Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:01 PM JST

PDB ID	:	7BTI / pdb_00007bti
EMDB ID	:	EMD-30179
Title	:	Phalloidin bound F-actin complex
Authors	:	Kumari, A.; Ragunath, V.K.; Sirajuddin, M.
Deposited on	:	2020-04-01
Resolution	:	3.60 Å(reported)
Based on initial model	:	5ONV

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:

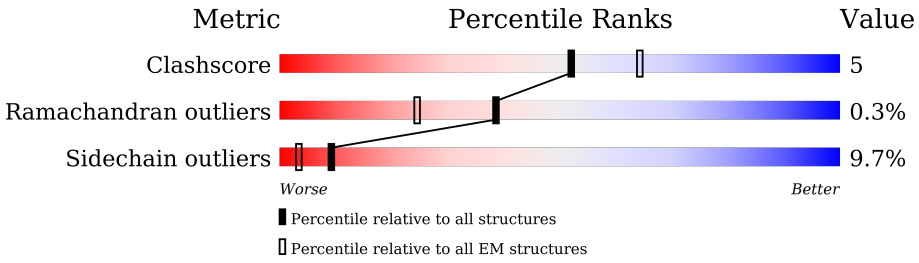
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	377	79% 17%
1	B	377	79% 17%
1	C	377	77% 20%
1	D	377	77% 17%
1	E	377	78% 16%
2	X	7	71% 29%
2	Y	7	43% 57%
2	Z	7	43% 57%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14650 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	366	Total	C	N	O	S	0	0
			2855	1808	483	543	21		
1	B	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		
1	C	369	Total	C	N	O	S	0	0
			2868	1816	485	546	21		
1	D	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		
1	E	366	Total	C	N	O	S	0	0
			2862	1814	484	543	21		

- Molecule 2 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	Y	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	Z	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	

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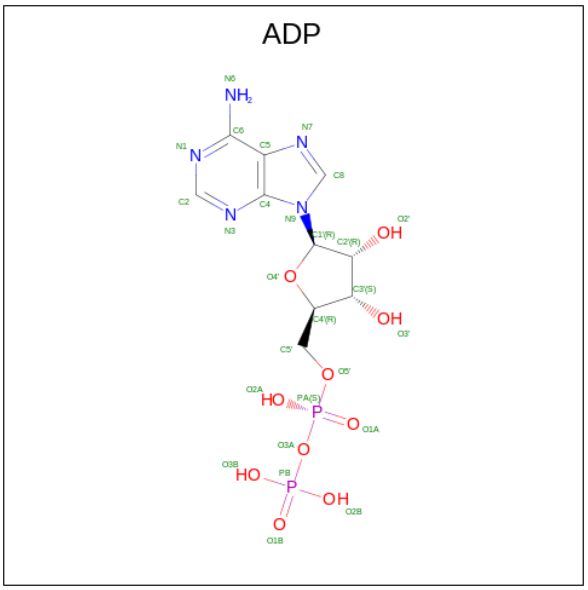
Mol	Chain	Residues	Atoms	AltConf
3	E	1	Total Mg 1 1	0

- 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).



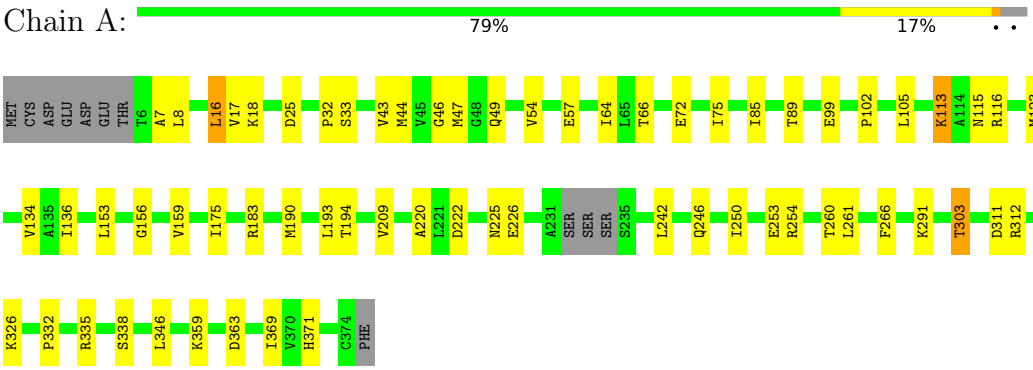
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O P 27 10 5 10 2	0
4	B	1	Total C N O P 27 10 5 10 2	0
4	C	1	Total C N O P 27 10 5 10 2	0
4	D	1	Total C N O P 27 10 5 10 2	0
4	E	1	Total C N O P 27 10 5 10 2	0

3 Residue-property plots (i)

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

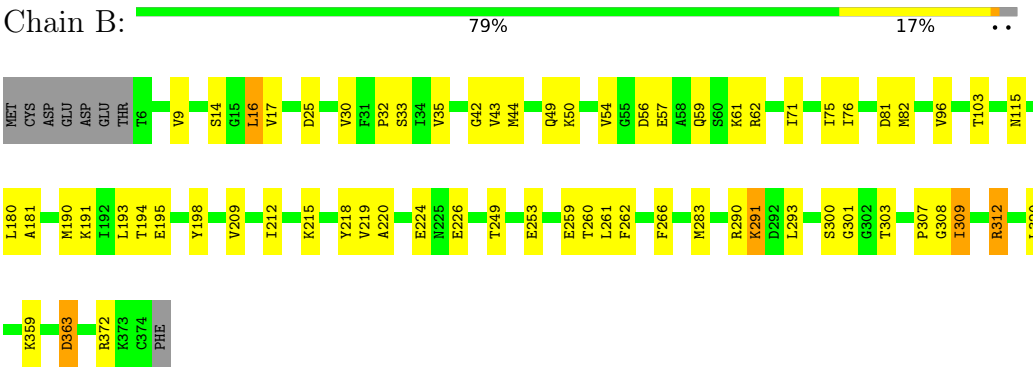
• Molecule 1: Actin, alpha skeletal muscle

Chain A:



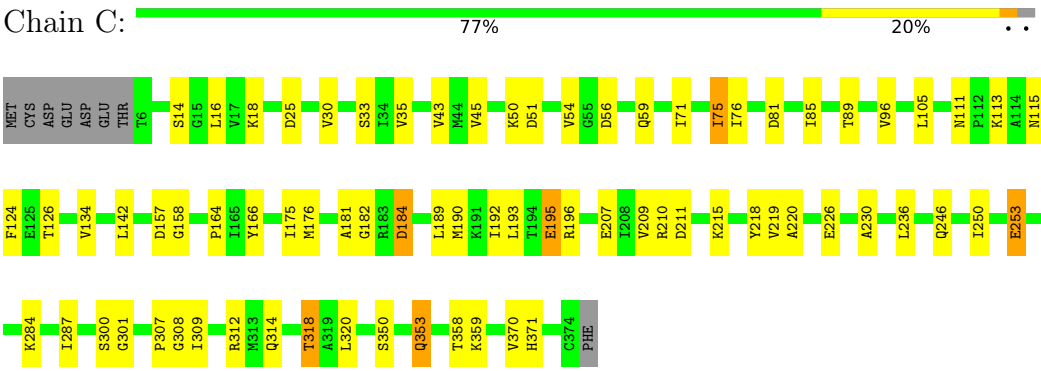
• Molecule 1: Actin, alpha skeletal muscle

