



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 27, 2018 – 11:07 am GMT

PDB ID : 6C1G
EMDB ID: : EMD-7330
Title : High-Resolution Cryo-EM Structures of Actin-bound Myosin States Reveal the Mechanism of Myosin Force Sensing
Authors : Menten, A.; Huehn, A.; Liu, X.; Zwolak, A.; Dominguez, R.; Shuman, H.; Ostap, E.M.; Sindelar, C.V.
Deposited on : 2018-01-04
Resolution : 3.80 Å (reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

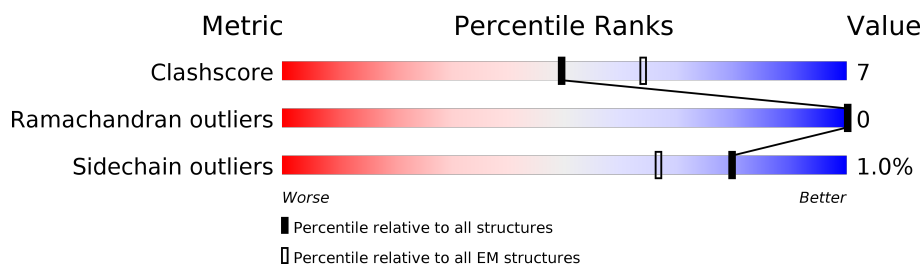
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	P	729	85% 15% .
2	R	148	99% .
3	A	375	81% 18% .
3	B	375	81% 18% .
3	C	375	80% 19% .
3	D	375	82% 17% .
3	E	375	81% 18% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20994 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 Unconventional myosin-Ib.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	729	Total	C	N	O	S	0	0
			5570	3489	987	1073	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	729	GLY	-	expression tag	UNP Q05096
P	730	LEU	-	expression tag	UNP Q05096
P	731	ASN	-	expression tag	UNP Q05096
P	732	ASP	-	expression tag	UNP Q05096
P	733	ILE	-	expression tag	UNP Q05096
P	734	PHE	-	expression tag	UNP Q05096

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	R	148	Total	C	N	O	0	0
			591	296	148	147		

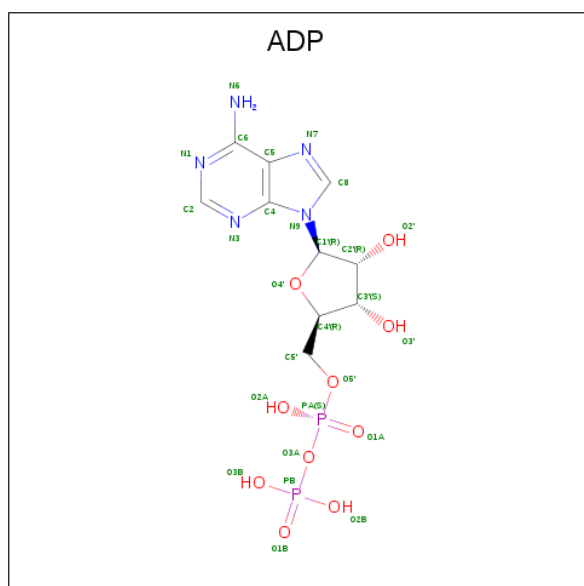
- Molecule 3 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
3	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
3	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
3	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
3	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	P	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0
4	E	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	A	1	Total Mg 1 1	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

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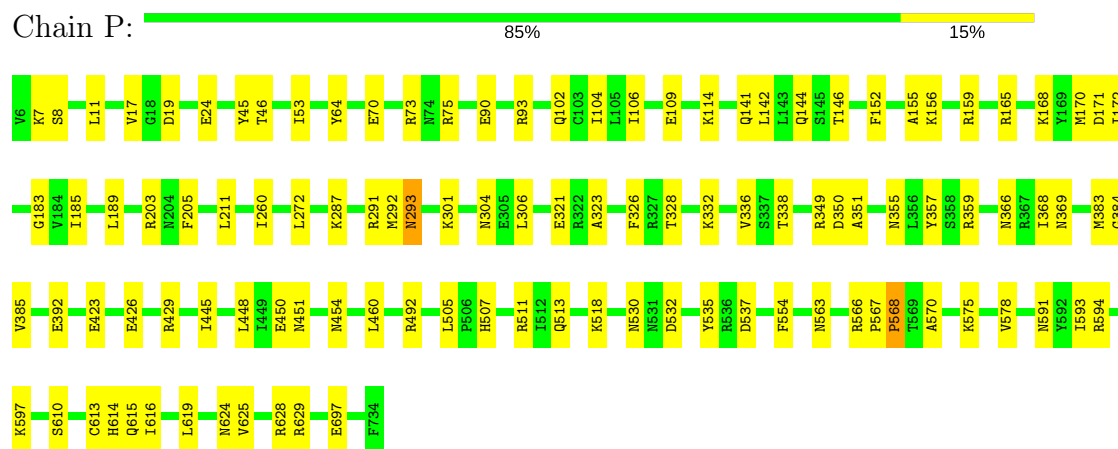
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Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

