



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 8, 2018 – 11:05 AM EDT

PDB ID : 6D8C  
EMDB ID: : EMD-7831  
Title : Cryo-EM structure of FLNaABD E254K bound to phalloidin-stabilized F-actin  
Authors : Iwamoto, D.V.; Huehn, A.R.; Simon, B.; Huet-Calderwood, C.; Baldassarre, M.; Sindelar, C.V.; Calderwood, D.A.  
Deposited on : 2018-04-26  
Resolution : 3.54 Å (reported)  
Based on PDB ID : 3HOC, 6C1D

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](mailto: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.

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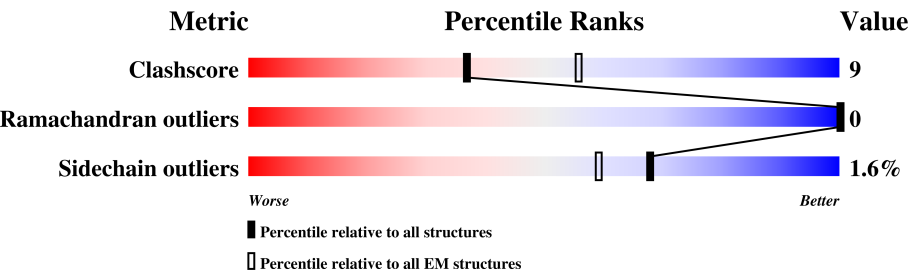
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.54 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	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  $\geq 3$ , 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	A	306	<div><div>36%</div><div>60%</div></div>
1	B	306	<div><div>38%</div><div>60%</div></div>
1	C	306	<div><div>36%</div><div>60%</div></div>
1	D	306	<div><div>36%</div><div>60%</div></div>
1	E	306	<div><div>36%</div><div>60%</div></div>
2	H	375	<div><div>76%</div><div>22%</div><div>..</div></div>
2	J	375	<div><div>79%</div><div>19%</div><div>..</div></div>
2	K	375	<div><div>77%</div><div>21%</div><div>..</div></div>
2	L	375	<div><div>78%</div><div>20%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	M	375	<div><div></div><div>78%</div><div>19%</div><div>..</div></div>
3	N	7	<div><div></div><div>57%</div><div>43%</div></div>
3	O	7	<div><div></div><div>71%</div><div>29%</div></div>
3	P	7	<div><div></div><div>57%</div><div>43%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39316 atoms, of which 19651 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 Filamin-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	121	Total 2012	C 627	H 1027	N 177	O 177	S 4	0	0
1	A	121	Total 2012	C 627	H 1027	N 177	O 177	S 4	0	0
1	B	121	Total 2012	C 627	H 1027	N 177	O 177	S 4	0	0
1	C	121	Total 2012	C 627	H 1027	N 177	O 177	S 4	0	0
1	E	121	Total 2012	C 627	H 1027	N 177	O 177	S 4	0	0

There are 145 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	MET	-	expression tag	UNP P21333
D	-26	HIS	-	expression tag	UNP P21333
D	-25	HIS	-	expression tag	UNP P21333
D	-24	HIS	-	expression tag	UNP P21333
D	-23	HIS	-	expression tag	UNP P21333
D	-22	HIS	-	expression tag	UNP P21333
D	-21	HIS	-	expression tag	UNP P21333
D	-20	GLY	-	expression tag	UNP P21333
D	-19	SER	-	expression tag	UNP P21333
D	-18	LEU	-	expression tag	UNP P21333
D	-17	VAL	-	expression tag	UNP P21333
D	-16	PRO	-	expression tag	UNP P21333
D	-15	ARG	-	expression tag	UNP P21333
D	-14	SER	-	expression tag	UNP P21333
D	-13	GLU	-	expression tag	UNP P21333
D	-12	ASN	-	expression tag	UNP P21333
D	-11	LEU	-	expression tag	UNP P21333
D	-10	TYR	-	expression tag	UNP P21333
D	-9	PHE	-	expression tag	UNP P21333
D	-8	GLN	-	expression tag	UNP P21333

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	GLY	-	expression tag	UNP P21333
D	-6	SER	-	expression tag	UNP P21333
D	-5	ASP	-	expression tag	UNP P21333
D	-4	ILE	-	expression tag	UNP P21333
D	-3	LEU	-	expression tag	UNP P21333
D	-2	GLN	-	expression tag	UNP P21333
D	-1	GLY	-	expression tag	UNP P21333
D	0	THR	-	expression tag	UNP P21333
D	254	LYS	GLU	engineered mutation	UNP P21333
A	-27	MET	-	expression tag	UNP P21333
A	-26	HIS	-	expression tag	UNP P21333
A	-25	HIS	-	expression tag	UNP P21333
A	-24	HIS	-	expression tag	UNP P21333
A	-23	HIS	-	expression tag	UNP P21333
A	-22	HIS	-	expression tag	UNP P21333
A	-21	HIS	-	expression tag	UNP P21333
A	-20	GLY	-	expression tag	UNP P21333
A	-19	SER	-	expression tag	UNP P21333
A	-18	LEU	-	expression tag	UNP P21333
A	-17	VAL	-	expression tag	UNP P21333
A	-16	PRO	-	expression tag	UNP P21333
A	-15	ARG	-	expression tag	UNP P21333
A	-14	SER	-	expression tag	UNP P21333
A	-13	GLU	-	expression tag	UNP P21333
A	-12	ASN	-	expression tag	UNP P21333
A	-11	LEU	-	expression tag	UNP P21333
A	-10	TYR	-	expression tag	UNP P21333
A	-9	PHE	-	expression tag	UNP P21333
A	-8	GLN	-	expression tag	UNP P21333
A	-7	GLY	-	expression tag	UNP P21333
A	-6	SER	-	expression tag	UNP P21333
A	-5	ASP	-	expression tag	UNP P21333
A	-4	ILE	-	expression tag	UNP P21333
A	-3	LEU	-	expression tag	UNP P21333
A	-2	GLN	-	expression tag	UNP P21333
A	-1	GLY	-	expression tag	UNP P21333
A	0	THR	-	expression tag	UNP P21333
A	254	LYS	GLU	engineered mutation	UNP P21333
B	-27	MET	-	expression tag	UNP P21333
B	-26	HIS	-	expression tag	UNP P21333
B	-25	HIS	-	expression tag	UNP P21333
B	-24	HIS	-	expression tag	UNP P21333

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	HIS	-	expression tag	UNP P21333
B	-22	HIS	-	expression tag	UNP P21333
B	-21	HIS	-	expression tag	UNP P21333
B	-20	GLY	-	expression tag	UNP P21333
B	-19	SER	-	expression tag	UNP P21333
B	-18	LEU	-	expression tag	UNP P21333
B	-17	VAL	-	expression tag	UNP P21333
B	-16	PRO	-	expression tag	UNP P21333
B	-15	ARG	-	expression tag	UNP P21333
B	-14	SER	-	expression tag	UNP P21333
B	-13	GLU	-	expression tag	UNP P21333
B	-12	ASN	-	expression tag	UNP P21333
B	-11	LEU	-	expression tag	UNP P21333
B	-10	TYR	-	expression tag	UNP P21333
B	-9	PHE	-	expression tag	UNP P21333
B	-8	GLN	-	expression tag	UNP P21333
B	-7	GLY	-	expression tag	UNP P21333
B	-6	SER	-	expression tag	UNP P21333
B	-5	ASP	-	expression tag	UNP P21333
B	-4	ILE	-	expression tag	UNP P21333
B	-3	LEU	-	expression tag	UNP P21333
B	-2	GLN	-	expression tag	UNP P21333
B	-1	GLY	-	expression tag	UNP P21333
B	0	THR	-	expression tag	UNP P21333
B	254	LYS	GLU	engineered mutation	UNP P21333
C	-27	MET	-	expression tag	UNP P21333
C	-26	HIS	-	expression tag	UNP P21333
C	-25	HIS	-	expression tag	UNP P21333
C	-24	HIS	-	expression tag	UNP P21333
C	-23	HIS	-	expression tag	UNP P21333
C	-22	HIS	-	expression tag	UNP P21333
C	-21	HIS	-	expression tag	UNP P21333
C	-20	GLY	-	expression tag	UNP P21333
C	-19	SER	-	expression tag	UNP P21333
C	-18	LEU	-	expression tag	UNP P21333
C	-17	VAL	-	expression tag	UNP P21333
C	-16	PRO	-	expression tag	UNP P21333
C	-15	ARG	-	expression tag	UNP P21333
C	-14	SER	-	expression tag	UNP P21333
C	-13	GLU	-	expression tag	UNP P21333
C	-12	ASN	-	expression tag	UNP P21333
C	-11	LEU	-	expression tag	UNP P21333

