:D:656:ASP:OD1	1:D:656:ASP:N	2.52	0.42
1:F:11:ARG:HH12	1:F:25:VAL:HG22	1.83	0.42
1:F:310:HIS:HA	1:F:313:GLN:HG2	2.02	0.42
1:E:6:PRO:HG3	1:E:36:GLU:HG3	2.02	0.42
1:A:218:ASP:O	1:A:222:ARG:HB2	2.20	0.42
1:C:656:ASP:OD1	1:C:656:ASP:N	2.53	0.42
1:E:13:THR:OG1	1:E:14:VAL:N	2.51	0.42
1:F:243:LEU:C	1:F:245:ASP:N	2.78	0.42
1:A:614:VAL:HG12	1:A:665:VAL:HG22	2.01	0.42
1:B:33:ALA:O	1:B:37:ALA:HB2	2.20	0.42
1:E:432:ARG:HH12	2:S:21:UNK:CA	2.32	0.42
1:F:603:THR:OG1	1:F:606:GLY:O	2.28	0.42
1:A:246:LEU:O	1:A:250:ARG:HB2	2.19	0.42
1:B:152:VAL:HG12	1:B:161:LEU:HD21	2.01	0.41
1:B:656:ASP:N	1:B:656:ASP:OD1	2.53	0.41
1:F:210:ALA:HA	1:F:213:VAL:HG12	2.01	0.41
1:E:134:LYS:O	1:E:138:ASN:HB2	2.19	0.41
1:A:224:TYR:O	1:A:228:GLU:HB2	2.20	0.41
1:A:402:PRO:HG3	1:A:455:TYR:CD2	2.55	0.41
1:B:358:GLY:HA3	1:B:539:GLY:HA3	2.01	0.41
1:C:244:SER:O	1:C:248:ALA:CB	2.68	0.41
1:C:625:LEU:HD23	1:C:665:VAL:HB	2.02	0.41
1:F:101:PRO:HA	1:F:102:TYR:HA	1.76	0.41
1:C:130:GLU:HA	1:C:133:GLU:HG2	2.01	0.41
1:F:118:GLU:OE2	1:F:122:ARG:NH2	2.54	0.41
1:F:656:ASP:OD1	1:F:656:ASP:N	2.53	0.41
1:B:242:GLY:HA2	1:B:246:LEU:CD2	2.51	0.41
1:C:44:ILE:HB	1:C:69:ALA:HB3	2.03	0.41
1:C:394:ARG:HG2	1:C:396:THR:HG23	2.02	0.41
1:D:722:LEU:HD12	1:D:754:LEU:HD13	2.03	0.41
1:E:502:ALA:HB2	1:E:543:LEU:HD21	2.03	0.41
1:E:693:ARG:HG3	1:E:778:PRO:HA	2.02	0.41
1:A:242:GLY:HA2	1:A:246:LEU:CD2	2.51	0.41
1:A:702:MET:HE3	1:A:702:MET:HB2	1.93	0.41
1:B:275:ARG:HH21	1:A:234:GLN:NE2	2.11	0.41
1:C:385:ARG:HD2	1:D:433:GLY:HA2	2.03	0.41
1:E:530:VAL:HA	1:E:534:TYR:HD2	1.85	0.41
1:C:17:PRO:HG3	1:C:88:ALA:HB3	2.03	0.41
1:D:668:PRO:HA	1:D:669:ASP:HA	1.74	0.41
1:A:10:LEU:HB2	1:A:48:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LEU:HD12	1:D:364:LEU:HA	1.91	0.41
1:E:128:LEU:HB2	1:E:193:LEU:HD21	2.02	0.41
1:B:260:GLU:HA	1:B:263:LYS:HG2	2.03	0.40
1:C:227:ARG:HA	1:C:230:MET:HG2	2.02	0.40
1:F:412:VAL:HG21	1:F:417:PRO:HG3	2.03	0.40
1:B:141:SER:HA	1:B:143:ARG:HH11	1.86	0.40
1:F:379:ILE:HD13	1:F:379:ILE:HA	1.81	0.40
1:F:559:LEU:HA	1:F:559:LEU:HD23	1.86	0.40
1:F:718:VAL:HG11	1:F:742:GLN:HB3	2.03	0.40
1:A:133:GLU:HG2	1:A:149:LEU:HD21	2.04	0.40
1:A:311:THR:HG23	1:A:371:SER:HB3	2.04	0.40
1:C:10:LEU:HD21	1:C:46:LEU:HD13	2.02	0.40
1:E:265:LYS:NZ	1:E:289:TYR:OH	2.50	0.40
1:B:10:LEU:H	1:B:48:ALA:HA	1.87	0.40
1:C:122:ARG:HA	1:C:125:VAL:HG12	2.03	0.40
1:D:143:ARG:HH21	1:A:124:LEU:HD22	1.86	0.40
1:E:223:GLU:OE2	1:E:227:ARG:HD2	2.21	0.40
1:F:425:ASP:OD2	1:F:473:THR:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	777/806 (96%)	738 (95%)	39 (5%)	0	100	100
1	B	777/806 (96%)	748 (96%)	28 (4%)	1 (0%)	48	59
1	C	777/806 (96%)	738 (95%)	39 (5%)	0	100	100
1	D	777/806 (96%)	744 (96%)	31 (4%)	2 (0%)	36	43
1	E	777/806 (96%)	744 (96%)	32 (4%)	1 (0%)	48	59
1	F	777/806 (96%)	748 (96%)	26 (3%)	3 (0%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4662/4836 (96%)	4460 (96%)	195 (4%)	7 (0%)	44	52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	LEU
1	D	241	ASP
1	E	241	ASP
1	F	380	SER
1	F	240	GLU
1	F	384	VAL
1	D	491	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	655/675 (97%)	648 (99%)	7 (1%)	65	79
1	B	655/675 (97%)	650 (99%)	5 (1%)	73	84
1	C	655/675 (97%)	649 (99%)	6 (1%)	70	82
1	D	655/675 (97%)	651 (99%)	4 (1%)	78	87
1	E	655/675 (97%)	649 (99%)	6 (1%)	70	82
1	F	655/675 (97%)	648 (99%)	7 (1%)	65	79
All	All	3930/4050 (97%)	3895 (99%)	35 (1%)	68	82

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	398	ILE
1	B	470	THR
1	B	674	LYS
1	B	678	SER
1	B	681	ILE

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Mol	Chain	Res	Type
1	C	165	ILE
1	C	196	LEU
1	C	237	LEU
1	C	243	LEU
1	C	331	GLU
1	C	674	LYS
1	D	361	LYS
1	D	422	ASP
1	D	544	GLU
1	D	674	LYS
1	E	178	GLU
1	E	195	LEU
1	E	196	LEU
1	E	215	GLU
1	E	240	GLU
1	E	243	LEU
1	F	237	LEU
1	F	243	LEU
1	F	379	ILE
1	F	405	LEU
1	F	406	ILE
1	F	594	VAL
1	F	678	SER
1	A	47	VAL
1	A	62	LEU
1	A	142	LEU
1	A	216	GLN
1	A	246	LEU
1	A	424	ILE
1	A	678	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	ASN
1	B	168	HIS
1	B	177	GLN
1	B	277	GLN
1	B	377	HIS
1	B	407	HIS
1	B	593	GLN
1	B	598	GLN

