



## wwPDB EM Map/Model Validation Report ⓘ

Oct 10, 2016 – 07:23 PM EDT

PDB ID : 5JLF  
EMDB ID: : EMD-8162  
Title : Structure of the F-actin-tropomyosin complex (reprocessed)  
Authors : von der Ecken, J.; Raunser, S.  
Deposited on : 2016-04-27  
Resolution : 3.60 Å(reported)  
Based on PDB ID : 3J8A

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

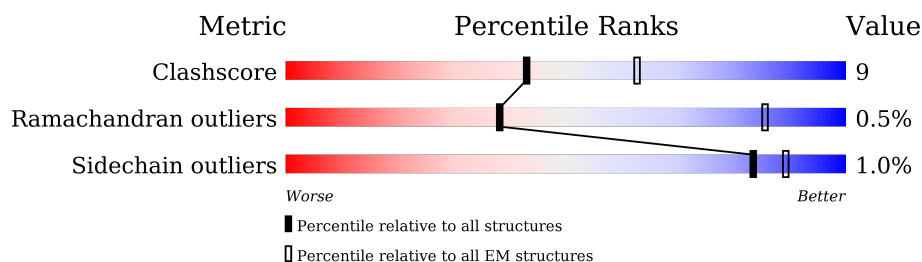
# 1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	375	75% 22% ..
1	B	375	77% 20% ..
1	C	375	77% 21% ..
1	D	375	76% 22% ..
1	E	375	76% 21% ..
2	F	135	99% .
2	G	135	99% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15800 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.

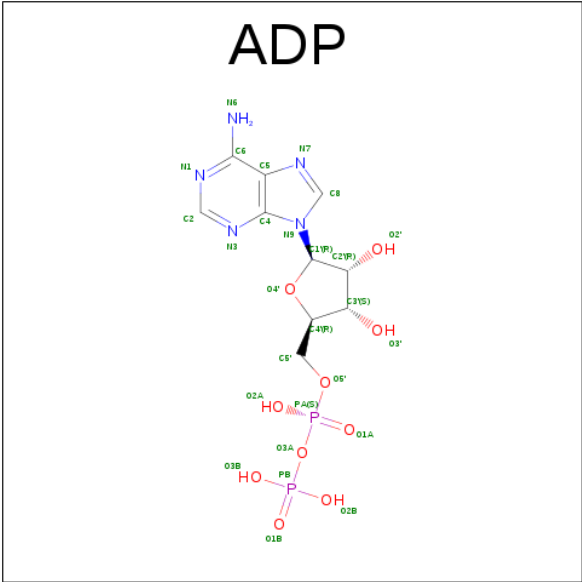
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
1	B	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
1	C	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
1	D	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
1	E	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		

- Molecule 2 is a protein called Tropomyosin Alpha-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	135	Total	C	N	O	0	0
			675	405	135	135		
2	G	135	Total	C	N	O	0	0
			675	405	135	135		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

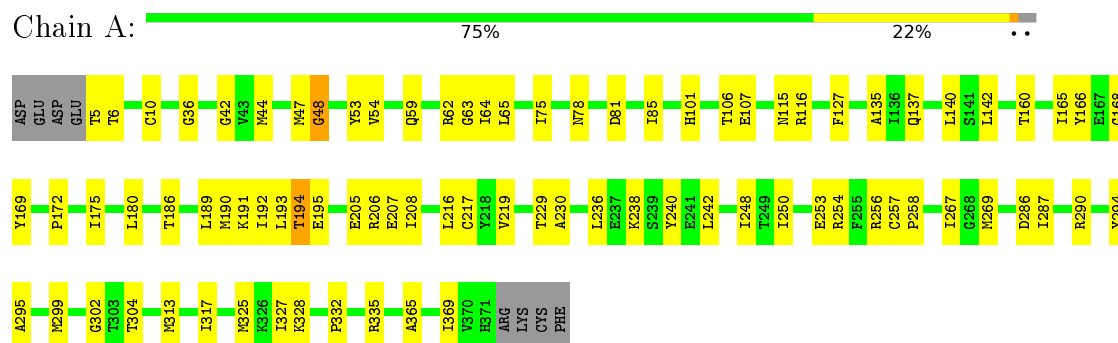
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