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	TYR	-	expression tag	UNP P21333
C	-9	PHE	-	expression tag	UNP P21333
C	-8	GLN	-	expression tag	UNP P21333
C	-7	GLY	-	expression tag	UNP P21333
C	-6	SER	-	expression tag	UNP P21333
C	-5	ASP	-	expression tag	UNP P21333
C	-4	ILE	-	expression tag	UNP P21333
C	-3	LEU	-	expression tag	UNP P21333
C	-2	GLN	-	expression tag	UNP P21333
C	-1	GLY	-	expression tag	UNP P21333
C	0	THR	-	expression tag	UNP P21333
C	254	LYS	GLU	engineered mutation	UNP P21333
E	-27	MET	-	expression tag	UNP P21333
E	-26	HIS	-	expression tag	UNP P21333
E	-25	HIS	-	expression tag	UNP P21333
E	-24	HIS	-	expression tag	UNP P21333
E	-23	HIS	-	expression tag	UNP P21333
E	-22	HIS	-	expression tag	UNP P21333
E	-21	HIS	-	expression tag	UNP P21333
E	-20	GLY	-	expression tag	UNP P21333
E	-19	SER	-	expression tag	UNP P21333
E	-18	LEU	-	expression tag	UNP P21333
E	-17	VAL	-	expression tag	UNP P21333
E	-16	PRO	-	expression tag	UNP P21333
E	-15	ARG	-	expression tag	UNP P21333
E	-14	SER	-	expression tag	UNP P21333
E	-13	GLU	-	expression tag	UNP P21333
E	-12	ASN	-	expression tag	UNP P21333
E	-11	LEU	-	expression tag	UNP P21333
E	-10	TYR	-	expression tag	UNP P21333
E	-9	PHE	-	expression tag	UNP P21333
E	-8	GLN	-	expression tag	UNP P21333
E	-7	GLY	-	expression tag	UNP P21333
E	-6	SER	-	expression tag	UNP P21333
E	-5	ASP	-	expression tag	UNP P21333
E	-4	ILE	-	expression tag	UNP P21333
E	-3	LEU	-	expression tag	UNP P21333
E	-2	GLN	-	expression tag	UNP P21333
E	-1	GLY	-	expression tag	UNP P21333
E	0	THR	-	expression tag	UNP P21333
E	254	LYS	GLU	engineered mutation	UNP P21333

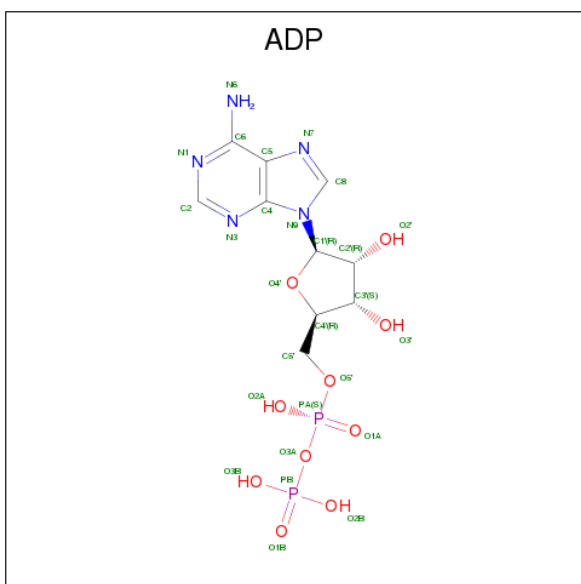
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	370	Total 5750	C 1827	H 2863	N 488	O 551	S 21	0	0
2	J	370	Total 5750	C 1827	H 2863	N 488	O 551	S 21	0	0
2	K	370	Total 5750	C 1827	H 2863	N 488	O 551	S 21	0	0
2	L	370	Total 5750	C 1827	H 2863	N 488	O 551	S 21	0	0
2	M	370	Total 5750	C 1827	H 2863	N 488	O 551	S 21	0	0

- Molecule 3 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	N	7	Total 102	C 35	H 47	N 8	O 11	S 1	0	0
3	O	7	Total 102	C 35	H 47	N 8	O 11	S 1	0	0
3	P	7	Total 102	C 35	H 47	N 8	O 11	S 1	0	0

- Molecule 4 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
4	H	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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Mol	Chain	Residues	Atoms						AltConf
4	J	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	K	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	L	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	M	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

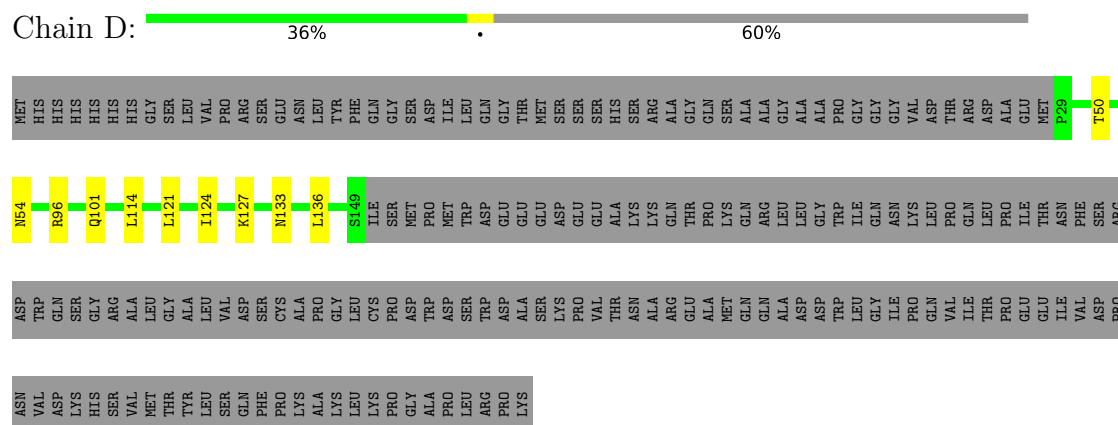
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	H	1	Total	Mg	0
			1	1	
5	J	1	Total	Mg	0
			1	1	
5	L	1	Total	Mg	0
			1	1	
5	K	1	Total	Mg	0
			1	1	
5	M	1	Total	Mg	0
			1	1	

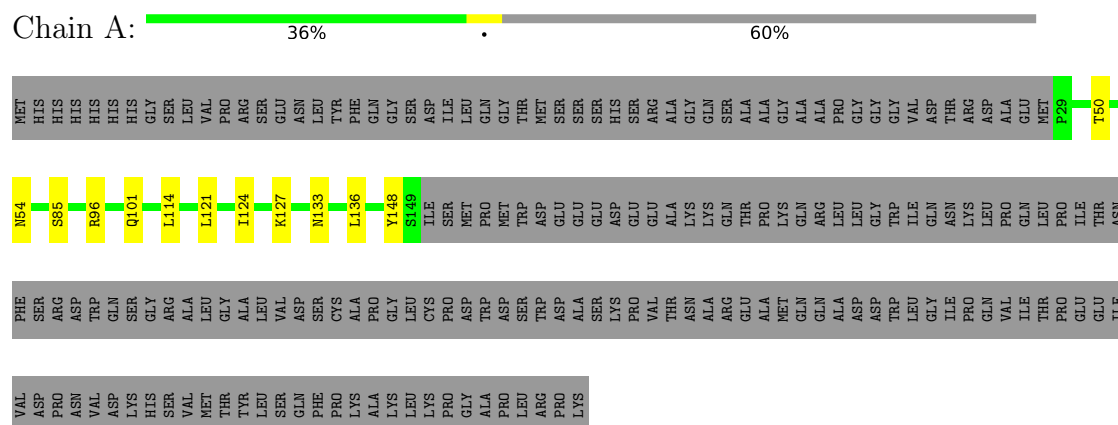
### 3 Residue-property plots [i](#)

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.