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Mol	Chain	Res	Type
1	C	12	ASN
1	C	49	GLN
1	C	73	GLN
1	C	148	GLN
1	C	177	GLN
1	C	220	ASN
1	C	393	HIS
1	C	407	HIS
1	C	454	HIS
1	D	68	GLN
1	D	73	GLN
1	D	168	HIS
1	D	277	GLN
1	D	499	GLN
1	D	504	GLN
1	D	510	GLN
1	D	598	GLN
1	D	628	GLN
1	D	739	ASN
1	E	49	GLN
1	E	83	GLN
1	E	177	GLN
1	E	216	GLN
1	E	220	ASN
1	E	234	GLN
1	E	340	GLN
1	E	475	GLN
1	E	593	GLN
1	E	731	HIS
1	F	18	HIS
1	F	234	GLN
1	F	319	HIS
1	F	449	ASN
1	F	628	GLN
1	F	726	HIS
1	A	12	ASN
1	A	234	GLN
1	A	337	GLN
1	A	377	HIS
1	A	598	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	B	901	-	32,33,33	1.09	4 (12%)	45,52,52	0.69	1 (2%)
4	ADP	E	901	-	28,29,29	0.54	0	43,45,45	0.60	0
4	ADP	F	901	-	28,29,29	0.55	0	43,45,45	0.59	0
3	AGS	A	901	-	32,33,33	0.93	3 (9%)	45,52,52	0.55	1 (2%)
3	AGS	C	901	-	32,33,33	0.77	2 (6%)	45,52,52	0.75	0
3	AGS	D	901	-	32,33,33	0.72	0	45,52,52	0.61	0

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	B	901	-	-	1/21/38/38	0/3/3/3
4	ADP	E	901	-	-	0/16/32/32	0/3/3/3
4	ADP	F	901	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	901	-	-	5/21/38/38	0/3/3/3
3	AGS	C	901	-	-	3/21/38/38	0/3/3/3
3	AGS	D	901	-	-	2/21/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	AGS	PA-O3A	-3.35	1.55	1.59
3	B	901	AGS	PB-O3B	-2.96	1.56	1.59
3	A	901	AGS	PA-O3A	-2.84	1.56	1.59
3	B	901	AGS	PB-O3A	-2.75	1.56	1.59
3	A	901	AGS	PB-O3A	-2.34	1.57	1.59
3	A	901	AGS	PB-O3B	-2.32	1.57	1.59
3	C	901	AGS	PG-O3G	-2.16	1.47	1.54
3	B	901	AGS	PG-S1G	2.10	1.95	1.90
3	C	901	AGS	PB-O2B	-2.10	1.45	1.55

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	AGS	PB-O3B-PG	-3.62	119.93	133.17
3	A	901	AGS	PB-O3B-PG	-2.24	124.97	133.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	901	AGS	O4'-C1'-N9-C4
3	D	901	AGS	O4'-C1'-N9-C4
4	F	901	ADP	O4'-C1'-N9-C4
3	D	901	AGS	O4'-C1'-N9-C8
3	C	901	AGS	O4'-C1'-N9-C8
4	F	901	ADP	O4'-C1'-N9-C8
3	A	901	AGS	O4'-C4'-C5'-O5'
3	A	901	AGS	C5'-O5'-PA-O1A
3	A	901	AGS	PA-O3A-PB-O1B
3	B	901	AGS	O4'-C4'-C5'-O5'
3	A	901	AGS	C3'-C4'-C5'-O5'
4	F	901	ADP	O4'-C4'-C5'-O5'
3	C	901	AGS	PA-O3A-PB-O2B
3	A	901	AGS	PA-O3A-PB-O2B

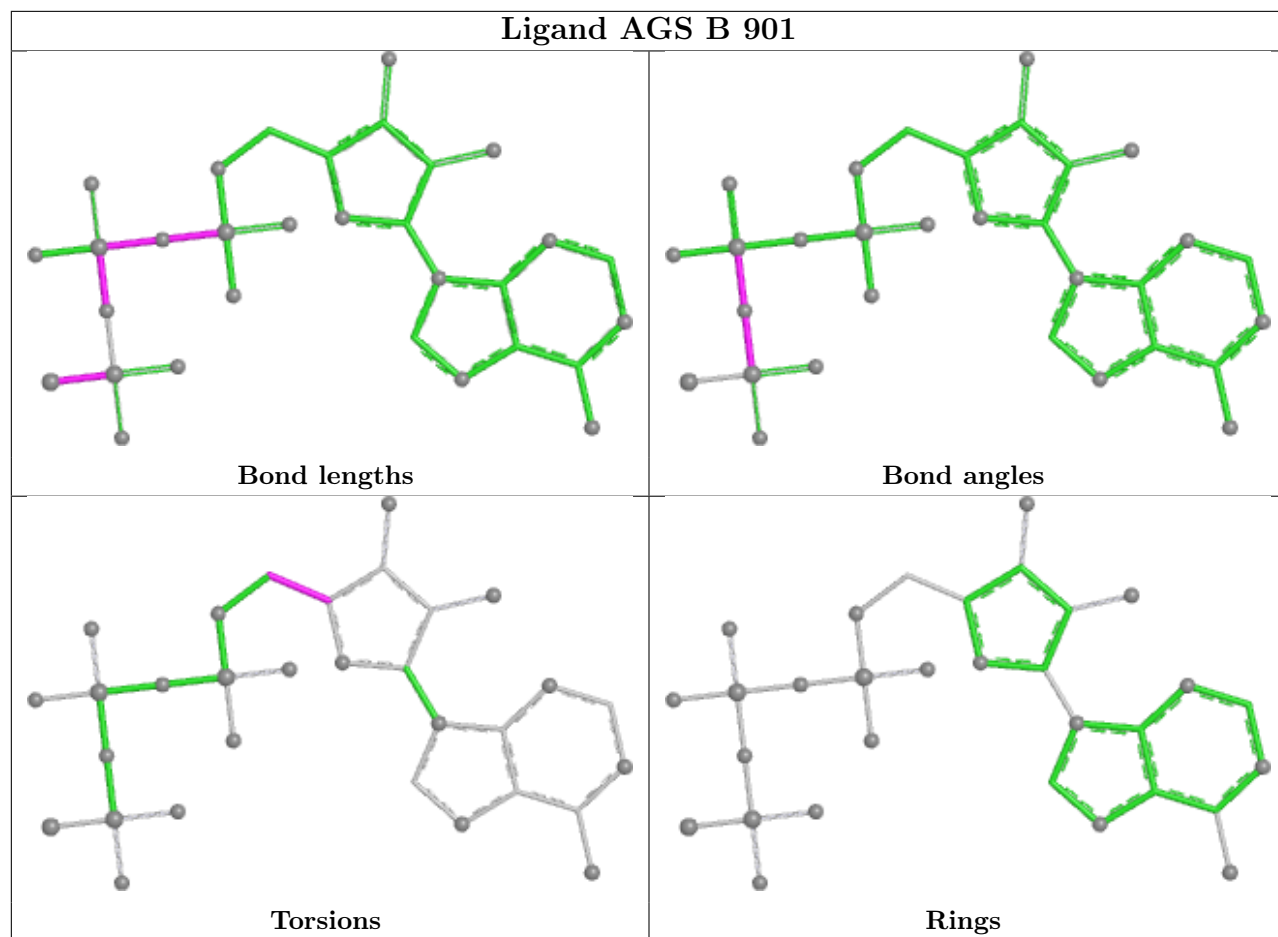
There are no ring outliers.

