



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:16 AM EST

PDB ID : 7JK6
EMDB ID : EMD-22363
Title : Structure of Drosophila ORC in the active conformation
Authors : Schmidt, J.M.; Bleichert, F.
Deposited on : 2020-07-27
Resolution : 4.00 Å(reported)

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

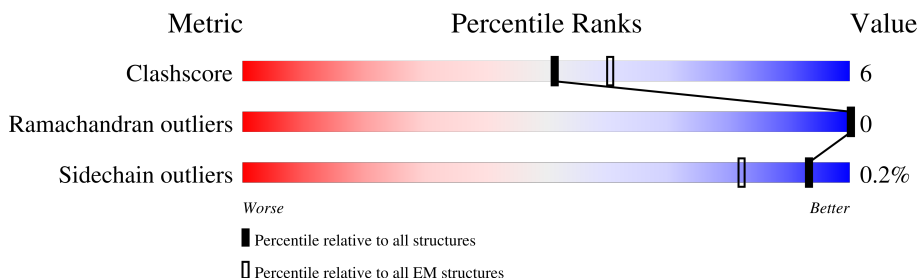
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	D	462	82% 13% 5%
2	E	460	67% 14% 19%
3	A	488	66% 10% 24%
4	B	618	23% 73%
5	C	721	60% 12% 28%
6	F	257	6% 93%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15161 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 Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	438	Total	C	N	O	S	0	0
			3528	2252	622	638	16		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q9W102
D	-1	ASN	-	expression tag	UNP Q9W102
D	0	ALA	-	expression tag	UNP Q9W102

- Molecule 2 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	374	Total	C	N	O	S	0	0
			2974	1909	502	547	16		

- Molecule 3 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	373	Total	C	N	O	S	0	0
			2919	1832	526	543	18		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	SER	-	expression tag	UNP O16810
A	438	ASN	-	expression tag	UNP O16810
A	439	ALA	-	expression tag	UNP O16810

- Molecule 4 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	165	Total	C	N	O	S	0	0
			1328	863	218	238	9		

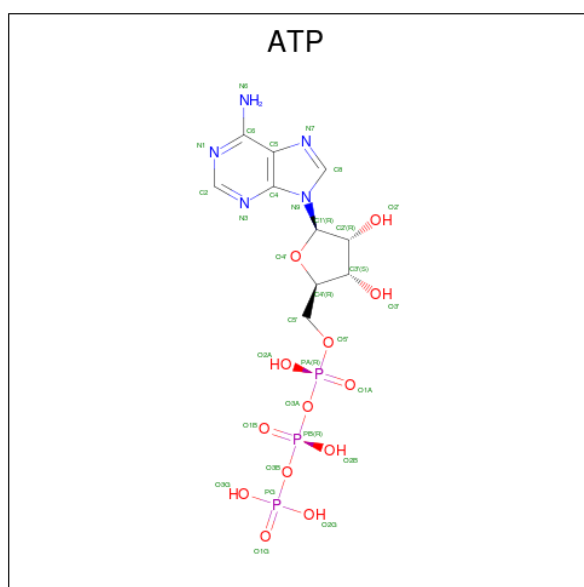
- Molecule 5 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	520	Total	C	N	O	S	0	0
			4173	2679	730	742	22		

- Molecule 6 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	17	Total	C	N	O	S	0	0
			143	92	25	25	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

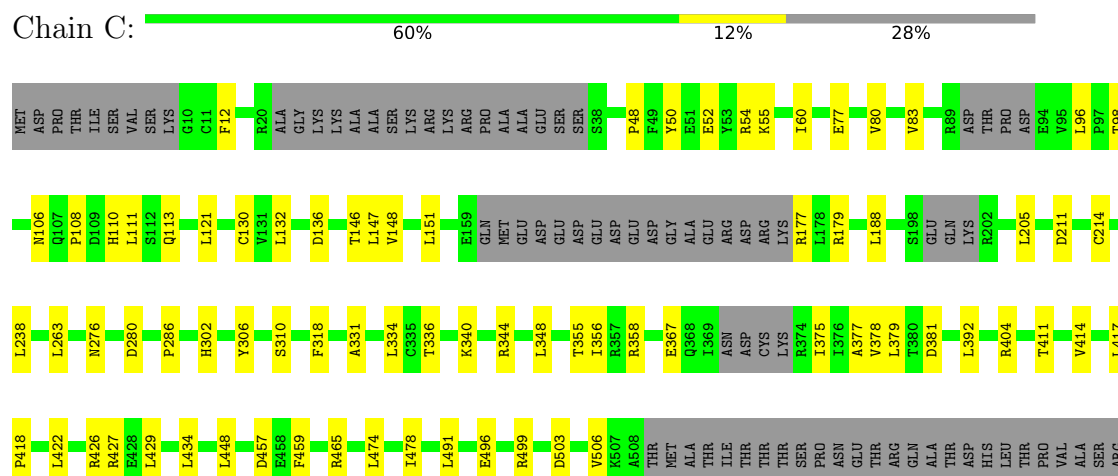
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total 1	Mg 1	0
8	E	1	Total 1	Mg 1	0
8	A	1	Total 1	Mg 1	0