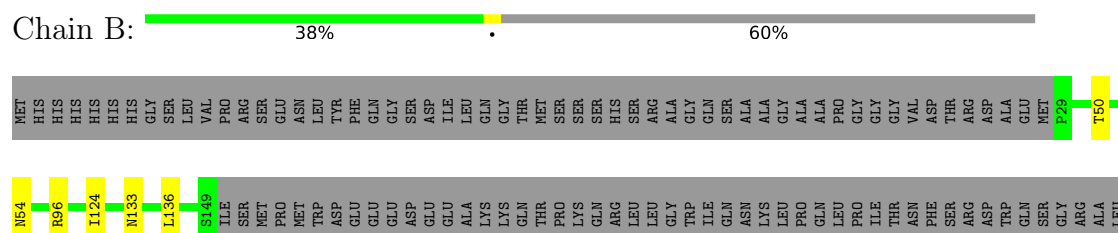
#### • Molecule 1: Filamin-A



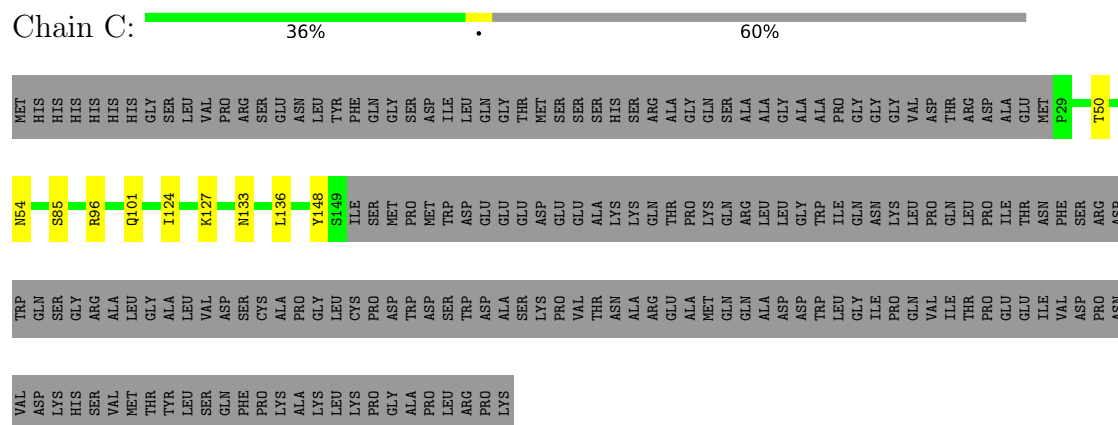
#### • Molecule 1: Filamin-A



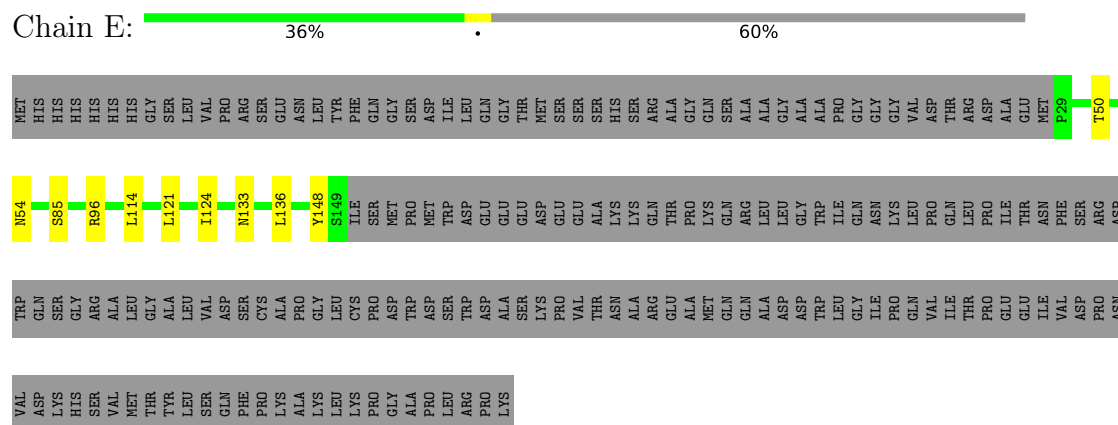
#### • Molecule 1: Filamin-A



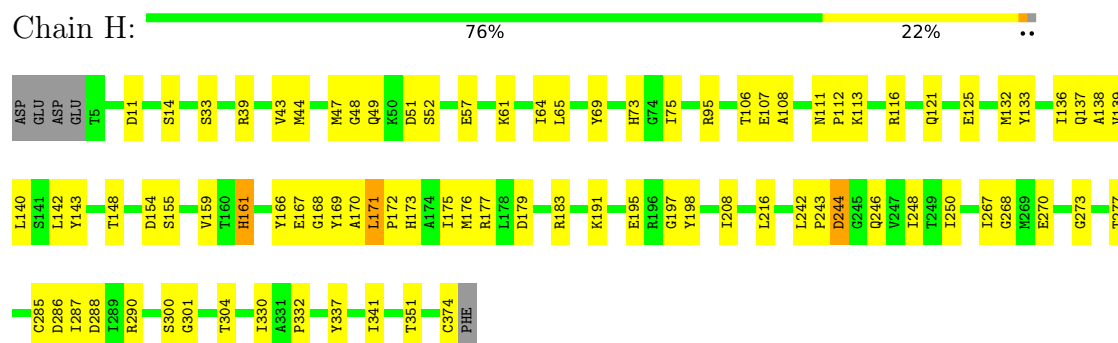
- Molecule 1: Filamin-A



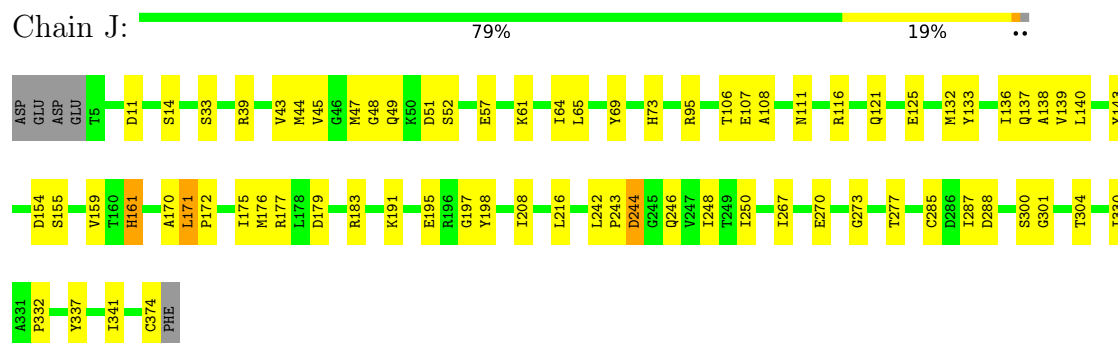
- Molecule 1: Filamin-A



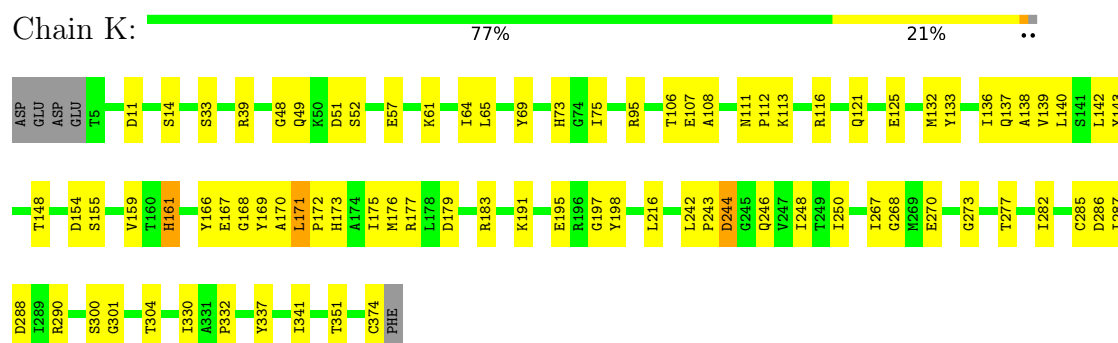
- Molecule 2: Actin, alpha skeletal muscle



