



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:23 PM UTC

PDB ID : 8DAR / pdb_00008dar
EMDB ID : EMD-27273
Title : Saccharomyces cerevisiae Ufd1/Npl4/Cdc48 complex unbound but in the presence of SUMO-ubiquitin(K48polyUb)-mEOS and ATP
Authors : Lee, H.G.; Lima, C.D.
Deposited on : 2022-06-14
Resolution : 3.00 Å(reported)

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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:

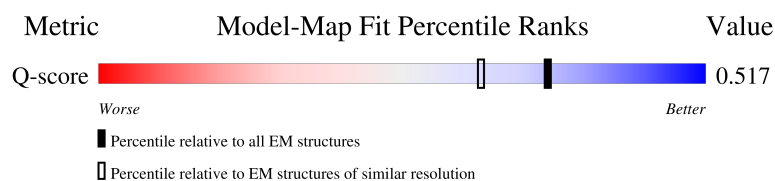
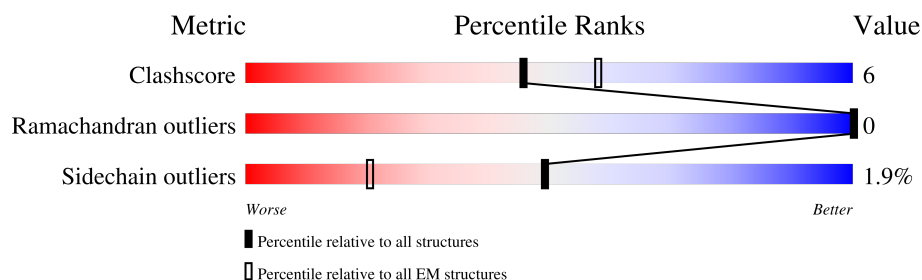
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	A	838	
1	B	838	
1	C	838	
1	D	838	

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Mol	Chain	Length	Quality of chain
1	E	838	56%8%36%
1	F	838	56%10%35%
2	G	583	67%13%19%
3	H	363	14%84%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30157 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 Cell division control protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	553	Total	C	N	O	S	0	0
			4294	2695	758	821	20		
1	B	555	Total	C	N	O	S	0	0
			4298	2698	756	824	20		
1	C	548	Total	C	N	O	S	0	0
			4248	2666	745	817	20		
1	D	554	Total	C	N	O	S	0	0
			4300	2697	756	827	20		
1	E	538	Total	C	N	O	S	0	0
			4166	2619	723	804	20		
1	F	548	Total	C	N	O	S	0	0
			4251	2669	745	817	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P25694
A	-1	SER	-	expression tag	UNP P25694
A	0	HIS	-	expression tag	UNP P25694
B	-2	GLY	-	expression tag	UNP P25694
B	-1	SER	-	expression tag	UNP P25694
B	0	HIS	-	expression tag	UNP P25694
C	-2	GLY	-	expression tag	UNP P25694
C	-1	SER	-	expression tag	UNP P25694
C	0	HIS	-	expression tag	UNP P25694
D	-2	GLY	-	expression tag	UNP P25694
D	-1	SER	-	expression tag	UNP P25694
D	0	HIS	-	expression tag	UNP P25694
E	-2	GLY	-	expression tag	UNP P25694
E	-1	SER	-	expression tag	UNP P25694
E	0	HIS	-	expression tag	UNP P25694
F	-2	GLY	-	expression tag	UNP P25694
F	-1	SER	-	expression tag	UNP P25694
F	0	HIS	-	expression tag	UNP P25694

- Molecule 2 is a protein called Nuclear protein localization protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	474	Total	C	N	O	S	0	0
			3815	2415	640	739	21		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP P33755
G	-1	SER	-	expression tag	UNP P33755
G	0	HIS	-	expression tag	UNP P33755

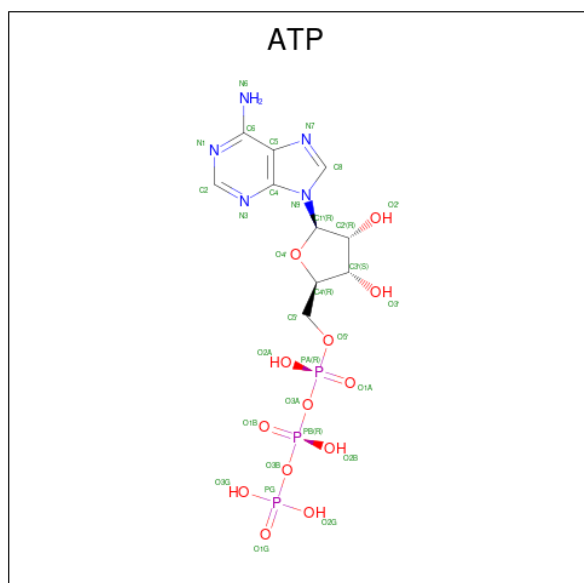
- Molecule 3 is a protein called Ubiquitin fusion degradation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	57	Total	C	N	O	S	0	0
			435	278	71	83	3		

There are 2 discrepancies between the modelled and reference sequences:

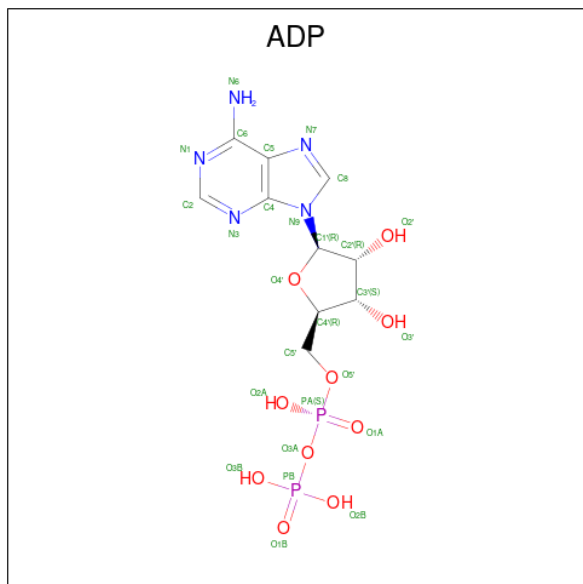
Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P53044
H	0	SER	-	expression tag	UNP P53044

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

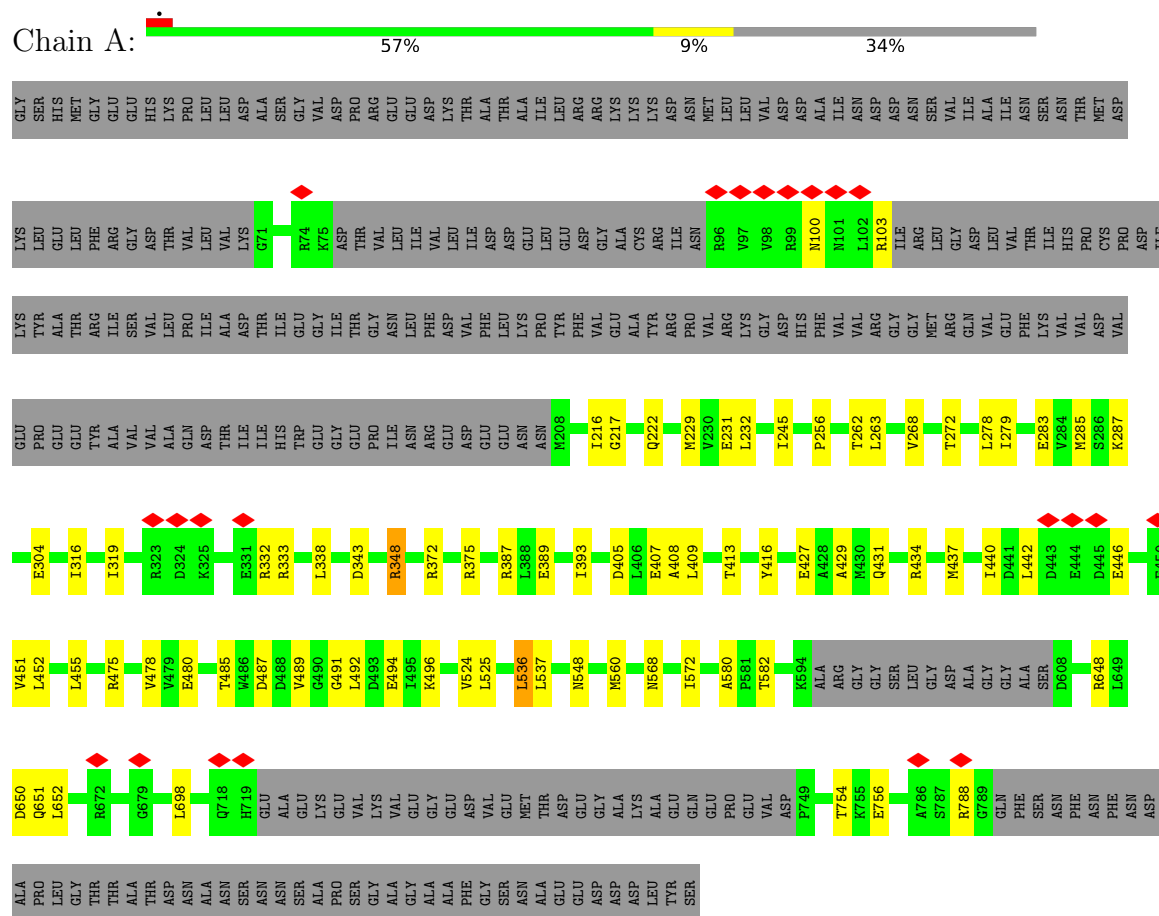
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	G	2	Total	Zn	0
			2	2	

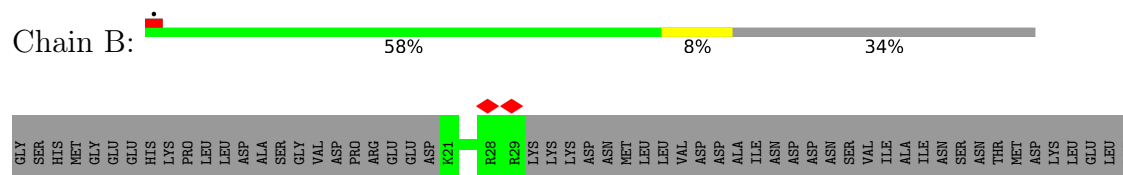
3 Residue-property plots

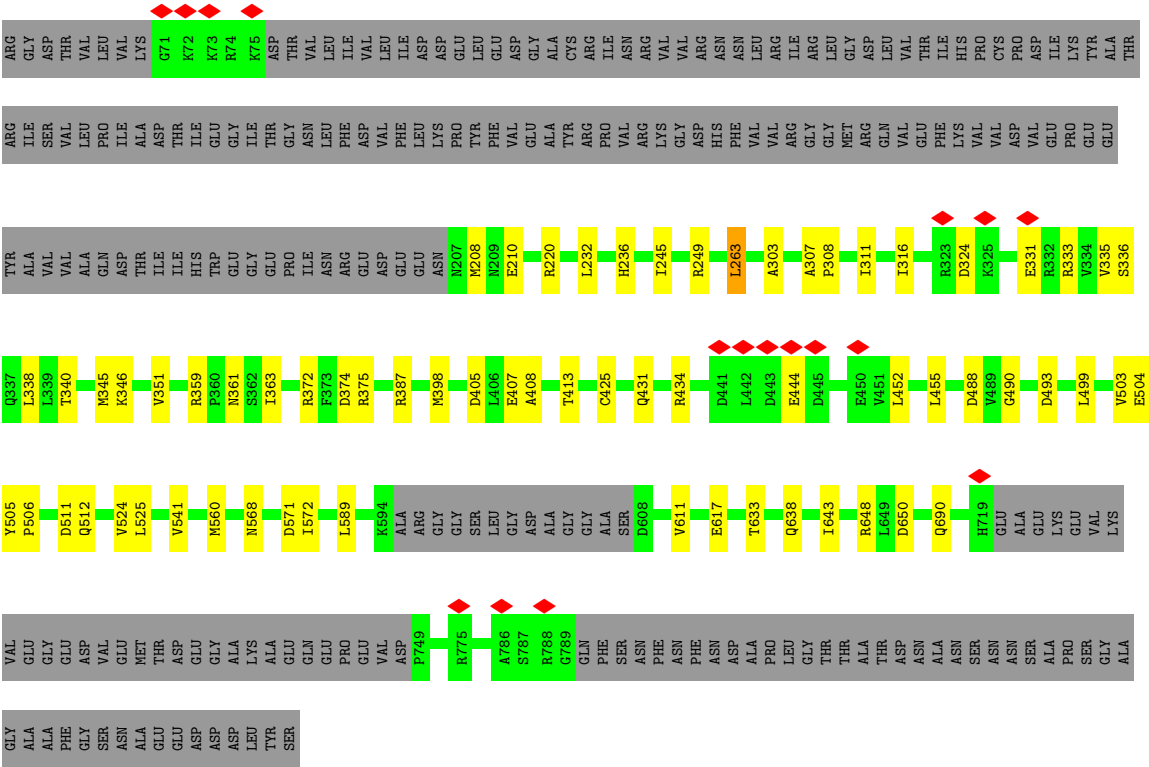
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cell division control protein 48

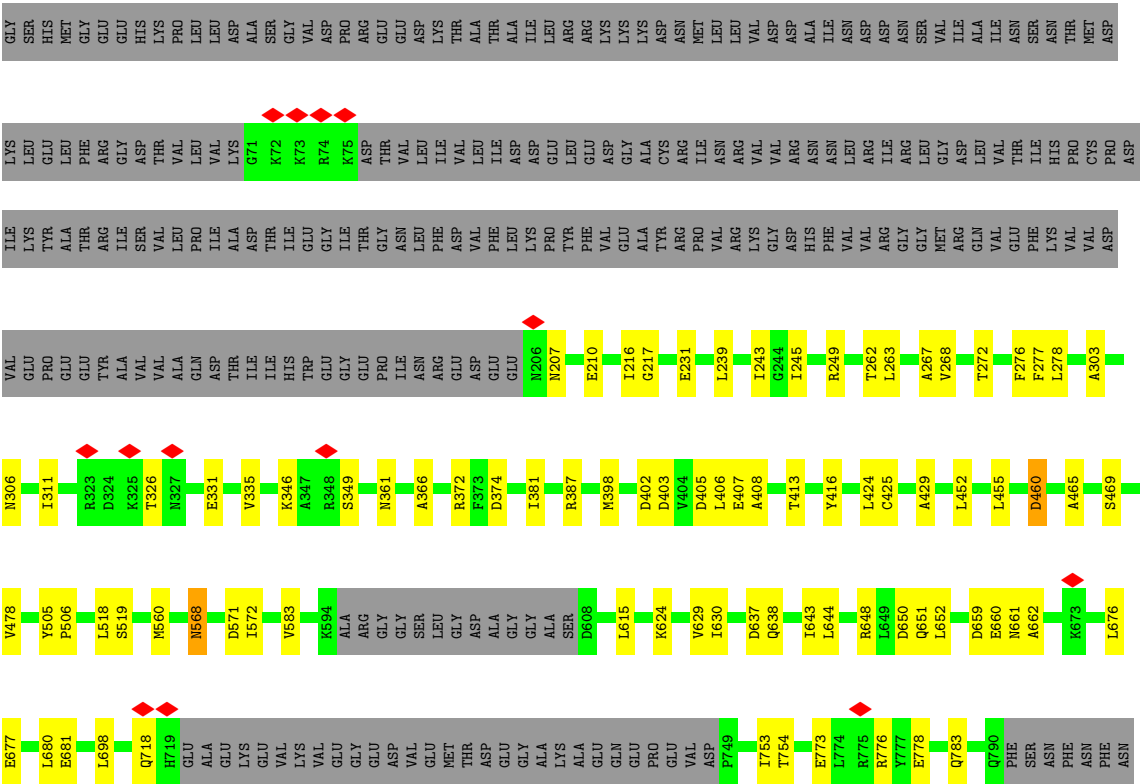


• Molecule 1: Cell division control protein 48





● Molecule 1: Cell division control protein 48



ASP
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PHE
GLY
SER

• Molecule 1: Cell division control protein 48

Chain D:



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SER
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LYS
G71
K72
K73
R74
K75
THR
VAL
LEU
LEU
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D324
K325
T326
N327
E331
V335
L339
K346
A347
R348
N361
A366
L367
R372
F373
D374
R375
R387
D405
L406
E407
A408
T413
R434
M437
D441
L442
D443
E444
D445
E446
I447
D448
L452
N470
V478

D488
V489
E494
I495
K496
L499
D511
L518
S519
F526
L537
N548
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D571
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• Molecule 1: Cell division control protein 48

Chain E:



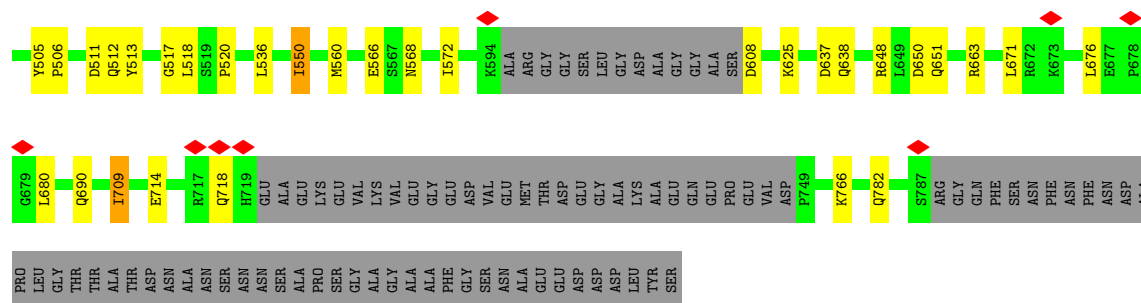
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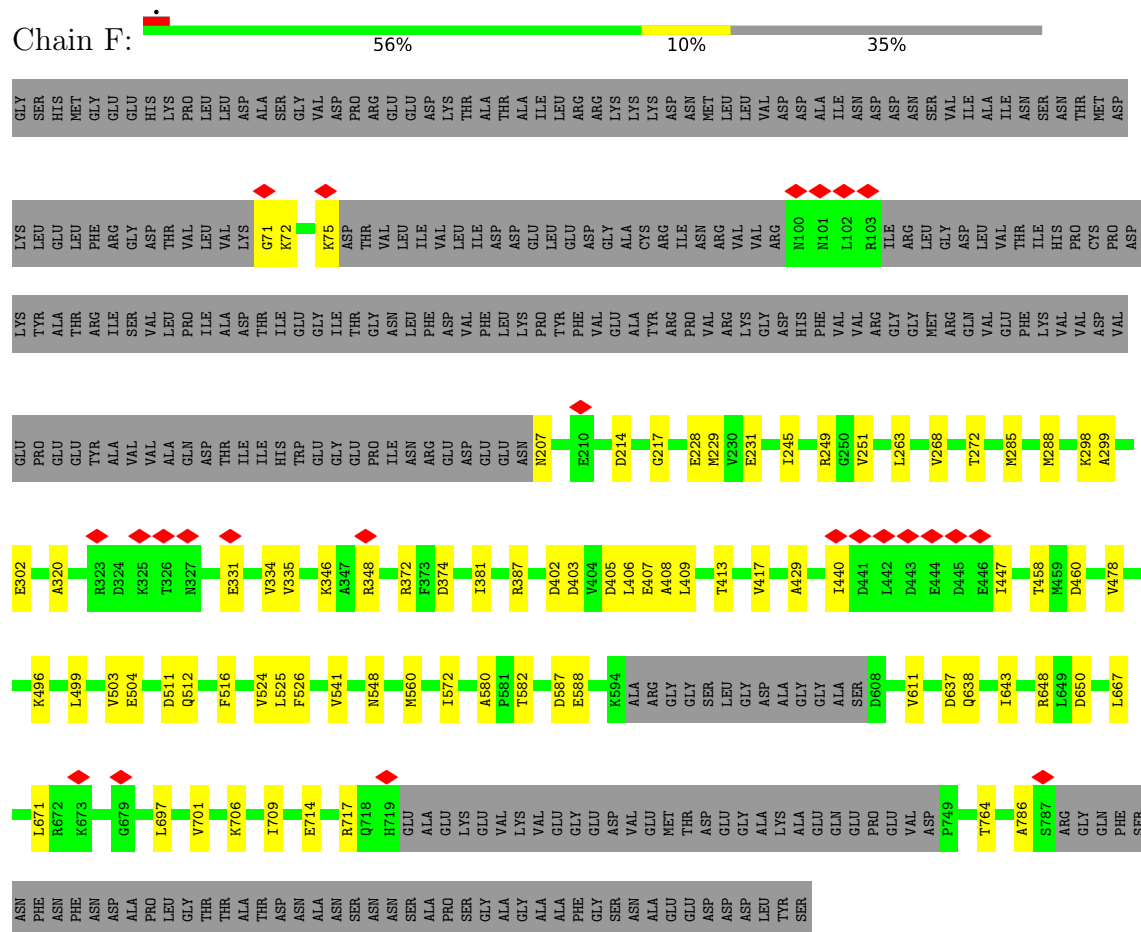
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GLU
ASN
ASN
R208
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G217
E228
M229
V230
E231
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I310
I311
R323
D324

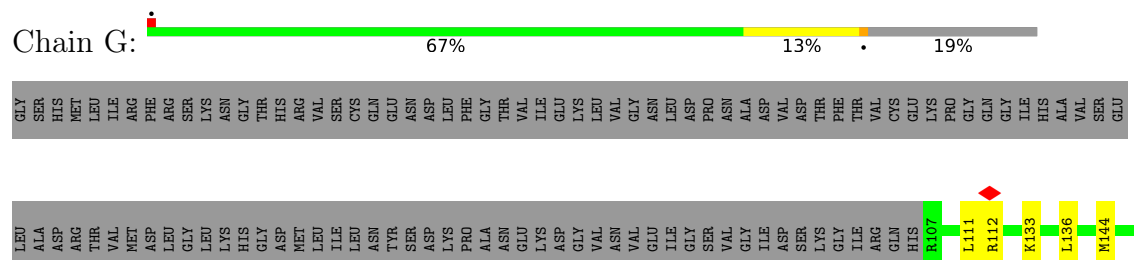
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E329
V330
E331
R332
R333
K346
N350
R359
P360
N361
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R375
R387
D405
L406
E407
A408
L409
T413
A429
R434
D441
L442
E444
D445
E446
I447
D448
L452
L455
E476
E480
D488
V489
G490
E498



• Molecule 1: Cell division control protein 48



• Molecule 2: Nuclear protein localization protein 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	346933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.577	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.358	Depositor
Minimum map value	-32.561	Depositor
Average map value	-0.029	Depositor
Map value standard deviation	1.015	Depositor
Recommended contour level	7	Depositor
Map size ($\text{\AA}$)	408.576, 408.576, 408.576	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.064, 1.064, 1.064	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: ATP, ZN, 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	0.13	0/4360	0.23	0/5883
1	B	0.14	0/4364	0.23	0/5890
1	C	0.13	0/4315	0.24	0/5825
1	D	0.13	0/4366	0.24	0/5892
1	E	0.12	0/4234	0.23	0/5723
1	F	0.12	0/4317	0.23	0/5827
2	G	0.15	0/3906	0.29	0/5275
3	H	0.14	0/443	0.28	0/594
All	All	0.13	0/30305	0.24	0/40909

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	4294	0	4340	63	0
1	B	4298	0	4340	47	0
1	C	4248	0	4281	59	0
1	D	4300	0	4333	60	0
1	E	4166	0	4191	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4251	0	4286	63	0
2	G	3815	0	3688	59	0
3	H	435	0	434	7	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0
4	C	31	0	12	2	0
4	D	31	0	12	1	0
4	E	31	0	12	3	0
4	F	31	0	12	1	0
5	A	27	0	12	2	0
5	B	27	0	12	1	0
5	C	27	0	12	1	0
5	D	27	0	12	0	0
5	E	27	0	12	2	0
5	F	27	0	12	2	0
6	G	2	0	0	0	0
All	All	30157	0	30037	373	0