Chain B:



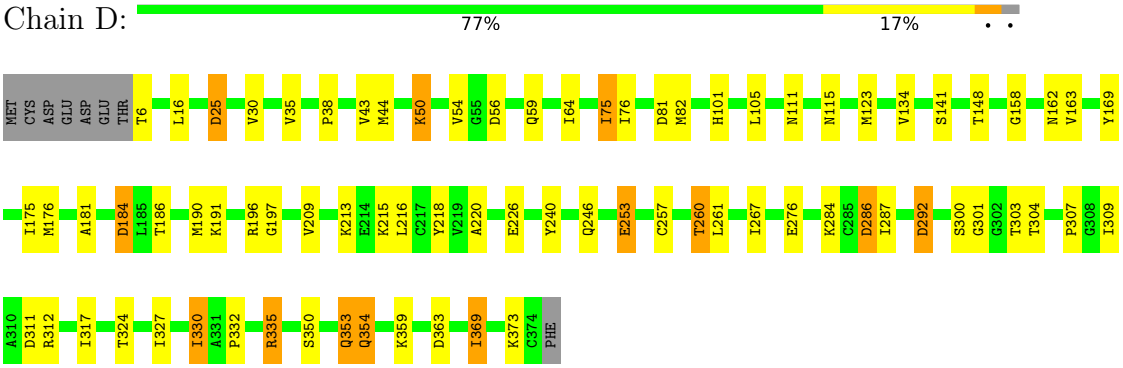
• Molecule 1: Actin, alpha skeletal muscle

Chain C:



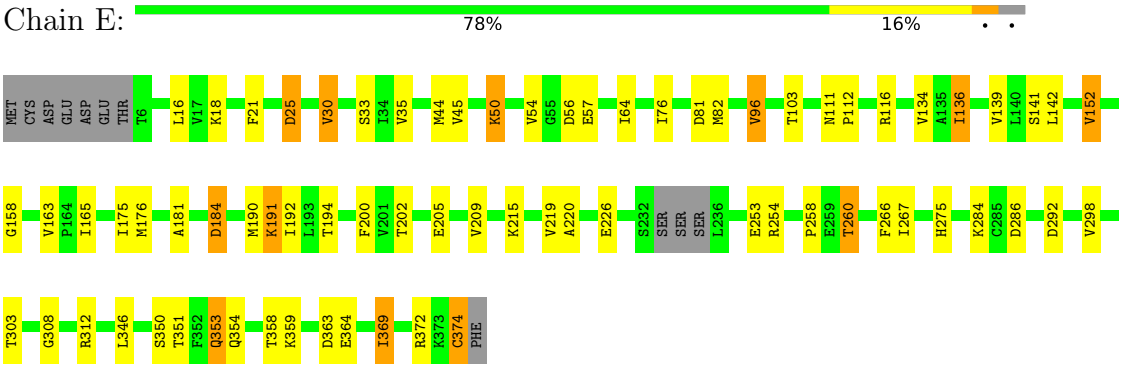
• Molecule 1: Actin, alpha skeletal muscle

Chain D:



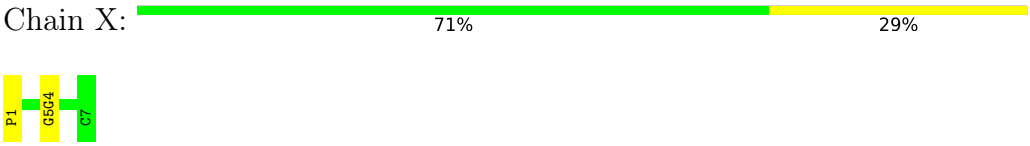
• Molecule 1: Actin, alpha skeletal muscle

Chain E:



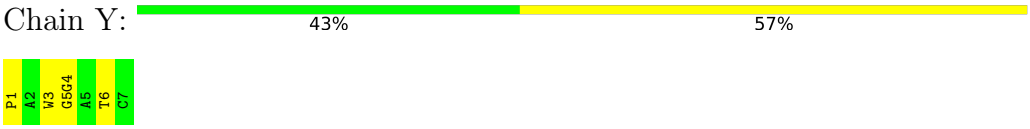
• Molecule 2: Phalloidin

Chain X:



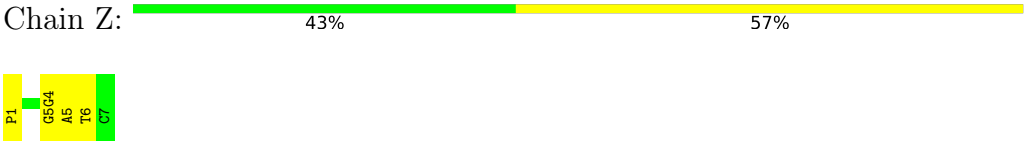
• Molecule 2: Phalloidin

Chain Y:



• Molecule 2: Phalloidin

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-167°, rise=27.89 Å, axial sym=C1	Depositor
Number of segments used	91245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; GCTF for CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (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: G5G, HYP, MG, ADP, ALO

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	0.29	0/2916	0.47	0/3951
1	B	0.31	0/2942	0.48	0/3986
1	C	0.31	0/2930	0.50	0/3972
1	D	0.31	0/2942	0.49	0/3986
1	E	0.31	0/2923	0.50	0/3959
2	X	0.46	0/29	0.45	0/36
2	Y	0.37	0/29	0.40	0/36
2	Z	0.43	0/29	0.38	0/36
All	All	0.31	0/14740	0.49	0/19962

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

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	2855	0	2819	24	0
1	B	2880	0	2855	30	0
1	C	2868	0	2834	35	0
1	D	2880	0	2855	35	0
1	E	2862	0	2839	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	55	0	39	0	0
2	Y	55	0	38	0	0
2	Z	55	0	39	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
All	All	14650	0	14378	150	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 5.