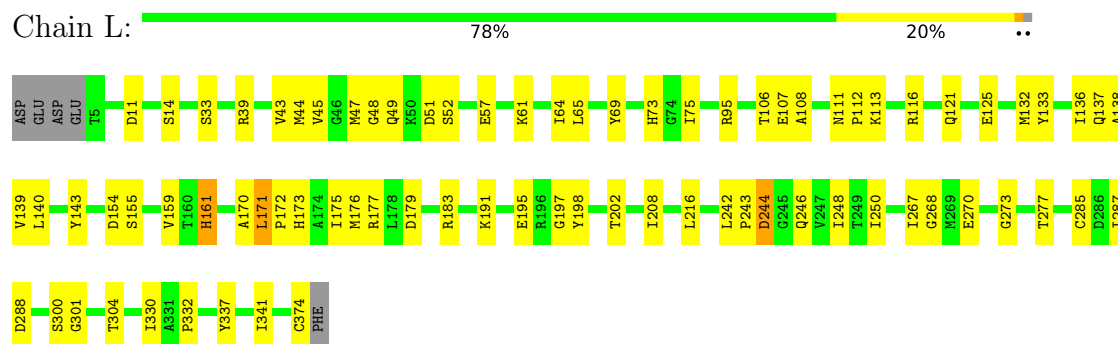
- Molecule 2: Actin, alpha skeletal muscle



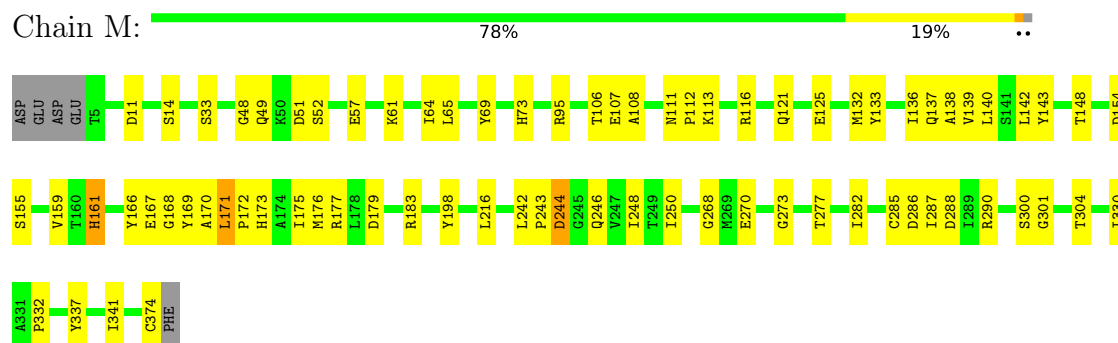
- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle

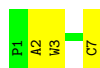


- Molecule 2: Actin, alpha skeletal muscle



- Molecule 3: Phalloidin

Chain N:  57% 43%



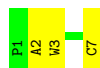
- Molecule 3: Phalloidin

Chain O:  71% 29%



- Molecule 3: Phalloidin

Chain P:  57% 43%



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.73°, rise=27.54 Å, axial sym=C1	Depositor
Number of segments used	67000	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)	1000	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	37500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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: HYP, ALO, MG, G5G, 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	A	0.25	0/1001	0.45	0/1349
1	B	0.24	0/1001	0.45	0/1349
1	C	0.24	0/1001	0.45	0/1349
1	D	0.24	0/1001	0.45	0/1349
1	E	0.25	0/1001	0.45	0/1349
2	H	0.27	0/2949	0.50	0/3996
2	J	0.27	0/2949	0.50	0/3996
2	K	0.27	0/2949	0.50	0/3996
2	L	0.27	0/2949	0.50	0/3996
2	M	0.27	0/2949	0.50	0/3996
3	N	1.78	0/29	1.78	0/36
3	O	1.80	0/29	1.77	0/36
3	P	1.78	0/29	1.78	0/36
All	All	0.29	0/19837	0.50	0/26833

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	985	1027	1027	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	985	1027	1027	3	0
1	C	985	1027	1027	8	0
1	D	985	1027	1027	7	0
1	E	985	1027	1027	5	0
2	H	2887	2863	2862	103	0
2	J	2887	2863	2862	72	0
2	K	2887	2863	2862	86	0
2	L	2887	2863	2862	84	0
2	M	2887	2863	2862	74	0
3	N	55	47	38	3	0
3	O	55	47	38	1	0
3	P	55	47	38	3	0
4	H	27	12	12	0	0
4	J	27	12	12	0	0
4	K	27	12	12	0	0
4	L	27	12	12	0	0
4	M	27	12	12	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
All	All	19665	19651	19619	355	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 9.