6 monomers are involved in 8 short contacts:

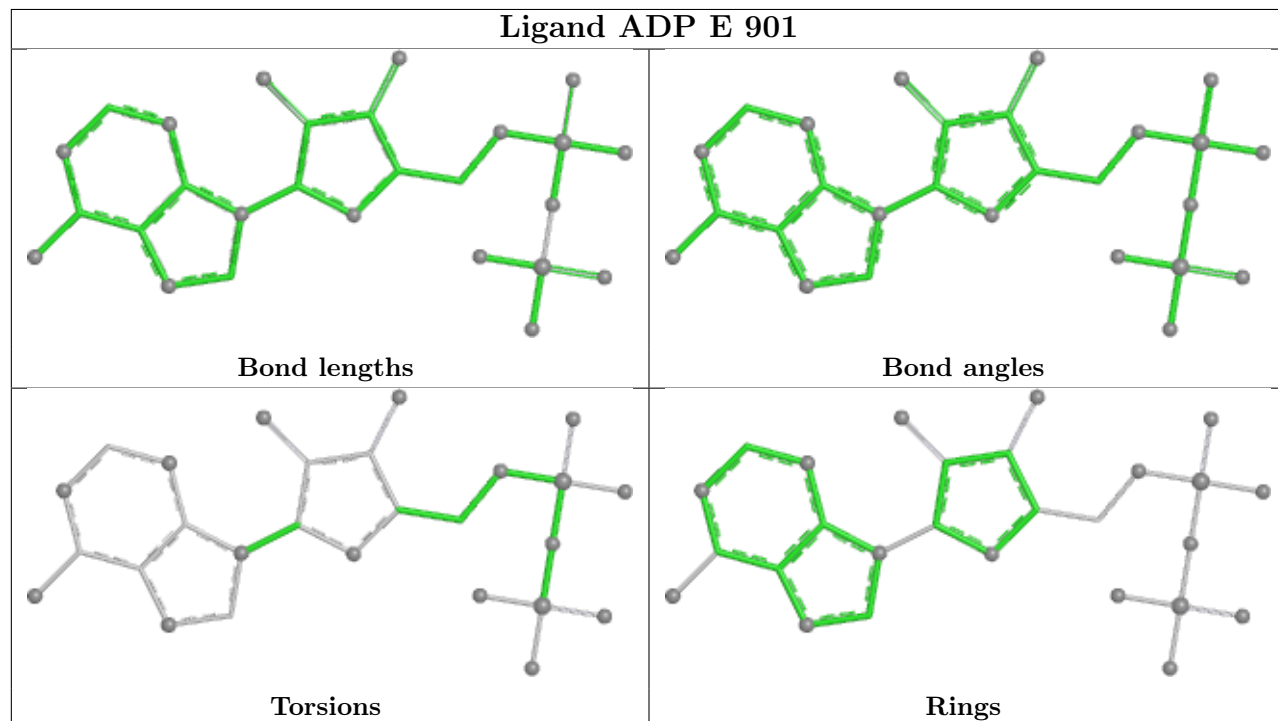
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	AGS	1	0
4	E	901	ADP	1	0
4	F	901	ADP	2	0
3	A	901	AGS	2	0
3	C	901	AGS	1	0
3	D	901	AGS	1	0

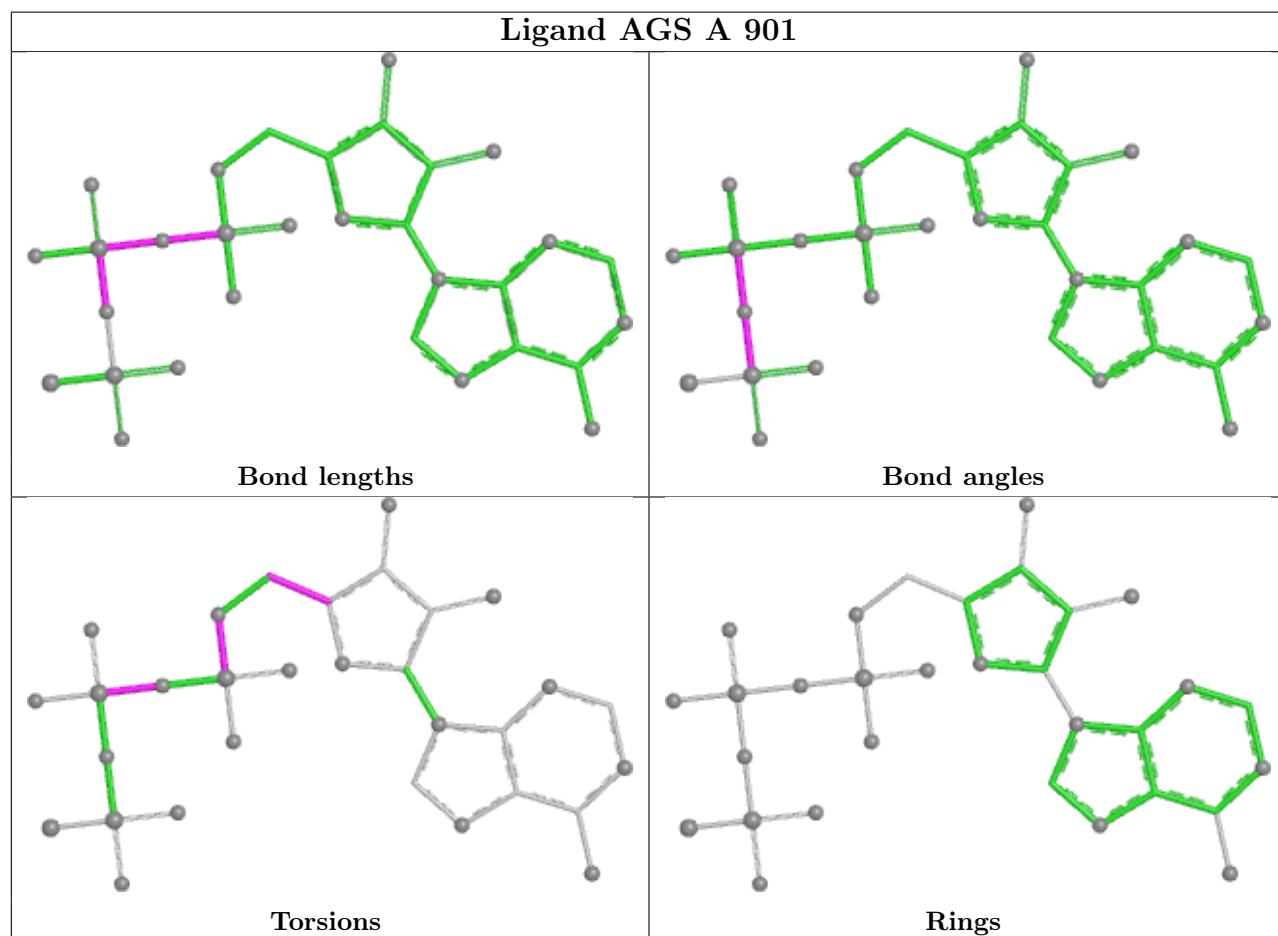
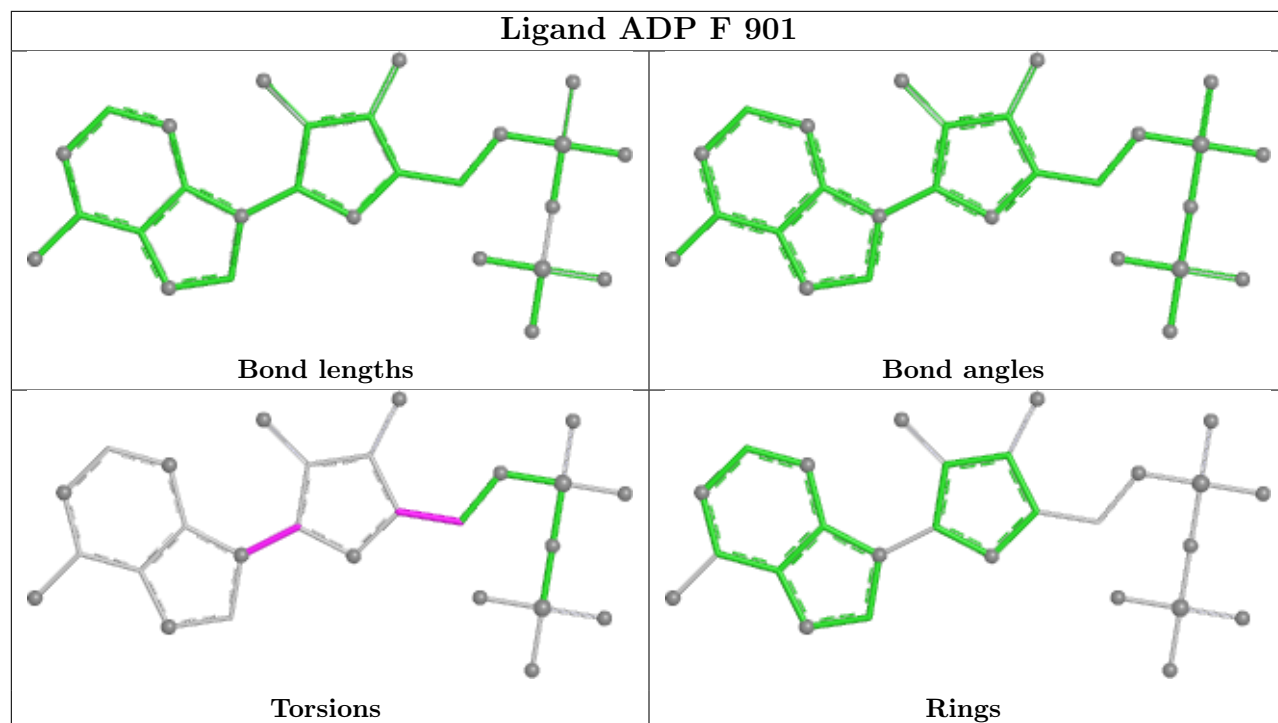
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