- Molecule 4: Origin recognition complex subunit 2



- Molecule 5: Origin recognition complex subunit 3



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	126560	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	0.38	0/3594	0.64	0/4847
2	E	0.42	0/3019	0.70	1/4079 (0.0%)
3	A	0.36	0/2961	0.65	1/4005 (0.0%)
4	B	0.35	0/1362	0.69	1/1851 (0.1%)
5	C	0.39	0/4253	0.69	3/5752 (0.1%)
6	F	0.31	0/145	0.62	0/192
All	All	0.38	0/15334	0.67	6/20726 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	153	LEU	CA-CB-CG	6.35	129.90	115.30
3	A	722	LEU	CB-CG-CD1	-6.35	100.21	111.00
5	C	626	GLN	CA-CB-CG	5.70	125.93	113.40
5	C	598	ASP	CB-CG-OD1	5.64	123.38	118.30
4	B	364	LEU	CA-CB-CG	5.56	128.09	115.30
5	C	96	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

There are no planarity outliers.

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	D	3528	0	3565	45	0
2	E	2974	0	3042	45	0
3	A	2919	0	2994	34	0
4	B	1328	0	1321	15	0
5	C	4173	0	4241	54	0
6	F	143	0	145	1	0
7	A	31	0	12	5	0
7	D	31	0	12	5	0
7	E	31	0	12	4	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
All	All	15161	0	15344	178	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 (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LYS:NZ	7:D:901:ATP:O2'	1.97	0.97
2:E:47:LYS:NZ	7:E:901:ATP:O1B	2.03	0.92
5:C:98:THR:O	5:C:263:LEU:HA	1.76	0.84
2:E:183:TYR:OH	7:E:901:ATP:N6	2.14	0.80
1:D:206:PHE:HB3	3:A:828:ASN:HD22	1.50	0.77
3:A:745:TYR:OH	7:A:1001:ATP:N6	2.17	0.74
3:A:698:TYR:O	3:A:702:ASP:HB2	1.93	0.69
5:C:48:PRO:HB3	5:C:344:ARG:NH1	2.10	0.67
3:A:605:THR:HB	7:A:1001:ATP:O1A	1.96	0.64
3:A:603:GLY:HA2	7:A:1001:ATP:O2A	1.99	0.63
2:E:15:ARG:NH2	2:E:181:ALA:O	2.30	0.63
1:D:43:THR:HG21	1:D:176:CYS:HB2	1.80	0.62
2:E:13:PRO:HG2	2:E:191:ILE:HG22	1.81	0.62
2:E:202:GLN:OE1	2:E:252:ARG:NH2	2.32	0.62
1:D:12:ARG:NH1	2:E:31:GLU:OE2	2.32	0.61
2:E:33:TYR:HB3	2:E:154:CYS:HB2	1.83	0.61
1:D:302:LYS:HE3	7:D:901:ATP:H1'	1.83	0.60
1:D:58:ARG:HG3	7:D:901:ATP:O2G	2.03	0.59
3:A:687:ASP:HB3	3:A:722:LEU:HD11	1.84	0.59
4:B:422:PHE:O	4:B:459:ASN:ND2	2.35	0.58
5:C:148:VAL:HG22	5:C:188:LEU:HD22	1.85	0.58
1:D:16:LYS:NZ	2:E:31:GLU:OE1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:CYS:SG	7:D:901:ATP:O2G	2.62	0.58
2:E:379:SER:HB2	2:E:431:ARG:HB3	1.84	0.58
2:E:162:PRO:HB2	2:E:164:GLU:HG2	1.85	0.57
4:B:457:ILE:HB	4:B:460:ILE:HG12	1.87	0.57
1:D:446:LEU:HD12	1:D:447:PRO:HD2	1.85	0.57
2:E:145:LEU:HB3	2:E:153:LEU:HD11	1.87	0.57
1:D:297:SER:OG	3:A:884:LYS:NZ	2.39	0.56
3:A:628:GLU:HB3	3:A:679:THR:HG22	1.86	0.56
5:C:177:ARG:HH12	5:C:179:ARG:HH21	1.54	0.56
5:C:286:PRO:HG3	5:C:404:ARG:HG2	1.87	0.56
2:E:174:GLU:OE2	3:A:880:ARG:NH1	2.39	0.56
3:A:789:ILE:HG12	3:A:817:MET:HG3	1.87	0.56
5:C:496:GLU:OE2	5:C:499:ARG:NH2	2.39	0.55
3:A:680:VAL:HG12	3:A:712:VAL:HB	1.89	0.55
5:C:392:LEU:HD11	5:C:589:PRO:HG2	1.87	0.54
2:E:123:ILE:HG23	2:E:155:VAL:HA	1.88	0.54
4:B:436:ASN:H	4:B:465:SER:HB3	1.73	0.54
5:C:110:HIS:HA	5:C:113:GLN:HG2	1.90	0.54
1:D:421:GLN:HG2	2:E:435:THR:HG23	1.89	0.53
1:D:289:GLN:NE2	1:D:293:ASP:OD1	2.42	0.53
5:C:302:HIS:O	5:C:306:TYR:HB2	2.08	0.53
5:C:151:LEU:HD13	5:C:205:LEU:HD23	1.91	0.53
4:B:391:LYS:O	4:B:395:ASP:HB2	2.09	0.53
5:C:474:LEU:HD23	5:C:478:ILE:HG13	1.90	0.53
1:D:13:ARG:HG2	2:E:31:GLU:HG2	1.91	0.53
1:D:48:GLU:OE2	3:A:791:ARG:NH2	2.42	0.53
5:C:130:CYS:HB2	5:C:151:LEU:HG	1.92	0.52
5:C:340:LYS:O	5:C:344:ARG:HG2	2.10	0.52