All (355) 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)
2:K:167:GLU:HG2	1:C:127:LYS:HE3	1.55	0.88
1:D:127:LYS:HE3	2:M:167:GLU:HG2	1.54	0.86
2:H:167:GLU:HG2	1:A:127:LYS:HE3	1.59	0.84
1:E:136:LEU:HD11	2:M:57:GLU:HG2	1.60	0.83
1:D:136:LEU:HD11	2:H:57:GLU:HG2	1.60	0.83
1:A:136:LEU:HD11	2:J:57:GLU:HG2	1.60	0.83
1:B:136:LEU:HD11	2:K:57:GLU:HG2	1.60	0.83
1:C:136:LEU:HD11	2:L:57:GLU:HG2	1.60	0.82
2:K:290:ARG:HD2	2:L:244:ASP:HB2	1.62	0.82
2:H:290:ARG:HD2	2:J:244:ASP:HB2	1.62	0.81
2:H:244:ASP:HB2	2:M:290:ARG:HD2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:MET:HE3	2:M:142:LEU:HD23	1.68	0.76
2:H:44:MET:CE	2:M:142:LEU:HD23	2.15	0.76
2:H:169:TYR:CD2	2:J:64:ILE:HD13	2.22	0.74
2:K:142:LEU:HD23	2:L:44:MET:CE	2.19	0.73
2:J:270:GLU:O	2:J:270:GLU:OE1	2.08	0.72
2:L:270:GLU:OE1	2:L:270:GLU:O	2.08	0.72
2:M:270:GLU:OE1	2:M:270:GLU:O	2.08	0.72
2:H:270:GLU:OE1	2:H:270:GLU:O	2.08	0.72
2:K:270:GLU:OE1	2:K:270:GLU:O	2.08	0.71
2:H:244:ASP:OD2	2:M:290:ARG:NH1	2.23	0.71
2:K:169:TYR:CD2	2:L:64:ILE:HD13	2.26	0.71
2:K:142:LEU:HD23	2:L:44:MET:HE3	1.74	0.70
2:H:286:ASP:OD1	2:J:39:ARG:NH2	2.25	0.69
2:H:290:ARG:NH1	2:J:244:ASP:OD2	2.25	0.69
2:H:142:LEU:HD23	2:J:44:MET:CE	2.23	0.68
2:H:143:TYR:CD1	1:A:101:GLN:HG3	2.27	0.68
2:H:142:LEU:HD23	2:J:44:MET:HE3	1.76	0.67
2:H:39:ARG:NH2	2:M:286:ASP:OD1	2.28	0.67
2:H:14:SER:O	2:H:183:ARG:NH2	2.29	0.66
2:K:14:SER:O	2:K:183:ARG:NH2	2.29	0.66
2:L:14:SER:O	2:L:183:ARG:NH2	2.29	0.66
2:J:14:SER:O	2:J:183:ARG:NH2	2.29	0.66
2:M:14:SER:O	2:M:183:ARG:NH2	2.28	0.66
1:E:85:SER:HG	1:E:148:TYR:HH	1.44	0.66
2:H:64:ILE:HD13	2:M:169:TYR:CD2	2.31	0.65
1:C:85:SER:HG	1:C:148:TYR:HH	1.42	0.65
2:H:287:ILE:HD11	2:J:208:ILE:HD13	1.79	0.65
2:H:139:VAL:HG13	2:H:140:LEU:HD12	1.80	0.64
2:J:139:VAL:HG13	2:J:140:LEU:HD12	1.80	0.64
2:K:143:TYR:CD1	1:C:101:GLN:HG3	2.33	0.64
2:M:139:VAL:HG13	2:M:140:LEU:HD12	1.80	0.64
2:K:139:VAL:HG13	2:K:140:LEU:HD12	1.80	0.64
2:L:139:VAL:HG13	2:L:140:LEU:HD12	1.80	0.63
2:H:143:TYR:HD1	1:A:101:GLN:HG3	1.63	0.63
2:L:137:GLN:CD	2:L:154:ASP:OD2	2.37	0.63
2:M:116:ARG:NH2	2:M:374:CYS:SG	2.72	0.63
2:M:137:GLN:CD	2:M:154:ASP:OD2	2.37	0.63
2:J:116:ARG:NH2	2:J:374:CYS:SG	2.72	0.63
2:K:116:ARG:NH2	2:K:374:CYS:SG	2.72	0.63
2:J:137:GLN:CD	2:J:154:ASP:OD2	2.37	0.63
2:K:286:ASP:OD1	2:L:39:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:137:GLN:CD	2:K:154:ASP:OD2	2.37	0.62
2:K:75:ILE:HG21	3:N:2:ALA:O	1.99	0.62
2:H:116:ARG:NH2	2:H:374:CYS:SG	2.72	0.62
2:K:287:ILE:HD11	2:L:208:ILE:HD13	1.82	0.62
2:H:137:GLN:CD	2:H:154:ASP:OD2	2.37	0.62
1:D:101:GLN:HG3	2:M:143:TYR:CD1	2.35	0.62
2:L:116:ARG:NH2	2:L:374:CYS:SG	2.72	0.62
2:H:43:VAL:HG12	2:M:168:GLY:O	1.99	0.62
2:H:197:GLY:HA2	2:K:112:PRO:HB3	1.82	0.61
2:H:173:HIS:HB3	2:L:267:ILE:O	2.01	0.60
2:K:170:ALA:C	2:K:171:LEU:HD23	2.22	0.60
2:L:170:ALA:C	2:L:171:LEU:HD23	2.22	0.60
2:J:170:ALA:C	2:J:171:LEU:HD23	2.22	0.60
2:K:33:SER:O	2:K:69:TYR:CD1	2.55	0.60
2:M:170:ALA:C	2:M:171:LEU:HD23	2.22	0.60
2:L:33:SER:O	2:L:69:TYR:CD1	2.55	0.60
2:K:168:GLY:O	2:L:43:VAL:HG12	2.02	0.60
1:D:50:THR:O	1:D:54:ASN:ND2	2.35	0.60
2:K:108:ALA:O	2:K:111:ASN:ND2	2.35	0.60
2:M:108:ALA:O	2:M:111:ASN:ND2	2.35	0.60
2:H:108:ALA:O	2:H:111:ASN:ND2	2.35	0.59
2:M:33:SER:O	2:M:69:TYR:CD1	2.55	0.59
1:C:50:THR:O	1:C:54:ASN:ND2	2.35	0.59
2:H:170:ALA:C	2:H:171:LEU:HD23	2.22	0.59
2:H:208:ILE:HD13	2:M:287:ILE:HD11	1.83	0.59
2:J:33:SER:O	2:J:69:TYR:CD1	2.55	0.59
1:B:50:THR:O	1:B:54:ASN:ND2	2.35	0.59
2:H:44:MET:CE	2:M:142:LEU:CD2	2.80	0.59
1:A:50:THR:O	1:A:54:ASN:ND2	2.35	0.59
2:J:11:ASP:O	2:J:106:THR:OG1	2.21	0.59
2:K:11:ASP:O	2:K:106:THR:OG1	2.21	0.59
2:H:112:PRO:HB3	2:L:197:GLY:HA2	1.85	0.59
2:H:33:SER:O	2:H:69:TYR:CD1	2.55	0.59
2:J:108:ALA:O	2:J:111:ASN:ND2	2.35	0.59
2:H:11:ASP:O	2:H:106:THR:OG1	2.21	0.59
2:H:136:ILE:O	2:H:139:VAL:HG12	2.02	0.59
2:M:136:ILE:O	2:M:139:VAL:HG12	2.02	0.59
2:L:108:ALA:O	2:L:111:ASN:ND2	2.35	0.59
1:E:50:THR:O	1:E:54:ASN:ND2	2.35	0.58
2:J:136:ILE:O	2:J:139:VAL:HG12	2.02	0.58
2:L:11:ASP:O	2:L:106:THR:OG1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:171:LEU:HD23	2:M:171:LEU:N	2.19	0.58
2:M:11:ASP:O	2:M:106:THR:OG1	2.21	0.58
2:L:140:LEU:HA	2:L:143:TYR:HD2	1.69	0.58
2:H:140:LEU:HA	2:H:143:TYR:HD2	1.69	0.58
2:L:136:ILE:O	2:L:139:VAL:HG12	2.02	0.58
2:M:140:LEU:HA	2:M:143:TYR:HD2	1.69	0.58
2:H:168:GLY:O	2:J:43:VAL:HG12	2.04	0.58
2:K:136:ILE:O	2:K:139:VAL:HG12	2.02	0.58
2:K:140:LEU:HA	2:K:143:TYR:HD2	1.69	0.58
2:K:171:LEU:HD23	2:K:171:LEU:N	2.19	0.57
2:H:75:ILE:HG21	3:P:2:ALA:O	2.04	0.57
2:H:171:LEU:N	2:H:171:LEU:HD23	2.19	0.57
2:K:142:LEU:CD2	2:L:44:MET:CE	2.83	0.57
2:L:171:LEU:N	2:L:171:LEU:HD23	2.19	0.57
2:J:140:LEU:HA	2:J:143:TYR:HD2	1.69	0.56
2:H:267:ILE:O	2:K:173:HIS:HB3	2.05	0.56
2:J:267:ILE:O	2:L:173:HIS:HB3	2.06	0.56
2:L:155:SER:OG	2:L:304:THR:HG23	2.05	0.56
2:H:173:HIS:CB	2:L:267:ILE:O	2.53	0.56
2:L:48:GLY:C	2:L:49:GLN:HG2	2.26	0.56
2:M:155:SER:OG	2:M:304:THR:HG23	2.06	0.56
2:J:171:LEU:N	2:J:171:LEU:HD23	2.19	0.56
2:K:155:SER:OG	2:K:304:THR:HG23	2.05	0.56
2:J:48:GLY:C	2:J:49:GLN:HG2	2.26	0.56
2:H:155:SER:OG	2:H:304:THR:HG23	2.06	0.56
2:J:155:SER:OG	2:J:304:THR:HG23	2.05	0.56
2:M:48:GLY:C	2:M:49:GLN:HG2	2.26	0.56
2:L:75:ILE:HG21	3:O:2:ALA:O	2.07	0.56
2:H:48:GLY:C	2:H:49:GLN:HG2	2.26	0.55
2:L:242:LEU:HD12	2:L:243:PRO:O	2.07	0.55
2:K:143:TYR:HD1	1:C:101:GLN:HG3	1.71	0.55
2:K:242:LEU:HD12	2:K:243:PRO:O	2.07	0.55
2:M:242:LEU:HD12	2:M:243:PRO:O	2.07	0.55
2:K:244:ASP:OD1	2:K:246:GLN:OE1	2.25	0.55
2:J:242:LEU:HD12	2:J:243:PRO:O	2.07	0.55
2:K:121:GLN:NE2	2:K:125:GLU:OE1	2.41	0.54