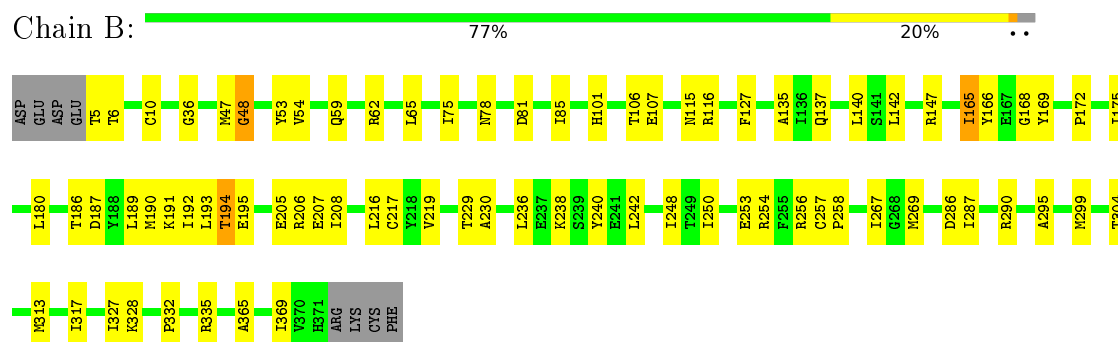
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

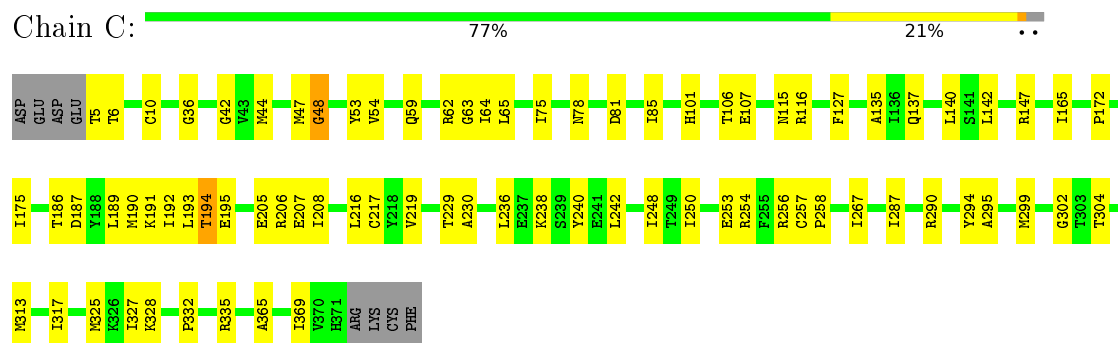
- Molecule 1: Actin, alpha skeletal muscle



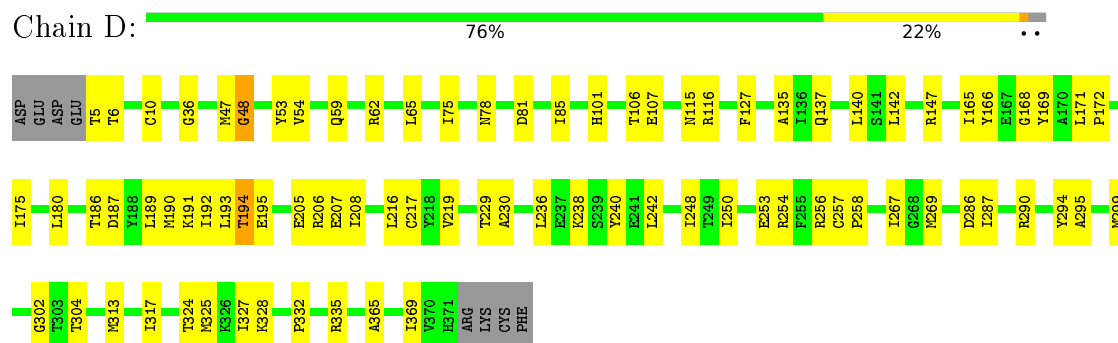
- Molecule 1: Actin, alpha skeletal muscle