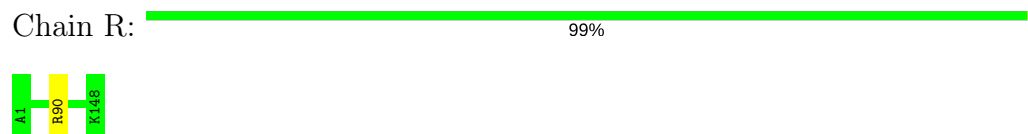
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

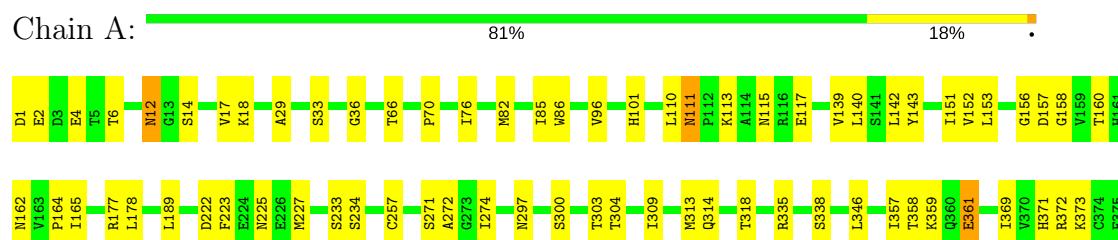
- Molecule 1: Unconventional myosin-Ib



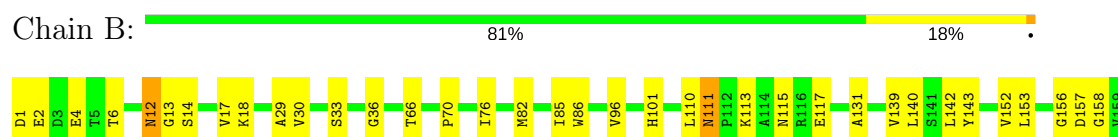
- Molecule 2: Calmodulin



- Molecule 3: Actin, alpha skeletal muscle



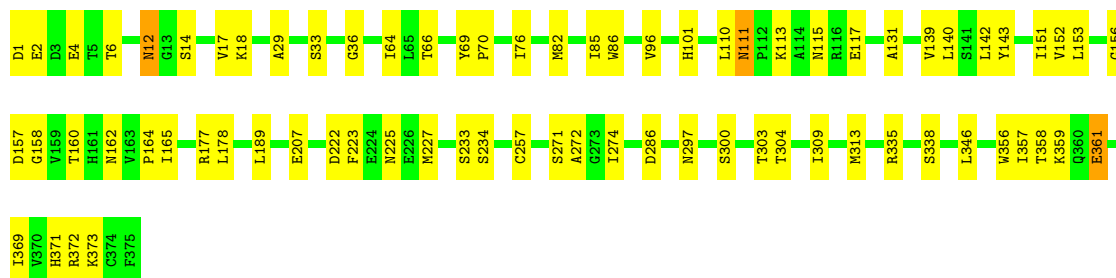
- Molecule 3: Actin, alpha skeletal muscle





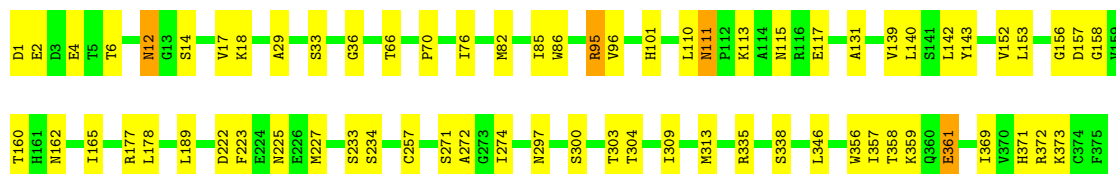
- Molecule 3: Actin, alpha skeletal muscle

Chain C: 80% 19%



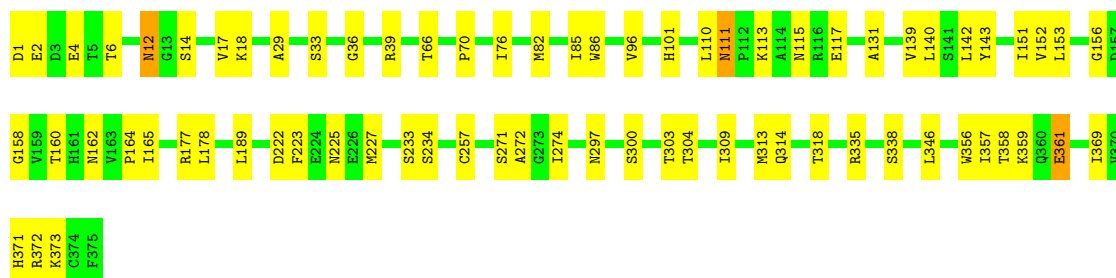
- Molecule 3: Actin, alpha skeletal muscle