2:E:393:LEU:HG	2:E:395:GLU:HB3	1.90	0.52
1:D:347:GLU:HG3	1:D:396:ALA:HB1	1.91	0.52
2:E:237:PHE:HE2	2:E:250:THR:HG21	1.74	0.52
2:E:126:ASP:HA	2:E:158:LEU:HB2	1.92	0.52
2:E:39:LEU:HA	2:E:178:LEU:O	2.10	0.51
2:E:379:SER:HA	2:E:432:LEU:O	2.10	0.51
5:C:564:ALA:HA	5:C:567:LYS:HG3	1.91	0.51
4:B:364:LEU:HD11	4:B:492:THR:HG21	1.93	0.51
5:C:148:VAL:HG13	5:C:188:LEU:HD13	1.93	0.51
4:B:398:THR:HG21	4:B:407:SER:HB3	1.91	0.51
4:B:382:ASN:HD21	5:C:12:PHE:HE2	1.59	0.51
5:C:474:LEU:HD11	5:C:491:LEU:HD23	1.93	0.50
2:E:334:LEU:HD21	2:E:452:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:GLU:HG3	1:D:50:ASN:HD21	1.76	0.50
5:C:375:ILE:O	5:C:378:VAL:N	2.44	0.50
5:C:132:LEU:HD11	5:C:147:LEU:HD12	1.94	0.50
5:C:60:ILE:HD13	5:C:318:PHE:HE2	1.77	0.50
5:C:276:ASN:OD1	5:C:427:ARG:NE	2.45	0.49
5:C:414:VAL:HG11	5:C:422:LEU:HB2	1.94	0.49
2:E:333:PHE:CG	2:E:441:VAL:HG21	2.46	0.49
5:C:108:PRO:HA	5:C:111:LEU:HD13	1.95	0.49
2:E:245:PRO:HG3	7:E:901:ATP:O4'	2.12	0.48
2:E:66:THR:O	2:E:87:SER:OG	2.28	0.48
2:E:121:PHE:HB2	2:E:153:LEU:HB3	1.95	0.48
5:C:177:ARG:HH12	5:C:179:ARG:HD2	1.79	0.48
1:D:429:LEU:HG	1:D:431:LEU:H	1.78	0.48
2:E:260:GLU:HG3	2:E:261:PRO:HD3	1.96	0.48
2:E:48:THR:OG1	7:E:901:ATP:O2B	2.32	0.47
5:C:280:ASP:HB3	5:C:426:ARG:HH21	1.79	0.47
3:A:565:PRO:HG2	3:A:568:LEU:HD23	1.96	0.47
5:C:50:TYR:OH	5:C:54:ARG:NH2	2.46	0.47
1:D:142:VAL:HB	1:D:175:ILE:HG22	1.96	0.47
1:D:223:LEU:HD21	1:D:305:LEU:HD22	1.97	0.47
1:D:238:ILE:HD12	1:D:255:HIS:HD1	1.79	0.47
1:D:313:ARG:NH1	2:E:24:GLU:HG2	2.30	0.46
3:A:592:GLY:O	3:A:712:VAL:HA	2.15	0.46
1:D:185:ASP:N	1:D:185:ASP:OD1	2.48	0.46
1:D:52:LEU:HD11	1:D:203:VAL:HG23	1.98	0.46
2:E:406:GLN:HA	2:E:409:THR:HG22	1.97	0.46
3:A:639:GLU:HB2	3:A:642:GLN:HG2	1.96	0.46
1:D:296:ILE:HG23	3:A:830:SER:HB3	1.98	0.46
1:D:235:ALA:HA	1:D:238:ILE:HG22	1.97	0.46
1:D:347:GLU:HB3	1:D:400:LEU:HD21	1.98	0.45
2:E:51:THR:HG21	2:E:158:LEU:HD21	1.98	0.45
4:B:347:LEU:HD22	4:B:461:HIS:HB3	1.98	0.45
1:D:36:VAL:HG12	1:D:69:VAL:HG11	1.98	0.45
1:D:295:ASP:OD1	3:A:884:LYS:NZ	2.48	0.45
5:C:106:ASN:HD22	5:C:310:SER:HB2	1.81	0.45
1:D:83:THR:HA	1:D:141:SER:O	2.17	0.45
3:A:574:GLU:HG3	3:A:740:LEU:HD11	1.99	0.45
1:D:169:GLN:HG3	1:D:197:ARG:HG2	1.97	0.45
1:D:218:LEU:HD21	1:D:298:GLU:HG3	1.99	0.45
3:A:559:LEU:HD21	3:A:754:VAL:HG13	1.99	0.45
5:C:136:ASP:HB3	5:C:146:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ILE:HA	1:D:241:LEU:HG	1.98	0.45
2:E:65:ARG:HE	2:E:90:PRO:HG3	1.81	0.45
5:C:52:GLU:OE2	5:C:336:THR:OG1	2.31	0.45
1:D:40:LEU:HD21	1:D:178:LEU:HD21	1.99	0.44
5:C:377:ALA:HA	5:C:381:ASP:HB2	1.98	0.44
2:E:321:LEU:HB2	2:E:326:LYS:HE3	1.99	0.44
3:A:775:LYS:HD2	3:A:814:LEU:HD13	1.98	0.44
5:C:411:THR:HG21	5:C:426:ARG:HG2	1.99	0.44
3:A:556:ARG:HB2	3:A:794:THR:HG21	1.99	0.44
3:A:640:PRO:HG2	3:A:693:ARG:HH11	1.82	0.44
5:C:355:THR:HA	5:C:358:ARG:HB2	1.98	0.44
5:C:422:LEU:HB3	5:C:429:LEU:HD21	1.99	0.44
3:A:892:ILE:HB	3:A:905:LEU:HB2	2.00	0.44
5:C:55:LYS:HA	5:C:55:LYS:HD2	1.77	0.44
2:E:239:LYS:HE2	2:E:239:LYS:HB3	1.84	0.44
1:D:344:SER:HB3	2:E:242:ARG:HG3	1.98	0.44
4:B:359:GLY:O	4:B:361:LYS:NZ	2.43	0.44
5:C:334:LEU:HD11	5:C:348:LEU:HD11	2.00	0.44
5:C:459:PHE:HE1	5:C:569:LEU:HD21	1.83	0.44
2:E:293:ARG:HD3	2:E:293:ARG:HA	1.85	0.44
5:C:465:ARG:HA	5:C:465:ARG:HD2	1.78	0.44
3:A:595:TYR:OH	3:A:719:THR:O	2.36	0.43
1:D:293:ASP:OD1	3:A:831:ARG:NH2	2.50	0.43