2:J:69:TYR:CD1	2:J:183:ARG:NH2	2.75	0.54
2:K:69:TYR:CD1	2:K:183:ARG:NH2	2.76	0.54
2:K:267:ILE:O	2:M:173:HIS:HB3	2.07	0.54
2:K:154:ASP:HB2	2:K:161:HIS:NE2	2.23	0.54
2:K:48:GLY:C	2:K:49:GLN:HG2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:ASP:HB2	2:H:161:HIS:NE2	2.23	0.54
2:H:242:LEU:HD12	2:H:243:PRO:O	2.07	0.54
2:J:197:GLY:HA2	2:L:112:PRO:HB3	1.89	0.54
2:L:121:GLN:NE2	2:L:125:GLU:OE1	2.40	0.54
2:L:244:ASP:OD1	2:L:246:GLN:OE1	2.25	0.54
2:K:198:TYR:CE1	2:K:248:ILE:HB	2.43	0.54
2:H:244:ASP:OD1	2:H:246:GLN:OE1	2.25	0.54
2:H:121:GLN:NE2	2:H:125:GLU:OE1	2.41	0.54
2:H:69:TYR:CD1	2:H:183:ARG:NH2	2.76	0.54
2:J:121:GLN:NE2	2:J:125:GLU:OE1	2.40	0.54
2:L:154:ASP:HB2	2:L:161:HIS:NE2	2.23	0.54
2:L:198:TYR:CE1	2:L:248:ILE:HB	2.43	0.54
2:M:121:GLN:NE2	2:M:125:GLU:OE1	2.40	0.54
2:J:244:ASP:OD1	2:J:246:GLN:OE1	2.25	0.54
2:L:69:TYR:CD1	2:L:183:ARG:NH2	2.76	0.54
2:M:69:TYR:CD1	2:M:183:ARG:NH2	2.76	0.54
2:H:167:GLU:OE2	2:J:61:LYS:HG2	2.08	0.53
2:H:142:LEU:CD2	2:J:44:MET:CE	2.86	0.53
2:J:154:ASP:HB2	2:J:161:HIS:NE2	2.23	0.53
2:M:154:ASP:HB2	2:M:161:HIS:NE2	2.23	0.53
2:M:244:ASP:OD1	2:M:246:GLN:OE1	2.25	0.53
2:K:197:GLY:HA2	2:M:112:PRO:HB3	1.91	0.53
2:J:195:GLU:OE1	2:L:113:LYS:HD2	2.08	0.52
2:J:198:TYR:CE1	2:J:248:ILE:HB	2.43	0.52
2:M:177:ARG:NH1	2:M:179:ASP:OD1	2.43	0.52
2:H:177:ARG:NH1	2:H:179:ASP:OD1	2.43	0.52
2:L:177:ARG:NH1	2:L:179:ASP:OD1	2.43	0.52
2:H:198:TYR:CE1	2:H:248:ILE:HB	2.43	0.52
2:J:177:ARG:NH1	2:J:179:ASP:OD1	2.43	0.52
2:K:177:ARG:NH1	2:K:179:ASP:OD1	2.43	0.52
2:M:198:TYR:CE1	2:M:248:ILE:HB	2.43	0.52
2:L:132:MET:SD	2:L:133:TYR:N	2.83	0.52
2:J:64:ILE:HD12	2:J:65:LEU:HD12	1.92	0.52
2:K:132:MET:SD	2:K:133:TYR:N	2.83	0.52
2:J:132:MET:SD	2:J:133:TYR:N	2.83	0.52
2:K:195:GLU:OE1	2:M:113:LYS:HD2	2.10	0.52
2:M:132:MET:SD	2:M:133:TYR:N	2.83	0.51
2:K:64:ILE:HD12	2:K:65:LEU:HD12	1.92	0.51
2:H:132:MET:SD	2:H:133:TYR:N	2.83	0.51
1:D:101:GLN:HG3	2:M:143:TYR:HD1	1.74	0.51
2:M:64:ILE:HD12	2:M:65:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:ILE:HD12	2:H:65:LEU:HD12	1.92	0.51
2:K:290:ARG:NH1	2:L:244:ASP:OD2	2.44	0.51
2:L:159:VAL:HG21	2:L:177:ARG:CZ	2.41	0.51
2:H:47:MET:CE	2:M:148:THR:OG1	2.59	0.51
2:K:159:VAL:HG21	2:K:177:ARG:CZ	2.41	0.51
2:L:64:ILE:HD12	2:L:65:LEU:HD12	1.92	0.50
2:K:48:GLY:O	2:K:49:GLN:HG2	2.12	0.50
2:H:48:GLY:O	2:H:49:GLN:HG2	2.12	0.50
2:K:142:LEU:CD2	2:L:44:MET:HE3	2.41	0.50
2:M:48:GLY:O	2:M:49:GLN:HG2	2.12	0.50
2:H:159:VAL:HG21	2:H:177:ARG:CZ	2.41	0.50
2:J:159:VAL:HG21	2:J:177:ARG:CZ	2.41	0.50
2:J:267:ILE:O	2:L:173:HIS:CB	2.60	0.50
2:K:148:THR:OG1	2:L:47:MET:CE	2.59	0.50
2:M:159:VAL:HG21	2:M:177:ARG:CZ	2.41	0.50
2:K:270:GLU:CD	2:K:270:GLU:O	2.51	0.49
2:L:270:GLU:O	2:L:270:GLU:CD	2.51	0.49
2:H:195:GLU:OE1	2:K:113:LYS:HD2	2.12	0.49
2:H:267:ILE:O	2:K:173:HIS:CB	2.60	0.49
2:L:107:GLU:OE2	2:L:116:ARG:NH1	2.45	0.49
2:H:148:THR:OG1	2:J:47:MET:CE	2.60	0.49
2:J:107:GLU:OE2	2:J:116:ARG:NH1	2.45	0.49
2:K:107:GLU:OE2	2:K:116:ARG:NH1	2.45	0.49
2:H:172:PRO:O	2:L:191:LYS:HE3	2.11	0.49
2:J:48:GLY:O	2:J:49:GLN:HG2	2.12	0.49
2:J:73:HIS:O	2:J:177:ARG:NH2	2.46	0.49
2:K:167:GLU:OE2	2:L:61:LYS:HG2	2.13	0.49
2:H:197:GLY:CA	2:K:112:PRO:HB3	2.42	0.49
2:H:113:LYS:HD2	2:L:195:GLU:OE1	2.13	0.49
2:K:73:HIS:O	2:K:177:ARG:NH2	2.45	0.49
2:M:107:GLU:OE2	2:M:116:ARG:NH1	2.45	0.49
2:M:73:HIS:O	2:M:177:ARG:NH2	2.46	0.49
2:M:51:ASP:OD1	2:M:52:SER:N	2.46	0.49
2:H:49:GLN:HB2	2:M:169:TYR:OH	2.12	0.49
2:J:51:ASP:OD1	2:J:52:SER:N	2.46	0.49
2:L:73:HIS:O	2:L:177:ARG:NH2	2.46	0.49
2:J:270:GLU:O	2:J:270:GLU:CD	2.51	0.49
2:L:48:GLY:O	2:L:49:GLN:HG2	2.12	0.49
2:H:268:GLY:O	2:L:39:ARG:NH1	2.46	0.48
2:M:270:GLU:O	2:M:270:GLU:CD	2.51	0.48
2:L:51:ASP:OD1	2:L:52:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:HIS:O	2:H:177:ARG:NH2	2.45	0.48
2:L:159:VAL:HG21	2:L:177:ARG:NE	2.29	0.48
2:H:107:GLU:OE2	2:H:116:ARG:NH1	2.45	0.48
2:K:51:ASP:OD1	2:K:52:SER:N	2.46	0.48
2:H:169:TYR:CE2	2:J:64:ILE:HD13	2.49	0.48
2:H:166:TYR:HD2	2:J:64:ILE:HG23	1.79	0.48
2:H:51:ASP:OD1	2:H:52:SER:N	2.46	0.48
2:H:270:GLU:CD	2:H:270:GLU:O	2.51	0.48
2:J:159:VAL:HG21	2:J:177:ARG:NE	2.29	0.48
2:K:267:ILE:O	2:M:173:HIS:CB	2.61	0.48
2:K:159:VAL:HG21	2:K:177:ARG:NE	2.29	0.48
2:M:159:VAL:HG21	2:M:177:ARG:NE	2.29	0.48
2:H:112:PRO:HB3	2:L:197:GLY:CA	2.44	0.47
2:H:159:VAL:HG21	2:H:177:ARG:NE	2.29	0.47
2:H:243:PRO:O	2:H:244:ASP:CB	2.63	0.47
2:J:243:PRO:O	2:J:244:ASP:CB	2.63	0.47
2:H:166:TYR:CD2	2:J:64:ILE:HG23	2.49	0.47
2:M:243:PRO:O	2:M:244:ASP:CB	2.62	0.47
2:L:243:PRO:O	2:L:244:ASP:CB	2.63	0.47
2:J:39:ARG:NH1	2:L:268:GLY:O	2.48	0.47
2:H:61:LYS:O	2:H:65:LEU:HD13	2.15	0.47
2:K:243:PRO:O	2:K:244:ASP:CB	2.63	0.47
2:H:44:MET:HG2	2:M:168:GLY:HA2	1.97	0.47
2:J:61:LYS:O	2:J:65:LEU:HD13	2.15	0.47
2:H:61:LYS:HG2	2:M:167:GLU:OE2	2.15	0.46
2:H:191:LYS:HE3	2:K:172:PRO:O	2.15	0.46
2:K:244:ASP:OD2	2:K:246:GLN:OE1	2.34	0.46
2:L:244:ASP:OD2	2:L:246:GLN:OE1	2.34	0.46
2:M:61:LYS:O	2:M:65:LEU:HD13	2.15	0.46
2:K:61:LYS:O	2:K:65:LEU:HD13	2.15	0.46
1:C:85:SER:OG	1:C:148:TYR:OH	2.24	0.46
2:K:169:TYR:CE2	2:L:64:ILE:HD13	2.51	0.46
2:K:282:ILE:HG22	2:K:290:ARG:HG2	1.98	0.45
2:L:61:LYS:O	2:L:65:LEU:HD13	2.15	0.45
2:M:244:ASP:OD2	2:M:246:GLN:OE1	2.34	0.45
2:J:216:LEU:HD23	2:J:250:ILE:HD11	1.98	0.45
2:L:171:LEU:HD12	2:L:285:CYS:SG	2.57	0.45
2:M:337:TYR:O	2:M:341:ILE:HD12	2.17	0.45
2:H:244:ASP:OD2	2:H:246:GLN:OE1	2.34	0.45
2:H:216:LEU:HD23	2:H:250:ILE:HD11	1.99	0.45
2:J:244:ASP:OD2	2:J:246:GLN:OE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:337:TYR:O	2:J:341:ILE:HD12	2.17	0.45