Chain D: 82% 17%



- Molecule 3: Actin, alpha skeletal muscle

Chain E: 81% 18%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-167.4°, rise=27.5 Å, axial sym=C1	Depositor
Number of segments used	7700	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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: MG, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	P	0.32	0/5667	0.53	0/7614
2	R	0.25	0/590	0.55	0/736
3	A	0.33	0/2996	0.51	0/4058
3	B	0.33	0/2996	0.51	0/4058
3	C	0.33	0/2996	0.51	0/4058
3	D	0.33	0/2996	0.57	1/4058 (0.0%)
3	E	0.33	0/2996	0.51	0/4058
All	All	0.32	0/21237	0.52	1/28640 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	95	ARG	CG-CD-NE	16.18	145.78	111.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	12	ASN	Peptide
3	A	361	GLU	Peptide
3	B	12	ASN	Peptide
3	B	361	GLU	Peptide
3	C	12	ASN	Peptide
3	C	361	GLU	Peptide
3	D	12	ASN	Peptide
3	D	361	GLU	Peptide
3	E	12	ASN	Peptide
3	E	361	GLU	Peptide
1	P	24	GLU	Peptide

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	P	5570	0	5326	71	0
2	R	591	0	170	1	0
3	A	2933	0	2894	38	0
3	B	2933	0	2894	42	0
3	C	2933	0	2894	43	0
3	D	2933	0	2894	40	0
3	E	2933	0	2894	40	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	P	1	0	0	0	0
5	A	27	0	12	1	0
5	B	27	0	12	4	0
5	C	27	0	12	2	0
5	D	27	0	12	2	0
5	E	27	0	12	0	0
5	P	27	0	12	0	0
All	All	20994	0	20038	270	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 7.