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

All (373) 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:F:560:MET:HE1	1:F:572:ILE:HD11	1.56	0.87
1:A:560:MET:HE1	1:A:572:ILE:HD11	1.58	0.84
1:E:307:ALA:HB3	1:E:308:PRO:HD3	1.63	0.80
1:E:359:ARG:NH1	1:E:566:GLU:O	2.15	0.79
2:G:311:ASP:OD2	2:G:321:ARG:NH1	2.16	0.78
1:C:398:MET:HE2	1:D:245:ILE:HG22	1.66	0.77
2:G:167:ILE:O	2:G:171:SER:OG	2.01	0.77
1:D:715:ALA:O	1:D:719:HIS:ND1	2.17	0.77
1:E:560:MET:HE1	1:E:572:ILE:HD11	1.68	0.76
2:G:243:GLU:OE1	2:G:243:GLU:N	2.18	0.76
1:B:249:ARG:NH2	1:B:346:LYS:O	2.19	0.75
1:D:71:GLY:N	1:D:75:LYS:O	2.20	0.75
2:G:313:GLN:NE2	2:G:534:ASN:OD1	2.20	0.74
1:C:231:GLU:HG2	1:C:272:THR:HG22	1.69	0.74
1:F:409:LEU:O	1:F:413:THR:HG22	1.88	0.74
1:A:231:GLU:HG2	1:A:272:THR:HG22	1.71	0.73
1:A:245:ILE:HD13	1:F:429:ALA:HB3	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:MET:HE1	1:C:572:ILE:HD11	1.70	0.73
1:E:498:GLU:OE2	1:E:651:GLN:NE2	2.21	0.73
1:A:494:GLU:N	1:A:494:GLU:OE1	2.21	0.73
1:B:444:GLU:OE1	1:B:444:GLU:N	2.23	0.72
1:C:249:ARG:NH2	1:C:349:SER:O	2.22	0.72
1:D:494:GLU:N	1:D:494:GLU:OE1	2.22	0.72
1:A:431:GLN:OE1	1:A:434:ARG:NH1	2.22	0.72
1:B:361:ASN:ND2	1:B:571:ASP:OD2	2.22	0.72
1:C:773:GLU:OE1	1:C:776:ARG:NH2	2.22	0.72
1:F:72:LYS:NZ	1:F:214:ASP:OD2	2.16	0.72
1:F:387:ARG:NE	1:F:413:THR:O	2.23	0.72
1:D:470:ASN:OD1	1:E:625:LYS:NZ	2.22	0.71
2:G:251:ALA:O	2:G:255:THR:HG22	1.90	0.71
1:D:361:ASN:ND2	1:D:571:ASP:OD2	2.22	0.71
1:D:434:ARG:NH1	1:E:228:GLU:OE2	2.23	0.71
1:F:458:THR:OG1	1:F:460:ASP:OD1	2.09	0.71
2:G:497:GLN:OE1	2:G:497:GLN:N	2.24	0.71
1:A:409:LEU:O	1:A:413:THR:HG22	1.90	0.71
1:B:331:GLU:OE1	1:B:331:GLU:N	2.23	0.71
2:G:417:SER:OG	2:G:422:MET:O	2.06	0.71
1:A:429:ALA:HB3	1:B:245:ILE:HD13	1.72	0.70
1:E:231:GLU:HG2	1:E:272:THR:HG22	1.73	0.70
1:B:690:GLN:N	1:B:690:GLN:OE1	2.24	0.70
1:A:387:ARG:NE	1:A:413:THR:O	2.25	0.70
1:A:437:MET:CE	1:B:232:LEU:HD11	2.22	0.69
1:D:231:GLU:HG2	1:D:272:THR:HG22	1.73	0.69
1:A:442:LEU:O	1:B:236:HIS:NE2	2.25	0.69
1:A:446:GLU:N	1:A:446:GLU:OE1	2.26	0.69
1:B:387:ARG:NE	1:B:413:THR:O	2.25	0.69
1:F:407:GLU:N	1:F:407:GLU:OE1	2.25	0.69
3:H:228:LEU:HD12	3:H:229:ASP:N	2.07	0.69
1:B:249:ARG:NH1	1:B:345:MET:O	2.24	0.68
1:D:387:ARG:NE	1:D:413:THR:O	2.26	0.68
1:E:766:LYS:NZ	1:F:786:ALA:O	2.16	0.68
1:D:339:LEU:HD21	1:D:367:LEU:HD12	1.75	0.68
1:B:307:ALA:HB1	1:B:308:PRO:HD2	1.74	0.68
2:G:344:HIS:NE2	2:G:346:ASP:OD1	2.26	0.68
1:C:387:ARG:NE	1:C:413:THR:O	2.26	0.67
1:A:475:ARG:NH2	1:B:617:GLU:OE1	2.27	0.67
1:C:407:GLU:N	1:C:407:GLU:OE1	2.28	0.67
1:D:405:ASP:O	1:D:408:ALA:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:OG1	1:A:487:ASP:OD1	2.12	0.67
1:A:491:GLY:C	1:A:492:LEU:HD23	2.20	0.66
1:A:754:THR:OG1	1:A:756:GLU:OE2	2.14	0.66
1:C:681:GLU:N	1:C:681:GLU:OE1	2.28	0.66
1:C:331:GLU:N	1:C:331:GLU:OE1	2.28	0.65
2:G:451:GLU:N	2:G:451:GLU:OE1	2.29	0.65
1:B:560:MET:HE1	1:B:572:ILE:HD11	1.78	0.65
1:D:577:ARG:HG2	1:D:621:MET:HE1	1.78	0.65
1:F:231:GLU:HG2	1:F:272:THR:HG22	1.77	0.65
1:E:387:ARG:NE	1:E:413:THR:O	2.29	0.65
1:D:407:GLU:OE1	1:D:407:GLU:N	2.30	0.64
1:E:405:ASP:O	1:E:408:ALA:N	2.29	0.64
1:D:499:LEU:CD1	1:D:537:LEU:HD21	2.28	0.64
1:F:302:GLU:N	1:F:302:GLU:OE1	2.30	0.64
1:D:548:ASN:HB2	1:D:582:THR:HG22	1.80	0.64
1:C:637:ASP:OD1	1:C:638:GLN:N	2.31	0.63
1:A:333:ARG:NH1	1:F:288:MET:SD	2.71	0.63
1:C:615:LEU:HD21	1:C:643:ILE:HD13	1.80	0.63
1:D:499:LEU:HD13	1:D:537:LEU:HD21	1.81	0.63
2:G:495:MET:SD	2:G:495:MET:N	2.72	0.63
1:A:440:ILE:HG23	1:A:451:VAL:HG11	1.82	0.62
1:E:480:GLU:N	1:E:480:GLU:OE1	2.32	0.62
1:D:366:ALA:O	1:D:372:ARG:NH1	2.32	0.62
1:F:503:VAL:HG21	1:F:541:VAL:HG13	1.81	0.62
1:F:405:ASP:O	1:F:408:ALA:N	2.32	0.61
1:E:409:LEU:O	1:E:413:THR:HG22	2.00	0.61
1:B:431:GLN:OE1	1:B:434:ARG:NH1	2.33	0.61
1:D:331:GLU:O	1:D:335:VAL:HG23	2.00	0.60
1:B:405:ASP:O	1:B:408:ALA:N	2.33	0.60
1:E:262:THR:OG1	4:E:901:ATP:O3G	2.18	0.60
1:A:548:ASN:HB2	1:A:582:THR:HG22	1.83	0.60
1:E:229:MET:HE3	1:E:375:ARG:HD3	1.84	0.60
1:C:568:ASN:N	1:C:568:ASN:OD1	2.34	0.60
1:B:503:VAL:HG21	1:B:541:VAL:HG13	1.82	0.60
1:A:343:ASP:OD2	1:A:372:ARG:NH2	2.34	0.60
1:F:637:ASP:OD1	1:F:638:GLN:N	2.35	0.59
1:F:331:GLU:N	1:F:331:GLU:OE1	2.33	0.59
1:B:490:GLY:H	5:B:902:ADP:HN61	1.50	0.59
1:E:671:LEU:HD21	1:E:676:LEU:HD13	1.85	0.59
1:E:676:LEU:HD11	1:E:680:LEU:HD23	1.85	0.59
1:E:429:ALA:HB3	1:F:245:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ALA:CB	1:F:245:ILE:HD13	2.32	0.59
1:E:434:ARG:NH1	1:F:228:GLU:OE2	2.35	0.58
1:C:676:LEU:HD12	1:C:680:LEU:HD23	1.84	0.58
1:D:705:ALA:HB3	1:E:518:LEU:HD11	1.84	0.58
1:E:513:TYR:O	1:E:517:GLY:N	2.36	0.58
1:C:676:LEU:HD12	1:C:680:LEU:CD2	2.33	0.58
1:F:490:GLY:H	5:F:902:ADP:N6	2.01	0.58
1:D:268:VAL:O	1:D:272:THR:HG23	2.02	0.58
1:E:413:THR:O	1:E:413:THR:HG23	2.04	0.58
1:A:343:ASP:OD1	1:A:372:ARG:NE	2.34	0.58
1:A:429:ALA:CB	1:B:245:ILE:HD13	2.33	0.58
1:A:283:GLU:HA	1:B:340:THR:HG21	1.86	0.58
1:A:332:ARG:NH2	1:F:331:GLU:OE2	2.37	0.58
1:A:480:GLU:N	1:A:480:GLU:OE1	2.37	0.58
1:A:222:GLN:N	1:A:222:GLN:OE1	2.35	0.58
1:F:268:VAL:O	1:F:272:THR:HG23	2.04	0.57
2:G:395:ASP:OD1	2:G:396:ILE:N	2.36	0.57
1:F:331:GLU:O	1:F:335:VAL:HG23	2.03	0.57
1:A:440:ILE:CG2	1:A:451:VAL:HG11	2.33	0.57
1:A:437:MET:HE2	1:B:232:LEU:HD11	1.87	0.57
1:C:429:ALA:CB	1:D:245:ILE:HG21	2.35	0.57
1:D:590:ASP:OD1	1:D:591:SER:N	2.37	0.57
1:F:231:GLU:CG	1:F:272:THR:HG22	2.33	0.57
2:G:555:GLU:OE1	2:G:555:GLU:N	2.38	0.57
1:F:207:ASN:O	1:F:207:ASN:ND2	2.38	0.57
1:A:413:THR:O	1:A:413:THR:HG23	2.05	0.56
1:E:303:ALA:CB	1:E:311:ILE:HD11	2.35	0.56
1:E:608:ASP:N	1:E:608:ASP:OD1	2.38	0.56
1:A:650:ASP:OD1	1:A:651:GLN:N	2.38	0.56
1:A:245:ILE:HD13	1:F:429:ALA:CB	2.36	0.56
1:E:303:ALA:HB3	1:E:311:ILE:HD11	1.87	0.56
1:E:229:MET:HE3	1:E:375:ARG:CD	2.35	0.56
2:G:490:SER:O	2:G:492:ARG:N	2.39	0.56
1:D:560:MET:HE1	1:D:572:ILE:HD11	1.88	0.56
2:G:346:ASP:OD1	2:G:347:SER:N	2.39	0.56
1:C:405:ASP:O	1:C:408:ALA:N	2.38	0.55
1:C:268:VAL:O	1:C:272:THR:HG23	2.06	0.55
1:D:320:ALA:HA	1:D:335:VAL:HG22	1.87	0.55
1:D:705:ALA:CB	1:E:518:LEU:HD11	2.37	0.55
1:E:361:ASN:ND2	1:E:568:ASN:OD1	2.40	0.55
1:D:231:GLU:CG	1:D:272:THR:HG22	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:540:SER:OG	2:G:542:ASP:OD1	2.25	0.55
1:D:73:LYS:NZ	1:D:210:GLU:O	2.29	0.55
1:E:709:ILE:HD11	1:F:512:GLN:O	2.07	0.55
2:G:260:PHE:CZ	2:G:324:LEU:HD12	2.42	0.55
1:F:488:ASP:OD1	1:F:488:ASP:N	2.39	0.54
1:E:429:ALA:CB	1:F:245:ILE:HG21	2.37	0.54
1:F:413:THR:O	1:F:413:THR:HG23	2.08	0.54
2:G:394:ILE:O	2:G:394:ILE:HG22	2.09	0.53
2:G:542:ASP:OD1	2:G:543:GLU:N	2.40	0.53
1:D:209:ASN:OD1	1:D:210:GLU:N	2.38	0.53
2:G:418:THR:HG22	3:H:290:ALA:H	1.73	0.53
1:B:407:GLU:OE1	1:B:407:GLU:N	2.39	0.53
1:C:429:ALA:CB	1:D:245:ILE:HD13	2.39	0.53
1:D:650:ASP:OD1	1:D:651:GLN:N	2.41	0.53
1:E:714:GLU:OE2	1:E:718:GLN:NE2	2.41	0.53
1:B:307:ALA:HB1	1:B:308:PRO:CD	2.38	0.53
1:B:499:LEU:O	1:B:503:VAL:HG22	2.09	0.53
1:D:279:ILE:HD11	1:D:299:ALA:CB	2.39	0.53
1:D:445:ASP:OD1	1:D:446:GLU:N	2.42	0.53
1:D:331:GLU:OE1	1:D:331:GLU:N	2.36	0.52
1:E:350:ASN:N	1:E:350:ASN:OD1	2.42	0.52
1:F:402:ASP:OD1	1:F:403:ASP:N	2.42	0.52
1:E:709:ILE:HD11	1:F:512:GLN:C	2.34	0.52
1:C:661:ASN:OD1	1:C:662:ALA:N	2.41	0.52
2:G:357:MET:SD	3:H:299:LEU:HD21	2.50	0.52
1:B:372:ARG:O	1:B:374:ASP:N	2.43	0.52
1:F:490:GLY:H	5:F:902:ADP:HN61	1.56	0.52
1:F:460:ASP:OD1	1:F:460:ASP:N	2.40	0.52
2:G:475:THR:HG22	2:G:477:THR:HG23	1.91	0.52
1:D:323:ARG:O	1:D:326:THR:OG1	2.24	0.52
1:D:488:ASP:OD1	1:D:488:ASP:N	2.43	0.52
1:D:526:PHE:CZ	1:D:537:LEU:HD22	2.45	0.52
1:E:263:LEU:HD23	1:E:263:LEU:O	2.10	0.52
1:C:372:ARG:O	1:C:374:ASP:N	2.43	0.51
1:F:499:LEU:O	1:F:503:VAL:HG22	2.10	0.51
1:A:231:GLU:CG	1:A:272:THR:HG22	2.38	0.51
1:F:525:LEU:HD23	1:F:526:PHE:N	2.25	0.51
1:E:452:LEU:HA	1:E:455:LEU:HD23	1.92	0.51
1:B:525:LEU:HD21	1:B:633:THR:HG22	1.93	0.51
2:G:281:VAL:HG12	2:G:322:ILE:HD11	1.92	0.51
1:C:398:MET:HE1	1:C:425:CYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:285:TYR:HD2	2:G:307:MET:HE1	1.76	0.51
1:D:709:ILE:HD11	1:E:512:GLN:HB2	1.92	0.51
1:E:663:ARG:NH2	1:E:690:GLN:OE1	2.41	0.51
1:A:648:ARG:O	1:A:650:ASP:N	2.44	0.51
1:C:455:LEU:HD12	1:D:243:ILE:HD11	1.92	0.51
2:G:475:THR:CG2	2:G:477:THR:HG23	2.41	0.51
1:B:648:ARG:O	1:B:650:ASP:N	2.44	0.51
1:B:511:ASP:OD1	1:B:512:GLN:N	2.44	0.51
1:A:316:ILE:HD11	1:A:338:LEU:HD21	1.94	0.50
2:G:360:ARG:NE	3:H:296:GLU:OE1	2.44	0.50
1:D:489:VAL:O	1:D:496:LYS:NZ	2.35	0.50
1:D:621:MET:HE2	1:D:627:VAL:HB	1.93	0.50
2:G:356:ILE:HD11	2:G:414:ILE:CG2	2.41	0.50
1:A:278:LEU:HD23	1:A:279:ILE:N	2.27	0.50
1:E:490:GLY:H	5:E:902:ADP:HN61	1.60	0.50
1:A:405:ASP:O	1:A:408:ALA:N	2.40	0.50
1:D:302:GLU:HG2	2:G:144:MET:HE1	1.92	0.50
1:F:548:ASN:HB2	1:F:582:THR:HG22	1.93	0.50
2:G:543:GLU:OE2	2:G:566:SER:OG	2.29	0.50
3:H:281:MET:HA	3:H:281:MET:HE2	1.93	0.50
1:B:374:ASP:OD1	1:B:375:ARG:N	2.44	0.50
1:C:429:ALA:HB3	1:D:245:ILE:HD13	1.93	0.50
1:B:303:ALA:CB	1:B:311:ILE:HD11	2.41	0.50
1:E:216:ILE:HG12	1:E:263:LEU:HD22	1.94	0.50
1:C:303:ALA:HB3	1:C:311:ILE:HD11	1.93	0.49
1:D:537:LEU:C	1:D:537:LEU:HD23	2.37	0.49
1:A:525:LEU:HD23	1:A:652:LEU:HD22	1.94	0.49
1:D:306:ASN:OD1	1:D:306:ASN:N	2.43	0.49
1:F:580:ALA:HA	1:F:582:THR:HG23	1.93	0.49
1:C:231:GLU:CG	1:C:272:THR:HG22	2.42	0.49
2:G:373:GLU:OE1	2:G:373:GLU:N	2.40	0.49
1:A:100:ASN:O	1:A:103:ARG:NH1	2.45	0.49
1:A:489:VAL:HG12	1:A:536:LEU:HD13	1.95	0.49
1:E:263:LEU:HD12	4:E:901:ATP:H2'	1.94	0.49
2:G:187:SER:OG	2:G:188:SER:N	2.44	0.49
2:G:230:GLU:OE1	2:G:230:GLU:N	2.46	0.49
2:G:262:TYR:CD1	2:G:307:MET:HE3	2.48	0.49
1:C:381:ILE:HG23	1:C:478:VAL:HG11	1.93	0.48
1:C:460:ASP:N	1:C:460:ASP:OD1	2.45	0.48
1:D:279:ILE:HD11	1:D:299:ALA:HB1	1.95	0.48
1:F:381:ILE:HG23	1:F:478:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLU:O	1:B:335:VAL:HG23	2.12	0.48
2:G:489:TRP:O	2:G:499:GLN:NE2	2.47	0.48
1:B:336:SER:O	1:B:340:THR:HG23	2.14	0.48
1:A:788:ARG:NH2	1:F:764:THR:OG1	2.47	0.48
2:G:548:ILE:O	2:G:552:VAL:HG12	2.13	0.48
1:A:268:VAL:O	1:A:272:THR:HG23	2.14	0.48
2:G:260:PHE:CE2	2:G:324:LEU:HD12	2.49	0.48
1:E:307:ALA:HB3	1:E:308:PRO:CD	2.41	0.47
1:E:709:ILE:HD12	1:F:516:PHE:CD1	2.49	0.47
1:A:407:GLU:OE1	1:A:407:GLU:N	2.38	0.47
1:B:452:LEU:HD22	1:C:239:LEU:HD23	1.96	0.47
1:D:72:LYS:NZ	1:D:103:ARG:O	2.38	0.47
2:G:434:VAL:HG23	2:G:434:VAL:O	2.13	0.47
1:C:207:ASN:O	1:C:210:GLU:N	2.48	0.47
1:C:366:ALA:O	1:C:372:ARG:NH1	2.38	0.47
1:C:644:LEU:HD12	1:C:652:LEU:HD11	1.96	0.47
1:C:648:ARG:O	1:C:650:ASP:N	2.45	0.47
2:G:357:MET:CE	3:H:299:LEU:HD21	2.45	0.47
1:A:287:LYS:O	1:B:333:ARG:NH1	2.48	0.47
1:C:659:ASP:OD1	1:C:660:GLU:N	2.41	0.47
1:B:493:ASP:N	1:B:493:ASP:OD1	2.47	0.47
1:C:650:ASP:OD1	1:C:651:GLN:N	2.48	0.47
1:D:648:ARG:O	1:D:650:ASP:N	2.48	0.47
1:F:372:ARG:O	1:F:374:ASP:N	2.48	0.46
1:C:402:ASP:OD1	1:C:403:ASP:N	2.48	0.46
1:E:306:ASN:OD1	1:E:306:ASN:N	2.48	0.46
1:F:285:MET:HE1	1:F:334:VAL:HG11	1.98	0.46
1:C:615:LEU:CD2	1:C:643:ILE:HD13	2.44	0.46
1:F:714:GLU:OE1	1:F:717:ARG:NH2	2.48	0.46
1:A:262:THR:OG1	4:A:901:ATP:O1G	2.33	0.46
1:F:671:LEU:HD21	1:F:701:VAL:HG23	1.97	0.46
2:G:461:TYR:C	2:G:462:LEU:HD12	2.40	0.46
1:A:580:ALA:HA	1:A:582:THR:HG23	1.97	0.46
1:E:263:LEU:HD23	1:E:263:LEU:C	2.41	0.46
2:G:255:THR:HG23	2:G:257:MET:H	1.81	0.46
2:G:357:MET:HE1	3:H:299:LEU:HD21	1.97	0.46
1:C:630:ILE:HD12	1:C:630:ILE:N	2.31	0.46
1:E:366:ALA:O	1:E:372:ARG:NH1	2.45	0.46
1:F:298:LYS:O	1:F:299:ALA:C	2.58	0.46
2:G:256:GLY:C	2:G:257:MET:HE2	2.41	0.46
1:C:452:LEU:HA	1:C:455:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:546:LEU:CD1	2:G:563:LEU:HD13	2.46	0.45
2:G:524:ILE:O	2:G:524:ILE:HG22	2.15	0.45
1:A:217:GLY:H	4:A:901:ATP:HN61	1.63	0.45
1:A:256:PRO:HG3	1:A:478:VAL:HG12	1.99	0.45
1:F:249:ARG:NH1	1:F:348:ARG:O	2.47	0.45
1:D:518:LEU:HD23	1:D:519:SER:N	2.31	0.45
2:G:292:GLU:N	2:G:295:GLY:O	2.49	0.45
1:F:667:LEU:HD21	1:F:697:LEU:HD12	1.98	0.45
1:C:518:LEU:HD23	1:C:519:SER:N	2.31	0.45
1:D:643:ILE:CG2	1:D:649:LEU:HD23	2.47	0.45
2:G:508:LEU:HD11	2:G:524:ILE:CD1	2.47	0.45
1:E:310:ILE:O	1:E:311:ILE:C	2.59	0.45
2:G:356:ILE:HD11	2:G:414:ILE:HG22	1.99	0.45
2:G:547:LEU:O	2:G:547:LEU:HD23	2.17	0.45
1:F:587:ASP:OD1	1:F:588:GLU:N	2.50	0.44
2:G:547:LEU:HD23	2:G:547:LEU:C	2.43	0.44
1:C:278:LEU:HD23	2:G:186:GLY:H	1.82	0.44
1:D:447:ILE:HD13	1:D:452:LEU:HD21	2.00	0.44
1:E:637:ASP:OD1	1:E:638:GLN:N	2.50	0.44
2:G:572:LEU:C	2:G:572:LEU:HD13	2.43	0.44
2:G:516:ASP:O	2:G:519:LEU:N	2.50	0.44
1:B:316:ILE:HG23	1:B:363:ILE:HD12	2.00	0.44
1:F:524:VAL:HG12	1:F:525:LEU:N	2.32	0.44
1:C:698:LEU:HD23	1:C:698:LEU:C	2.42	0.43
1:C:629:VAL:C	1:C:630:ILE:HD12	2.43	0.43
1:A:536:LEU:HD12	1:A:537:LEU:H	1.83	0.43
1:A:229:MET:SD	1:A:375:ARG:NH1	2.92	0.43
1:A:389:GLU:O	1:A:393:ILE:HD13	2.19	0.43
1:C:424:LEU:HD12	1:C:465:ALA:HB1	2.00	0.43
2:G:324:LEU:HD23	2:G:324:LEU:H	1.83	0.43
2:G:412:ASP:OD2	2:G:432:ARG:NH1	2.42	0.43
1:B:524:VAL:HG12	1:B:525:LEU:N	2.34	0.43
1:D:374:ASP:OD1	1:D:375:ARG:N	2.47	0.43
1:A:698:LEU:HD12	5:A:902:ADP:O3'	2.19	0.43
1:E:511:ASP:OD1	1:E:512:GLN:N	2.52	0.43
1:F:440:ILE:HG23	1:F:447:ILE:CD1	2.48	0.43
2:G:429:THR:HG23	2:G:431:GLU:H	1.83	0.43
1:C:217:GLY:H	4:C:901:ATP:HN61	1.67	0.43
1:C:331:GLU:O	1:C:335:VAL:HG23	2.19	0.43
1:B:452:LEU:CD2	1:C:239:LEU:HD23	2.49	0.43
1:C:416:TYR:OH	1:C:469:SER:OG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLU:OE2	1:B:375:ARG:NH2	2.52	0.42
1:D:372:ARG:O	1:D:374:ASP:N	2.51	0.42
1:F:229:MET:SD	1:F:251:VAL:HG22	2.59	0.42
2:G:529:LEU:HD23	2:G:529:LEU:C	2.44	0.42
1:A:536:LEU:HD21	5:A:902:ADP:C8	2.54	0.42
1:D:288:MET:HE1	1:E:333:ARG:NH1	2.34	0.42
1:D:499:LEU:HD11	1:D:537:LEU:HD21	2.01	0.42
1:E:310:ILE:O	1:E:310:ILE:HG13	2.19	0.42
1:E:648:ARG:O	1:E:650:ASP:N	2.52	0.42
1:F:503:VAL:HG23	1:F:504:GLU:N	2.35	0.42
1:F:648:ARG:O	1:F:650:ASP:N	2.50	0.42
1:A:489:VAL:HG23	1:A:496:LYS:HE2	2.02	0.42
1:D:256:PRO:HD2	1:D:259:THR:HG21	2.01	0.42
1:F:511:ASP:OD1	1:F:512:GLN:N	2.52	0.42
2:G:112:ARG:NE	2:G:112:ARG:O	2.52	0.42
1:A:285:MET:HG2	1:A:319:ILE:HG22	2.01	0.42
1:A:348:ARG:HE	1:A:348:ARG:HA	1.85	0.42
1:C:243:ILE:O	1:C:243:ILE:HG22	2.20	0.42
1:A:452:LEU:HA	1:A:455:LEU:HD23	2.01	0.42
1:C:505:TYR:HB2	1:C:506:PRO:HD3	2.01	0.42
1:F:217:GLY:H	4:F:901:ATP:HN61	1.66	0.42
1:A:524:VAL:HG12	1:A:525:LEU:N	2.34	0.42
1:A:698:LEU:C	1:A:698:LEU:HD23	2.45	0.42
1:C:583:VAL:HG13	1:C:630:ILE:HD13	2.02	0.42
1:C:753:ILE:HG22	1:C:754:THR:N	2.34	0.42
1:B:611:VAL:HG13	1:B:643:ILE:HD11	2.02	0.42
1:C:277:PHE:O	1:C:278:LEU:C	2.63	0.42
1:D:256:PRO:HG3	1:D:478:VAL:HG12	2.01	0.42
1:A:788:ARG:NH1	1:F:764:THR:O	2.53	0.41
1:B:324:ASP:OD1	1:B:324:ASP:N	2.53	0.41
1:E:506:PRO:HB3	1:E:520:PRO:HB3	2.02	0.41
1:F:489:VAL:HG23	1:F:496:LYS:HE2	2.02	0.41
1:B:505:TYR:HB2	1:B:506:PRO:HD3	2.01	0.41
1:C:303:ALA:CB	1:C:311:ILE:HD11	2.50	0.41
1:A:413:THR:OG1	1:A:416:TYR:CG	2.74	0.41
1:F:320:ALA:HA	1:F:335:VAL:HG22	2.01	0.41
1:D:511:ASP:OD1	1:D:511:ASP:N	2.54	0.41
1:F:71:GLY:N	1:F:75:LYS:O	2.53	0.41
2:G:263:MET:HE2	2:G:281:VAL:HG11	2.02	0.41
1:B:263:LEU:HD12	4:B:901:ATP:H2'	2.02	0.41
1:A:216:ILE:HG12	1:A:263:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:VAL:HG23	1:B:504:GLU:N	2.35	0.41
1:C:216:ILE:HD11	1:C:267:ALA:HB2	2.03	0.41
1:D:217:GLY:H	4:D:901:ATP:HN61	1.69	0.41
1:D:637:ASP:OD1	1:D:638:GLN:N	2.53	0.41
1:E:550:ILE:HD11	1:E:572:ILE:HG23	2.03	0.41
1:A:405:ASP:O	1:A:407:GLU:N	2.54	0.41
1:C:276:PHE:CE2	1:C:278:LEU:HB2	2.56	0.41
1:D:706:LYS:HA	1:D:709:ILE:HG22	2.03	0.41
1:E:405:ASP:O	1:E:406:LEU:C	2.64	0.41
1:E:217:GLY:H	4:E:901:ATP:HN61	1.69	0.41
1:F:405:ASP:O	1:F:406:LEU:C	2.64	0.41
1:F:706:LYS:HA	1:F:709:ILE:HG22	2.03	0.41
1:A:278:LEU:HD23	1:A:278:LEU:C	2.46	0.40
1:B:452:LEU:HA	1:B:455:LEU:HD23	2.02	0.40
1:B:488:ASP:OD1	1:B:488:ASP:N	2.54	0.40
1:C:262:THR:OG1	4:C:901:ATP:O2G	2.23	0.40
1:C:361:ASN:ND2	1:C:571:ASP:OD2	2.54	0.40
2:G:524:ILE:O	2:G:524:ILE:CG2	2.69	0.40
1:B:351:VAL:HG13	1:B:351:VAL:O	2.20	0.40
1:B:398:MET:HE1	1:B:425:CYS:HB3	2.03	0.40
1:E:505:TYR:HB2	1:E:506:PRO:HD3	2.03	0.40
2:G:429:THR:HG22	2:G:432:ARG:HE	1.85	0.40
1:C:405:ASP:O	1:C:406:LEU:C	2.65	0.40
1:E:429:ALA:HB1	1:F:245:ILE:HD13	2.03	0.40
1:E:536:LEU:HD11	5:E:902:ADP:H2'	2.04	0.40
1:F:611:VAL:HG13	1:F:643:ILE:HD11	2.03	0.40
1:C:698:LEU:HD12	5:C:902:ADP:O3'	2.21	0.40
1:E:232:LEU:HB2	1:E:233:PRO:HD3	2.03	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	543/838 (65%)	519 (96%)	24 (4%)	0	100	100
1	B	545/838 (65%)	524 (96%)	21 (4%)	0	100	100
1	C	540/838 (64%)	518 (96%)	22 (4%)	0	100	100
1	D	544/838 (65%)	522 (96%)	22 (4%)	0	100	100
1	E	532/838 (64%)	513 (96%)	19 (4%)	0	100	100
1	F	538/838 (64%)	520 (97%)	18 (3%)	0	100	100
2	G	472/583 (81%)	426 (90%)	46 (10%)	0	100	100
3	H	53/363 (15%)	49 (92%)	4 (8%)	0	100	100
All	All	3767/5974 (63%)	3591 (95%)	176 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	460/697 (66%)	455 (99%)	5 (1%)	65	83
1	B	459/697 (66%)	450 (98%)	9 (2%)	48	76
1	C	455/697 (65%)	443 (97%)	12 (3%)	40	72
1	D	461/697 (66%)	451 (98%)	10 (2%)	45	74
1	E	447/697 (64%)	439 (98%)	8 (2%)	51	77
1	F	456/697 (65%)	452 (99%)	4 (1%)	70	85
2	G	425/518 (82%)	412 (97%)	13 (3%)	35	68
3	H	48/315 (15%)	47 (98%)	1 (2%)	47	75
All	All	3211/5015 (64%)	3149 (98%)	62 (2%)	49	76