2:K:171:LEU:HD12	2:K:285:CYS:SG	2.57	0.45
2:M:216:LEU:HD23	2:M:250:ILE:HD11	1.99	0.45
2:L:139:VAL:HG22	2:L:143:TYR:HE2	1.82	0.44
2:L:216:LEU:HD23	2:L:250:ILE:HD11	1.98	0.44
2:K:139:VAL:HG22	2:K:143:TYR:HE2	1.82	0.44
2:L:287:ILE:HG13	2:L:288:ASP:N	2.33	0.44
2:L:337:TYR:O	2:L:341:ILE:HD12	2.17	0.44
2:M:171:LEU:HD12	2:M:285:CYS:SG	2.57	0.44
2:K:75:ILE:CG2	3:N:2:ALA:O	2.65	0.44
2:L:154:ASP:CB	2:L:161:HIS:CE1	3.01	0.44
2:M:154:ASP:CB	2:M:161:HIS:CE1	3.01	0.44
2:H:171:LEU:HD12	2:H:285:CYS:SG	2.57	0.44
2:H:330:ILE:HG22	2:H:332:PRO:HD3	2.00	0.44
2:J:171:LEU:HD12	2:J:285:CYS:SG	2.57	0.44
2:K:216:LEU:HD23	2:K:250:ILE:HD11	1.99	0.44
2:K:337:TYR:O	2:K:341:ILE:HD12	2.17	0.44
2:M:287:ILE:HG13	2:M:288:ASP:N	2.33	0.44
2:K:148:THR:OG1	2:L:47:MET:HE2	2.17	0.44
2:H:287:ILE:HG13	2:H:288:ASP:N	2.33	0.44
2:K:154:ASP:CB	2:K:161:HIS:CE1	3.01	0.44
2:H:154:ASP:CB	2:H:161:HIS:CE1	3.01	0.43
2:L:330:ILE:HG22	2:L:332:PRO:HD3	2.00	0.43
1:E:124:ILE:HG23	1:E:124:ILE:O	2.18	0.43
2:H:337:TYR:O	2:H:341:ILE:HD12	2.17	0.43
2:J:287:ILE:HG13	2:J:288:ASP:N	2.33	0.43
2:K:287:ILE:HG13	2:K:288:ASP:N	2.33	0.43
2:M:330:ILE:HG22	2:M:332:PRO:HD3	2.00	0.43
1:B:124:ILE:HG23	1:B:124:ILE:O	2.18	0.43
2:H:169:TYR:CD2	2:J:64:ILE:CD1	2.98	0.43
2:J:139:VAL:HG22	2:J:143:TYR:HE2	1.82	0.43
2:H:44:MET:CG	2:M:168:GLY:HA2	2.47	0.43
1:A:85:SER:OG	1:A:148:TYR:OH	2.24	0.43
2:H:161:HIS:O	2:H:176:MET:O	2.37	0.43
2:J:154:ASP:CB	2:J:161:HIS:CE1	3.01	0.43
2:K:169:TYR:OH	2:L:49:GLN:HB2	2.19	0.43
2:K:330:ILE:HG22	2:K:332:PRO:HD3	2.00	0.43
2:H:139:VAL:HG22	2:H:143:TYR:HE2	1.82	0.43
2:H:64:ILE:HG23	2:M:166:TYR:CD2	2.53	0.43
2:J:161:HIS:O	2:J:176:MET:O	2.37	0.43
2:L:161:HIS:O	2:L:176:MET:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ILE:HG23	1:C:124:ILE:O	2.19	0.43
1:D:124:ILE:HG23	1:D:124:ILE:O	2.19	0.43
2:H:39:ARG:NH1	2:K:268:GLY:O	2.52	0.43
2:K:39:ARG:NH1	2:M:268:GLY:O	2.50	0.43
2:L:172:PRO:O	2:L:175:ILE:HG22	2.19	0.43
2:M:139:VAL:HG22	2:M:143:TYR:HE2	1.82	0.43
2:K:172:PRO:O	2:K:175:ILE:HG22	2.19	0.42
2:K:166:TYR:CD2	2:L:64:ILE:HG23	2.54	0.42
2:M:161:HIS:O	2:M:176:MET:O	2.37	0.42
2:H:172:PRO:O	2:H:175:ILE:HG22	2.19	0.42
2:J:330:ILE:HG22	2:J:332:PRO:HD3	2.00	0.42
2:J:172:PRO:O	2:J:175:ILE:HG22	2.19	0.42
1:A:124:ILE:HG23	1:A:124:ILE:O	2.18	0.42
2:K:136:ILE:HG22	2:K:138:ALA:H	1.85	0.42
2:H:136:ILE:HG22	2:H:138:ALA:H	1.85	0.42
2:H:351:THR:CG2	2:J:45:VAL:HG12	2.50	0.42
2:L:288:ASP:OD1	2:L:288:ASP:O	2.38	0.42
2:J:288:ASP:O	2:J:288:ASP:OD1	2.38	0.42
2:H:270:GLU:OE1	2:L:202:THR:HA	2.20	0.42
2:M:172:PRO:O	2:M:175:ILE:HG22	2.19	0.42
2:H:288:ASP:O	2:H:288:ASP:OD1	2.38	0.42
2:H:64:ILE:HG23	2:M:166:TYR:HD2	1.85	0.42
2:J:191:LYS:HE3	2:L:172:PRO:O	2.19	0.42
2:M:282:ILE:HG22	2:M:290:ARG:HG2	2.01	0.42
2:M:288:ASP:OD1	2:M:288:ASP:O	2.38	0.42
2:H:273:GLY:O	2:H:277:THR:HG23	2.20	0.42
2:K:161:HIS:O	2:K:176:MET:O	2.37	0.42
2:K:288:ASP:OD1	2:K:288:ASP:O	2.38	0.41
2:K:166:TYR:HD2	2:L:64:ILE:HG23	1.84	0.41
2:H:300:SER:OG	2:H:301:GLY:N	2.54	0.41
2:J:273:GLY:O	2:J:277:THR:HG23	2.20	0.41
2:K:273:GLY:O	2:K:277:THR:HG23	2.20	0.41
2:L:273:GLY:O	2:L:277:THR:HG23	2.20	0.41
2:M:273:GLY:O	2:M:277:THR:HG23	2.20	0.41
2:H:166:TYR:HD2	2:J:64:ILE:CG2	2.33	0.41
2:M:136:ILE:HG22	2:M:138:ALA:H	1.85	0.41
2:J:136:ILE:HG22	2:J:138:ALA:H	1.85	0.41
2:J:197:GLY:CA	2:L:112:PRO:HB3	2.49	0.41
2:H:169:TYR:OH	2:J:49:GLN:HB2	2.21	0.41
2:K:168:GLY:HA2	2:L:44:MET:HG2	2.03	0.41
2:L:300:SER:OG	2:L:301:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:300:SER:OG	2:M:301:GLY:N	2.54	0.41
2:H:197:GLY:O	3:N:3:TRP:HE3	2.04	0.41
2:L:136:ILE:HG22	2:L:138:ALA:H	1.85	0.41
1:E:114:LEU:HD22	1:E:121:LEU:HD11	2.03	0.41
2:L:139:VAL:HG22	2:L:143:TYR:CE2	2.56	0.41
2:K:300:SER:OG	2:K:301:GLY:N	2.54	0.40
1:D:114:LEU:HD22	1:D:121:LEU:HD11	2.03	0.40
2:M:139:VAL:HG22	2:M:143:TYR:CE2	2.56	0.40
1:A:114:LEU:HD22	1:A:121:LEU:HD11	2.03	0.40
2:J:300:SER:OG	2:J:301:GLY:N	2.53	0.40
2:L:197:GLY:O	3:P:3:TRP:HE3	2.04	0.40
2:H:139:VAL:HG22	2:H:143:TYR:CE2	2.56	0.40
2:K:139:VAL:HG22	2:K:143:TYR:CE2	2.56	0.40
2:K:191:LYS:HE3	2:M:172:PRO:O	2.20	0.40
2:K:351:THR:CG2	2:L:45:VAL:HG12	2.51	0.40
2:H:75:ILE:CG2	3:P:2:ALA:O	2.69	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	119/306 (39%)	116 (98%)	3 (2%)	0	100	100
1	B	119/306 (39%)	116 (98%)	3 (2%)	0	100	100
1	C	119/306 (39%)	116 (98%)	3 (2%)	0	100	100
1	D	119/306 (39%)	116 (98%)	3 (2%)	0	100	100
1	E	119/306 (39%)	116 (98%)	3 (2%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
2	J	368/375 (98%)	357 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
2	L	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
2	M	368/375 (98%)	356 (97%)	12 (3%)	0	100	100
3	N	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
3	O	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
3	P	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
All	All	2444/3426 (71%)	2367 (97%)	77 (3%)	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	111/266 (42%)	109 (98%)	2 (2%)	62	84
1	B	111/266 (42%)	109 (98%)	2 (2%)	62	84
1	C	111/266 (42%)	109 (98%)	2 (2%)	62	84
1	D	111/266 (42%)	109 (98%)	2 (2%)	62	84
1	E	111/266 (42%)	109 (98%)	2 (2%)	62	84
2	H	313/318 (98%)	309 (99%)	4 (1%)	71	88
2	J	313/318 (98%)	309 (99%)	4 (1%)	71	88
2	K	313/318 (98%)	309 (99%)	4 (1%)	71	88
2	L	313/318 (98%)	309 (99%)	4 (1%)	71	88
2	M	313/318 (98%)	309 (99%)	4 (1%)	71	88
3	N	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	O	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	P	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	2126/2926 (73%)	2093 (98%)	33 (2%)	68	85