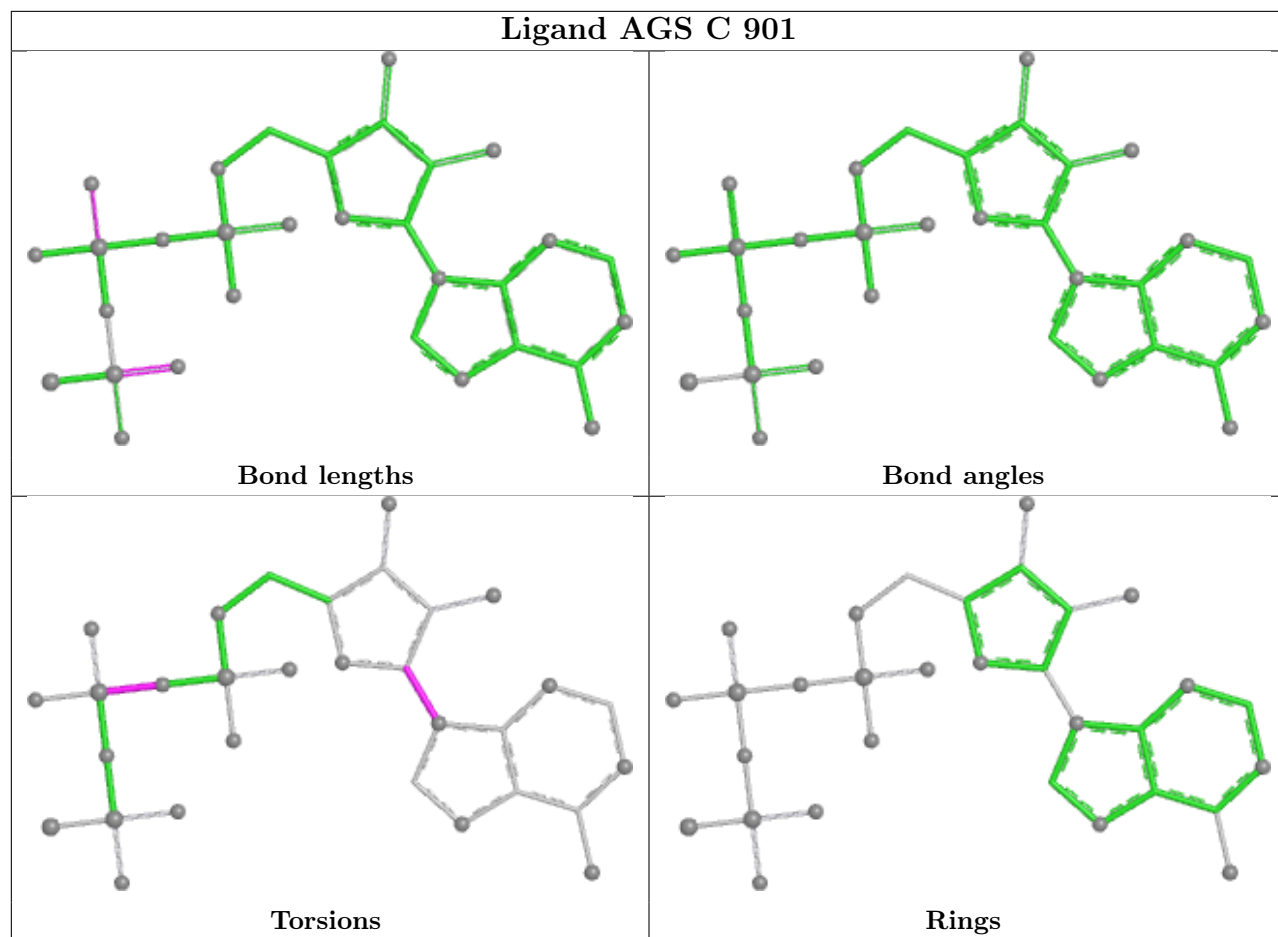
Ligand AGS B 901

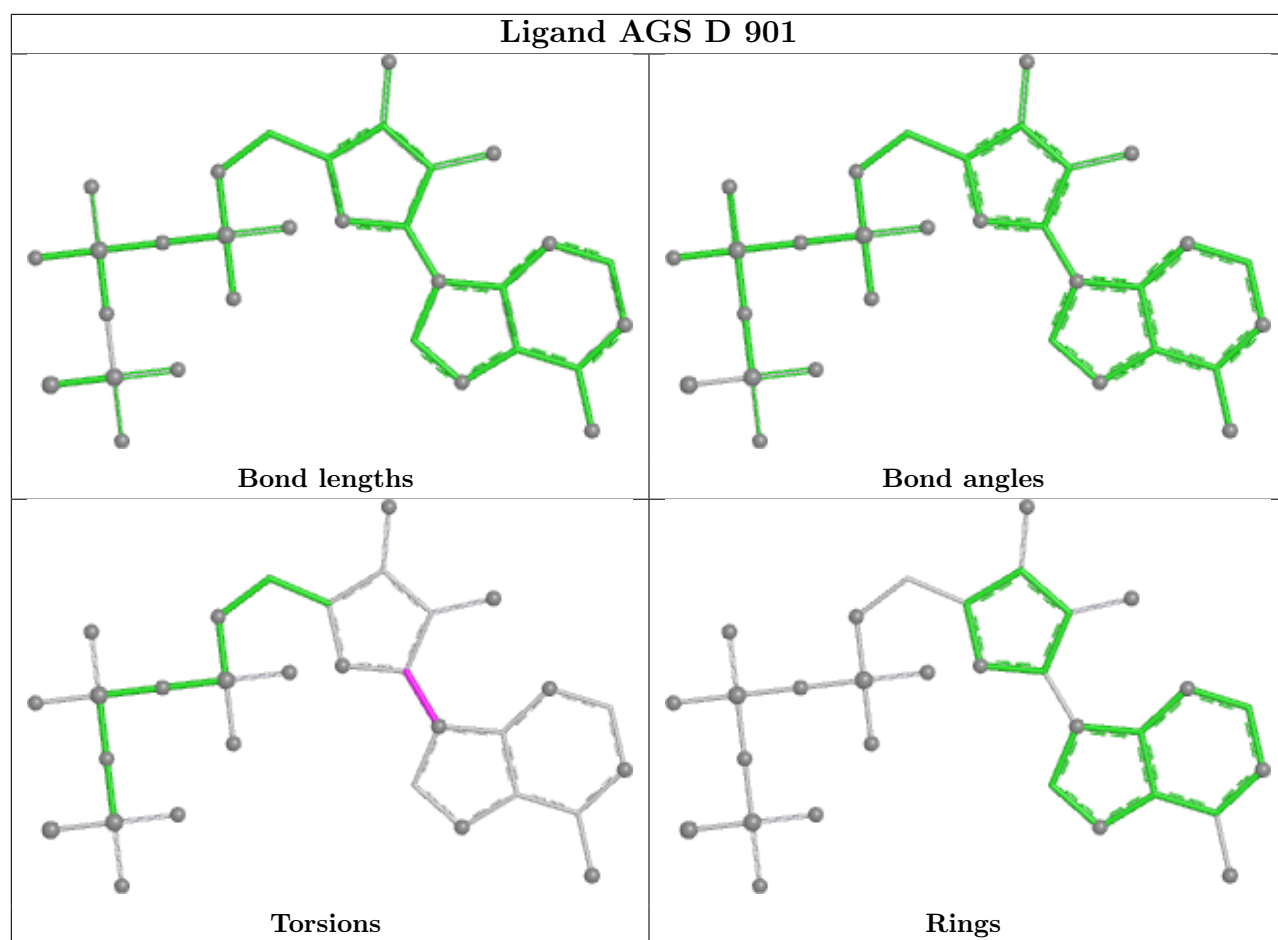


Ligand ADP E 901









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.

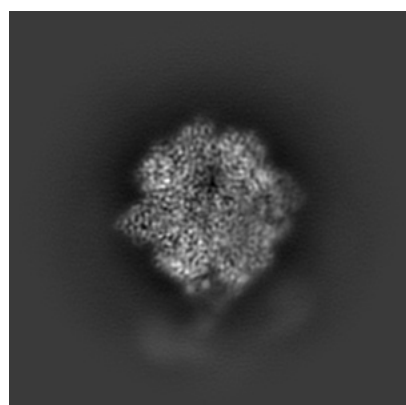
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31590. These allow visual inspection of the internal detail of the map and identification of artifacts.

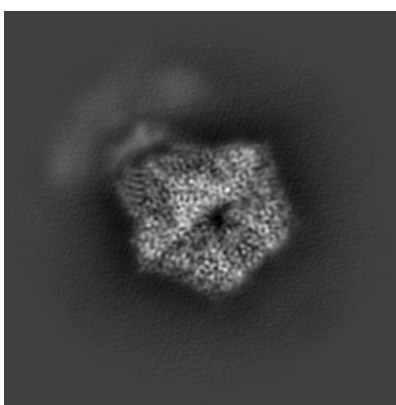
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

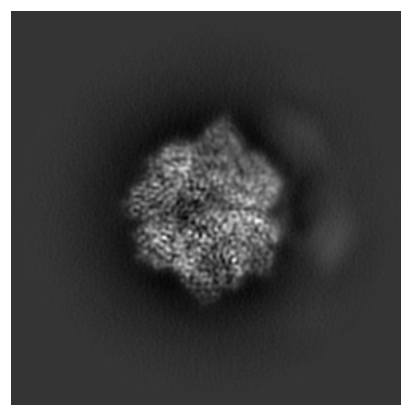
6.1.1 Primary map



X



Y

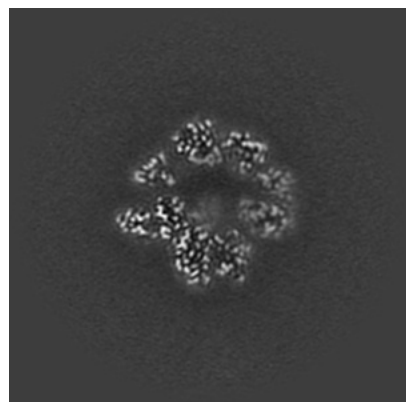


Z