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	LEU
1	A	304	GLU

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Mol	Chain	Res	Type
1	A	348	ARG
1	A	536	LEU
1	A	568	ASN
1	B	208	MET
1	B	210	GLU
1	B	220	ARG
1	B	263	LEU
1	B	338	LEU
1	B	359	ARG
1	B	568	ASN
1	B	589	LEU
1	B	638	GLN
1	C	245	ILE
1	C	263	LEU
1	C	306	ASN
1	C	326	THR
1	C	346	LYS
1	C	460	ASP
1	C	568	ASN
1	C	624	LYS
1	C	677	GLU
1	C	718	GLN
1	C	778	GLU
1	C	783	GLN
1	D	249	ARG
1	D	263	LEU
1	D	278	LEU
1	D	285	MET
1	D	306	ASN
1	D	346	LYS
1	D	437	MET
1	D	488	ASP
1	D	624	LYS
1	D	702	GLN
1	E	228	GLU
1	E	278	LEU
1	E	306	ASN
1	E	350	ASN
1	E	476	GLU
1	E	550	ILE
1	E	709	ILE
1	E	782	GLN

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Mol	Chain	Res	Type
1	F	263	LEU
1	F	346	LYS
1	F	417	VAL
1	F	488	ASP
2	G	111	LEU
2	G	133	LYS
2	G	136	LEU
2	G	211	TRP
2	G	215	ILE
2	G	331	ASP
2	G	354	GLU
2	G	357	MET
2	G	396	ILE
2	G	464	VAL
2	G	495	MET
2	G	505	LYS
2	G	543	GLU
3	H	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	548	ASN
1	A	612	ASN
1	B	716	HIS
1	C	414	HIS
1	C	626	ASN
1	D	414	HIS
1	D	670	GLN
1	E	651	GLN
1	E	782	GLN
1	F	414	HIS
2	G	159	HIS
2	G	177	ASN
2	G	313	GLN
2	G	367	ASN

5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
5	ADP	B	902	-	28,29,29	0.46	0	43,45,45	0.55	0
4	ATP	B	901	-	32,33,33	0.38	0	48,52,52	0.70	0
5	ADP	A	902	-	28,29,29	0.48	0	43,45,45	0.59	0
4	ATP	A	901	-	32,33,33	0.40	0	48,52,52	0.69	0
4	ATP	E	901	-	32,33,33	0.35	0	48,52,52	0.69	0
5	ADP	F	902	-	28,29,29	0.48	0	43,45,45	0.60	0
5	ADP	C	902	-	28,29,29	0.46	0	43,45,45	0.54	0
4	ATP	C	901	-	32,33,33	0.36	0	48,52,52	0.69	0
4	ATP	F	901	-	32,33,33	0.37	0	48,52,52	0.69	1 (2%)
5	ADP	D	902	-	28,29,29	0.46	0	43,45,45	0.53	0
4	ATP	D	901	-	32,33,33	0.40	0	48,52,52	0.69	1 (2%)
5	ADP	E	902	-	28,29,29	0.46	0	43,45,45	0.55	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
5	ADP	B	902	-	-	3/16/32/32	0/3/3/3
4	ATP	B	901	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	902	-	-	3/16/32/32	0/3/3/3
4	ATP	A	901	-	-	5/22/38/38	0/3/3/3
4	ATP	E	901	-	-	3/22/38/38	0/3/3/3
5	ADP	F	902	-	-	6/16/32/32	0/3/3/3
5	ADP	C	902	-	-	2/16/32/32	0/3/3/3
4	ATP	C	901	-	-	10/22/38/38	0/3/3/3
4	ATP	F	901	-	-	6/22/38/38	0/3/3/3
5	ADP	D	902	-	-	3/16/32/32	0/3/3/3
4	ATP	D	901	-	-	6/22/38/38	0/3/3/3
5	ADP	E	902	-	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	ATP	O3'-C3'-C2'	-2.02	105.33	111.82
4	F	901	ATP	O3'-C3'-C2'	-2.01	105.38	111.82

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	901	ATP	C5'-O5'-PA-O1A
4	C	901	ATP	C5'-O5'-PA-O2A
4	C	901	ATP	C5'-O5'-PA-O3A
4	C	901	ATP	O4'-C1'-N9-C8
4	C	901	ATP	O4'-C1'-N9-C4
4	D	901	ATP	O4'-C1'-N9-C4
4	F	901	ATP	O4'-C1'-N9-C8
4	F	901	ATP	O4'-C1'-N9-C4
5	F	902	ADP	C5'-O5'-PA-O1A
5	F	902	ADP	C5'-O5'-PA-O2A
5	F	902	ADP	C5'-O5'-PA-O3A
5	F	902	ADP	O4'-C1'-N9-C8
5	F	902	ADP	O4'-C1'-N9-C4
4	A	901	ATP	O4'-C1'-N9-C8
4	B	901	ATP	O4'-C1'-N9-C8
4	D	901	ATP	O4'-C1'-N9-C8
4	E	901	ATP	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
4	A	901	ATP	O4'-C1'-N9-C4
4	B	901	ATP	O4'-C1'-N9-C4
4	E	901	ATP	O4'-C1'-N9-C4
5	B	902	ADP	O4'-C1'-N9-C4
5	C	902	ADP	O4'-C1'-N9-C4
5	D	902	ADP	O4'-C1'-N9-C4
4	C	901	ATP	O4'-C4'-C5'-O5'
4	C	901	ATP	C3'-C4'-C5'-O5'
5	B	902	ADP	O4'-C1'-N9-C8
4	B	901	ATP	PA-O3A-PB-O1B
4	A	901	ATP	PB-O3B-PG-O3G
5	C	902	ADP	O4'-C1'-N9-C8
5	D	902	ADP	O4'-C1'-N9-C8
5	A	902	ADP	C2'-C1'-N9-C8
5	E	902	ADP	C2'-C1'-N9-C8
4	E	901	ATP	PA-O3A-PB-O1B
4	F	901	ATP	PA-O3A-PB-O3B
4	C	901	ATP	PA-O3A-PB-O3B
5	A	902	ADP	O4'-C1'-N9-C8
5	E	902	ADP	O4'-C1'-N9-C8
4	D	901	ATP	PA-O3A-PB-O3B
5	A	902	ADP	O4'-C1'-N9-C4
5	E	902	ADP	O4'-C1'-N9-C4
4	C	901	ATP	PA-O3A-PB-O1B
5	F	902	ADP	PA-O3A-PB-O1B
4	A	901	ATP	PA-O3A-PB-O3B
4	D	901	ATP	PA-O3A-PB-O1B
5	D	902	ADP	C2'-C1'-N9-C8
5	B	902	ADP	C2'-C1'-N9-C8
4	D	901	ATP	O4'-C4'-C5'-O5'
4	A	901	ATP	PA-O3A-PB-O1B
4	C	901	ATP	PA-O3A-PB-O2B
4	D	901	ATP	PA-O3A-PB-O2B
4	F	901	ATP	PA-O3A-PB-O1B
4	F	901	ATP	PA-O3A-PB-O2B
4	F	901	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 18 short contacts:

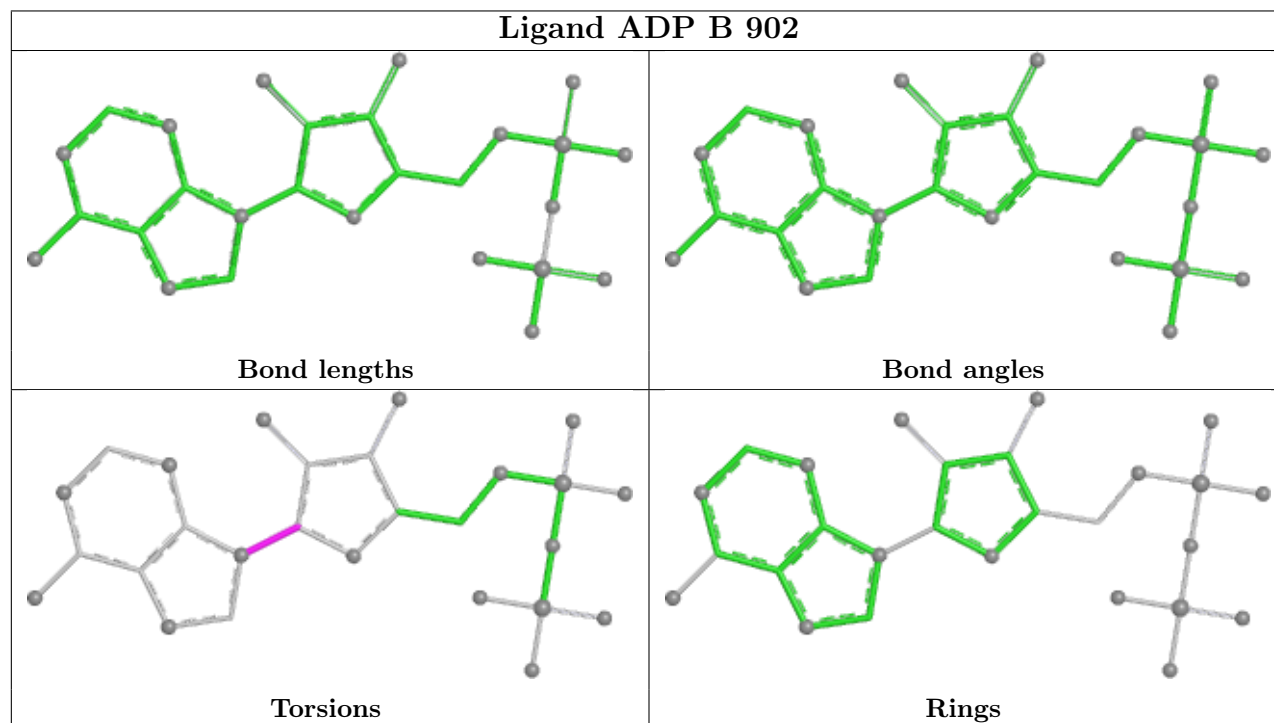
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	ADP	1	0

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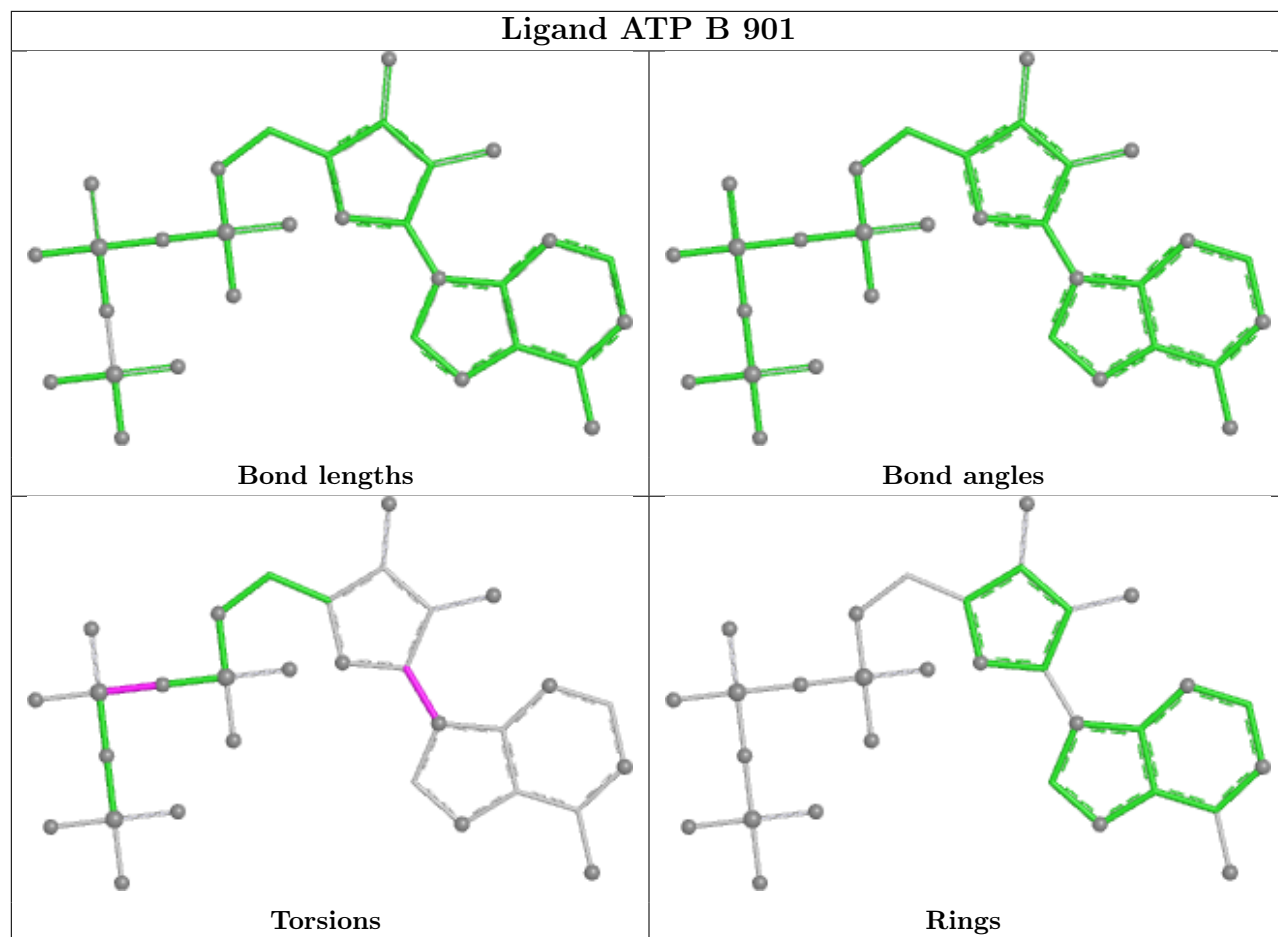
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	ATP	1	0
5	A	902	ADP	2	0
4	A	901	ATP	2	0
4	E	901	ATP	3	0
5	F	902	ADP	2	0
5	C	902	ADP	1	0
4	C	901	ATP	2	0
4	F	901	ATP	1	0
4	D	901	ATP	1	0
5	E	902	ADP	2	0

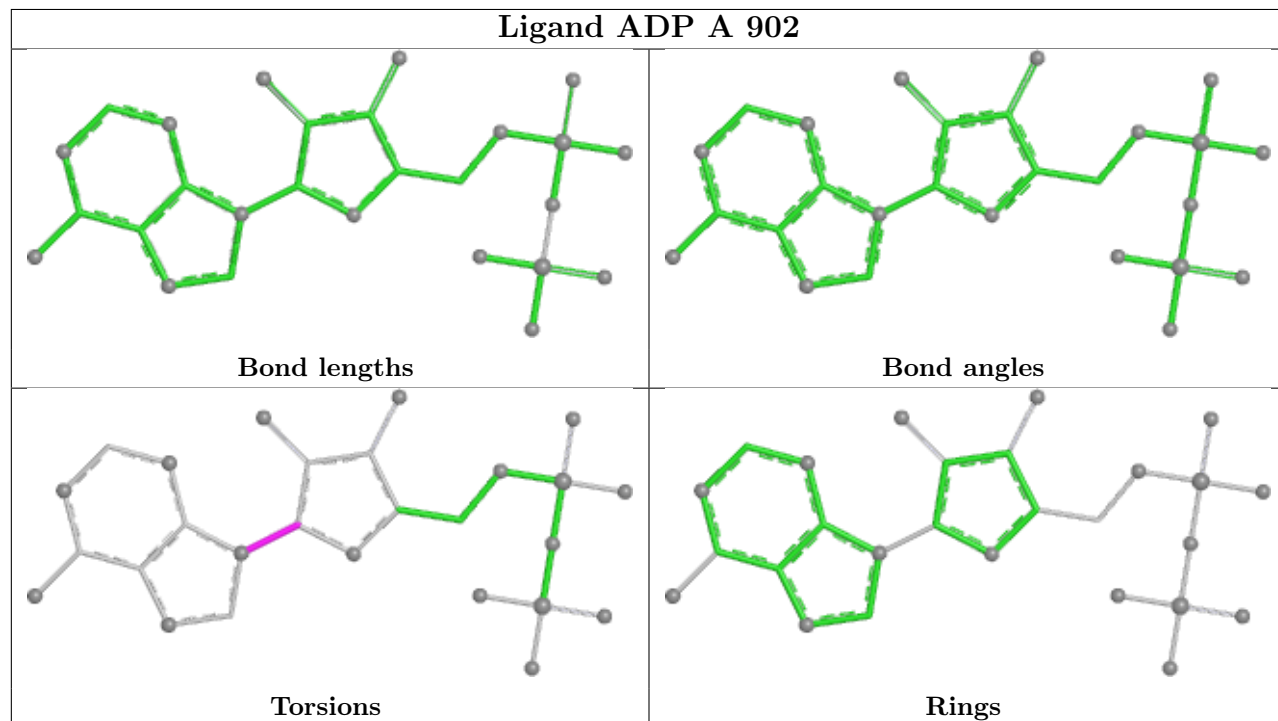
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