All (150) 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:B:158:GLY:H	1:B:181:ALA:HB3	1.55	0.72
1:E:158:GLY:H	1:E:181:ALA:HB3	1.55	0.71
1:C:219:VAL:HB	1:C:308:GLY:HA3	1.78	0.66
1:E:219:VAL:HB	1:E:308:GLY:HA3	1.78	0.65
1:A:75:ILE:HA	1:A:115:ASN:HD21	1.62	0.64
1:A:105:LEU:HD11	1:A:123:MET:HG3	1.80	0.64
1:E:35:VAL:HG21	1:E:81:ASP:HB2	1.81	0.62
1:C:105:LEU:HD11	1:C:123:MET:HG3	1.85	0.59
1:C:71:ILE:HG12	1:C:76:ILE:HG12	1.83	0.59
1:D:158:GLY:H	1:D:181:ALA:HB3	1.68	0.58
1:B:219:VAL:HB	1:B:308:GLY:HA3	1.86	0.57
1:D:25:ASP:N	1:D:25:ASP:OD1	2.37	0.57
1:E:163:VAL:HA	1:E:175:ILE:HG22	1.85	0.57
1:B:44:MET:HG2	1:D:148:THR:HG22	1.87	0.56
1:C:196:ARG:NE	1:C:253:GLU:OE2	2.37	0.56
1:E:350:SER:O	1:E:353:GLN:NE2	2.39	0.56
1:A:222:ASP:OD2	1:A:225:ASN:ND2	2.39	0.56
1:B:57:GLU:OE2	1:B:61:LYS:NZ	2.40	0.55
1:D:369:ILE:O	1:D:373:LYS:HB2	2.07	0.55
1:C:207:GLU:OE1	1:C:210:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:MET:SD	1:C:284:LYS:NZ	2.79	0.55
1:E:260:THR:HG23	1:E:266:PHE:HB2	1.89	0.55
1:C:211:ASP:OD1	1:C:215:LYS:NZ	2.39	0.55
1:C:184:ASP:N	1:C:184:ASP:OD1	2.41	0.54
1:D:350:SER:O	1:D:353:GLN:NE2	2.41	0.54
1:D:35:VAL:HG21	1:D:81:ASP:HB2	1.89	0.54
1:C:350:SER:O	1:C:353:GLN:NE2	2.40	0.54
1:D:75:ILE:HA	1:D:115:ASN:HD21	1.73	0.53
1:D:359:LYS:NZ	1:D:363:ASP:OD1	2.41	0.53
1:E:200:PHE:HB3	1:E:205:GLU:HB3	1.90	0.53
1:E:359:LYS:NZ	1:E:363:ASP:OD1	2.42	0.53
1:D:286:ASP:N	1:D:286:ASP:OD1	2.42	0.53
1:A:16:LEU:O	1:A:18:LYS:NZ	2.42	0.53
1:E:190:MET:HB3	1:E:209:VAL:HG11	1.90	0.53
1:B:75:ILE:HA	1:B:115:ASN:HD21	1.75	0.52
1:E:25:ASP:N	1:E:25:ASP:OD1	2.39	0.52
1:A:46:GLY:O	1:A:49:GLN:NE2	2.43	0.52
1:C:35:VAL:HG21	1:C:81:ASP:HB2	1.92	0.52
1:D:196:ARG:NH1	1:D:253:GLU:OE2	2.43	0.52
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.92	0.52
1:B:190:MET:HB3	1:B:209:VAL:HG11	1.92	0.51
1:E:116:ARG:NH1	1:E:374:CYS:SG	2.83	0.51
1:B:359:LYS:NZ	1:B:363:ASP:OD2	2.44	0.51
1:D:163:VAL:HA	1:D:175:ILE:HG22	1.92	0.51
1:E:76:ILE:HD13	1:E:82:MET:HG2	1.93	0.51
1:B:16:LEU:HA	1:B:32:PRO:HA	1.93	0.51
1:C:25:ASP:N	1:C:25:ASP:OD1	2.41	0.51
1:C:230:ALA:HB2	1:C:236:LEU:HD22	1.93	0.51
1:E:56:ASP:N	1:E:56:ASP:OD1	2.44	0.50
1:B:198:TYR:HD1	2:Z:5:ALA:HB2	1.75	0.50
1:D:176:MET:SD	1:D:284:LYS:NZ	2.83	0.50
1:B:25:ASP:N	1:B:25:ASP:OD1	2.44	0.50
1:C:158:GLY:H	1:C:181:ALA:HB3	1.76	0.50
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.94	0.50
1:C:157:ASP:H	1:C:182:GLY:H	1.60	0.50
1:D:300:SER:OG	1:D:301:GLY:N	2.44	0.50
1:B:42:GLY:HA2	1:D:169:TYR:HA	1.93	0.49
1:B:283:MET:SD	1:B:290:ARG:NH1	2.85	0.49
1:A:116:ARG:HH21	1:A:136:ILE:HD11	1.77	0.49
1:C:117:GLU:OE2	1:C:371:HIS:NE2	2.44	0.49
1:A:190:MET:HB3	1:A:209:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.93	0.48
1:B:71:ILE:HG12	1:B:76:ILE:HG12	1.94	0.48
1:A:16:LEU:HA	1:A:32:PRO:HA	1.96	0.48
1:C:16:LEU:O	1:C:18:LYS:NZ	2.47	0.48
1:D:197:GLY:HA2	1:E:112:PRO:HG3	1.96	0.48
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.95	0.48
1:C:56:ASP:OD1	1:C:56:ASP:N	2.47	0.47
1:C:81:ASP:N	1:C:81:ASP:OD1	2.41	0.47
1:A:99:GLU:HG3	1:A:128:ASN:HB2	1.95	0.47
1:E:176:MET:SD	1:E:284:LYS:NZ	2.79	0.47
1:C:359:LYS:NZ	1:C:359:LYS:O	2.46	0.47
1:D:324:THR:O	1:D:324:THR:OG1	2.31	0.47
1:A:156:GLY:O	1:A:303:THR:OG1	2.32	0.47
1:B:218:TYR:HA	1:B:307:PRO:HD2	1.97	0.47
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.97	0.46
1:E:184:ASP:N	1:E:184:ASP:OD1	2.47	0.46
1:B:260:THR:HG23	1:B:266:PHE:HB2	1.97	0.46
1:E:136:ILE:HG22	1:E:139:VAL:H	1.80	0.46
1:D:105:LEU:HD11	1:D:123:MET:HG3	1.98	0.46
1:C:189:LEU:HD13	1:C:257:CYS:HB2	1.97	0.46
1:D:220:ALA:HB1	1:D:226:GLU:HG3	1.98	0.46
1:A:85:ILE:O	1:A:89:THR:OG1	2.29	0.45
1:D:304:THR:O	1:D:335:ARG:NH2	2.50	0.45
1:B:259:GLU:OE2	1:B:312:ARG:NH1	2.49	0.45
1:C:219:VAL:HG22	1:C:258:PRO:HB2	1.98	0.45
1:B:209:VAL:HA	1:B:212:ILE:HD12	1.99	0.45
1:C:300:SER:OG	1:C:301:GLY:N	2.50	0.45
1:C:218:TYR:HA	1:C:307:PRO:HD2	1.99	0.45
1:D:215:LYS:HB3	1:D:215:LYS:HE2	1.81	0.44
1:C:195:GLU:H	1:C:195:GLU:HG3	1.58	0.44
1:D:218:TYR:HA	1:D:307:PRO:HD2	1.99	0.44
1:E:142:LEU:HD13	1:E:298:VAL:HG21	2.00	0.44
1:A:113:LYS:HB2	1:A:371:HIS:CE1	2.52	0.44
1:C:85:ILE:O	1:C:89:THR:OG1	2.32	0.44
1:A:17:VAL:HG23	1:A:33:SER:HB2	1.99	0.44
1:A:359:LYS:NZ	1:A:363:ASP:OD1	2.50	0.44
1:A:25:ASP:OD1	1:A:25:ASP:N	2.49	0.44
1:B:76:ILE:HD13	1:B:82:MET:HG2	1.99	0.44
1:B:300:SER:OG	1:B:301:GLY:N	2.51	0.44
1:D:304:THR:HA	1:D:309:ILE:HD13	1.99	0.44
1:E:18:LYS:HG2	1:E:30:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:ILE:HG12	1:E:372:ARG:HH11	1.83	0.44
1:B:35:VAL:HG21	1:B:81:ASP:HB2	2.00	0.44
1:A:7:ALA:HA	1:A:102:PRO:HD2	2.00	0.44
1:D:257:CYS:O	1:D:260:THR:OG1	2.35	0.44
1:E:192:ILE:HD12	1:E:192:ILE:HA	1.85	0.43
1:B:291:LYS:HB3	1:B:291:LYS:HE3	1.82	0.43
1:D:292:ASP:OD1	1:D:292:ASP:N	2.47	0.43
1:E:141:SER:HB2	1:E:152:VAL:HG11	1.99	0.43
1:B:56:ASP:N	1:B:56:ASP:OD1	2.52	0.43
1:A:332:PRO:O	1:A:335:ARG:NH1	2.43	0.43
1:E:21:PHE:HZ	1:E:96:VAL:HG11	1.84	0.43
1:C:314:GLN:O	1:C:318:THR:OG1	2.32	0.43
1:D:184:ASP:OD1	1:D:184:ASP:N	2.52	0.43
1:C:189:LEU:HA	1:C:192:ILE:HG22	2.01	0.42
1:D:216:LEU:HD11	1:D:240:TYR:HB2	2.00	0.42
1:D:186:THR:HG1	1:D:213:LYS:HZ3	1.67	0.42
1:A:242:LEU:N	1:A:246:GLN:O	2.48	0.42
1:E:369:ILE:HG12	1:E:372:ARG:HD2	2.01	0.42
1:B:195:GLU:HG3	1:C:113:LYS:HB3	2.01	0.42
1:C:190:MET:HB3	1:C:209:VAL:HG11	2.02	0.42
1:D:190:MET:HB3	1:D:209:VAL:HG11	2.01	0.42
1:D:330:ILE:HD12	1:D:332:PRO:HD3	2.01	0.41
1:B:220:ALA:HB1	1:B:226:GLU:HG3	2.01	0.41
1:C:192:ILE:HD12	1:C:192:ILE:HA	1.89	0.41
1:D:50:LYS:HE2	1:D:50:LYS:HB3	1.91	0.41
1:B:191:LYS:HE3	1:B:191:LYS:HB3	1.91	0.41
1:D:6:THR:O	1:D:101:HIS:ND1	2.46	0.41
1:D:317:ILE:HG22	1:D:327:ILE:HD13	2.02	0.41
1:E:33:SER:O	1:E:33:SER:OG	2.36	0.41
1:D:287:ILE:H	1:D:287:ILE:HG12	1.66	0.41
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.94	0.41
1:E:191:LYS:HE3	1:E:191:LYS:HB3	1.85	0.41
1:A:335:ARG:HA	1:A:338:SER:HB3	2.02	0.41
1:B:9:VAL:O	1:B:340:TRP:NE1	2.45	0.41
1:E:50:LYS:NZ	1:E:57:GLU:OE2	2.52	0.41
1:C:75:ILE:HA	1:C:115:ASN:HD21	1.86	0.41
1:C:287:ILE:H	1:C:287:ILE:HG12	1.72	0.40
1:D:353:GLN:OE1	1:D:354:GLN:NE2	2.54	0.40
1:A:64:ILE:HD11	1:C:166:TYR:HB3	2.04	0.40
1:A:72:GLU:OE2	1:A:183:ARG:NH1	2.55	0.40
1:B:215:LYS:HE2	1:B:215:LYS:HB3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:HZ	1:B:309:ILE:HG13	1.86	0.40
1:C:164:PRO:HD2	1:C:175:ILE:HG22	2.02	0.40
1:C:220:ALA:HB1	1:C:226:GLU:HG3	2.03	0.40
1:E:215:LYS:HB3	1:E:215:LYS:HE2	1.81	0.40
1:E:220:ALA:HB1	1:E:226:GLU:HG3	2.03	0.40
1:B:17:VAL:HG23	1:B:33:SER:HB3	2.03	0.40
1:E:50:LYS:H	1:E:50:LYS:HG3	1.56	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	362/377 (96%)	343 (95%)	19 (5%)	0	100 100
1	B	367/377 (97%)	349 (95%)	17 (5%)	1 (0%)	37 67
1	C	367/377 (97%)	346 (94%)	19 (5%)	2 (0%)	25 59
1	D	367/377 (97%)	341 (93%)	26 (7%)	0	100 100
1	E	362/377 (96%)	338 (93%)	23 (6%)	1 (0%)	37 67
2	X	3/7 (43%)	1 (33%)	2 (67%)	0	100 100
2	Y	3/7 (43%)	1 (33%)	1 (33%)	1 (33%)	0 0
2	Z	3/7 (43%)	0	3 (100%)	0	100 100
All	All	1834/1906 (96%)	1719 (94%)	110 (6%)	5 (0%)	38 67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	3	TRP
1	C	50	LYS
1	E	50	LYS