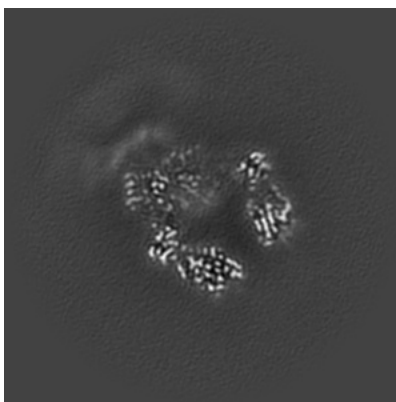
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

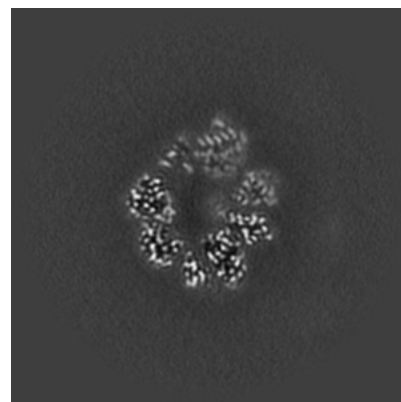
6.2.1 Primary map



X Index: 168



Y Index: 168

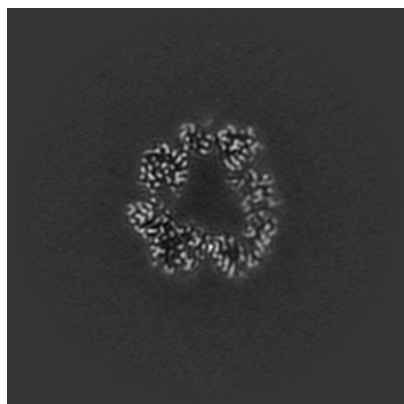


Z Index: 168

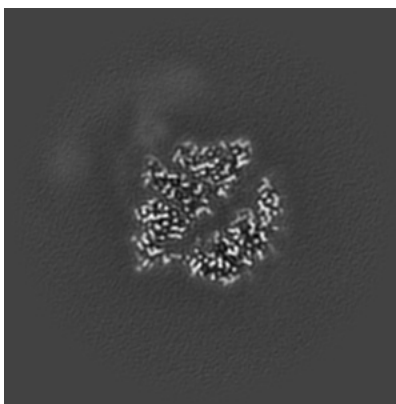
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

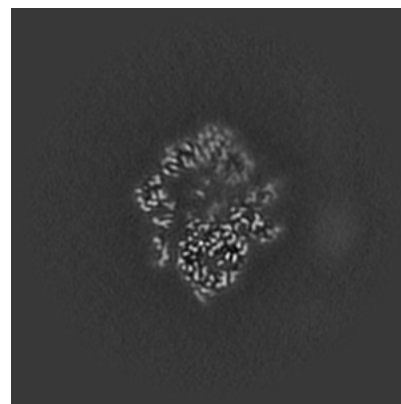
6.3.1 Primary map



X Index: 148



Y Index: 143

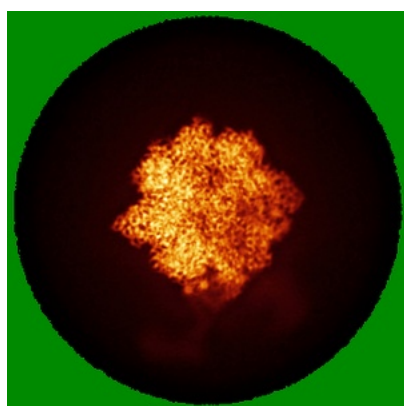


Z Index: 151

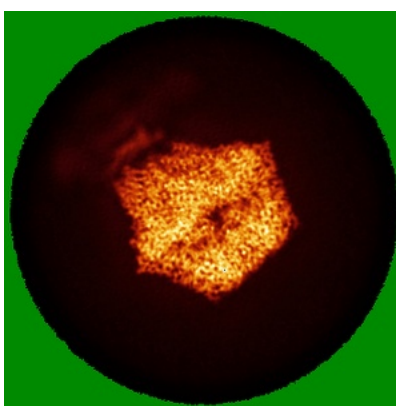
The images above show the largest variance slices of the map in three orthogonal directions.