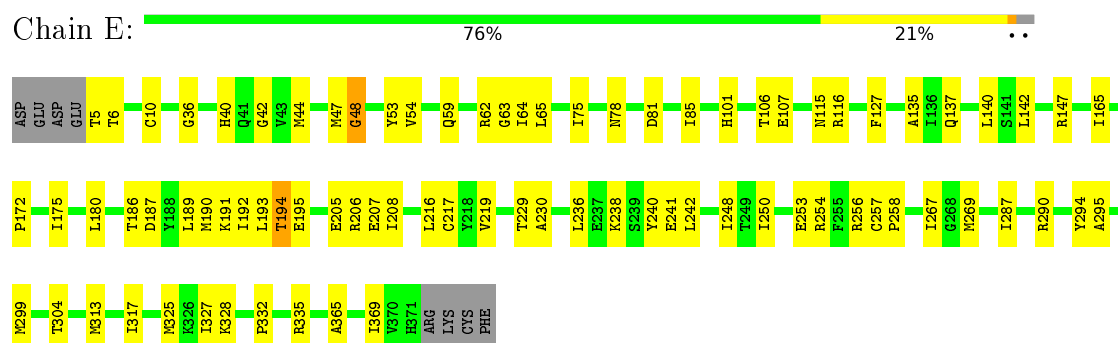
- Molecule 1: Actin, alpha skeletal muscle



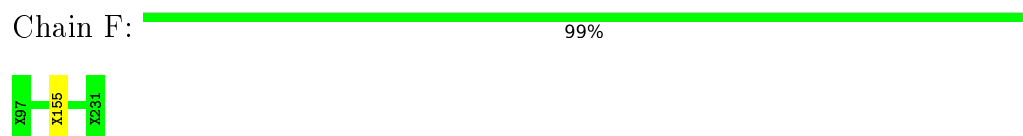
- Molecule 1: Actin, alpha skeletal muscle



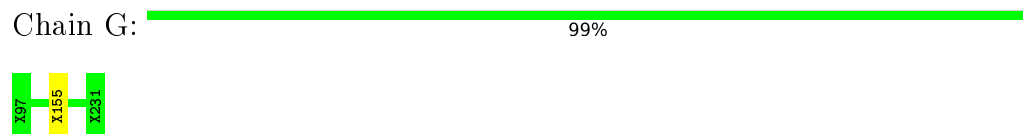
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Tropomyosin Alpha-1



- Molecule 2: Tropomyosin Alpha-1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	91000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	Not provided	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, HIC, 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	0.65	0/2911	0.88	3/3945 (0.1%)
1	B	0.64	0/2911	0.87	4/3945 (0.1%)
1	C	0.64	0/2911	0.87	4/3945 (0.1%)
1	D	0.65	0/2911	0.87	4/3945 (0.1%)
1	E	0.65	0/2911	0.87	4/3945 (0.1%)
All	All	0.65	0/14555	0.87	19/19725 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	62	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	62	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	62	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	62	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	E	62	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	62	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	D	62	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	62	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	E	62	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	E	147	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	147	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	147	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	E	127	PHE	N-CA-C	-5.19	96.98	111.00
1	C	127	PHE	N-CA-C	-5.18	97.02	111.00
1	C	147	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	127	PHE	N-CA-C	-5.14	97.12	111.00
1	D	127	PHE	N-CA-C	-5.11	97.21	111.00
1	B	127	PHE	N-CA-C	-5.07	97.30	111.00