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Mol	Chain	Res	Type
1	B	309	ILE
1	C	309	ILE

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	307/320 (96%)	279 (91%)	28 (9%)	7 31
1	B	312/320 (98%)	286 (92%)	26 (8%)	9 34
1	C	309/320 (97%)	281 (91%)	28 (9%)	7 31
1	D	312/320 (98%)	278 (89%)	34 (11%)	5 25
1	E	309/320 (97%)	274 (89%)	35 (11%)	4 24
2	X	2/2 (100%)	2 (100%)	0	100 100
2	Y	2/2 (100%)	2 (100%)	0	100 100
2	Z	2/2 (100%)	2 (100%)	0	100 100
All	All	1555/1606 (97%)	1404 (90%)	151 (10%)	9 29

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	16	LEU
1	A	43	VAL
1	A	44	MET
1	A	47	MET
1	A	54	VAL
1	A	57	GLU
1	A	66	THR
1	A	113	LYS
1	A	134	VAL
1	A	153	LEU
1	A	159	VAL
1	A	175	ILE

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	194	THR
1	A	250	ILE
1	A	253	GLU
1	A	254	ARG
1	A	261	LEU
1	A	291	LYS
1	A	303	THR
1	A	311	ASP
1	A	312	ARG
1	A	315	LYS
1	A	320	LEU
1	A	326	LYS
1	A	346	LEU
1	A	369	ILE
1	B	14	SER
1	B	16	LEU
1	B	30	VAL
1	B	43	VAL
1	B	49	GLN
1	B	50	LYS
1	B	54	VAL
1	B	59	GLN
1	B	62	ARG
1	B	96	VAL
1	B	103	THR
1	B	134	VAL
1	B	180	LEU
1	B	193	LEU
1	B	194	THR
1	B	224	GLU
1	B	249	THR
1	B	253	GLU
1	B	261	LEU
1	B	291	LYS
1	B	303	THR
1	B	312	ARG
1	B	320	LEU
1	B	335	ARG
1	B	363	ASP
1	B	372	ARG
1	C	14	SER