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

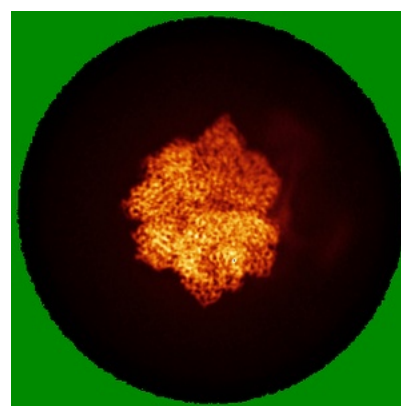
6.4.1 Primary map



X



Y

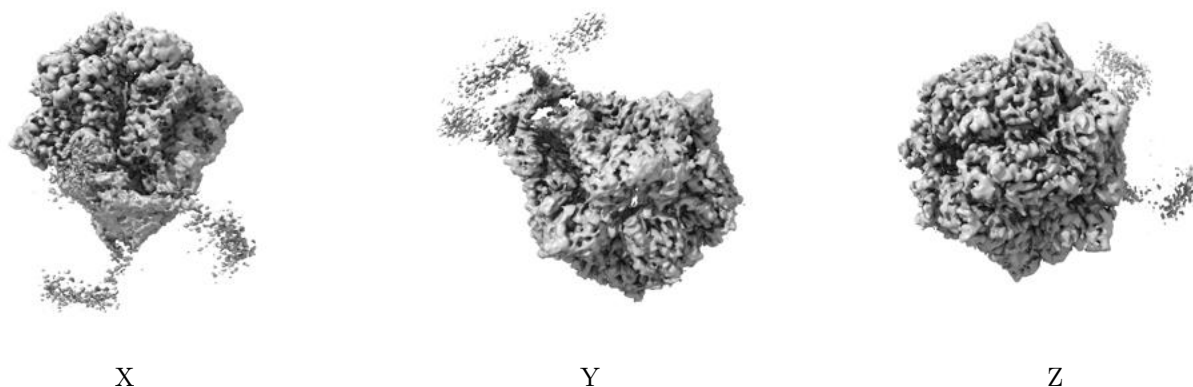


Z

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



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.

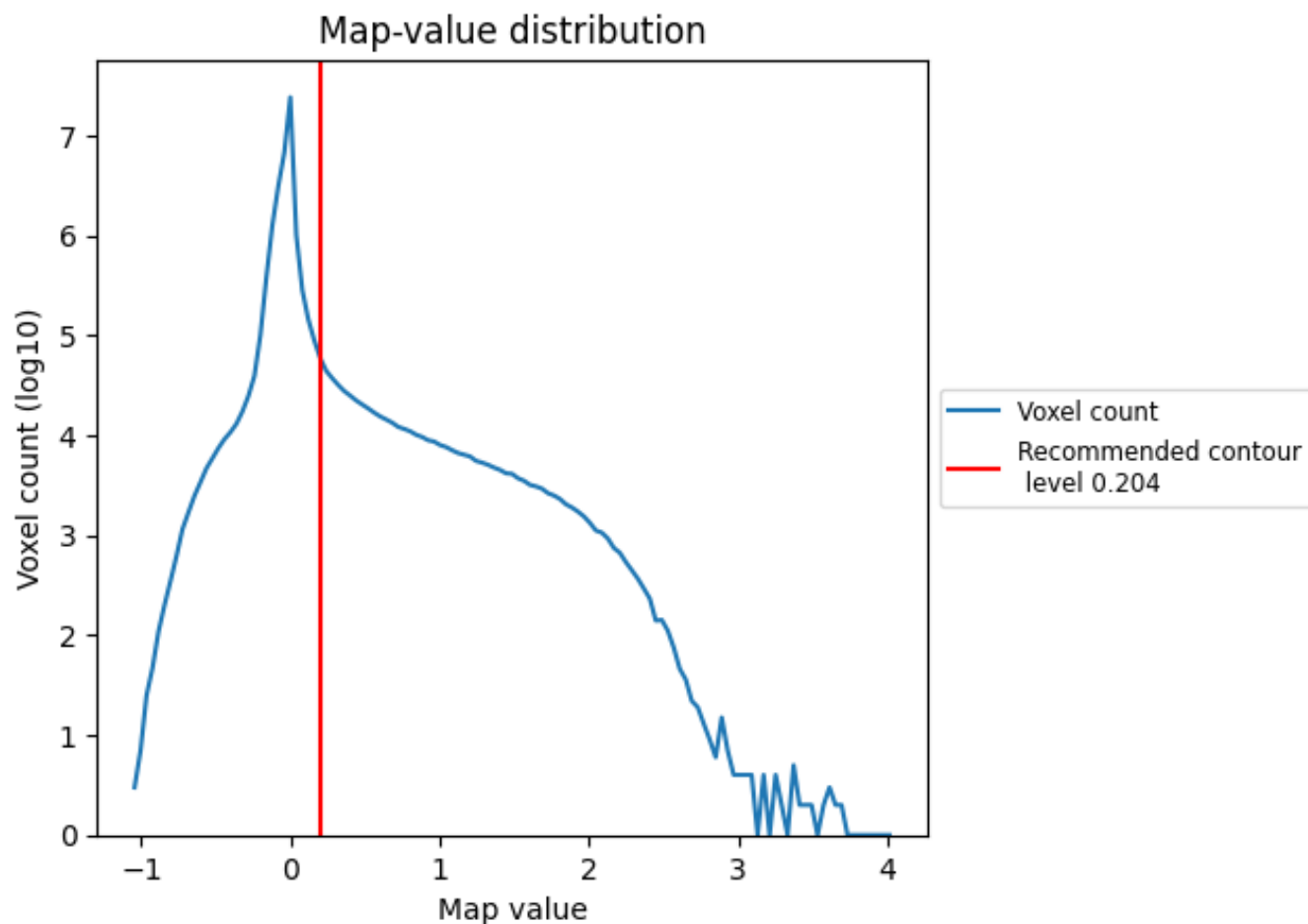
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