All (270) 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:P:142:LEU:HD21	1:P:170:MET:SD	1.46	1.53
1:P:142:LEU:CD2	1:P:170:MET:SD	2.01	1.45
1:P:142:LEU:CD1	1:P:170:MET:SD	2.48	1.02
1:P:142:LEU:HD22	1:P:170:MET:SD	1.99	0.98
1:P:142:LEU:HD11	1:P:170:MET:SD	2.06	0.96
3:B:13:GLY:HA3	5:B:401:ADP:O1B	1.74	0.87
1:P:142:LEU:CG	1:P:170:MET:SD	2.71	0.79
1:P:142:LEU:HD21	1:P:170:MET:CE	2.12	0.78
1:P:326:PHE:HA	1:P:338:THR:O	1.86	0.74
1:P:597:LYS:HB3	1:P:615:GLN:HE22	1.53	0.73
1:P:328:THR:HA	1:P:336:VAL:O	1.88	0.73
1:P:104:ILE:HA	1:P:591:ASN:O	1.97	0.64
3:E:223:PHE:O	3:E:227:MET:HB2	1.97	0.64
3:C:223:PHE:O	3:C:227:MET:HB2	1.97	0.64
3:D:223:PHE:O	3:D:227:MET:HB2	1.97	0.64
3:B:223:PHE:O	3:B:227:MET:HB2	1.97	0.63
1:P:172:ILE:HB	1:P:383:MET:O	1.98	0.63
3:A:223:PHE:O	3:A:227:MET:HB2	1.97	0.63
3:A:36:GLY:HA2	3:A:66:THR:O	1.99	0.63
1:P:170:MET:HE2	1:P:385:VAL:HG23	1.80	0.63
3:C:36:GLY:HA2	3:C:66:THR:O	1.99	0.63
3:D:36:GLY:HA2	3:D:66:THR:O	1.99	0.63
3:B:359:LYS:O	3:B:361:GLU:N	2.32	0.63
3:B:36:GLY:HA2	3:B:66:THR:O	1.99	0.62
3:E:36:GLY:HA2	3:E:66:THR:O	1.99	0.62
1:P:70:GLU:HG2	1:P:73:ARG:HH12	1.64	0.62
3:A:359:LYS:O	3:A:361:GLU:N	2.32	0.61
1:P:8:SER:OG	1:P:75:ARG:NH2	2.34	0.61
3:C:359:LYS:O	3:C:361:GLU:N	2.32	0.60
3:E:359:LYS:O	3:E:361:GLU:N	2.32	0.60
1:P:165:ARG:NH2	1:P:392:GLU:OE2	2.34	0.60
1:P:594:ARG:HD2	1:P:619:LEU:HD23	1.84	0.60
3:D:359:LYS:O	3:D:361:GLU:N	2.32	0.59
1:P:170:MET:HE3	1:P:385:VAL:HG21	1.84	0.59
3:D:357:ILE:HG12	3:D:373:LYS:HE3	1.85	0.58
3:B:357:ILE:HG12	3:B:373:LYS:HE3	1.86	0.58
1:P:610:SER:O	1:P:614:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:369:ILE:HD12	3:E:372:ARG:HD2	1.87	0.57
3:A:369:ILE:HD12	3:A:372:ARG:HD2	1.87	0.57
3:C:369:ILE:HD12	3:C:372:ARG:HD2	1.87	0.57
3:E:357:ILE:HG12	3:E:373:LYS:HE3	1.85	0.57
3:B:369:ILE:HD12	3:B:372:ARG:HD2	1.87	0.57
3:C:17:VAL:HG23	3:C:33:SER:HB2	1.87	0.57
3:A:17:VAL:HG23	3:A:33:SER:HB2	1.87	0.57
3:A:357:ILE:HG12	3:A:373:LYS:HE3	1.85	0.57
3:B:17:VAL:HG23	3:B:33:SER:HB2	1.87	0.57
1:P:46:THR:O	1:P:53:ILE:HB	2.05	0.57
3:D:17:VAL:HG23	3:D:33:SER:HB2	1.87	0.57
3:D:152:VAL:O	3:D:162:ASN:HA	2.05	0.56
3:D:369:ILE:HD12	3:D:372:ARG:HD2	1.87	0.56
3:E:17:VAL:HG23	3:E:33:SER:HB2	1.87	0.56
3:A:6:THR:O	3:A:101:HIS:ND1	2.35	0.56
3:C:357:ILE:HG12	3:C:373:LYS:HE3	1.86	0.56
1:P:141:GLN:HE21	1:P:368:ILE:HG23	1.71	0.56
3:A:304:THR:O	3:A:335:ARG:NH2	2.39	0.56
1:P:171:ASP:O	1:P:183:GLY:CA	2.54	0.56
1:P:211:LEU:HD13	1:P:272:LEU:HD22	1.87	0.56
3:C:304:THR:O	3:C:335:ARG:NH2	2.39	0.56
1:P:625:VAL:O	1:P:629:ARG:HB2	2.07	0.56
3:D:304:THR:O	3:D:335:ARG:NH2	2.39	0.55
3:B:304:THR:O	3:B:335:ARG:NH2	2.39	0.55
3:E:304:THR:O	3:E:335:ARG:NH2	2.39	0.55
1:P:7:LYS:NZ	2:R:90:ARG:O	2.38	0.55
3:A:152:VAL:O	3:A:162:ASN:HA	2.05	0.55
3:E:152:VAL:O	3:E:162:ASN:HA	2.06	0.55
3:C:152:VAL:O	3:C:162:ASN:HA	2.05	0.55
1:P:349:ARG:NH1	1:P:350:ASP:OD1	2.40	0.55
3:B:152:VAL:O	3:B:162:ASN:HA	2.05	0.55
1:P:170:MET:CE	1:P:385:VAL:CG2	2.84	0.55
3:A:157:ASP:OD1	5:A:401:ADP:O3'	2.25	0.54
1:P:566:ARG:HB3	1:P:568:PRO:HD2	1.88	0.54
1:P:513:GLN:HG2	1:P:518:LYS:HG2	1.90	0.54
3:A:222:ASP:OD2	3:A:225:ASN:ND2	2.41	0.54
3:E:222:ASP:OD2	3:E:225:ASN:ND2	2.41	0.54
3:C:6:THR:O	3:C:101:HIS:ND1	2.36	0.54
3:D:222:ASP:OD2	3:D:225:ASN:ND2	2.41	0.54
1:P:171:ASP:O	1:P:183:GLY:HA2	2.07	0.54
3:B:222:ASP:OD2	3:B:225:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:18:LYS:NZ	5:B:401:ADP:O3B	2.41	0.54
1:P:142:LEU:HD13	1:P:170:MET:SD	2.46	0.53
1:P:170:MET:HE3	1:P:385:VAL:CG2	2.38	0.53
3:C:222:ASP:OD2	3:C:225:ASN:ND2	2.41	0.53
1:P:323:ALA:O	1:P:535:TYR:OH	2.23	0.53
1:P:613:CYS:HA	1:P:616:ILE:HD12	1.91	0.53
1:P:170:MET:O	1:P:384:GLY:HA2	2.09	0.52
1:P:291:ARG:HD2	1:P:292:MET:HA	1.91	0.52
3:E:300:SER:HA	3:E:335:ARG:HG2	1.92	0.52
1:P:532:ASP:HB2	1:P:570:ALA:HB2	1.90	0.52
3:C:300:SER:HA	3:C:335:ARG:HG2	1.92	0.52
1:P:45:TYR:OH	1:P:64:TYR:OH	2.25	0.52
1:P:451:ASN:ND2	1:P:454:ASN:OD1	2.43	0.52
3:A:300:SER:HA	3:A:335:ARG:HG2	1.92	0.52
3:B:110:LEU:O	3:B:177:ARG:NH1	2.43	0.52
3:B:6:THR:O	3:B:101:HIS:ND1	2.35	0.52
1:P:423:GLU:OE2	1:P:628:ARG:NH1	2.42	0.51
3:D:110:LEU:O	3:D:177:ARG:NH1	2.43	0.51
3:E:358:THR:OG1	3:E:359:LYS:N	2.44	0.51