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	2862	0	2832	58	0
1	B	2862	0	2832	52	0
1	C	2862	0	2832	53	0
1	D	2862	0	2832	57	0
1	E	2862	0	2832	57	0
2	F	675	0	137	1	0
2	G	675	0	137	1	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	0	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
All	All	15800	0	14494	261	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 (261) 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:299:MET:HB3	1:B:304:THR:HG21	1.60	0.83
1:C:299:MET:HB3	1:C:304:THR:HG21	1.61	0.83
1:D:299:MET:HB3	1:D:304:THR:HG21	1.61	0.82
1:A:299:MET:HB3	1:A:304:THR:HG21	1.61	0.81
1:E:299:MET:HB3	1:E:304:THR:HG21	1.62	0.80
1:D:216:LEU:HD12	1:D:250:ILE:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD12	1:A:250:ILE:HD11	1.68	0.73
1:C:216:LEU:HD12	1:C:250:ILE:HD11	1.67	0.73
1:D:75:ILE:HA	1:D:115:ASN:HD21	1.54	0.73
1:D:169:TYR:HA	1:E:42:GLY:HA3	1.71	0.73
1:E:216:LEU:HD12	1:E:250:ILE:HD11	1.68	0.73
1:B:216:LEU:HD12	1:B:250:ILE:HD11	1.69	0.72
1:E:75:ILE:HA	1:E:115:ASN:HD21	1.55	0.71
1:B:75:ILE:HA	1:B:115:ASN:HD21	1.56	0.71
1:C:75:ILE:HA	1:C:115:ASN:HD21	1.56	0.71
1:A:75:ILE:HA	1:A:115:ASN:HD21	1.54	0.70
1:D:166:TYR:HB3	1:E:64:ILE:HD11	1.73	0.70
1:E:142:LEU:HD22	1:E:165:ILE:HG21	1.73	0.69
1:C:142:LEU:HD22	1:C:165:ILE:HG21	1.73	0.69
1:A:142:LEU:HD22	1:A:165:ILE:HG21	1.73	0.68
1:D:142:LEU:HD22	1:D:165:ILE:HG21	1.75	0.68
1:A:166:TYR:HB3	1:C:64:ILE:HD11	1.74	0.68
1:B:190:MET:CE	1:B:206:ARG:HG2	2.24	0.68
1:C:190:MET:CE	1:C:206:ARG:HG2	2.24	0.68
1:B:142:LEU:HD22	1:B:165:ILE:HG21	1.75	0.67
1:E:190:MET:CE	1:E:206:ARG:HG2	2.24	0.67
1:D:190:MET:CE	1:D:206:ARG:HG2	2.24	0.67
1:A:64:ILE:HD11	1:B:166:TYR:HB3	1.77	0.66
1:A:190:MET:CE	1:A:206:ARG:HG2	2.25	0.66
1:A:169:TYR:HA	1:C:42:GLY:HA3	1.78	0.65
1:A:106:THR:CG2	1:A:137:GLN:HG2	2.30	0.62
1:A:42:GLY:HA3	1:B:169:TYR:HA	1.82	0.62
1:D:106:THR:CG2	1:D:137:GLN:HG2	2.30	0.61
1:D:168:GLY:HA2	1:E:44:MET:HG3	1.81	0.61
1:E:106:THR:CG2	1:E:137:GLN:HG2	2.31	0.61
1:D:286:ASP:OD2	1:E:63:GLY:O	2.18	0.61
1:B:365:ALA:HB1	1:B:369:ILE:HG21	1.83	0.60
1:C:365:ALA:HB1	1:C:369:ILE:HG21	1.83	0.60
1:B:106:THR:CG2	1:B:137:GLN:HG2	2.32	0.60
1:A:365:ALA:HB1	1:A:369:ILE:HG21	1.83	0.60
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.84	0.60
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.84	0.60
1:C:106:THR:CG2	1:C:137:GLN:HG2	2.32	0.59
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.85	0.59