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	96	ARG
1	D	133	ASN
2	H	95	ARG
2	H	161	HIS
2	H	171	LEU
2	H	244	ASP
1	A	96	ARG
1	A	133	ASN
2	J	95	ARG
2	J	161	HIS
2	J	171	LEU
2	J	244	ASP
1	B	96	ARG
1	B	133	ASN
2	K	95	ARG
2	K	161	HIS
2	K	171	LEU
2	K	244	ASP
1	C	96	ARG
1	C	133	ASN
2	L	95	ARG
2	L	161	HIS
2	L	171	LEU
2	L	244	ASP
1	E	96	ARG
1	E	133	ASN
2	M	95	ARG
2	M	161	HIS
2	M	171	LEU
2	M	244	ASP
3	N	7	CYS
3	O	7	CYS
3	P	7	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	133	ASN
2	H	40	HIS
2	H	111	ASN
2	H	137	GLN

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Mol	Chain	Res	Type
1	A	133	ASN
2	J	40	HIS
2	J	137	GLN
1	B	133	ASN
2	K	137	GLN
1	C	133	ASN
2	L	137	GLN
1	E	133	ASN
2	M	137	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	$\# Z  > 2$
3	HYP	N	1	3	7,8,9	1.36	0	5,10,12	1.56	1 (20%)
3	G5G	N	4	3	8,9,10	1.53	2 (25%)	8,12,14	1.12	1 (12%)
3	ALO	N	6	3	6,6,7	0.74	0	6,7,9	1.44	1 (16%)
3	HYP	O	1	3	7,8,9	1.34	0	5,10,12	1.55	1 (20%)
3	G5G	O	4	3	8,9,10	1.54	2 (25%)	8,12,14	1.10	1 (12%)
3	ALO	O	6	3	6,6,7	0.73	0	6,7,9	1.44	1 (16%)
3	HYP	P	1	3	7,8,9	1.35	0	5,10,12	1.55	1 (20%)
3	G5G	P	4	3	8,9,10	1.52	2 (25%)	8,12,14	1.11	1 (12%)
3	ALO	P	6	3	6,6,7	0.71	0	6,7,9	1.43	1 (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
3	HYP	N	1	3	-	0/0/11/13	0/1/1/1
3	G5G	N	4	3	-	0/8/10/12	0/0/0/0
3	ALO	N	6	3	-	0/4/6/8	0/0/0/0
3	HYP	O	1	3	-	0/0/11/13	0/1/1/1
3	G5G	O	4	3	-	0/8/10/12	0/0/0/0
3	ALO	O	6	3	-	0/4/6/8	0/0/0/0
3	HYP	P	1	3	-	0/0/11/13	0/1/1/1
3	G5G	P	4	3	-	0/8/10/12	0/0/0/0
3	ALO	P	6	3	-	0/4/6/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	4	G5G	O1-CG	-2.88	1.40	1.44
3	N	4	G5G	O1-CG	-2.85	1.40	1.44
3	P	4	G5G	O1-CG	-2.81	1.40	1.44
3	P	4	G5G	CA-C	2.40	1.53	1.50
3	N	4	G5G	CA-C	2.41	1.53	1.50
3	O	4	G5G	CA-C	2.42	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	HYP	O-C-CA	-3.42	117.12	125.09
3	P	1	HYP	O-C-CA	-3.40	117.17	125.09
3	O	1	HYP	O-C-CA	-3.40	117.17	125.09
3	O	6	ALO	O-C-CA	-2.93	118.26	125.09
3	N	6	ALO	O-C-CA	-2.91	118.31	125.09
3	P	6	ALO	O-C-CA	-2.87	118.39	125.09
3	N	4	G5G	O-C-CA	-2.18	118.98	124.96
3	P	4	G5G	O-C-CA	-2.17	119.00	124.96
3	O	4	G5G	O-C-CA	-2.17	119.01	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	H	401	5	25,29,29	0.99	1 (4%)	25,45,45	1.95	4 (16%)
4	ADP	J	401	5	25,29,29	0.99	1 (4%)	25,45,45	1.95	4 (16%)
4	ADP	K	401	5	25,29,29	0.98	1 (4%)	25,45,45	1.93	4 (16%)
4	ADP	L	401	5	25,29,29	0.99	1 (4%)	25,45,45	1.96	4 (16%)
4	ADP	M	401	5	25,29,29	0.99	1 (4%)	25,45,45	1.96	4 (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
4	ADP	H	401	5	-	0/12/32/32	0/3/3/3
4	ADP	J	401	5	-	0/12/32/32	0/3/3/3
4	ADP	K	401	5	-	0/12/32/32	0/3/3/3
4	ADP	L	401	5	-	0/12/32/32	0/3/3/3
4	ADP	M	401	5	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	401	ADP	C5-C4	2.97	1.47	1.40
4	M	401	ADP	C5-C4	2.98	1.47	1.40
4	L	401	ADP	C5-C4	2.98	1.47	1.40
4	H	401	ADP	C5-C4	2.99	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	401	ADP	C5-C4	3.00	1.47	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	401	ADP	N3-C2-N1	-7.07	122.81	128.86
4	M	401	ADP	N3-C2-N1	-7.06	122.82	128.86
4	J	401	ADP	N3-C2-N1	-6.99	122.88	128.86
4	H	401	ADP	N3-C2-N1	-6.98	122.89	128.86
4	K	401	ADP	N3-C2-N1	-6.93	122.93	128.86
4	K	401	ADP	PA-O3A-PB	-3.81	119.82	132.63
4	H	401	ADP	PA-O3A-PB	-3.81	119.83	132.63
4	J	401	ADP	PA-O3A-PB	-3.80	119.84	132.63
4	M	401	ADP	PA-O3A-PB	-3.80	119.86	132.63
4	L	401	ADP	PA-O3A-PB	-3.79	119.90	132.63
4	J	401	ADP	C4-C5-N7	-2.96	106.55	109.41
4	M	401	ADP	C4-C5-N7	-2.95	106.56	109.41
4	H	401	ADP	C4-C5-N7	-2.88	106.63	109.41
4	L	401	ADP	C4-C5-N7	-2.88	106.63	109.41
4	K	401	ADP	C4-C5-N7	-2.85	106.66	109.41
4	K	401	ADP	C2-N1-C6	2.08	122.28	118.75
4	M	401	ADP	C2-N1-C6	2.09	122.31	118.75
4	H	401	ADP	C2-N1-C6	2.10	122.32	118.75
4	J	401	ADP	C2-N1-C6	2.11	122.33	118.75
4	L	401	ADP	C2-N1-C6	2.11	122.34	118.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.