3:C:358:THR:OG1	3:C:359:LYS:N	2.44	0.51
3:D:300:SER:HA	3:D:335:ARG:HG2	1.92	0.51
1:P:507:HIS:HB2	3:D:95:ARG:HH21	1.76	0.51
3:B:358:THR:OG1	3:B:359:LYS:N	2.44	0.51
1:P:332:LYS:HD2	3:B:30:VAL:H	1.75	0.51
3:B:300:SER:HA	3:B:335:ARG:HG2	1.92	0.51
3:C:2:GLU:HG3	3:C:4:GLU:H	1.76	0.51
3:B:2:GLU:HG3	3:B:4:GLU:H	1.76	0.50
3:A:358:THR:OG1	3:A:359:LYS:N	2.44	0.50
3:D:6:THR:O	3:D:101:HIS:ND1	2.36	0.50
1:P:351:ALA:O	1:P:355:ASN:HB2	2.11	0.50
1:P:535:TYR:HE2	1:P:537:ASP:HB2	1.76	0.50
3:E:2:GLU:HG3	3:E:4:GLU:H	1.76	0.50
3:A:2:GLU:HG3	3:A:4:GLU:H	1.76	0.50
3:B:113:LYS:NZ	3:B:117:GLU:OE2	2.39	0.50
3:D:358:THR:OG1	3:D:359:LYS:N	2.44	0.50
3:D:2:GLU:HG3	3:D:4:GLU:H	1.76	0.50
3:C:110:LEU:O	3:C:177:ARG:NH1	2.43	0.50
3:C:76:ILE:HD13	3:C:82:MET:HG2	1.94	0.50
3:E:6:THR:O	3:E:101:HIS:ND1	2.36	0.50
3:A:110:LEU:O	3:A:177:ARG:NH1	2.43	0.49
3:E:110:LEU:O	3:E:177:ARG:NH1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:76:ILE:HD13	3:A:82:MET:HG2	1.94	0.49
3:C:113:LYS:NZ	3:C:117:GLU:OE2	2.39	0.49
3:E:76:ILE:HD13	3:E:82:MET:HG2	1.94	0.49
1:P:17:VAL:HG12	1:P:19:ASP:H	1.78	0.49
3:D:12:ASN:HD22	3:D:86:TRP:HE1	1.61	0.49
3:C:12:ASN:HD22	3:C:86:TRP:HE1	1.61	0.49
3:A:12:ASN:HD22	3:A:86:TRP:HE1	1.61	0.49
3:C:157:ASP:OD1	5:C:401:ADP:O3'	2.31	0.49
3:A:189:LEU:HD13	3:A:257:CYS:HB2	1.95	0.48
3:D:189:LEU:HD13	3:D:257:CYS:HB2	1.95	0.48
3:E:189:LEU:HD13	3:E:257:CYS:HB2	1.95	0.48
3:B:76:ILE:HD13	3:B:82:MET:HG2	1.94	0.48
1:P:144:GLN:HG3	1:P:260:ILE:HG21	1.96	0.48
1:P:156:LYS:HB3	1:P:203:ARG:HB3	1.94	0.48
3:B:12:ASN:HD22	3:B:86:TRP:HE1	1.61	0.48
3:B:189:LEU:HD13	3:B:257:CYS:HB2	1.95	0.48
3:E:142:LEU:HB2	3:E:152:VAL:HG21	1.95	0.48
3:A:300:SER:O	3:A:338:SER:OG	2.32	0.48
3:B:300:SER:O	3:B:338:SER:OG	2.32	0.48
3:E:12:ASN:HD22	3:E:86:TRP:HE1	1.61	0.48
3:D:157:ASP:OD1	5:D:401:ADP:O3'	2.32	0.47
3:E:300:SER:O	3:E:338:SER:OG	2.32	0.47
3:C:142:LEU:HB2	3:C:152:VAL:HG21	1.95	0.47
3:C:300:SER:O	3:C:338:SER:OG	2.32	0.47
3:D:76:ILE:HD13	3:D:82:MET:HG2	1.94	0.47
1:P:146:THR:HG23	1:P:168:LYS:NZ	2.29	0.47
3:A:153:LEU:HD13	3:A:274:ILE:HD11	1.96	0.47
3:D:153:LEU:HD13	3:D:274:ILE:HD11	1.97	0.47
3:C:189:LEU:HD13	3:C:257:CYS:HB2	1.95	0.47
1:P:185:ILE:O	1:P:369:ASN:ND2	2.45	0.47
3:B:157:ASP:HB2	5:B:401:ADP:H4'	1.97	0.47
3:B:153:LEU:HD13	3:B:274:ILE:HD11	1.97	0.47
3:C:153:LEU:HD13	3:C:274:ILE:HD11	1.97	0.47
3:D:142:LEU:HB2	3:D:152:VAL:HG21	1.95	0.47
1:P:511:ARG:HD3	1:P:518:LYS:HB3	1.96	0.47
3:A:139:VAL:HG22	3:A:165:ILE:HD11	1.97	0.47
3:A:142:LEU:HB2	3:A:152:VAL:HG21	1.95	0.47
3:B:142:LEU:HB2	3:B:152:VAL:HG21	1.95	0.47
3:E:139:VAL:HG22	3:E:165:ILE:HD11	1.97	0.47
3:D:113:LYS:NZ	3:D:117:GLU:OE2	2.39	0.46
3:E:153:LEU:HD13	3:E:274:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:GLN:O	1:P:383:MET:HA	2.16	0.46
3:D:300:SER:O	3:D:338:SER:OG	2.32	0.46
1:P:492:ARG:HB2	1:P:505:LEU:HD22	1.96	0.46
3:E:113:LYS:NZ	3:E:117:GLU:OE2	2.39	0.46
1:P:306:LEU:HD21	1:P:321:GLU:HB2	1.96	0.46
3:C:139:VAL:HG22	3:C:165:ILE:HD11	1.97	0.46
3:C:233:SER:OG	3:C:234:SER:N	2.49	0.46
3:D:233:SER:OG	3:D:234:SER:N	2.49	0.45
3:E:14:SER:OG	3:E:158:GLY:N	2.49	0.45
3:E:233:SER:OG	3:E:234:SER:N	2.49	0.45
3:B:139:VAL:HG22	3:B:165:ILE:HD11	1.97	0.45
3:B:309:ILE:O	3:B:313:MET:HB2	2.17	0.45
3:B:14:SER:OG	3:B:158:GLY:N	2.49	0.45
1:P:109:GLU:OE2	1:P:159:ARG:NH1	2.44	0.45
1:P:109:GLU:O	1:P:114:LYS:NZ	2.50	0.45
3:A:309:ILE:O	3:A:313:MET:HB2	2.17	0.45
3:C:18:LYS:HA	3:C:29:ALA:O	2.17	0.45
3:D:14:SER:OG	3:D:158:GLY:N	2.49	0.45
1:P:90:GLU:OE1	1:P:93:ARG:NH2	2.49	0.45
3:A:18:LYS:HA	3:A:29:ALA:O	2.17	0.45
3:C:69:TYR:OH	3:C:207:GLU:OE2	2.31	0.45
3:E:309:ILE:O	3:E:313:MET:HB2	2.17	0.45
1:P:152:PHE:O	1:P:357:TYR:OH	2.35	0.45
3:A:14:SER:OG	3:A:158:GLY:N	2.49	0.45
3:B:18:LYS:HA	3:B:29:ALA:O	2.17	0.45
3:D:309:ILE:O	3:D:313:MET:HB2	2.17	0.45
3:B:233:SER:OG	3:B:234:SER:N	2.49	0.45
1:P:287:LYS:HD3	1:P:301:LYS:HG2	1.99	0.45
1:P:359:ARG:HD2	1:P:554:PHE:HE1	1.81	0.45
3:A:233:SER:OG	3:A:234:SER:N	2.49	0.45
3:E:18:LYS:HA	3:E:29:ALA:O	2.17	0.45
3:A:113:LYS:NZ	3:A:117:GLU:OE2	2.39	0.45
3:D:139:VAL:HG22	3:D:165:ILE:HD11	1.97	0.45
3:C:286:ASP:OD2	3:E:39:ARG:NH2	2.50	0.45
3:C:14:SER:OG	3:C:158:GLY:N	2.49	0.44