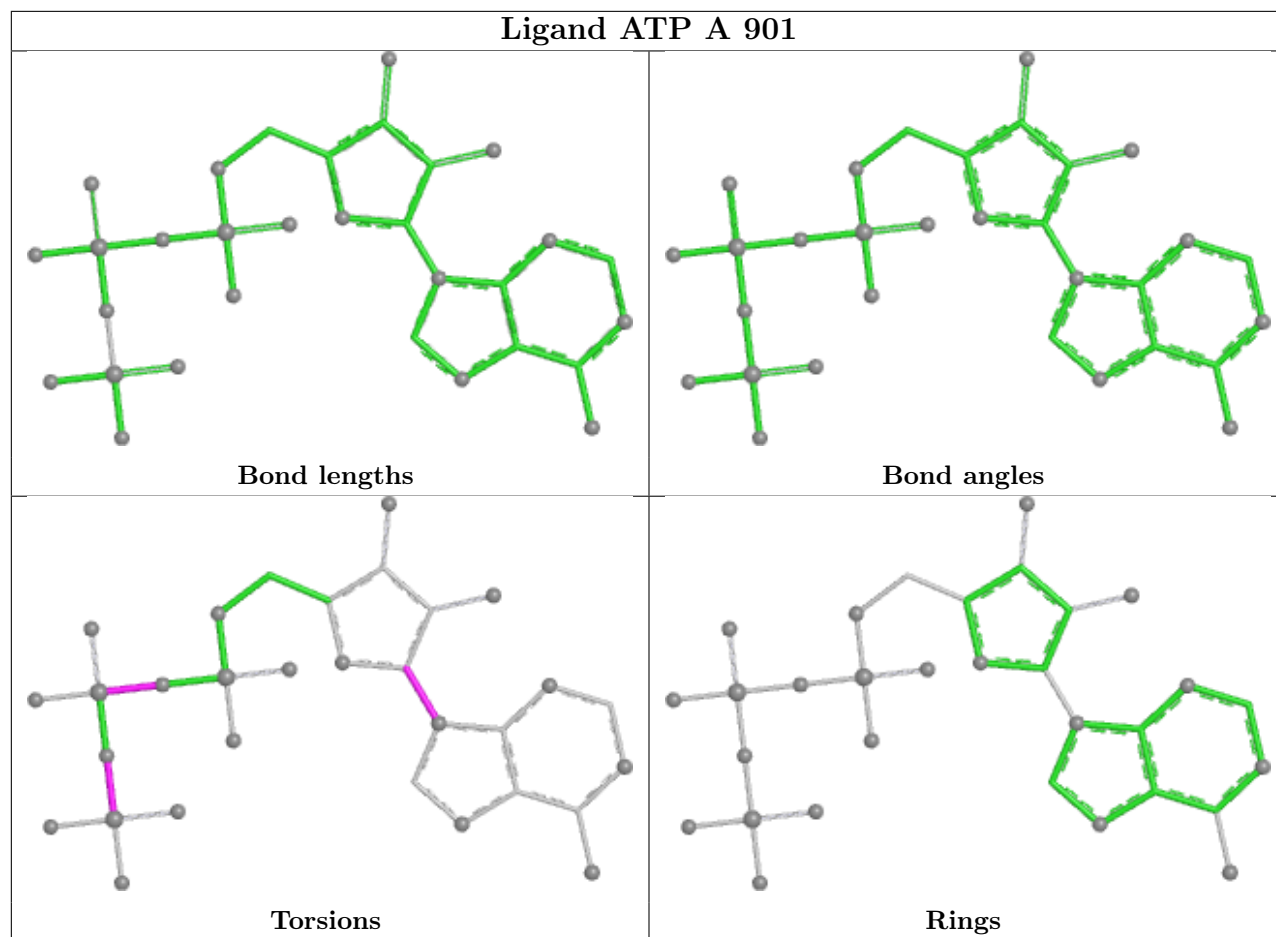


Ligand ATP B 901

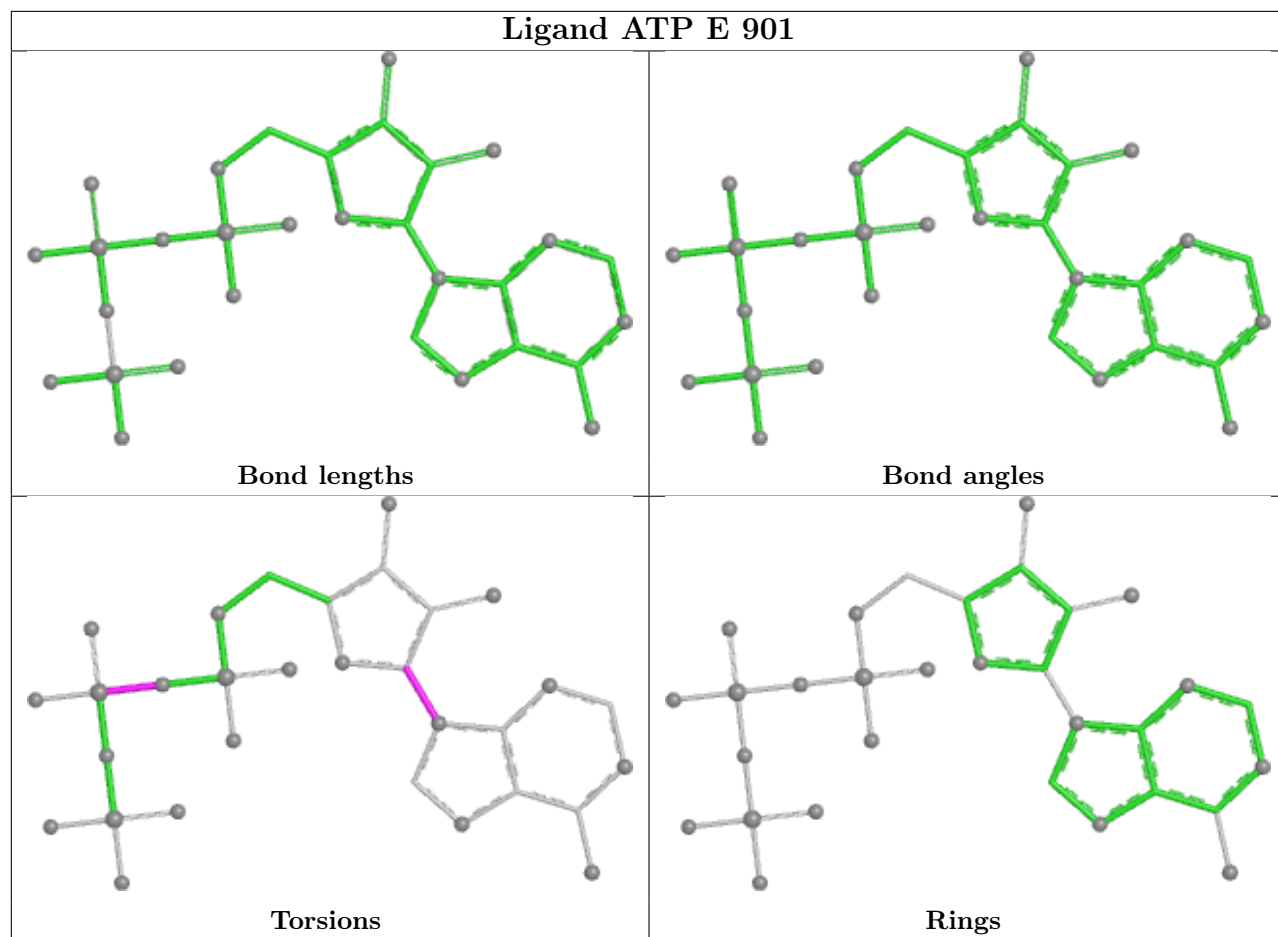


Ligand ADP A 902

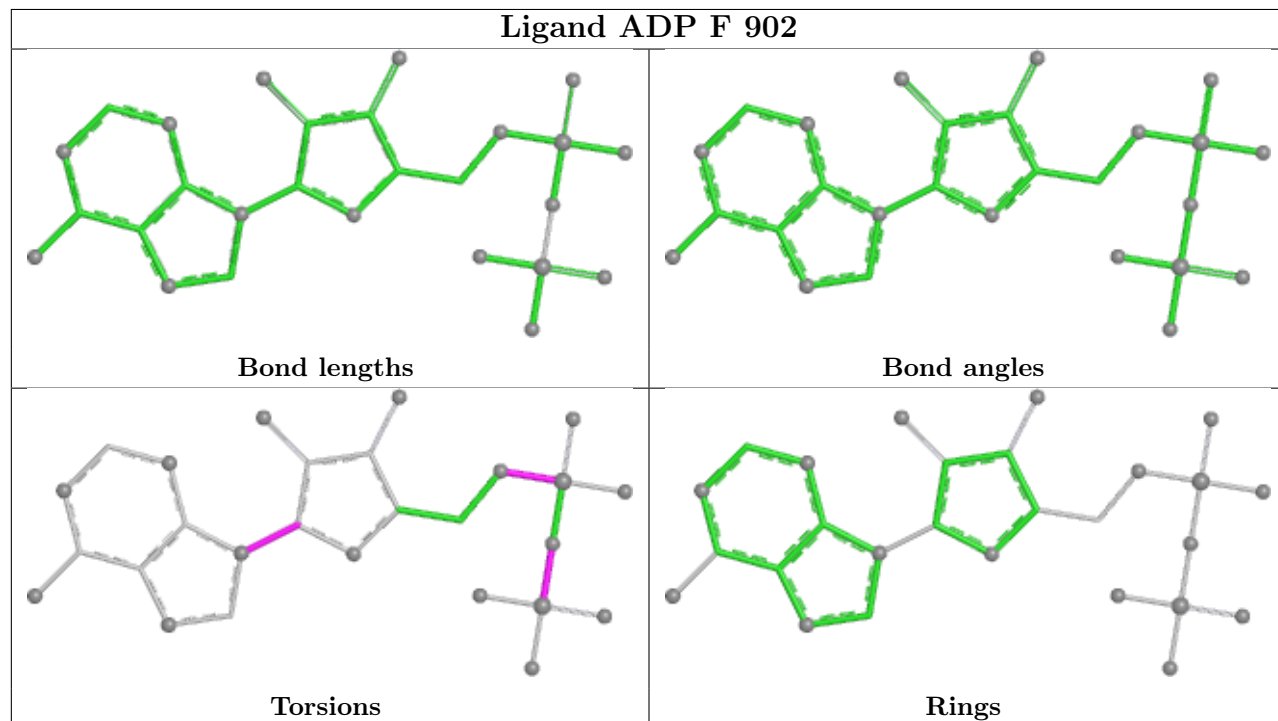


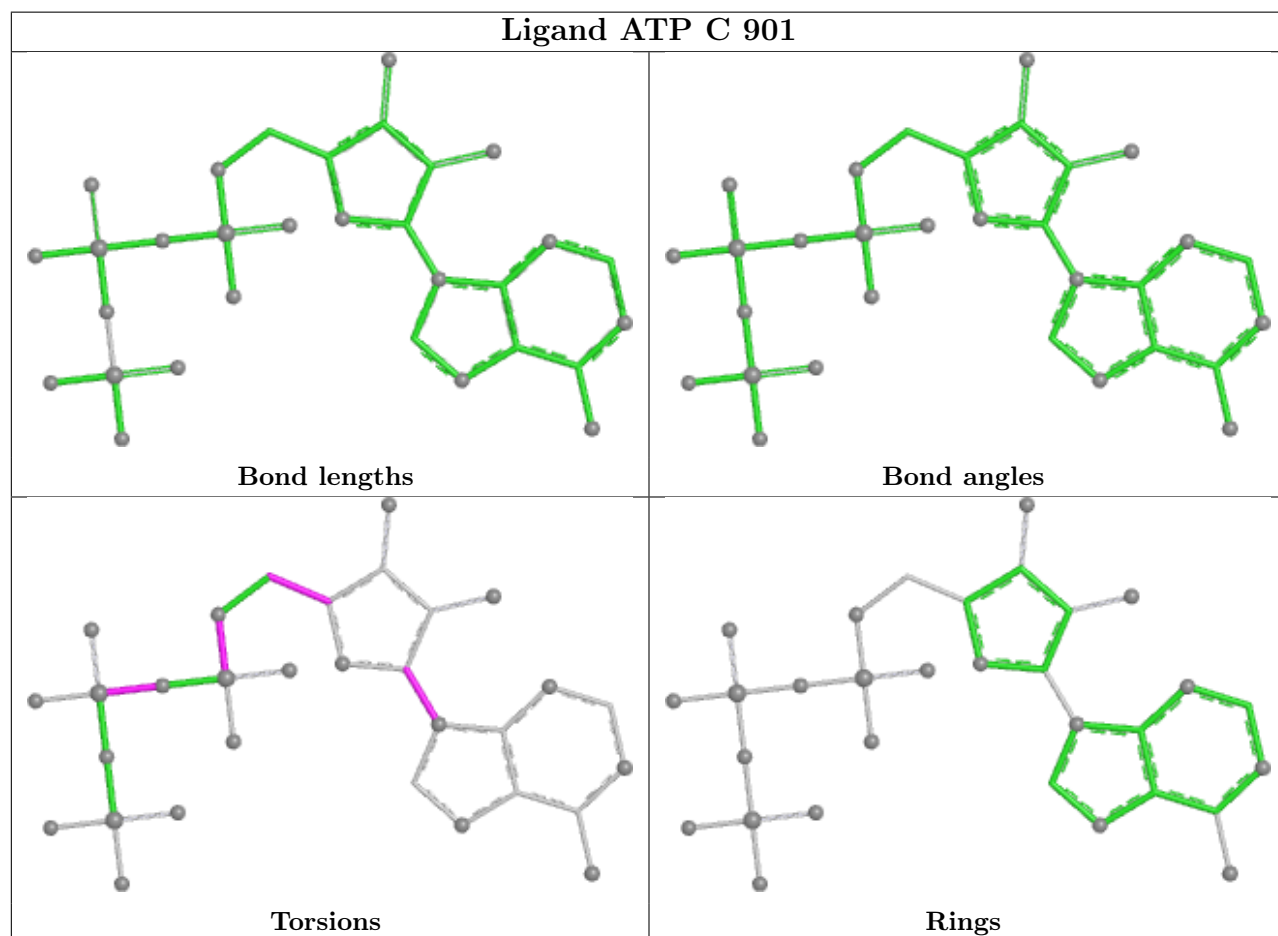
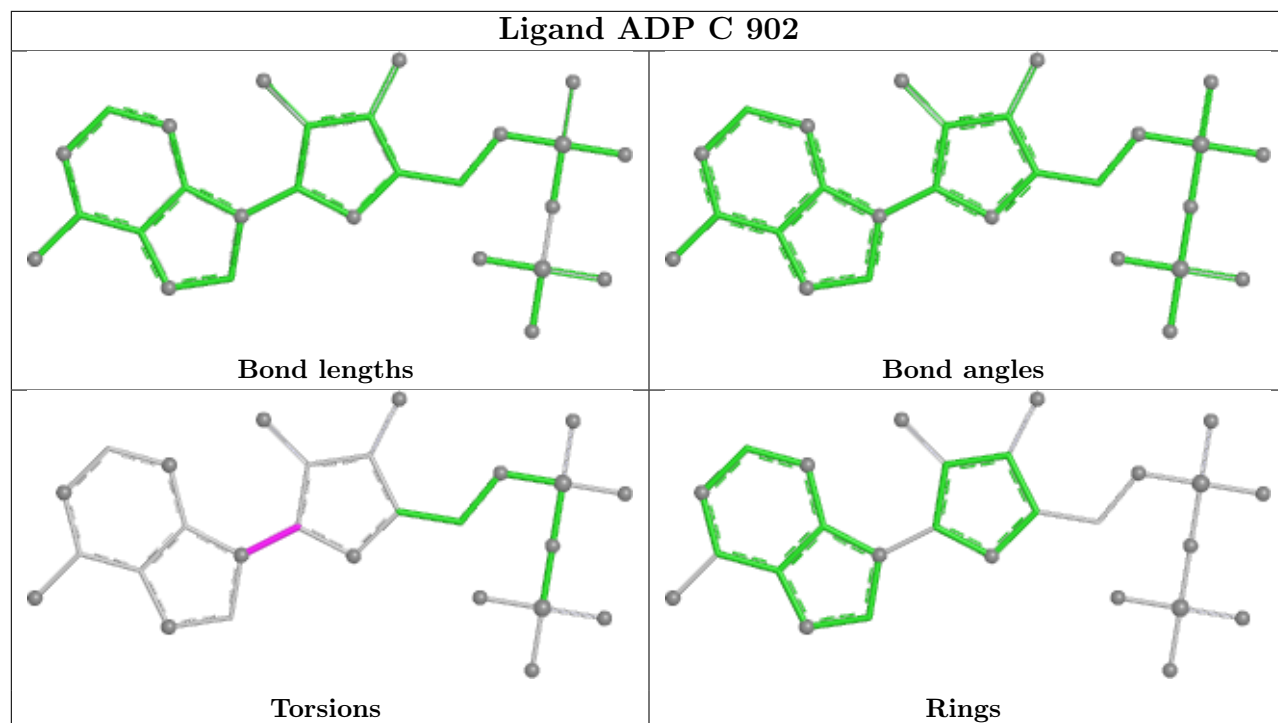