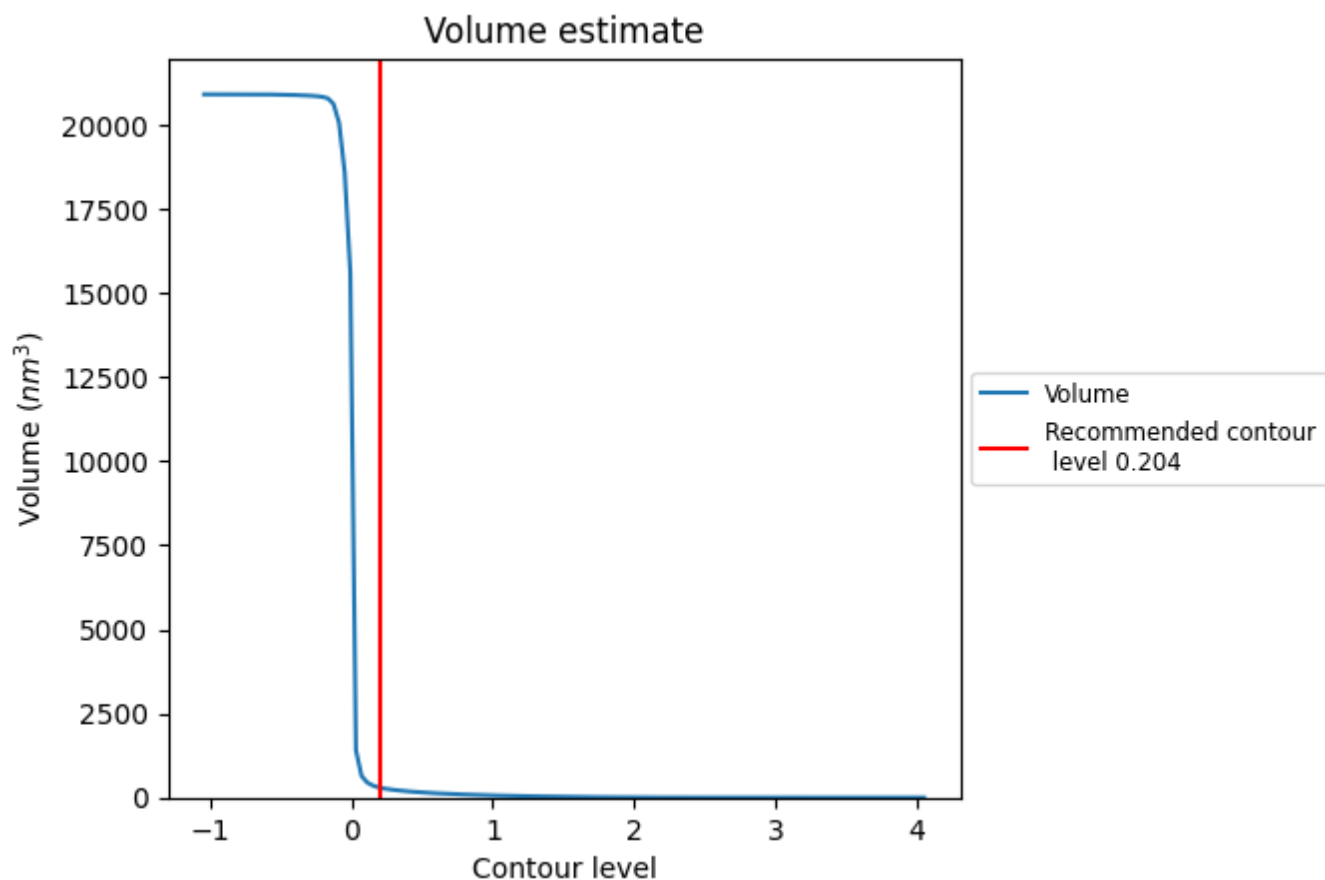
This section contains the results of statistical analysis of the map.

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.

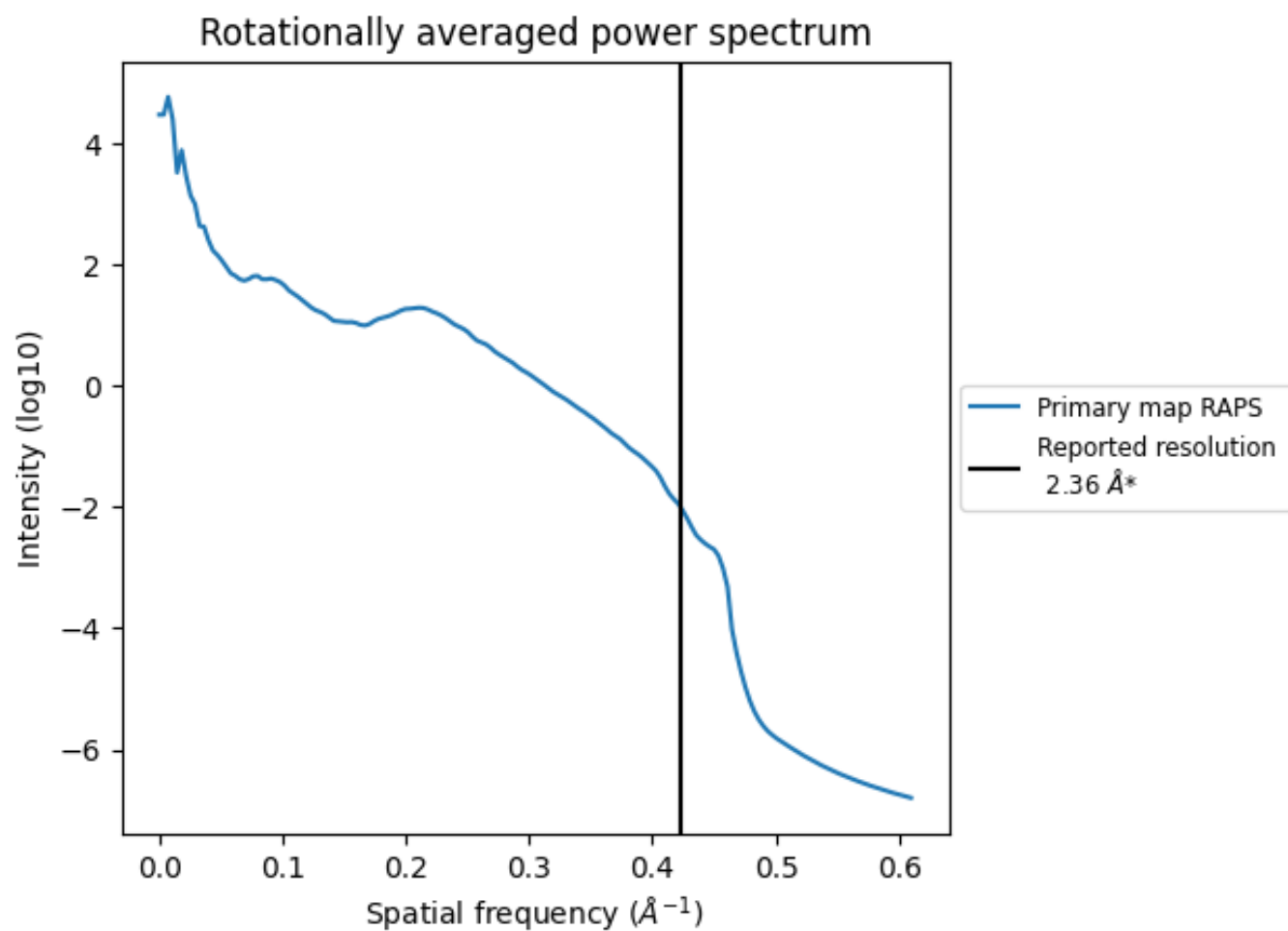
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 263 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 0.424 Å⁻¹

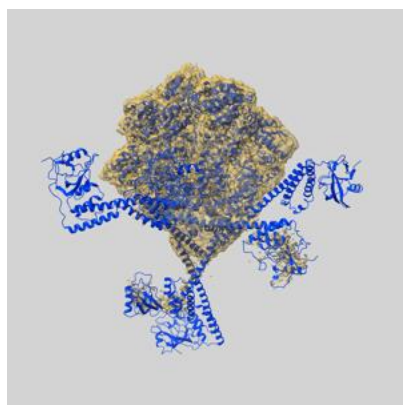
8 Fourier-Shell correlation

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

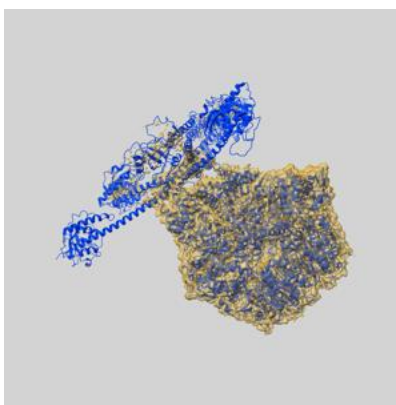
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31590 and PDB model 7FIE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

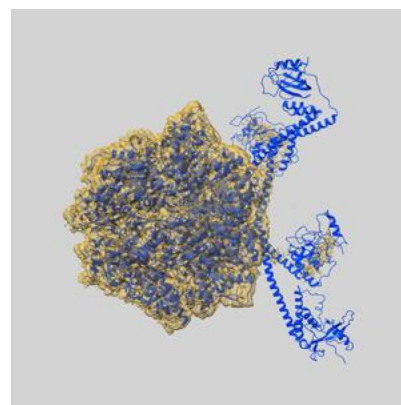
9.1 Map-model overlay [i](#)