3:D:18:LYS:HA	3:D:29:ALA:O	2.17	0.44
3:C:111:ASN:HD22	3:C:111:ASN:HA	1.56	0.44
3:D:18:LYS:NZ	5:D:401:ADP:O3B	2.50	0.44
1:P:450:GLU:O	1:P:575:LYS:NZ	2.45	0.44
3:C:309:ILE:O	3:C:313:MET:HB2	2.17	0.44
3:C:271:SER:OG	3:C:272:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:314:GLN:O	3:A:318:THR:OG1	2.33	0.43
3:D:156:GLY:O	3:D:303:THR:OG1	2.36	0.43
3:B:156:GLY:O	3:B:303:THR:OG1	2.36	0.43
3:B:113:LYS:HG3	3:B:371:HIS:CE1	2.54	0.43
1:P:189:LEU:HD21	1:P:578:VAL:HG23	2.01	0.43
3:D:113:LYS:HG3	3:D:371:HIS:CE1	2.54	0.43
3:E:271:SER:OG	3:E:272:ALA:N	2.51	0.43
3:D:111:ASN:HA	3:D:111:ASN:HD22	1.56	0.43
3:D:1:ASP:HA	3:D:96:VAL:HG23	2.00	0.43
3:E:156:GLY:O	3:E:303:THR:OG1	2.36	0.43
3:D:271:SER:OG	3:D:272:ALA:N	2.51	0.43
1:P:426:GLU:OE2	1:P:429:ARG:NH2	2.52	0.43
3:A:70:PRO:HG3	3:A:85:ILE:HG13	2.01	0.43
3:B:1:ASP:HA	3:B:96:VAL:HG23	2.00	0.43
3:B:70:PRO:HG3	3:B:85:ILE:HG13	2.01	0.43
3:C:70:PRO:HG3	3:C:85:ILE:HG13	2.01	0.43
3:E:70:PRO:HG3	3:E:85:ILE:HG13	2.01	0.43
1:P:155:ALA:HB2	1:P:205:PHE:HA	2.01	0.43
3:A:271:SER:OG	3:A:272:ALA:N	2.51	0.42
3:B:160:THR:HG23	3:B:178:LEU:HB3	2.01	0.42
3:B:271:SER:OG	3:B:272:ALA:N	2.51	0.42
3:C:1:ASP:HA	3:C:96:VAL:HG23	2.00	0.42
3:D:160:THR:HG23	3:D:178:LEU:HB3	2.01	0.42
3:A:113:LYS:HG3	3:A:371:HIS:CE1	2.54	0.42
3:B:18:LYS:NZ	5:B:401:ADP:O2A	2.36	0.42
3:A:160:THR:HG23	3:A:178:LEU:HB3	2.01	0.42
3:C:160:THR:HG23	3:C:178:LEU:HB3	2.01	0.42
3:A:156:GLY:O	3:A:303:THR:OG1	2.36	0.42
3:B:111:ASN:HD22	3:B:177:ARG:HH12	1.67	0.42
3:C:113:LYS:HG3	3:C:371:HIS:CE1	2.54	0.42
3:C:140:LEU:HA	3:C:143:TYR:HD2	1.85	0.42
3:D:70:PRO:HG3	3:D:85:ILE:HG13	2.01	0.42
3:E:113:LYS:HG3	3:E:371:HIS:CE1	2.54	0.42
3:E:140:LEU:HA	3:E:143:TYR:HD2	1.85	0.42
3:E:314:GLN:O	3:E:318:THR:OG1	2.33	0.42
1:P:11:LEU:HD13	1:P:697:GLU:HG3	2.01	0.42
3:A:1:ASP:HA	3:A:96:VAL:HG23	2.00	0.42
3:E:1:ASP:HA	3:E:96:VAL:HG23	2.00	0.42
1:P:293:ASN:ND2	3:B:328:LYS:HG3	2.35	0.42
3:E:111:ASN:HD22	3:E:177:ARG:HH12	1.67	0.42
3:C:156:GLY:O	3:C:303:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:160:THR:HG23	3:E:178:LEU:HB3	2.01	0.42
1:P:566:ARG:HA	1:P:567:PRO:HD3	1.90	0.42
3:A:111:ASN:HD22	3:A:177:ARG:HH12	1.67	0.42
1:P:460:LEU:HG	1:P:530:ASN:HD22	1.84	0.42
3:C:151:ILE:HA	3:C:164:PRO:HA	2.02	0.42
3:A:140:LEU:HA	3:A:143:TYR:HD2	1.85	0.41
3:B:140:LEU:HA	3:B:143:TYR:HD2	1.85	0.41
3:D:140:LEU:HA	3:D:143:TYR:HD2	1.85	0.41
1:P:445:ILE:O	1:P:448:LEU:HB3	2.21	0.41
3:B:131:ALA:HB1	3:B:356:TRP:HB3	2.03	0.41
1:P:625:VAL:O	1:P:629:ARG:CB	2.68	0.41
3:C:18:LYS:NZ	5:C:401:ADP:O3B	2.53	0.41
3:D:131:ALA:HB1	3:D:356:TRP:HB3	2.03	0.41
3:E:111:ASN:HD22	3:E:111:ASN:HA	1.56	0.41
3:A:143:TYR:CZ	3:A:346:LEU:HD13	2.56	0.41
3:D:143:TYR:CZ	3:D:346:LEU:HD13	2.56	0.41
1:P:170:MET:HE2	1:P:385:VAL:CG2	2.46	0.41
3:E:151:ILE:HA	3:E:164:PRO:HA	2.02	0.41
3:E:131:ALA:HB1	3:E:356:TRP:HB3	2.03	0.41
3:A:151:ILE:HA	3:A:164:PRO:HA	2.02	0.41
3:B:143:TYR:CZ	3:B:346:LEU:HD13	2.56	0.41
3:C:143:TYR:CZ	3:C:346:LEU:HD13	2.56	0.41
3:D:111:ASN:HD22	3:D:177:ARG:HH12	1.67	0.41
1:P:106:ILE:HG12	1:P:593:ILE:HB	2.02	0.41
3:C:111:ASN:HD22	3:C:177:ARG:HH12	1.67	0.41
3:C:64:ILE:H	3:C:64:ILE:HG13	1.78	0.41
3:E:143:TYR:CZ	3:E:346:LEU:HD13	2.56	0.40
3:C:131:ALA:HB1	3:C:356:TRP:HB3	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	P	727/729 (100%)	702 (97%)	25 (3%)	0	100	100
2	R	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
3	A	373/375 (100%)	348 (93%)	25 (7%)	0	100	100
3	B	373/375 (100%)	348 (93%)	25 (7%)	0	100	100
3	C	373/375 (100%)	348 (93%)	25 (7%)	0	100	100
3	D	373/375 (100%)	348 (93%)	25 (7%)	0	100	100
3	E	373/375 (100%)	347 (93%)	26 (7%)	0	100	100
All	All	2738/2752 (100%)	2582 (94%)	156 (6%)	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	P	581/651 (89%)	575 (99%)	6 (1%)	78	89
3	A	318/318 (100%)	315 (99%)	3 (1%)	81	91
3	B	318/318 (100%)	315 (99%)	3 (1%)	81	91
3	C	318/318 (100%)	315 (99%)	3 (1%)	81	91
3	D	318/318 (100%)	315 (99%)	3 (1%)	81	91
3	E	318/318 (100%)	315 (99%)	3 (1%)	81	91
All	All	2171/2241 (97%)	2150 (99%)	21 (1%)	80	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	293	ASN
1	P	304	ASN
1	P	366	ASN
1	P	563	ASN
1	P	568	PRO
1	P	624	ASN