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Mol	Chain	Res	Type
1	C	30	VAL
1	C	33	SER
1	C	43	VAL
1	C	45	VAL
1	C	51	ASP
1	C	54	VAL
1	C	59	GLN
1	C	75	ILE
1	C	96	VAL
1	C	111	ASN
1	C	124	PHE
1	C	126	THR
1	C	134	VAL
1	C	142	LEU
1	C	184	ASP
1	C	193	LEU
1	C	195	GLU
1	C	246	GLN
1	C	250	ILE
1	C	253	GLU
1	C	267	ILE
1	C	312	ARG
1	C	318	THR
1	C	320	LEU
1	C	353	GLN
1	C	358	THR
1	C	370	VAL
1	D	16	LEU
1	D	25	ASP
1	D	30	VAL
1	D	38	PRO
1	D	43	VAL
1	D	44	MET
1	D	50	LYS
1	D	54	VAL
1	D	56	ASP
1	D	59	GLN
1	D	64	ILE
1	D	75	ILE
1	D	111	ASN
1	D	134	VAL
1	D	141	SER

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Mol	Chain	Res	Type
1	D	162	ASN
1	D	184	ASP
1	D	191	LYS
1	D	246	GLN
1	D	253	GLU
1	D	260	THR
1	D	261	LEU
1	D	267	ILE
1	D	276	GLU
1	D	286	ASP
1	D	292	ASP
1	D	303	THR
1	D	311	ASP
1	D	312	ARG
1	D	330	ILE
1	D	335	ARG
1	D	353	GLN
1	D	354	GLN
1	D	369	ILE
1	E	16	LEU
1	E	25	ASP
1	E	30	VAL
1	E	44	MET
1	E	45	VAL
1	E	54	VAL
1	E	64	ILE
1	E	96	VAL
1	E	103	THR
1	E	111	ASN
1	E	134	VAL
1	E	136	ILE
1	E	152	VAL
1	E	165	ILE
1	E	184	ASP
1	E	191	LYS
1	E	194	THR
1	E	202	THR
1	E	253	GLU
1	E	254	ARG
1	E	260	THR
1	E	267	ILE
1	E	275	HIS

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Mol	Chain	Res	Type
1	E	286	ASP
1	E	292	ASP
1	E	303	THR
1	E	312	ARG
1	E	346	LEU
1	E	351	THR
1	E	353	GLN
1	E	354	GLN
1	E	358	THR
1	E	364	GLU
1	E	369	ILE
1	E	374	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	137	GLN
1	A	161	HIS
1	A	354	GLN
1	B	12	ASN
1	B	49	GLN
1	B	111	ASN
1	B	115	ASN
1	B	162	ASN
1	B	246	GLN
1	C	12	ASN
1	C	111	ASN
1	C	115	ASN
1	C	246	GLN
1	C	314	GLN
1	C	360	GLN
1	D	115	ASN
1	D	246	GLN
1	D	314	GLN
1	E	59	GLN
1	E	111	ASN
1	E	314	GLN
1	E	353	GLN
1	E	354	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	ALO	Z	6	2	5,6,7	0.72	0	6,7,9	1.09	1 (16%)
2	ALO	Y	6	2	5,6,7	0.76	0	6,7,9	1.18	1 (16%)
2	G5G	Z	4	2	8,9,10	2.85	2 (25%)	5,12,14	0.82	0
2	HYP	X	1	2	6,8,9	0.87	0	5,10,12	1.79	3 (60%)
2	G5G	X	4	2	8,9,10	2.87	2 (25%)	5,12,14	0.82	0
2	HYP	Z	1	2	6,8,9	0.91	0	5,10,12	1.75	2 (40%)
2	ALO	X	6	2	5,6,7	0.69	0	6,7,9	1.12	0
2	G5G	Y	4	2	8,9,10	2.85	2 (25%)	5,12,14	0.83	0
2	HYP	Y	1	2	6,8,9	0.88	0	5,10,12	1.61	1 (20%)

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
2	ALO	Z	6	2	-	1/5/6/8	-
2	ALO	Y	6	2	-	1/5/6/8	-
2	G5G	Z	4	2	-	8/9/10/12	-
2	HYP	X	1	2	-	0/0/11/13	0/1/1/1
2	G5G	X	4	2	-	8/9/10/12	-
2	HYP	Z	1	2	-	0/0/11/13	0/1/1/1
2	ALO	X	6	2	-	3/5/6/8	-
2	G5G	Y	4	2	-	8/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	Y	1	2	-	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	4	G5G	CA-N	-6.73	1.27	1.48
2	X	4	G5G	CA-N	-6.67	1.28	1.48
2	Z	4	G5G	CA-N	-6.56	1.28	1.48
2	Z	4	G5G	CD2-CG	-3.59	1.48	1.52
2	X	4	G5G	CD2-CG	-3.54	1.48	1.52
2	Y	4	G5G	CD2-CG	-3.47	1.48	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	6	ALO	CB-CA-C	-2.38	107.97	111.77
2	Z	1	HYP	OD1-CG-CB	2.29	115.70	110.03
2	X	1	HYP	OD1-CG-CB	2.24	115.58	110.03
2	Y	1	HYP	OD1-CG-CB	2.24	115.58	110.03
2	Z	1	HYP	O-C-CA	-2.20	119.02	124.78
2	X	1	HYP	CB-CG-CD	-2.08	100.71	103.27
2	Z	6	ALO	CB-CA-C	-2.05	108.51	111.77
2	X	1	HYP	O-C-CA	-2.02	119.48	124.78

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	4	G5G	CA-CB-CG-CD1
2	X	4	G5G	O2-CD1-CG-O1
2	X	4	G5G	O2-CD1-CG-CD2
2	X	4	G5G	N-CA-CB-CG
2	Y	4	G5G	CA-CB-CG-CD1
2	Y	4	G5G	O2-CD1-CG-O1
2	Y	4	G5G	O2-CD1-CG-CD2
2	Y	4	G5G	N-CA-CB-CG
2	Y	4	G5G	C-CA-CB-CG
2	Z	4	G5G	CA-CB-CG-CD1
2	Z	4	G5G	N-CA-CB-CG
2	X	4	G5G	CA-CB-CG-O1
2	Z	4	G5G	CA-CB-CG-O1