3:A:633:ASN:HB3	3:A:636:ARG:HD2	2.00	0.43
5:C:331:ALA:HB1	5:C:356:ILE:HG13	2.00	0.43
5:C:457:ASP:N	5:C:457:ASP:OD1	2.52	0.43
3:A:674:PRO:HA	3:A:676:ARG:H	1.82	0.43
1:D:74:LEU:HD23	1:D:74:LEU:HA	1.91	0.43
3:A:571:ARG:NH2	3:A:743:GLN:O	2.43	0.43
1:D:100:LEU:HD12	1:D:100:LEU:HA	1.85	0.43
3:A:591:GLY:HA2	3:A:712:VAL:HG22	2.01	0.43
4:B:415:VAL:HG21	4:B:450:ILE:HG23	2.01	0.43
5:C:77:GLU:HA	5:C:80:VAL:HG12	2.00	0.43
2:E:222:THR:OG1	2:E:223:GLU:N	2.51	0.43
5:C:434:LEU:HD22	5:C:584:LEU:HD13	2.01	0.43
4:B:342:LYS:HA	4:B:342:LYS:HD3	1.89	0.43
1:D:26:LEU:HA	7:D:901:ATP:C2	2.54	0.43
2:E:213:ARG:HA	2:E:216:ILE:HG22	2.00	0.43
3:A:745:TYR:OH	7:A:1001:ATP:N7	2.44	0.43
5:C:417:LEU:HD12	5:C:418:PRO:HD2	2.01	0.42
1:D:425:GLU:H	1:D:425:GLU:HG2	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:569:PRO:HD2	7:A:1001:ATP:N1	2.34	0.42
5:C:601:THR:HA	5:C:604:ARG:HG2	2.01	0.42
2:E:100:ASN:N	2:E:100:ASN:OD1	2.51	0.42
5:C:121:LEU:HD23	5:C:121:LEU:HA	1.87	0.42
5:C:80:VAL:HA	5:C:83:VAL:HG22	2.00	0.42
5:C:434:LEU:HD23	5:C:434:LEU:HA	1.86	0.42
1:D:49:SER:OG	1:D:168:SER:O	2.35	0.42
2:E:332:ALA:HA	2:E:385:LEU:HD21	2.00	0.42
4:B:395:ASP:HA	4:B:398:THR:HG22	2.02	0.42
1:D:240:ASN:HD22	1:D:240:ASN:HA	1.71	0.42
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.90	0.42
5:C:375:ILE:O	5:C:379:LEU:N	2.44	0.42
5:C:503:ASP:HA	5:C:506:VAL:HG12	2.01	0.42
1:D:111:ASN:ND2	1:D:118:PHE:O	2.53	0.41
3:A:552:LEU:HG	3:A:794:THR:HG23	2.02	0.41
5:C:98:THR:OG1	5:C:238:LEU:O	2.34	0.41
2:E:404:LEU:HD12	4:B:472:PRO:HG2	2.02	0.41
4:B:361:LYS:HA	4:B:364:LEU:HD13	2.02	0.41
1:D:392:ILE:HD13	2:E:287:LEU:HG	2.03	0.41
3:A:596:VAL:HG12	3:A:740:LEU:HB3	2.03	0.41
4:B:430:LEU:HB3	4:B:460:ILE:HG22	2.03	0.41
2:E:279:ILE:HD12	2:E:279:ILE:HA	1.94	0.40
6:F:228:TRP:CZ2	6:F:232:MET:HG3	2.56	0.40
1:D:21:ARG:NH1	1:D:254:ASN:OD1	2.55	0.40
3:A:556:ARG:HE	3:A:794:THR:HG22	1.86	0.40
5:C:211:ASP:HB2	5:C:214:CYS:SG	2.61	0.40
5:C:563:ARG:HD3	5:C:563:ARG:HA	1.79	0.40
2:E:108:LEU:HD23	2:E:108:LEU:HA	1.87	0.40
1:D:222:LEU:HD23	1:D:222:LEU:HA	1.94	0.40
2:E:101:MET:HE2	2:E:101:MET:HB3	1.91	0.40
5:C:367:GLU:O	5:C:367:GLU:HG2	2.21	0.40
5:C:448:LEU:HD12	5:C:448:LEU:HA	1.87	0.40
5:C:603:ARG:O	5:C:607:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	430/462 (93%)	411 (96%)	19 (4%)	0	100	100
2	E	362/460 (79%)	345 (95%)	17 (5%)	0	100	100
3	A	369/488 (76%)	357 (97%)	12 (3%)	0	100	100
4	B	161/618 (26%)	157 (98%)	4 (2%)	0	100	100
5	C	506/721 (70%)	477 (94%)	29 (6%)	0	100	100
6	F	15/257 (6%)	15 (100%)	0	0	100	100
All	All	1843/3006 (61%)	1762 (96%)	81 (4%)	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	D	387/400 (97%)	386 (100%)	1 (0%)	92	95
2	E	328/402 (82%)	328 (100%)	0	100	100
3	A	317/422 (75%)	315 (99%)	2 (1%)	86	92
4	B	148/545 (27%)	147 (99%)	1 (1%)	84	90
5	C	455/636 (72%)	455 (100%)	0	100	100
6	F	13/227 (6%)	13 (100%)	0	100	100
All	All	1648/2632 (63%)	1644 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	95	ASP
3	A	693	ARG
3	A	918	ARG
4	B	441	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	172	GLN
1	D	240	ASN
1	D	243	ASN
2	E	137	ASN
2	E	433	GLN
4	B	382	ASN
4	B	459	ASN
5	C	182	GLN
5	C	615	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
7	ATP	D	901	8	26,33,33	0.90	1 (3%)	31,52,52	1.62	5 (16%)
7	ATP	A	1001	8	26,33,33	0.91	1 (3%)	31,52,52	1.57	6 (19%)
7	ATP	E	901	8	26,33,33	0.91	1 (3%)	31,52,52	1.54	5 (16%)