Ligand ATP E 901

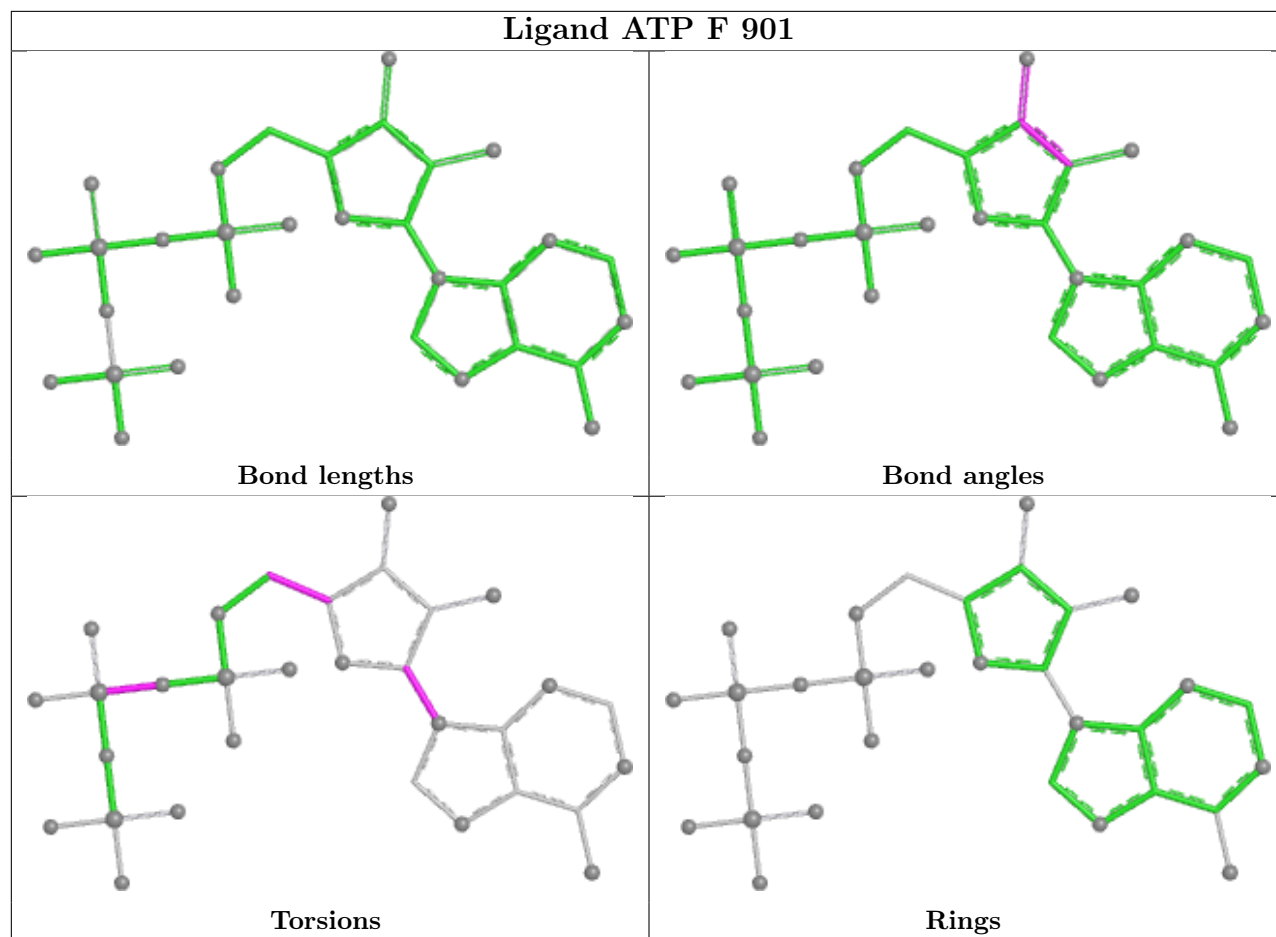


Ligand ADP F 902

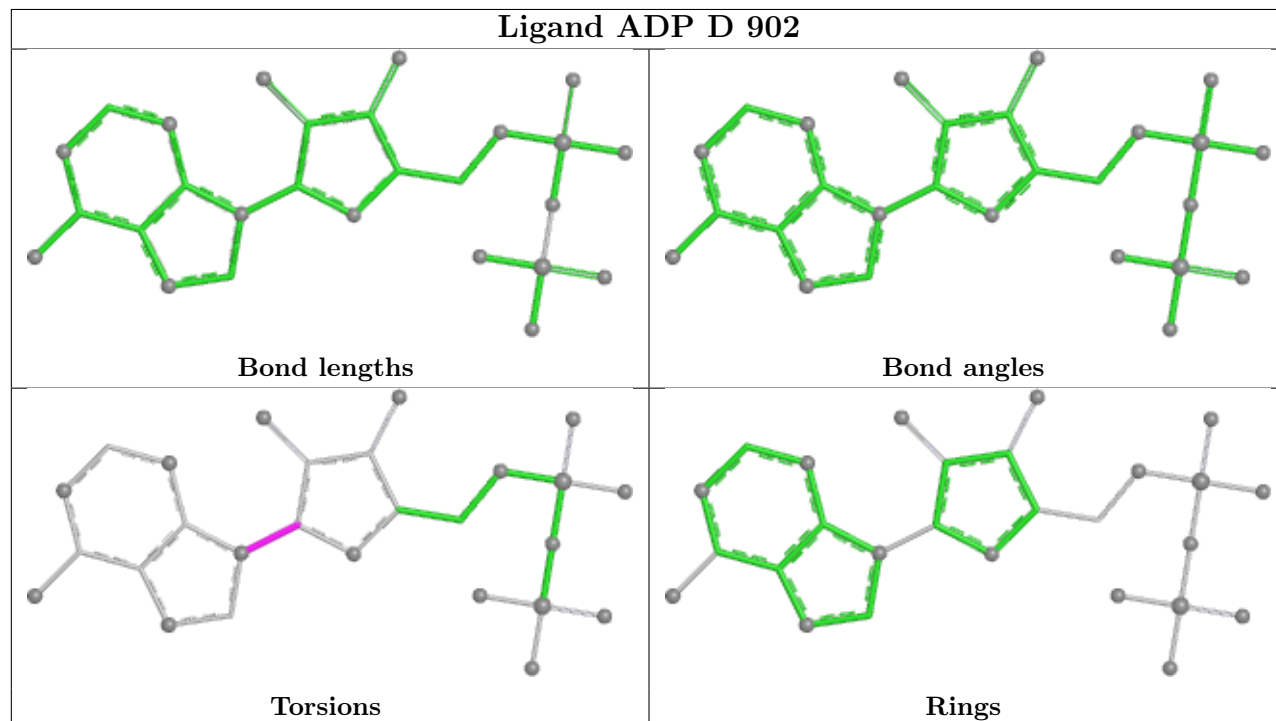




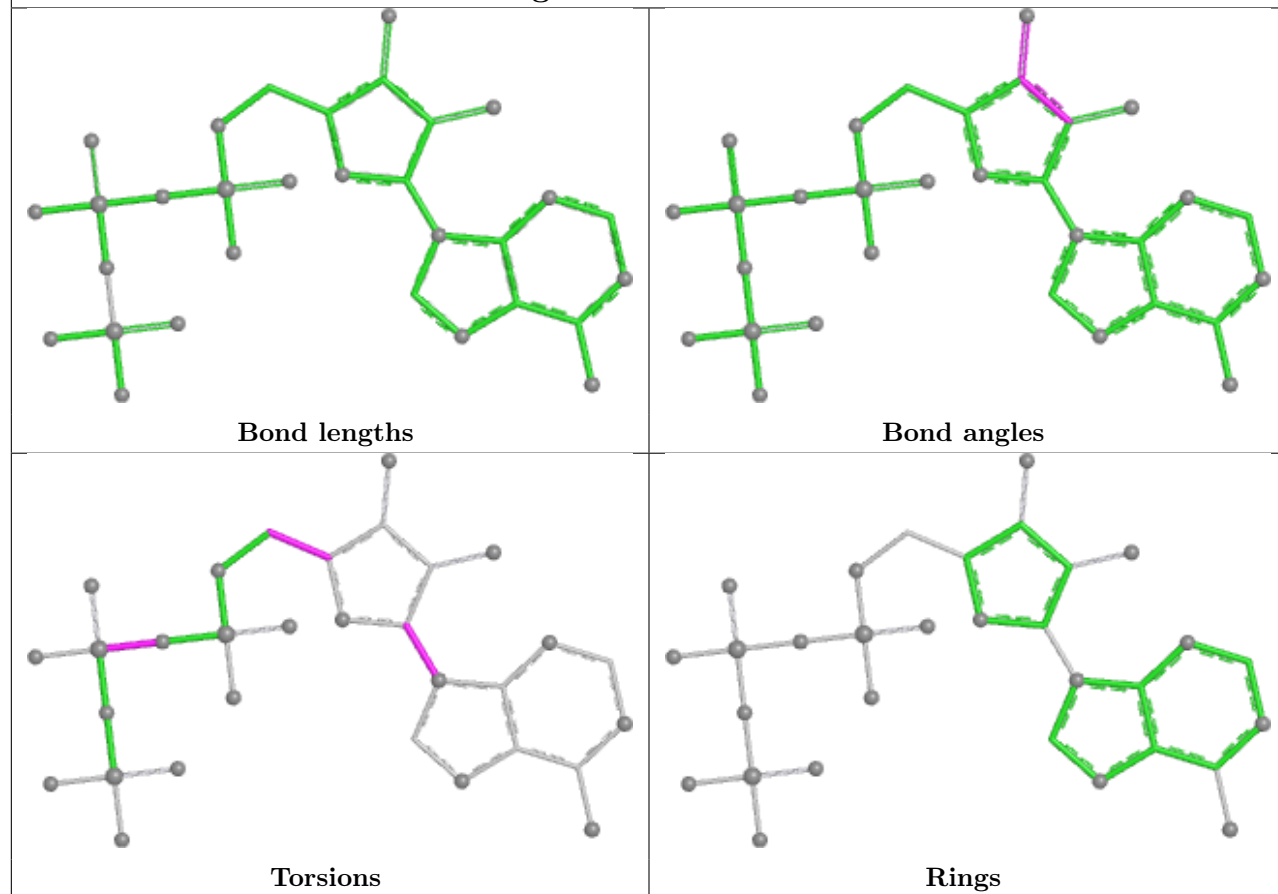
Ligand ATP F 901



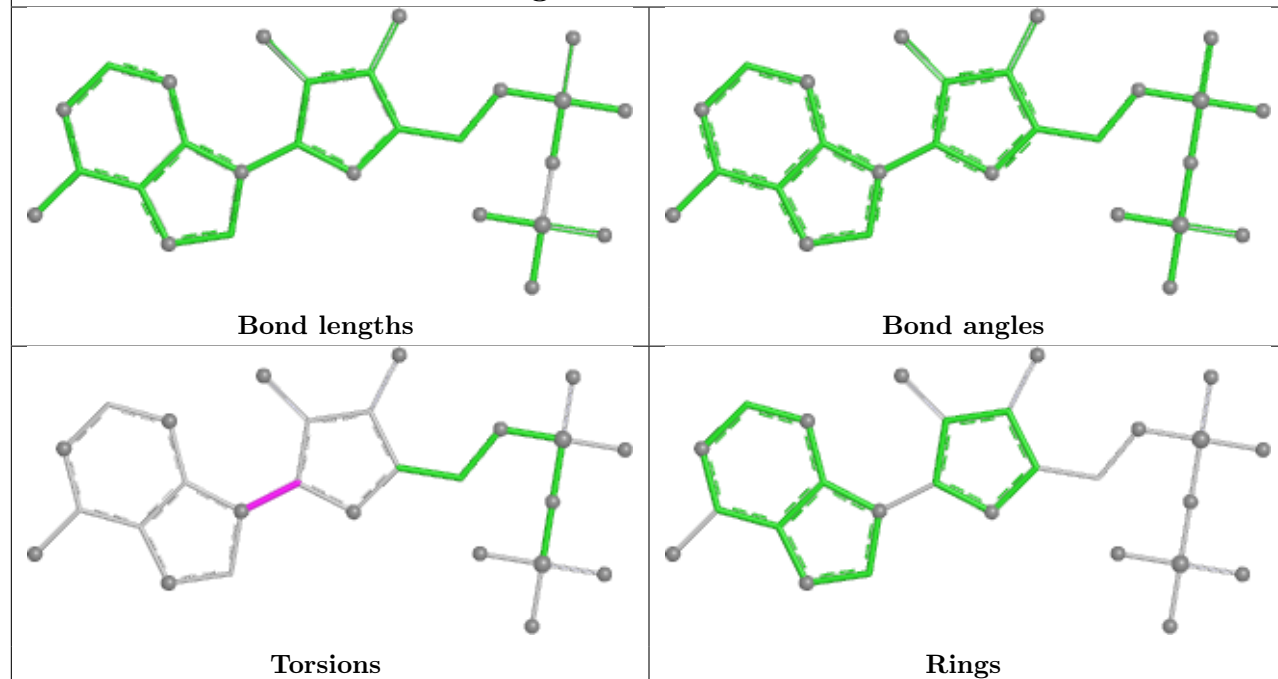
Ligand ADP D 902



Ligand ATP D 901



Ligand ADP E 902



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.

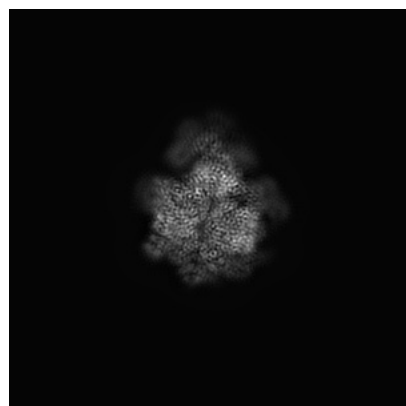
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27273. These allow visual inspection of the internal detail of the map and identification of artifacts.

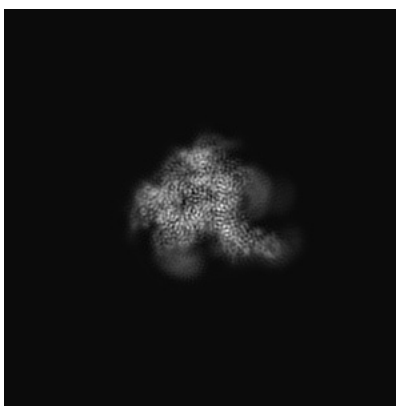
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

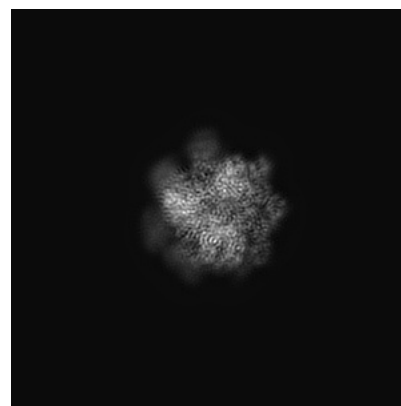
6.1.1 Primary map



X

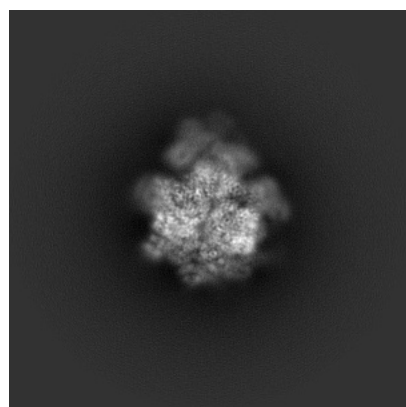


Y

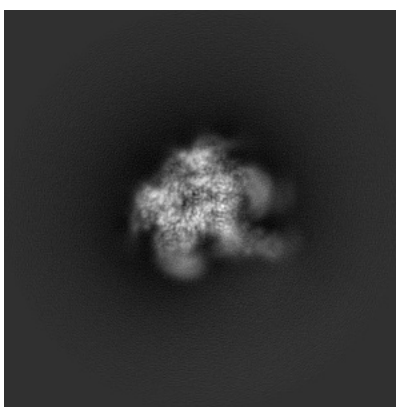


Z

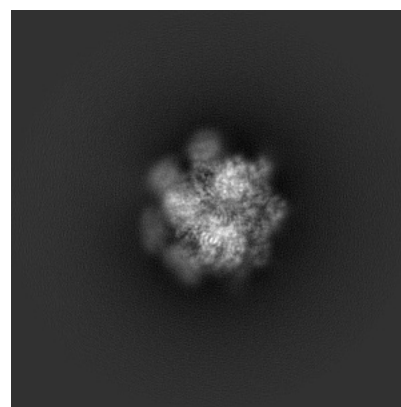
6.1.2 Raw map



X



Y

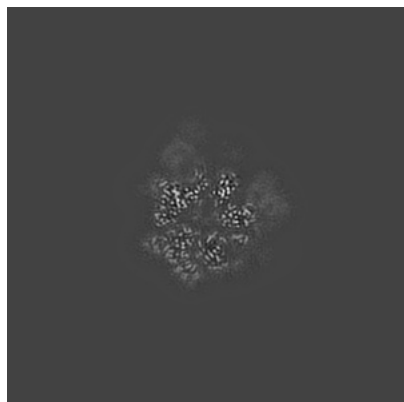


Z

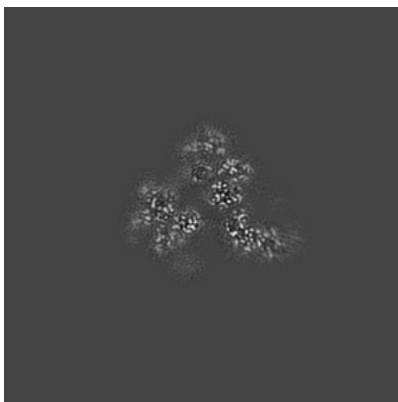
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