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Mol	Chain	Res	Type	Atoms
2	X	4	G5G	CA-CB-CG-CD2
2	Y	4	G5G	CA-CB-CG-CD2
2	Z	4	G5G	CA-CB-CG-CD2
2	Y	4	G5G	CA-CB-CG-O1
2	X	6	ALO	N-CA-CB-CG2
2	X	6	ALO	C-CA-CB-CG2
2	X	4	G5G	C-CA-CB-CG
2	X	4	G5G	O2-CD1-CG-CB
2	Y	4	G5G	O2-CD1-CG-CB
2	Z	4	G5G	O2-CD1-CG-CB
2	Z	4	G5G	O2-CD1-CG-O1
2	Z	4	G5G	O2-CD1-CG-CD2
2	Z	4	G5G	C-CA-CB-CG
2	X	6	ALO	O-C-CA-CB
2	Y	6	ALO	O-C-CA-CB
2	Z	6	ALO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	A	402	3	24,29,29	4.81	10 (41%)	29,45,45	1.82	5 (17%)
4	ADP	C	402	3	24,29,29	4.82	10 (41%)	29,45,45	1.78	5 (17%)
4	ADP	B	402	3	24,29,29	4.79	9 (37%)	29,45,45	1.80	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ADP	E	402	3	24,29,29	4.83	9 (37%)	29,45,45	1.87	5 (17%)
4	ADP	D	402	3	24,29,29	4.84	9 (37%)	29,45,45	1.78	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	402	3	-	5/12/32/32	0/3/3/3
4	ADP	C	402	3	-	5/12/32/32	0/3/3/3
4	ADP	B	402	3	-	5/12/32/32	0/3/3/3
4	ADP	E	402	3	-	3/12/32/32	0/3/3/3
4	ADP	D	402	3	-	3/12/32/32	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	ADP	C2'-C1'	-15.72	1.29	1.53
4	E	402	ADP	C2'-C1'	-15.72	1.29	1.53
4	C	402	ADP	C2'-C1'	-15.62	1.30	1.53
4	A	402	ADP	C2'-C1'	-15.51	1.30	1.53
4	B	402	ADP	C2'-C1'	-15.47	1.30	1.53
4	D	402	ADP	O4'-C1'	14.77	1.61	1.41
4	E	402	ADP	O4'-C1'	14.71	1.61	1.41
4	A	402	ADP	O4'-C1'	14.68	1.61	1.41
4	C	402	ADP	O4'-C1'	14.66	1.61	1.41
4	B	402	ADP	O4'-C1'	14.55	1.61	1.41
4	B	402	ADP	O4'-C4'	-5.79	1.32	1.45
4	D	402	ADP	O4'-C4'	-5.73	1.32	1.45
4	E	402	ADP	O4'-C4'	-5.73	1.32	1.45
4	C	402	ADP	O4'-C4'	-5.69	1.32	1.45
4	A	402	ADP	O4'-C4'	-5.65	1.32	1.45
4	A	402	ADP	O2'-C2'	3.54	1.51	1.43
4	C	402	ADP	O2'-C2'	3.44	1.51	1.43
4	B	402	ADP	O2'-C2'	3.42	1.51	1.43
4	E	402	ADP	O2'-C2'	3.36	1.50	1.43
4	D	402	ADP	O2'-C2'	3.36	1.50	1.43
4	D	402	ADP	C6-N6	3.31	1.46	1.34
4	B	402	ADP	C6-N6	3.29	1.46	1.34
4	C	402	ADP	C6-N6	3.29	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	ADP	C6-N6	3.27	1.46	1.34
4	E	402	ADP	C6-N6	3.26	1.45	1.34
4	E	402	ADP	C5-C4	-2.81	1.33	1.40
4	D	402	ADP	C5-C4	-2.78	1.33	1.40
4	B	402	ADP	C5-C4	-2.77	1.33	1.40
4	A	402	ADP	C5-C4	-2.75	1.33	1.40
4	C	402	ADP	C5-C4	-2.73	1.33	1.40
4	C	402	ADP	PB-O2B	-2.59	1.44	1.54
4	A	402	ADP	PB-O2B	-2.53	1.45	1.54
4	E	402	ADP	O3'-C3'	-2.50	1.37	1.43
4	D	402	ADP	C2-N3	2.49	1.36	1.32
4	A	402	ADP	C2-N3	2.48	1.36	1.32
4	C	402	ADP	O3'-C3'	-2.47	1.37	1.43
4	C	402	ADP	C2-N3	2.45	1.36	1.32
4	B	402	ADP	C2-N3	2.44	1.36	1.32
4	D	402	ADP	O3'-C3'	-2.41	1.37	1.43
4	B	402	ADP	O3'-C3'	-2.41	1.37	1.43
4	A	402	ADP	O3'-C3'	-2.41	1.37	1.43
4	A	402	ADP	PA-O5'	2.35	1.68	1.59
4	E	402	ADP	C2-N3	2.33	1.35	1.32
4	D	402	ADP	PA-O5'	2.29	1.68	1.59
4	B	402	ADP	PA-O5'	2.25	1.68	1.59
4	C	402	ADP	PA-O5'	2.23	1.68	1.59
4	E	402	ADP	PA-O5'	2.21	1.68	1.59

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	402	ADP	N3-C2-N1	-5.59	119.94	128.68
4	A	402	ADP	N3-C2-N1	-5.54	120.01	128.68
4	B	402	ADP	N3-C2-N1	-5.50	120.08	128.68
4	D	402	ADP	N3-C2-N1	-5.48	120.12	128.68
4	C	402	ADP	N3-C2-N1	-5.42	120.20	128.68
4	A	402	ADP	C3'-C2'-C1'	4.27	107.41	100.98
4	E	402	ADP	C5-C6-N6	4.22	126.77	120.35
4	C	402	ADP	C5-C6-N6	4.17	126.69	120.35
4	A	402	ADP	C5-C6-N6	4.09	126.57	120.35
4	D	402	ADP	C5-C6-N6	4.07	126.53	120.35
4	B	402	ADP	C5-C6-N6	4.05	126.51	120.35
4	B	402	ADP	C3'-C2'-C1'	3.95	106.93	100.98
4	C	402	ADP	C3'-C2'-C1'	3.94	106.91	100.98
4	E	402	ADP	PA-O3A-PB	-3.88	119.50	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	402	ADP	C3'-C2'-C1'	3.73	106.59	100.98
4	E	402	ADP	C3'-C2'-C1'	3.50	106.25	100.98
4	B	402	ADP	PA-O3A-PB	-3.27	121.60	132.83
4	D	402	ADP	PA-O3A-PB	-3.13	122.10	132.83
4	C	402	ADP	PA-O3A-PB	-2.91	122.83	132.83
4	A	402	ADP	PA-O3A-PB	-2.84	123.07	132.83
4	E	402	ADP	N6-C6-N1	-2.59	113.19	118.57
4	D	402	ADP	N6-C6-N1	-2.48	113.42	118.57
4	C	402	ADP	N6-C6-N1	-2.48	113.43	118.57
4	A	402	ADP	N6-C6-N1	-2.46	113.47	118.57
4	B	402	ADP	N6-C6-N1	-2.37	113.66	118.57

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	ADP	C5'-O5'-PA-O3A
4	A	402	ADP	C3'-C4'-C5'-O5'
4	B	402	ADP	C5'-O5'-PA-O3A
4	B	402	ADP	C3'-C4'-C5'-O5'
4	C	402	ADP	C5'-O5'-PA-O3A
4	C	402	ADP	C3'-C4'-C5'-O5'
4	D	402	ADP	C5'-O5'-PA-O1A
4	D	402	ADP	C3'-C4'-C5'-O5'
4	E	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C3'-C4'-C5'-O5'
4	A	402	ADP	O4'-C4'-C5'-O5'
4	B	402	ADP	O4'-C4'-C5'-O5'
4	C	402	ADP	O4'-C4'-C5'-O5'
4	D	402	ADP	O4'-C4'-C5'-O5'
4	E	402	ADP	O4'-C4'-C5'-O5'
4	A	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	C5'-O5'-PA-O2A
4	B	402	ADP	C5'-O5'-PA-O1A
4	B	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O1A
4	C	402	ADP	C5'-O5'-PA-O2A