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
7	ATP	D	901	8	-	0/18/38/38	0/3/3/3
7	ATP	A	1001	8	-	1/18/38/38	0/3/3/3
7	ATP	E	901	8	-	6/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	901	ATP	C5-C4	2.31	1.47	1.40
7	E	901	ATP	C5-C4	2.26	1.46	1.40
7	A	1001	ATP	C5-C4	2.25	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	901	ATP	PB-O3B-PG	-4.12	118.70	132.83
7	D	901	ATP	PA-O3A-PB	-3.83	119.69	132.83
7	E	901	ATP	PA-O3A-PB	-3.58	120.55	132.83
7	A	1001	ATP	C3'-C2'-C1'	3.56	106.33	100.98
7	E	901	ATP	PB-O3B-PG	-3.45	120.99	132.83
7	A	1001	ATP	N3-C2-N1	-3.31	123.51	128.68
7	D	901	ATP	N3-C2-N1	-3.22	123.65	128.68
7	E	901	ATP	N3-C2-N1	-3.17	123.73	128.68
7	A	1001	ATP	PB-O3B-PG	-2.90	122.88	132.83
7	E	901	ATP	C4-C5-N7	-2.61	106.67	109.40
7	A	1001	ATP	PA-O3A-PB	-2.61	123.86	132.83
7	E	901	ATP	C3'-C2'-C1'	2.54	104.81	100.98
7	D	901	ATP	C3'-C2'-C1'	2.51	104.75	100.98
7	A	1001	ATP	C4-C5-N7	-2.36	106.94	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	901	ATP	C4-C5-N7	-2.34	106.96	109.40
7	A	1001	ATP	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