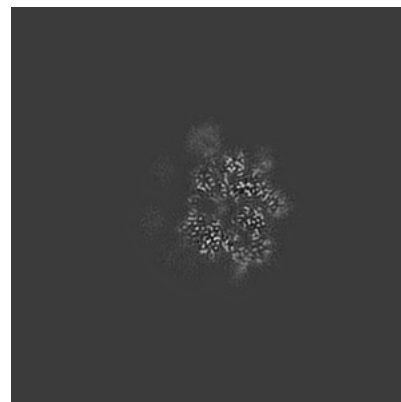
6.2.1 Primary map



X Index: 192

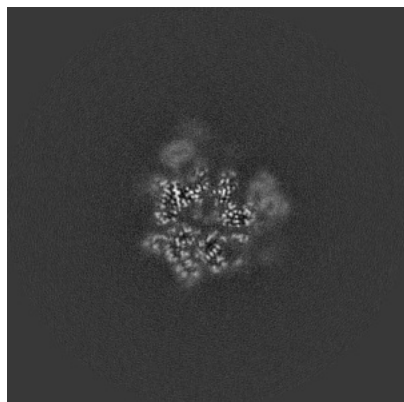


Y Index: 192

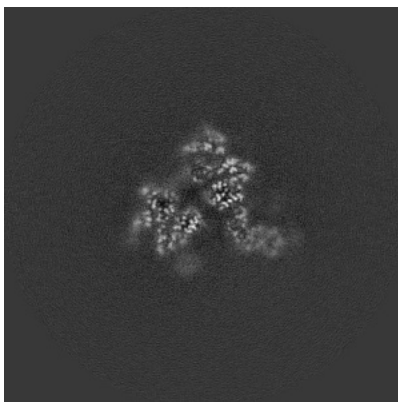


Z Index: 192

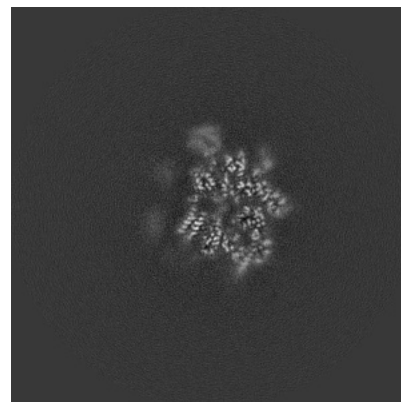
6.2.2 Raw map



X Index: 192



Y Index: 192

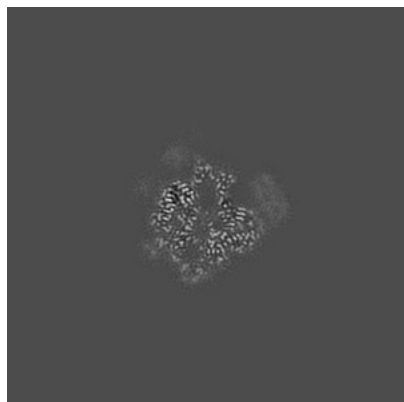


Z Index: 192

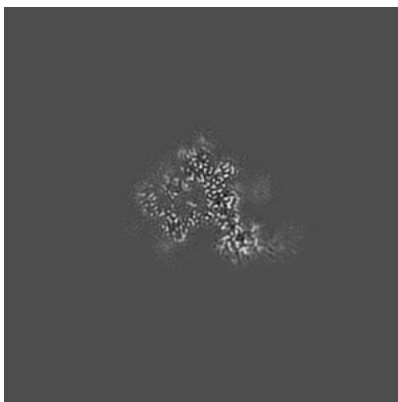
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

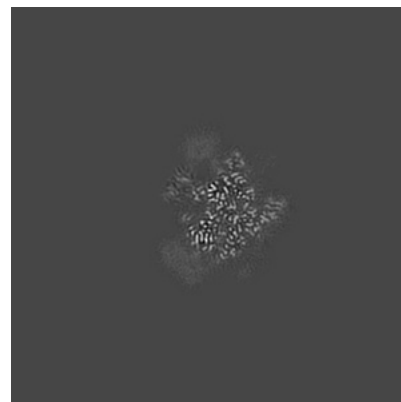
6.3.1 Primary map



X Index: 184

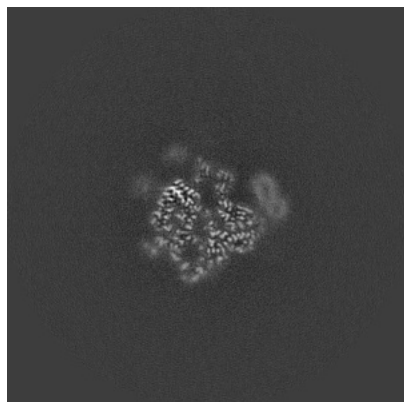


Y Index: 206

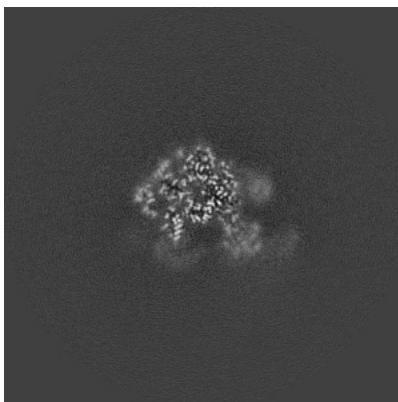


Z Index: 206

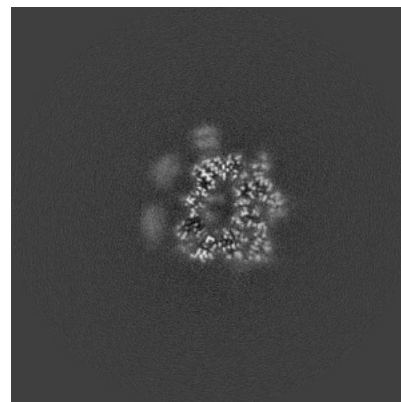
6.3.2 Raw map



X Index: 183



Y Index: 210

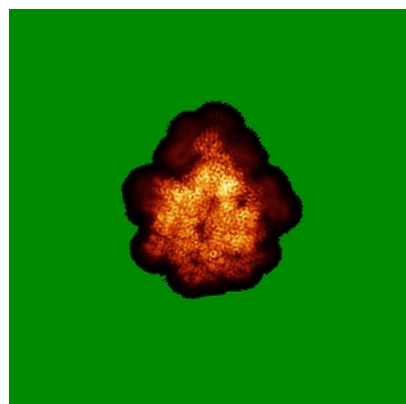


Z Index: 186

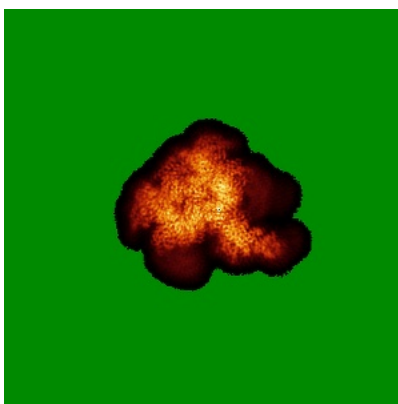
The images above show the largest variance slices of the map in three orthogonal directions.

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

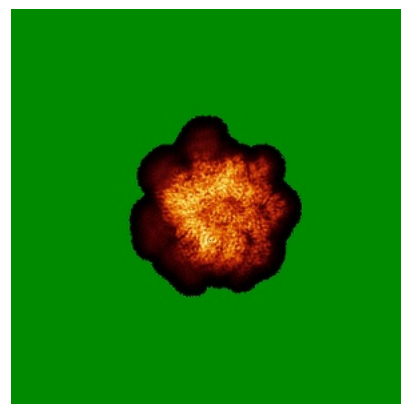
6.4.1 Primary map



X

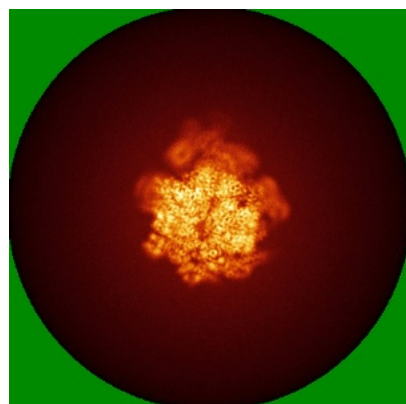


Y

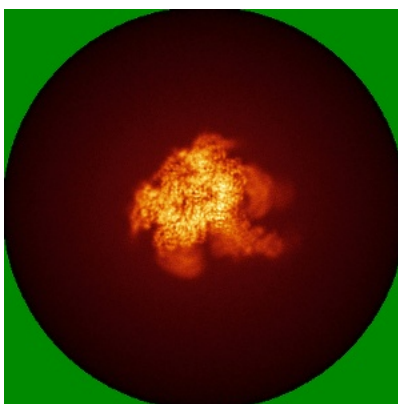


Z

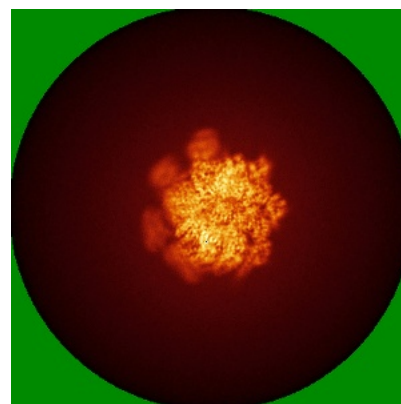
6.4.2 Raw map



X



Y

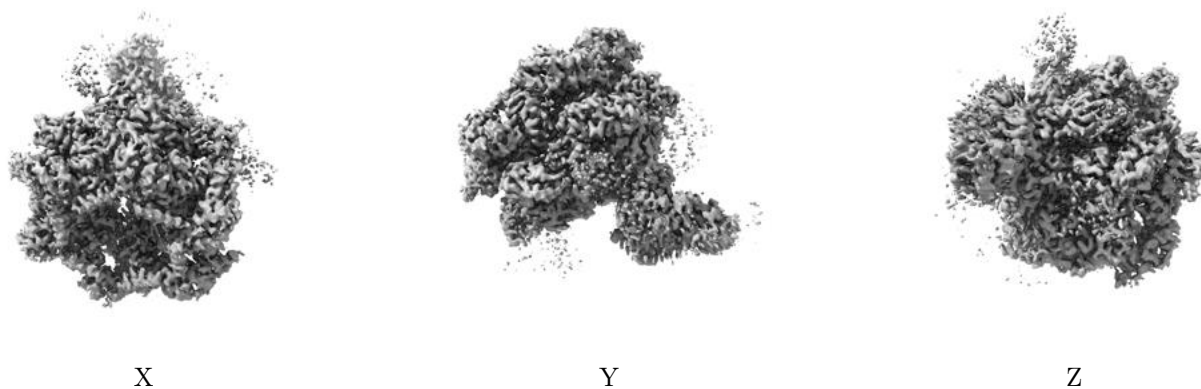


Z

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.

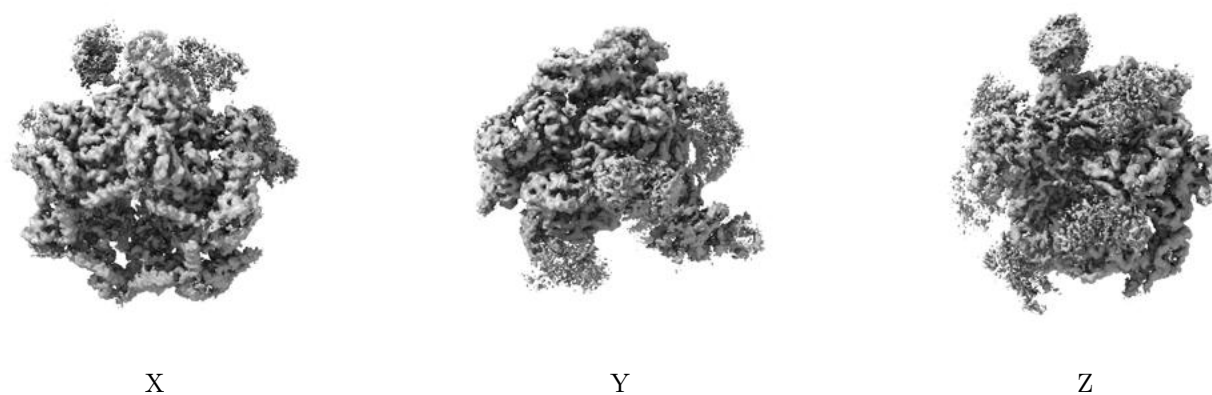
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

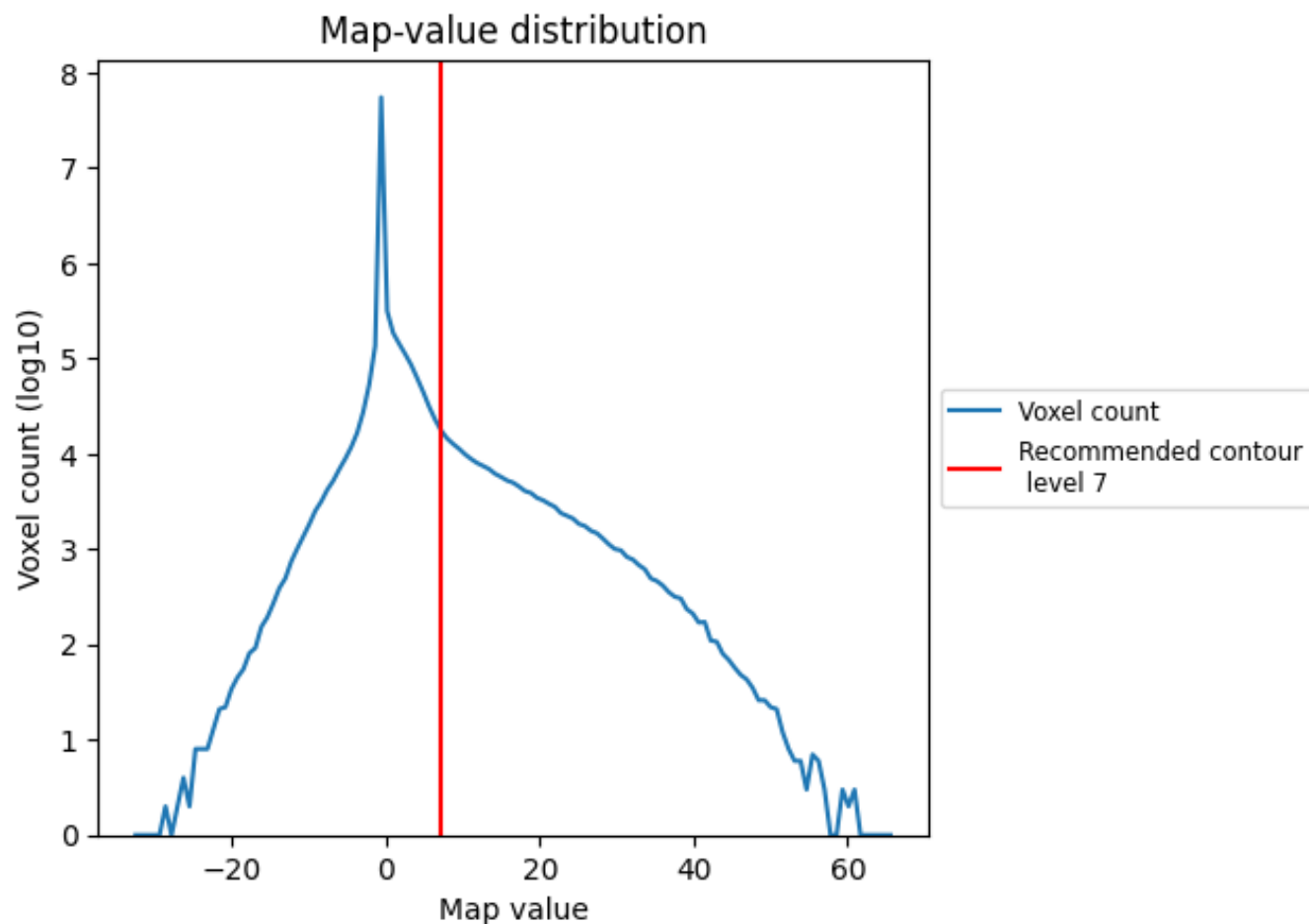
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

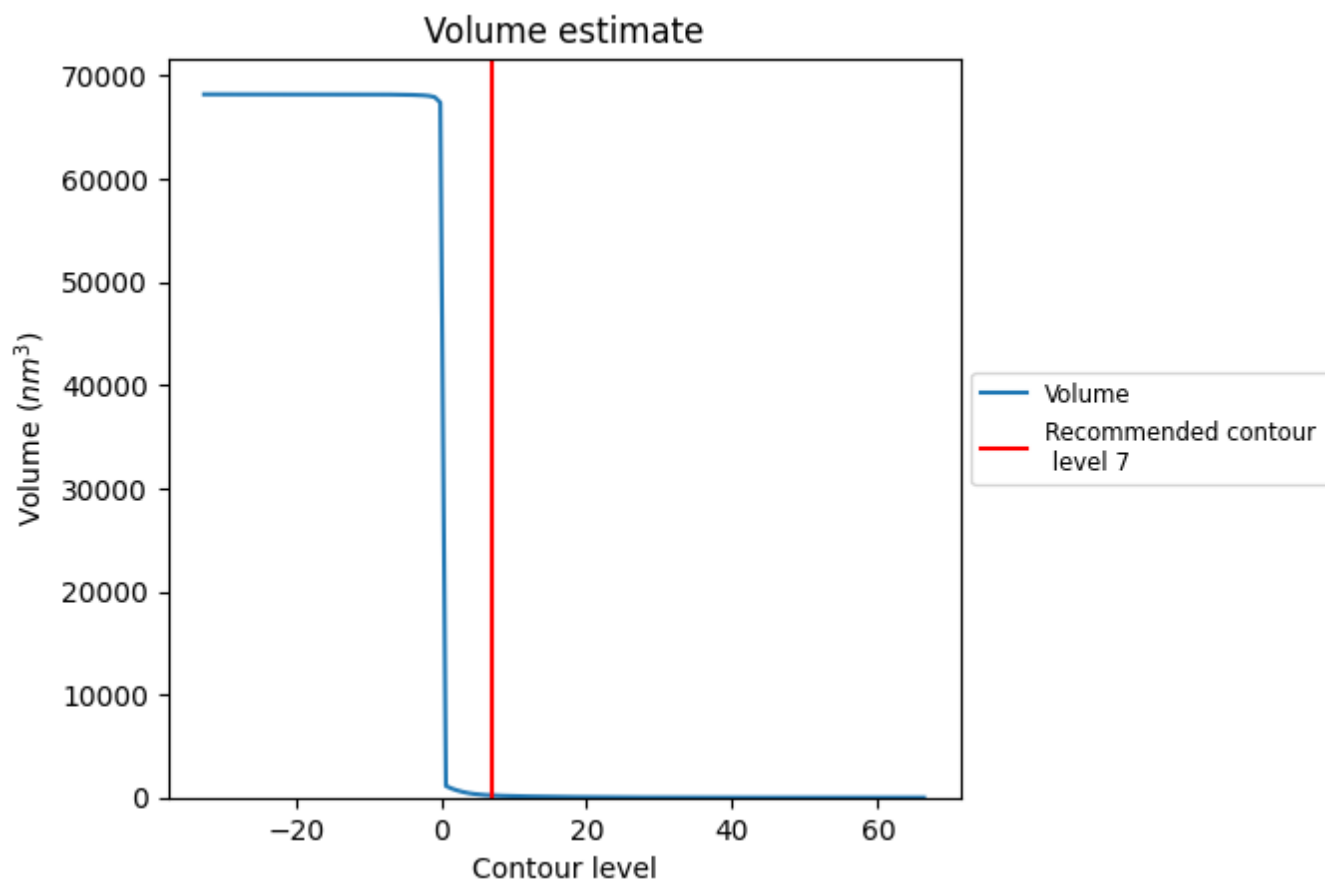
This section contains the results of statistical analysis of the map.