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Mol	Chain	Res	Type
3	A	111	ASN
3	A	115	ASN
3	A	297	ASN
3	B	111	ASN
3	B	115	ASN
3	B	297	ASN
3	C	111	ASN
3	C	115	ASN
3	C	297	ASN
3	D	111	ASN
3	D	115	ASN
3	D	297	ASN
3	E	111	ASN
3	E	115	ASN
3	E	297	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	102	GLN
1	P	141	GLN
1	P	293	ASN
1	P	304	ASN
1	P	366	ASN
1	P	408	ASN
1	P	486	HIS
1	P	563	ASN
1	P	589	ASN
1	P	591	ASN
3	A	111	ASN
3	A	115	ASN
3	A	162	ASN
3	A	225	ASN
3	A	297	ASN
3	B	111	ASN
3	B	115	ASN
3	B	162	ASN
3	B	225	ASN
3	B	297	ASN
3	C	111	ASN
3	C	115	ASN
3	C	162	ASN

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Mol	Chain	Res	Type
3	C	225	ASN
3	C	297	ASN
3	D	87	HIS
3	D	111	ASN
3	D	115	ASN
3	D	162	ASN
3	D	225	ASN
3	D	297	ASN
3	E	111	ASN
3	E	115	ASN
3	E	162	ASN
3	E	225	ASN
3	E	297	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	A	401	4	25,29,29	0.98	1 (4%)	25,45,45	1.66	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	B	401	4	25,29,29	1.36	2 (8%)	25,45,45	1.68	7 (28%)
5	ADP	C	401	4	25,29,29	1.00	2 (8%)	25,45,45	1.78	3 (12%)
5	ADP	D	401	4	25,29,29	0.97	1 (4%)	25,45,45	1.74	3 (12%)
5	ADP	E	401	4	25,29,29	0.98	1 (4%)	25,45,45	1.83	3 (12%)
5	ADP	P	802	4	25,29,29	1.06	2 (8%)	25,45,45	1.81	3 (12%)