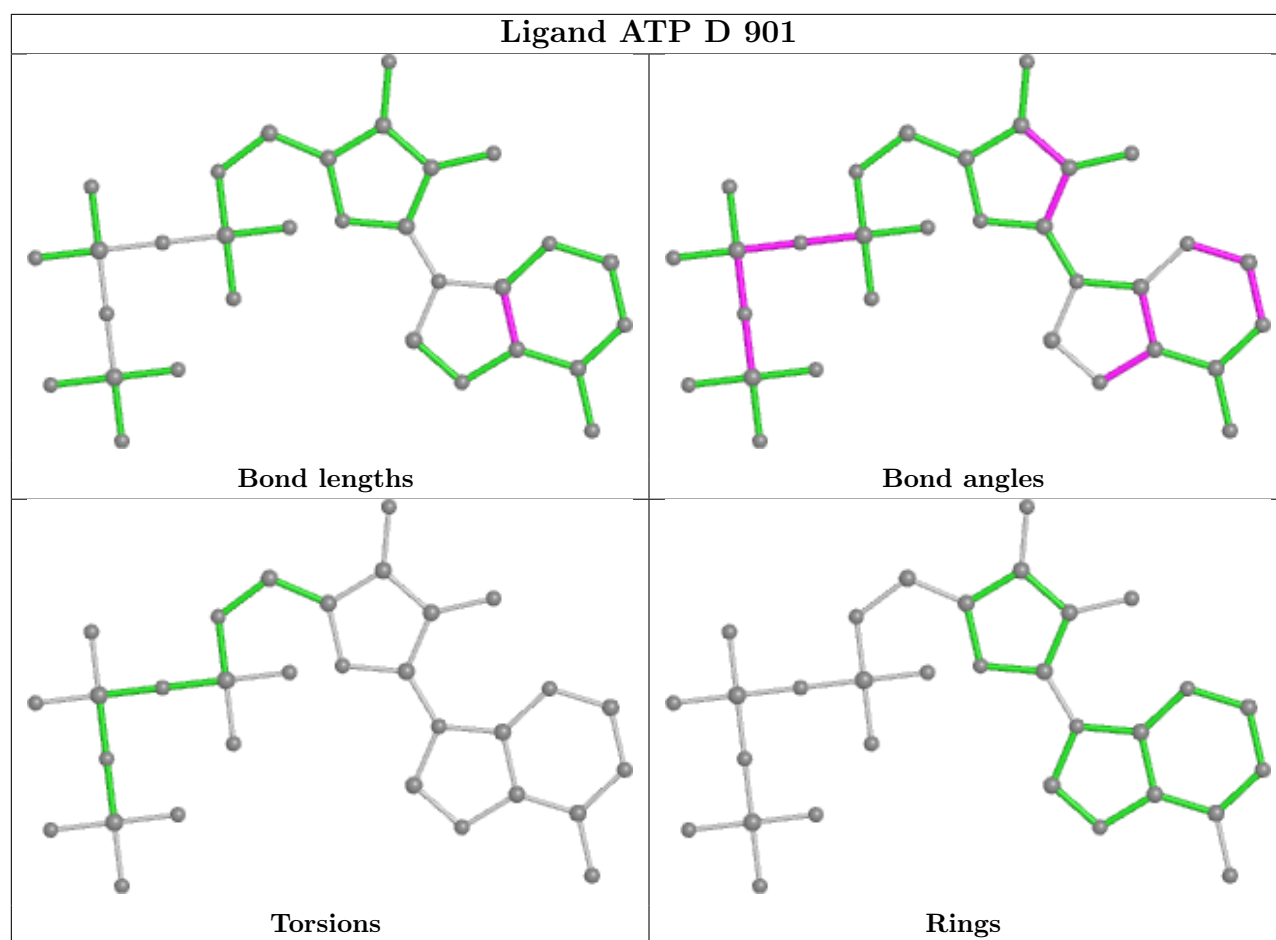
Mol	Chain	Res	Type	Atoms
7	E	901	ATP	C5'-O5'-PA-O2A
7	E	901	ATP	C5'-O5'-PA-O3A
7	E	901	ATP	O4'-C4'-C5'-O5'
7	E	901	ATP	C3'-C4'-C5'-O5'
7	E	901	ATP	PA-O3A-PB-O2B
7	E	901	ATP	PA-O3A-PB-O1B
7	A	1001	ATP	O4'-C4'-C5'-O5'