X



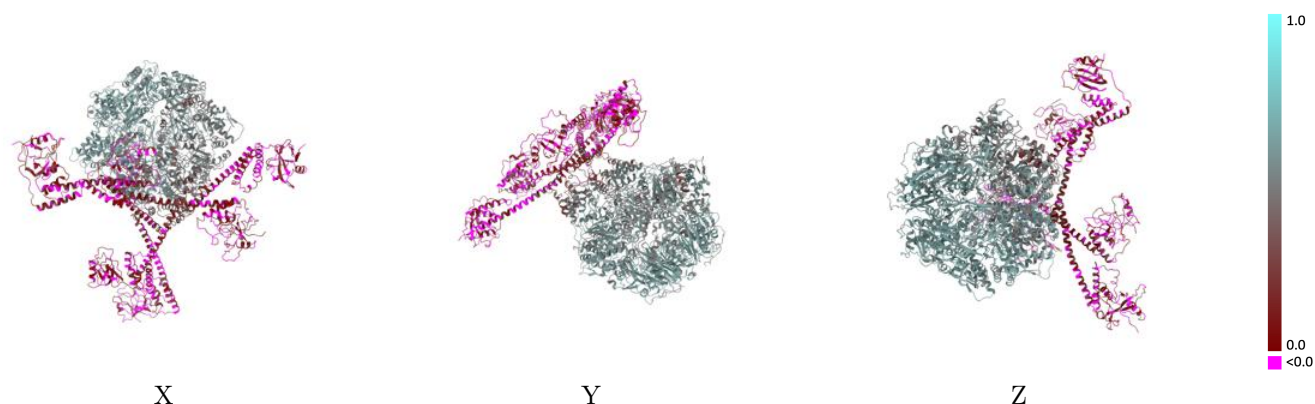
Y



Z

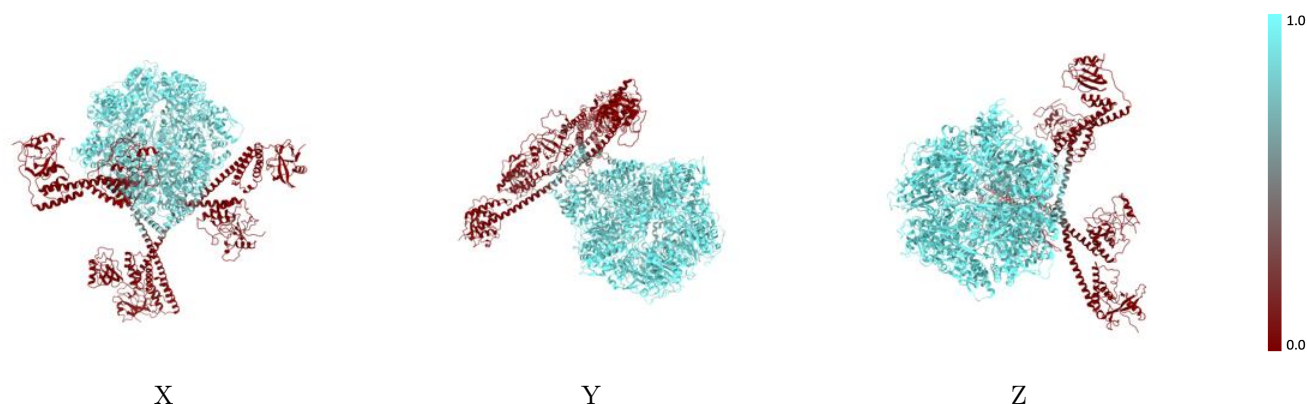
The images above show the 3D surface view of the map at the recommended contour level 0.204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



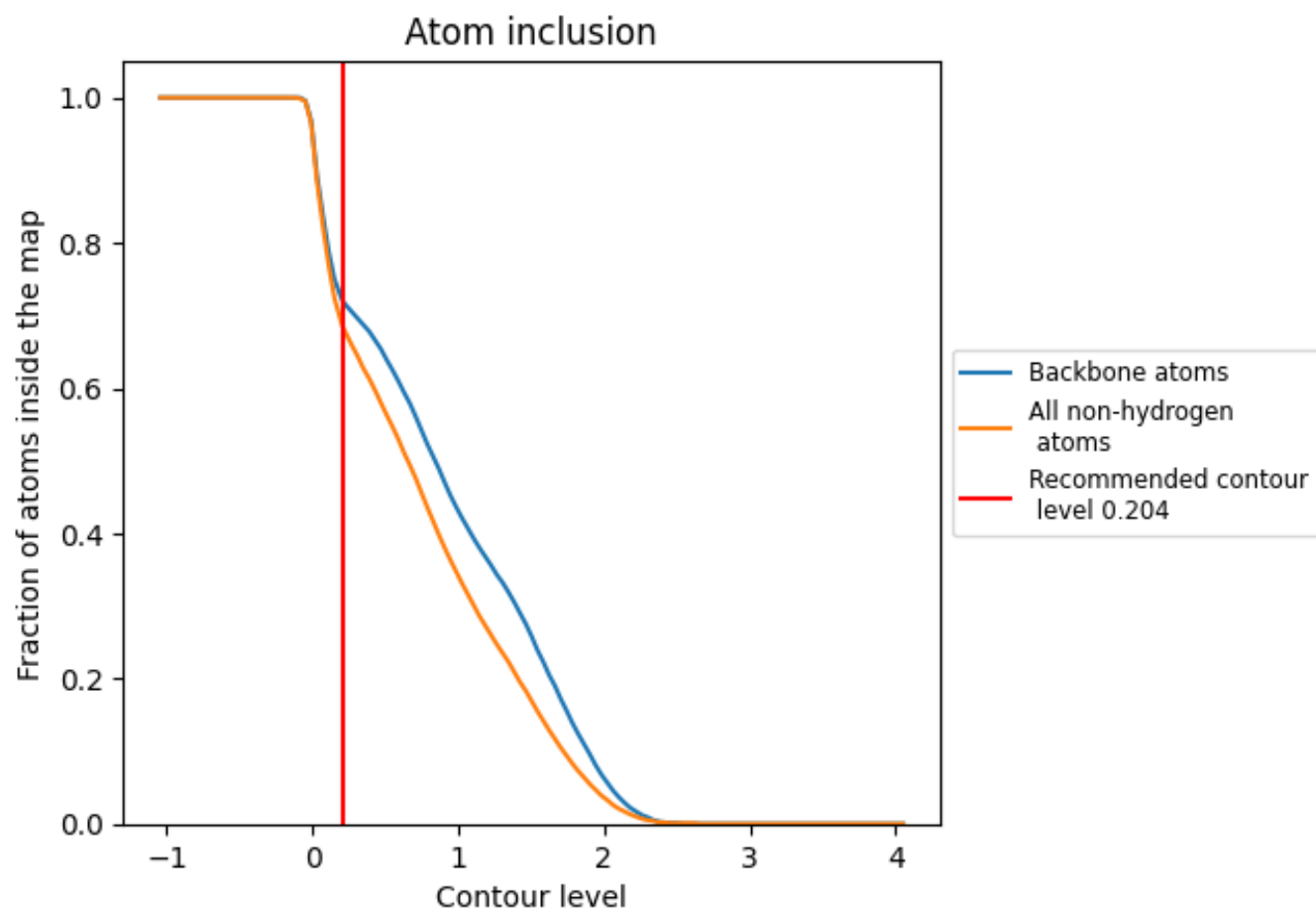
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.204).

9.4 Atom inclusion [i](#)



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	0.6860	0.4000
A	0.6980	0.4030
B	0.6780	0.4130
C	0.7050	0.4240
D	0.6810	0.4240
E	0.6870	0.3770
F	0.6660	0.3590
S	0.7840	0.4700

1.0

0.0

<0.0