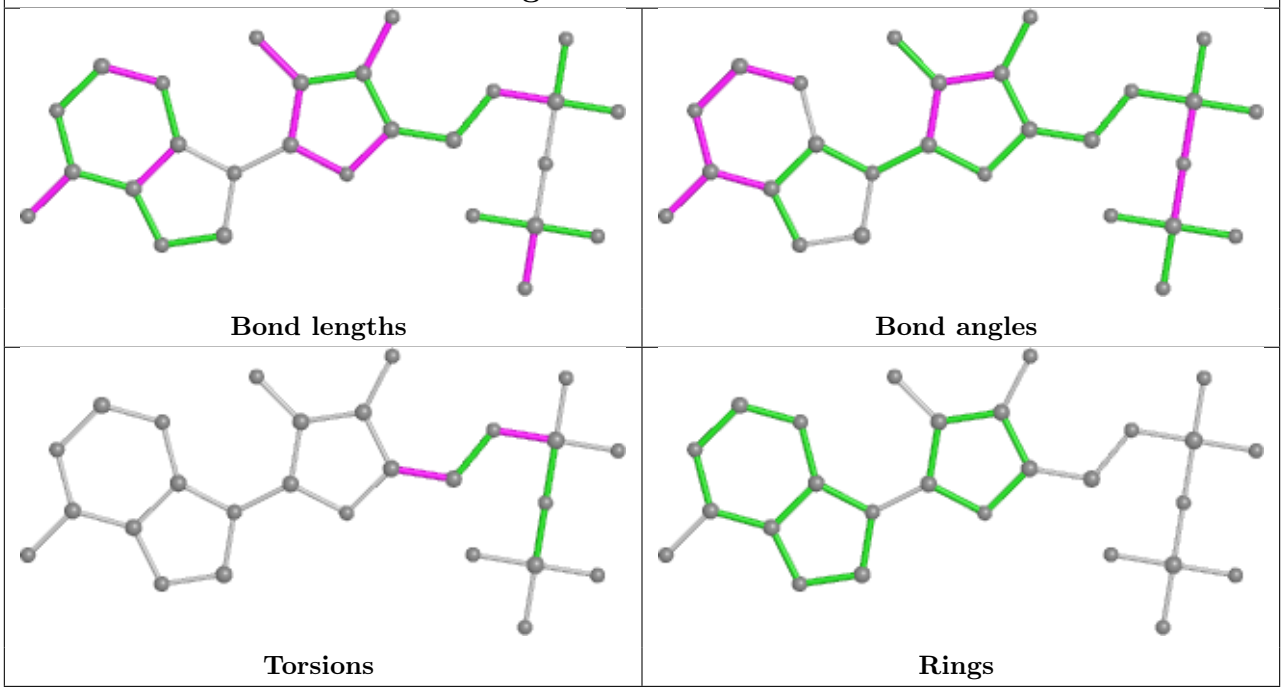
There are no ring outliers.

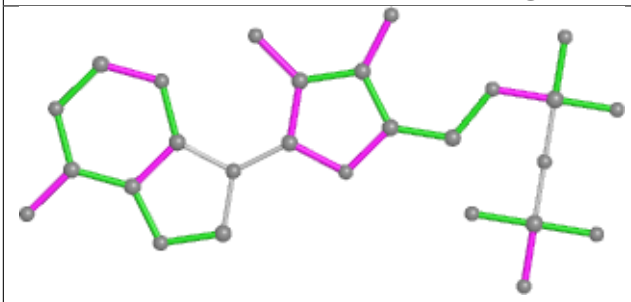
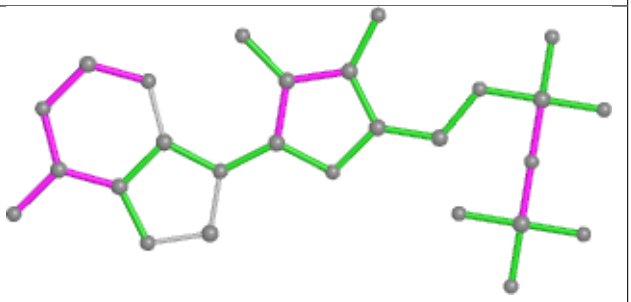
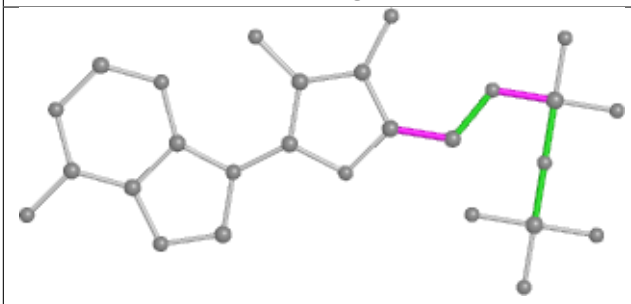
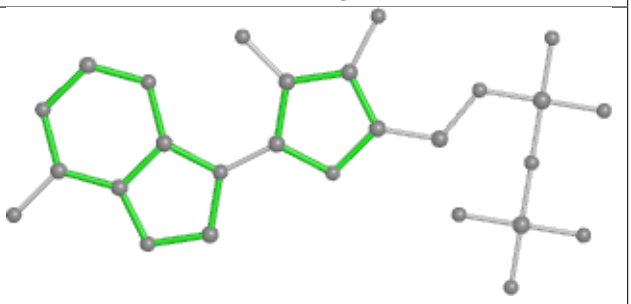
No monomer is involved in short contacts.

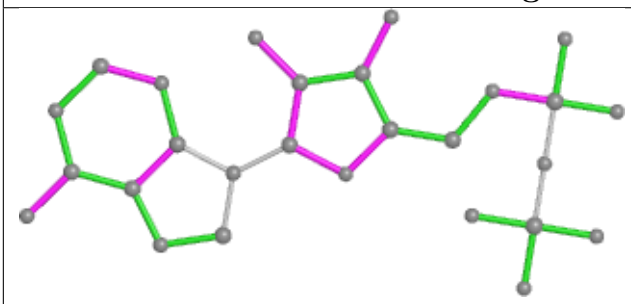
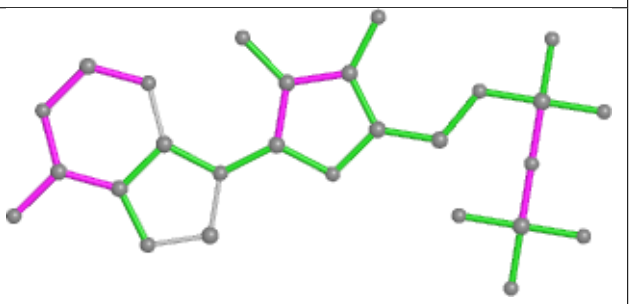
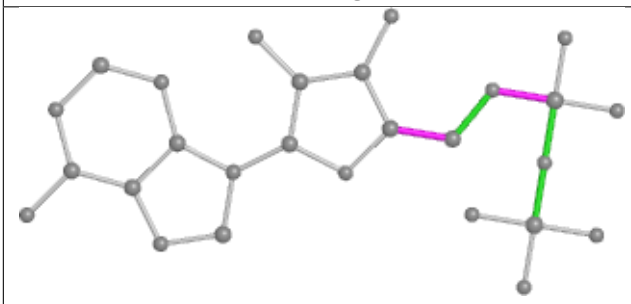
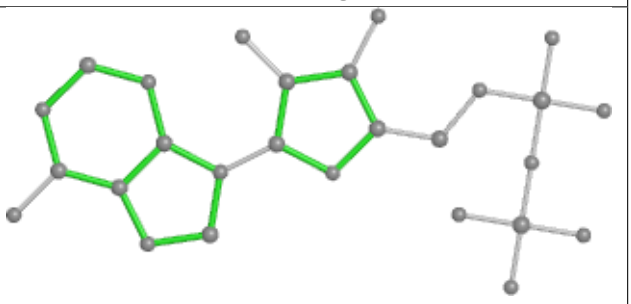
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