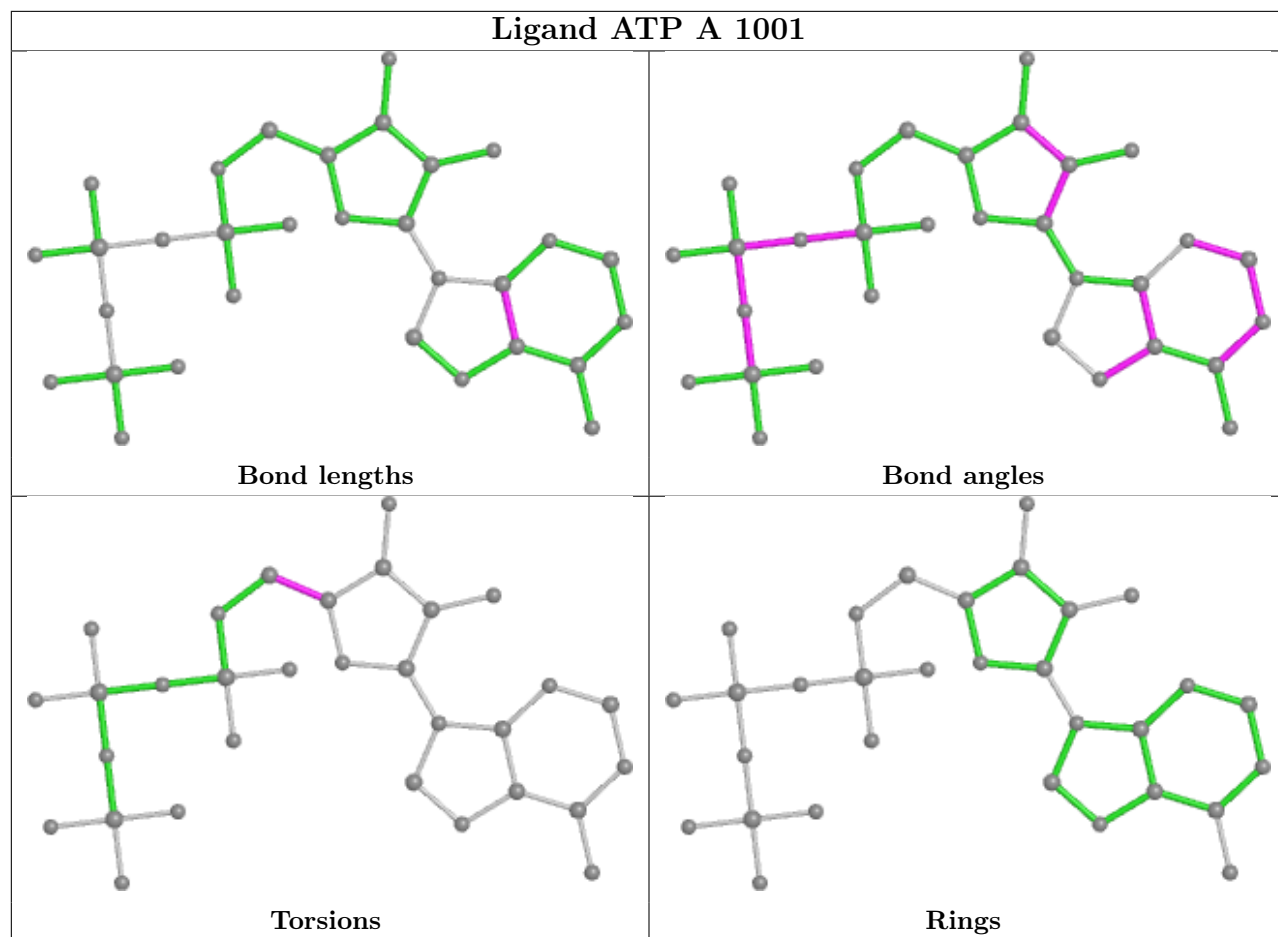
There are no ring outliers.