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.

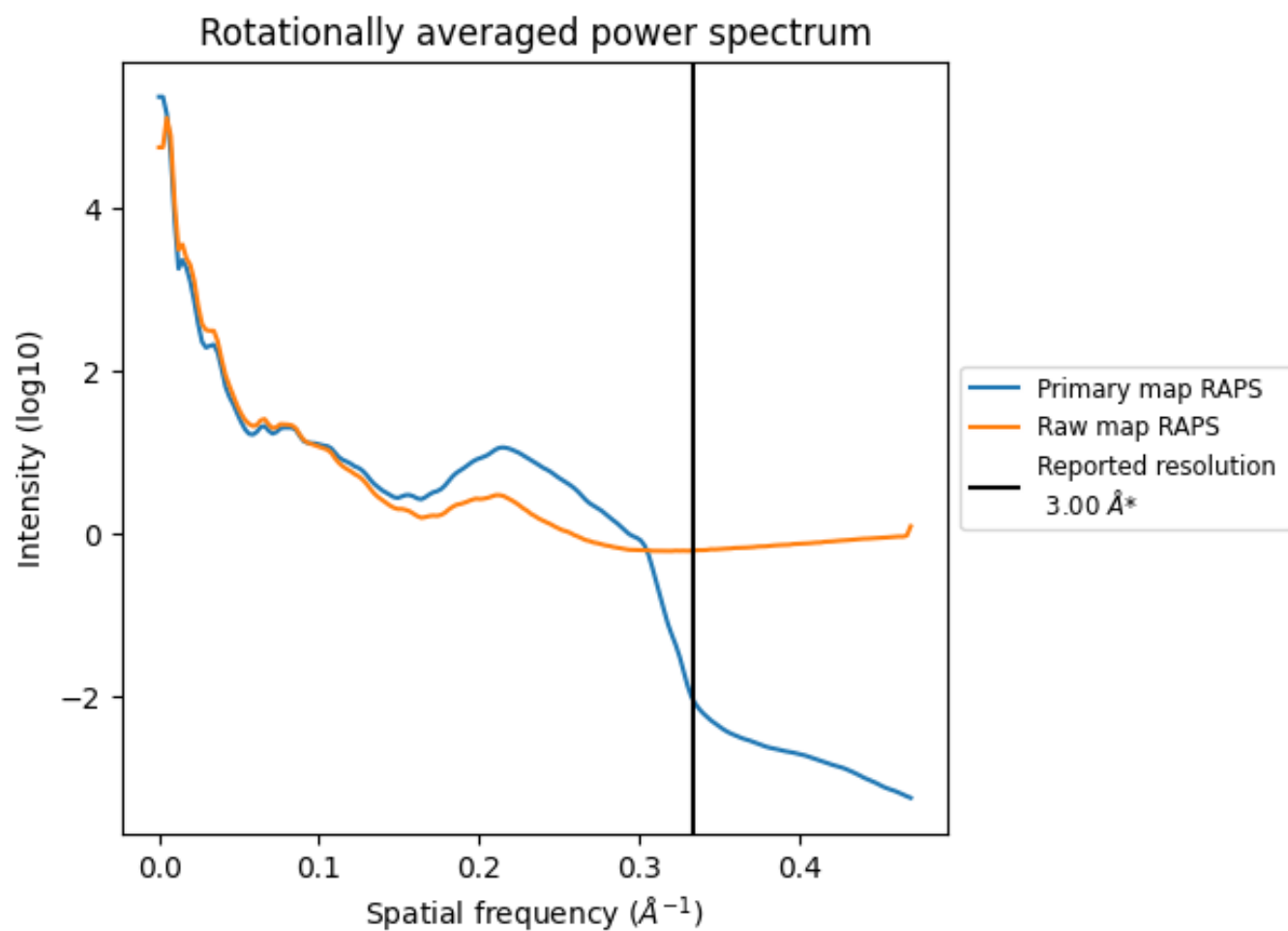
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm^3 ; this corresponds to an approximate mass of 189 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 ⓘ

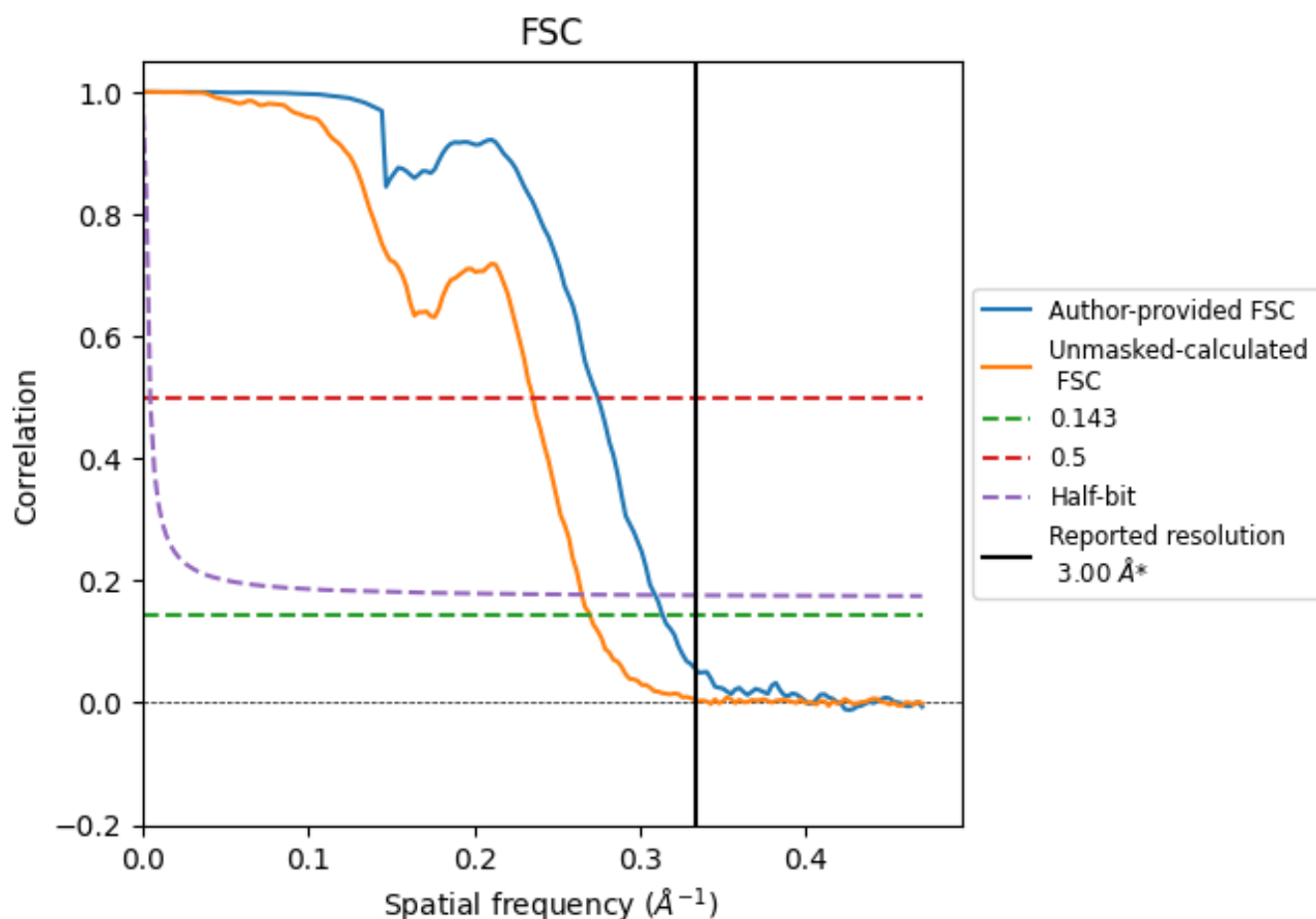


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

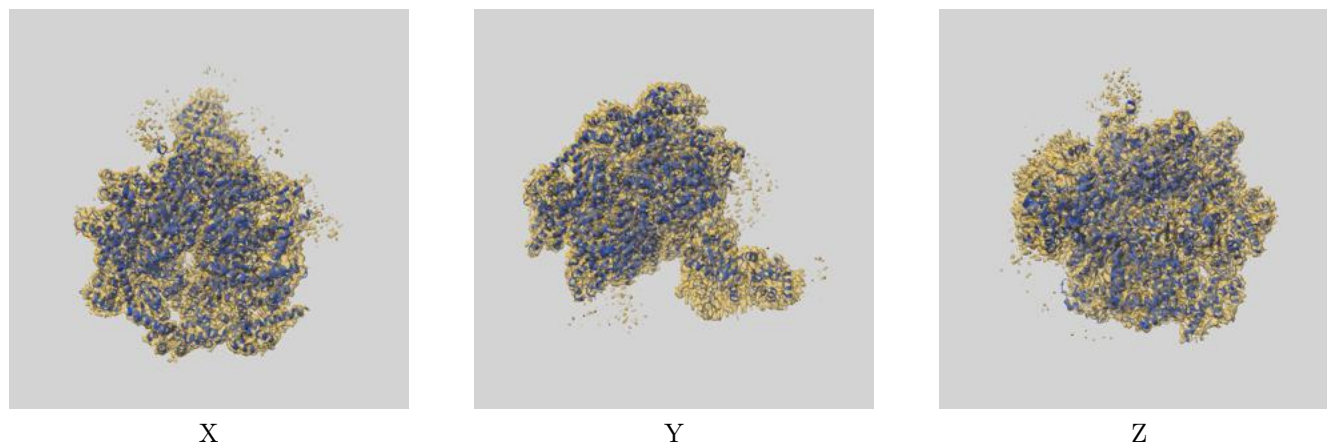
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.19	3.64	3.24
Unmasked-calculated*	3.71	4.25	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

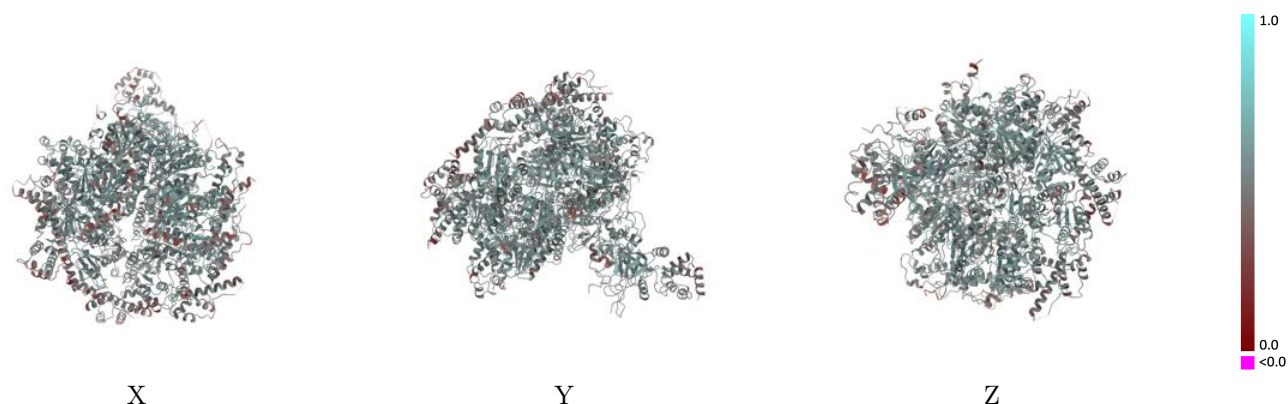
This section contains information regarding the fit between EMDB map EMD-27273 and PDB model 8DAR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



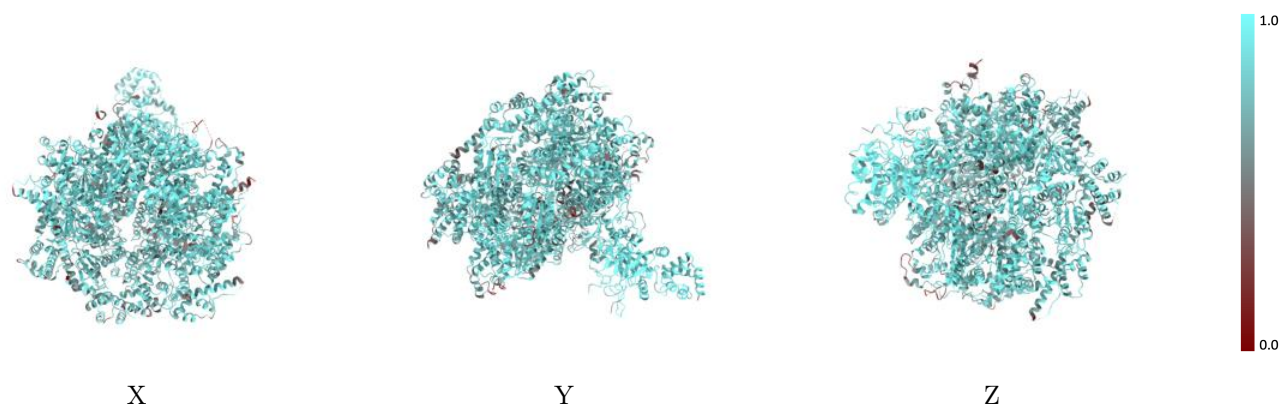
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



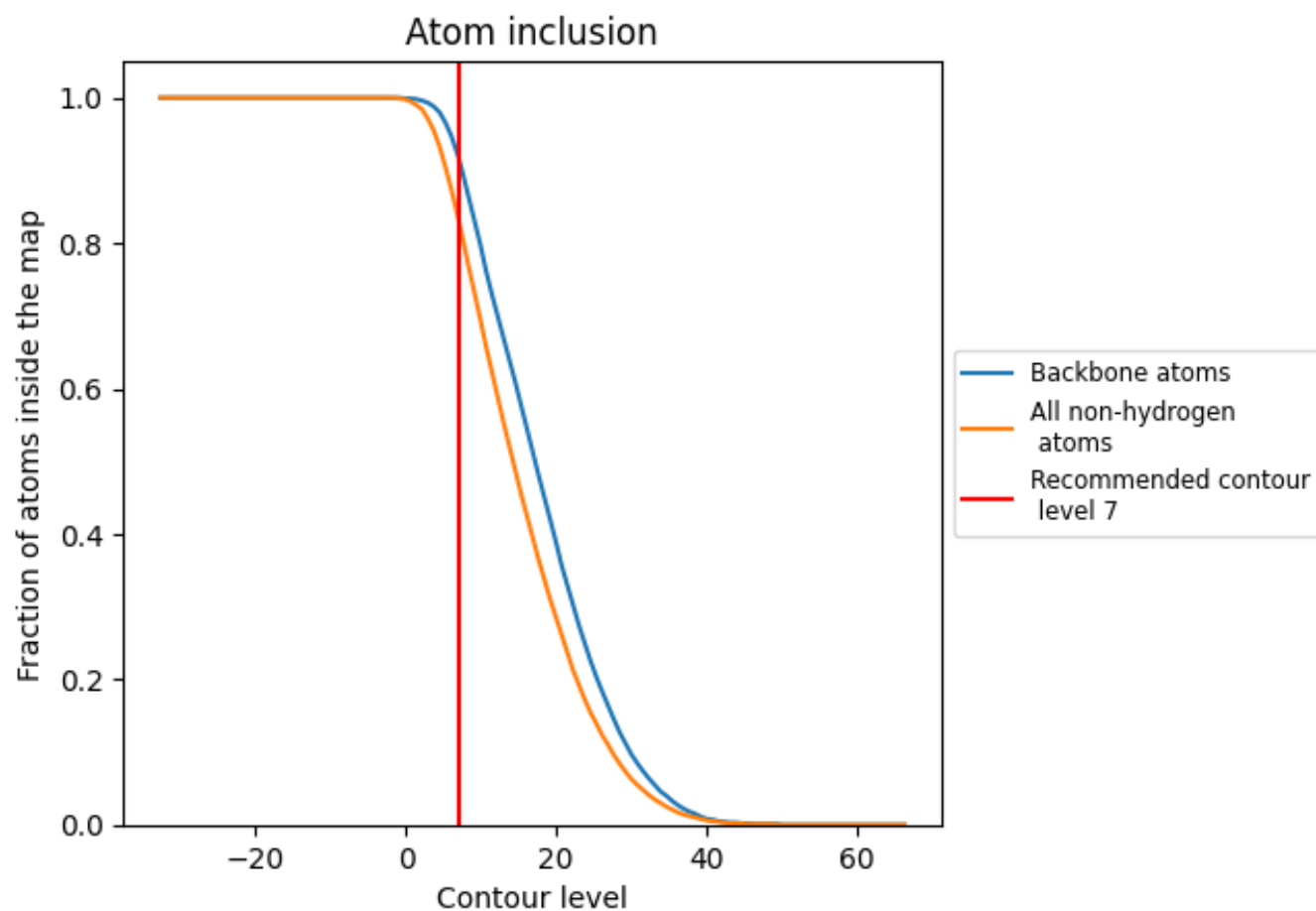
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5170
A	0.8290	0.5200
B	0.8360	0.5240
C	0.8470	0.5250
D	0.8190	0.5140
E	0.8200	0.5130
F	0.8160	0.5160
G	0.8830	0.5080
H	0.8610	0.4720

1.0

0.0

<0.0