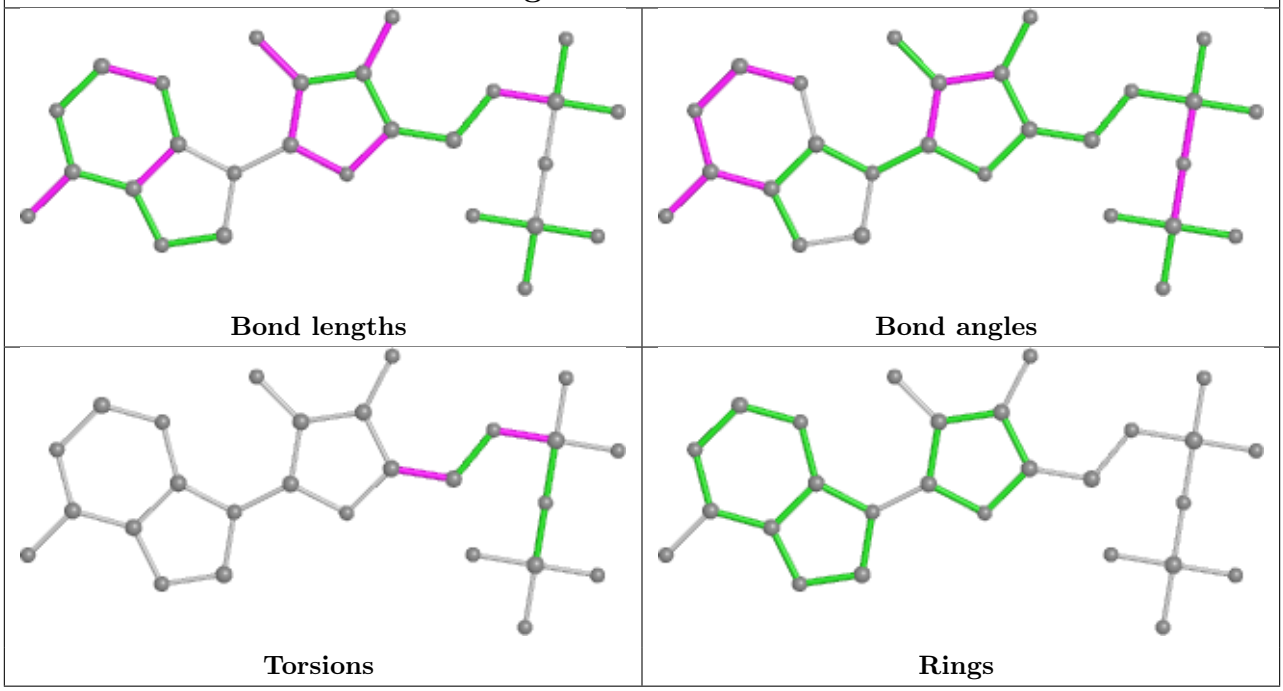
Ligand ADP A 402



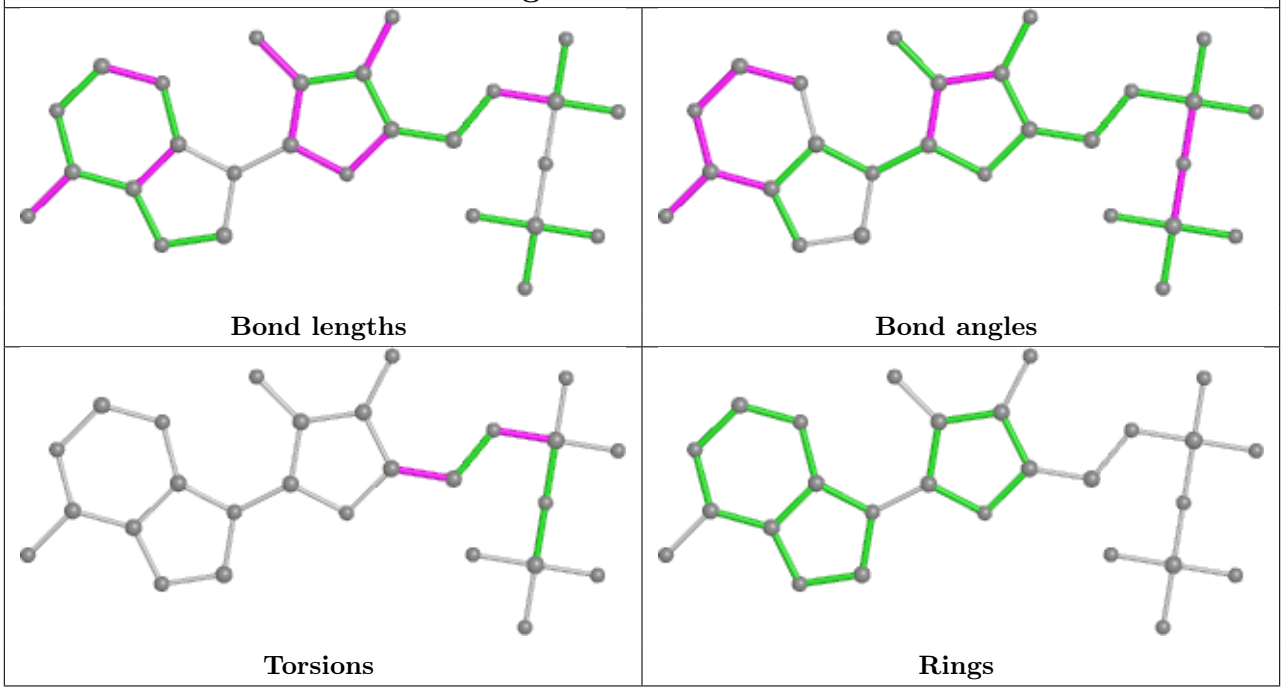
Ligand ADP C 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 402



Ligand ADP D 402



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-30179. 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

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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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 (i)

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

9 Map-model fit

This section was not generated.