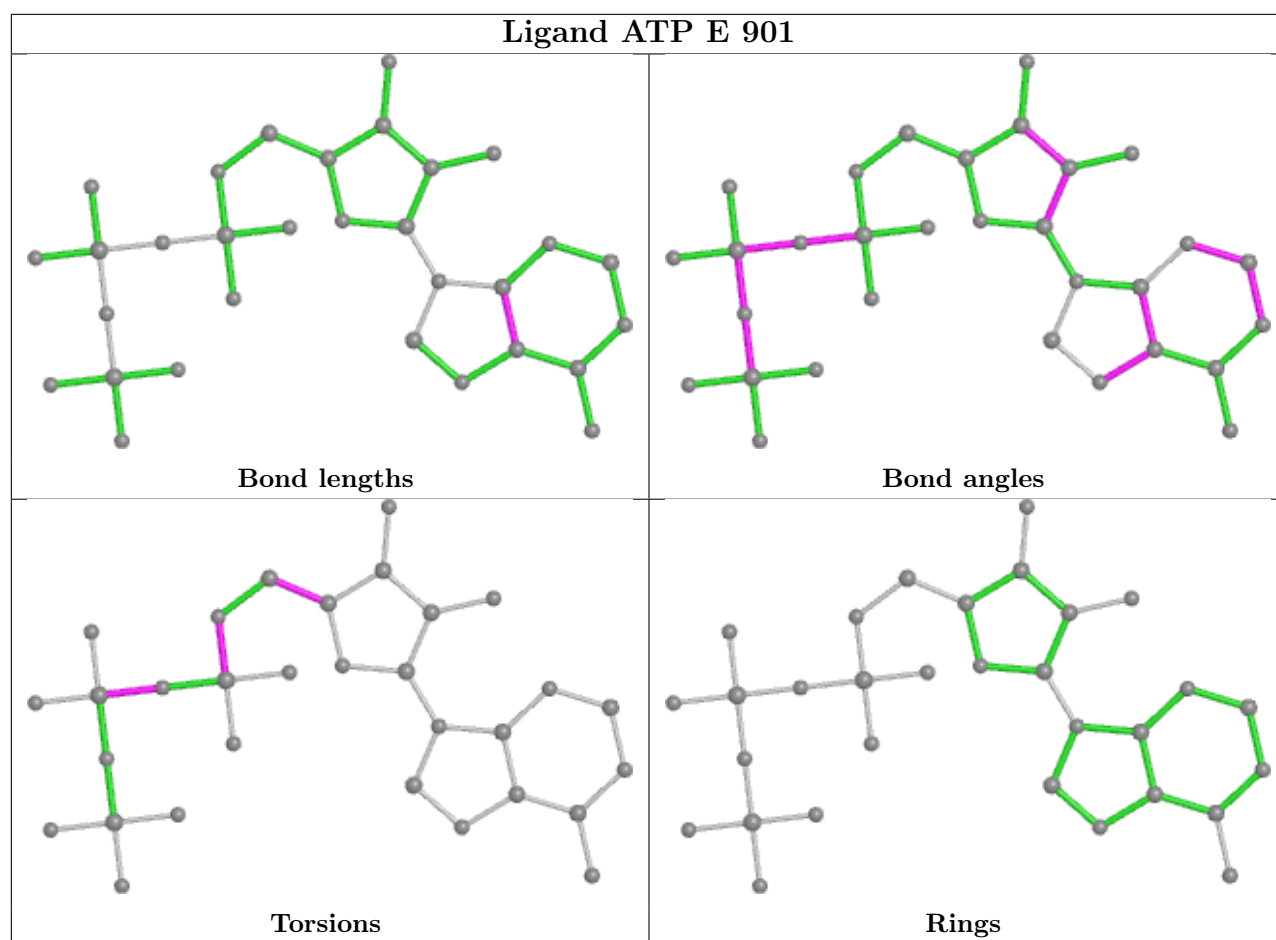
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	901	ATP	5	0
7	A	1001	ATP	5	0
7	E	901	ATP	4	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.







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

This section contains visualisations of the EMDB entry EMD-22363. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.