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	A	401	4	-	0/12/32/32	0/3/3/3
5	ADP	B	401	4	-	0/12/32/32	0/3/3/3
5	ADP	C	401	4	-	0/12/32/32	0/3/3/3
5	ADP	D	401	4	-	0/12/32/32	0/3/3/3
5	ADP	E	401	4	-	0/12/32/32	0/3/3/3
5	ADP	P	802	4	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	802	ADP	C8-N9	-2.17	1.34	1.36
5	B	401	ADP	PA-O1A	-2.12	1.43	1.50
5	C	401	ADP	C8-N9	-2.03	1.34	1.36
5	A	401	ADP	C5-C4	2.76	1.46	1.40
5	C	401	ADP	C5-C4	2.78	1.46	1.40
5	E	401	ADP	C5-C4	2.90	1.47	1.40
5	D	401	ADP	C5-C4	2.99	1.47	1.40
5	P	802	ADP	C5-C4	3.10	1.47	1.40
5	B	401	ADP	O4'-C1'	4.54	1.47	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	401	ADP	N3-C2-N1	-6.21	123.55	128.86
5	P	802	ADP	N3-C2-N1	-5.84	123.87	128.86
5	C	401	ADP	N3-C2-N1	-5.76	123.93	128.86
5	D	401	ADP	N3-C2-N1	-5.58	124.09	128.86
5	A	401	ADP	N3-C2-N1	-4.62	124.91	128.86
5	P	802	ADP	PA-O3A-PB	-3.79	119.89	132.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	ADP	PA-O3A-PB	-3.72	120.12	132.63
5	C	401	ADP	PA-O3A-PB	-3.60	120.55	132.63
5	E	401	ADP	PA-O3A-PB	-3.40	121.20	132.63
5	B	401	ADP	O3B-PB-O1B	-3.15	98.31	110.60
5	A	401	ADP	PA-O3A-PB	-2.97	122.64	132.63
5	A	401	ADP	C4-C5-N7	-2.77	106.74	109.41
5	P	802	ADP	C4-C5-N7	-2.70	106.80	109.41
5	C	401	ADP	C4-C5-N7	-2.69	106.81	109.41
5	B	401	ADP	C4'-O4'-C1'	-2.65	107.07	109.83
5	D	401	ADP	C4-C5-N7	-2.54	106.96	109.41
5	B	401	ADP	C5'-C4'-C3'	-2.50	105.88	115.29
5	E	401	ADP	C4-C5-N7	-2.49	107.00	109.41
5	A	401	ADP	C2'-C3'-C4'	2.09	106.62	102.62
5	B	401	ADP	O4'-C4'-C5'	2.15	116.55	109.39
5	B	401	ADP	C1'-N9-C4	2.28	130.57	126.64
5	B	401	ADP	C5-C6-N6	3.13	126.85	120.47
5	B	401	ADP	O3B-PB-O2B	3.54	121.60	107.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	ADP	1	0
5	B	401	ADP	4	0
5	C	401	ADP	2	0
5	D	401	ADP	2	0

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.