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.85	0.58
1:E:365:ALA:HB1	1:E:369:ILE:HG21	1.83	0.58
1:A:216:LEU:HD11	1:A:240:TYR:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD11	1:B:240:TYR:HB2	1.86	0.58
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.86	0.58
1:D:365:ALA:HB1	1:D:369:ILE:HG21	1.84	0.58
1:D:189:LEU:O	1:D:193:LEU:HB2	2.04	0.58
1:D:216:LEU:HD11	1:D:240:TYR:HB2	1.85	0.57
1:A:189:LEU:O	1:A:193:LEU:HB2	2.04	0.57
1:E:216:LEU:HD11	1:E:240:TYR:HB2	1.86	0.57
1:B:172:PRO:HA	1:B:175:ILE:HD12	1.87	0.57
1:C:216:LEU:HD11	1:C:240:TYR:HB2	1.87	0.57
1:E:189:LEU:O	1:E:193:LEU:HB2	2.04	0.57
1:B:189:LEU:O	1:B:193:LEU:HB2	2.05	0.57
1:C:189:LEU:O	1:C:193:LEU:HB2	2.04	0.56
1:C:54:VAL:HG23	1:C:85:ILE:HG22	1.87	0.56
1:E:172:PRO:HA	1:E:175:ILE:HD12	1.86	0.56
1:D:190:MET:HE1	1:D:206:ARG:HG2	1.86	0.56
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.87	0.55
1:C:190:MET:HE1	1:C:206:ARG:HG2	1.87	0.55
1:A:192:ILE:O	1:A:195:GLU:HG2	2.07	0.55
1:D:54:VAL:HG23	1:D:85:ILE:HG22	1.87	0.55
1:C:172:PRO:HA	1:C:175:ILE:HD12	1.88	0.54
1:E:54:VAL:HG23	1:E:85:ILE:HG22	1.88	0.54
1:B:192:ILE:O	1:B:195:GLU:HG2	2.07	0.54
1:A:54:VAL:HG23	1:A:85:ILE:HG22	1.88	0.54
1:D:192:ILE:O	1:D:195:GLU:HG2	2.07	0.54
1:E:192:ILE:O	1:E:195:GLU:HG2	2.07	0.54
1:A:168:GLY:HA2	1:C:44:MET:HG3	1.89	0.54
1:D:267:ILE:O	1:D:267:ILE:HG22	2.07	0.54
1:B:54:VAL:HG23	1:B:85:ILE:HG22	1.89	0.54
1:C:192:ILE:O	1:C:195:GLU:HG2	2.08	0.53
1:A:189:LEU:HA	1:A:192:ILE:HG22	1.90	0.53
1:B:189:LEU:HA	1:B:192:ILE:HG22	1.90	0.53
1:C:304:THR:HG22	1:C:304:THR:O	2.08	0.53
1:D:172:PRO:HA	1:D:175:ILE:HD12	1.89	0.53
1:D:189:LEU:HA	1:D:192:ILE:HG22	1.90	0.53
1:E:189:LEU:HA	1:E:192:ILE:HG22	1.90	0.53
1:E:190:MET:HE1	1:E:206:ARG:HG2	1.90	0.53
1:A:267:ILE:O	1:A:267:ILE:HG22	2.09	0.53
1:C:189:LEU:HA	1:C:192:ILE:HG22	1.90	0.53
1:A:190:MET:HE1	1:A:206:ARG:HG2	1.90	0.53
1:B:304:THR:HG22	1:B:304:THR:O	2.08	0.53
1:D:169:TYR:HA	1:E:42:GLY:CA	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HG22	1:A:304:THR:O	2.08	0.52
1:C:191:LYS:O	1:C:194:THR:HG22	2.10	0.52
1:B:5:THR:O	1:B:101:HIS:ND1	2.42	0.52
1:B:191:LYS:O	1:B:194:THR:HG22	2.10	0.52
1:B:190:MET:HE1	1:B:206:ARG:HG2	1.90	0.52
1:E:191:LYS:O	1:E:194:THR:HG22	2.10	0.52
1:D:304:THR:O	1:D:304:THR:HG22	2.09	0.52
1:B:267:ILE:HG22	1:B:267:ILE:O	2.09	0.51
1:A:191:LYS:O	1:A:194:THR:HG22	2.11	0.51
1:D:191:LYS:O	1:D:194:THR:HG22	2.10	0.51
1:D:317:ILE:HG22	1:D:327:ILE:HD13	1.91	0.51
1:B:190:MET:HE1	1:B:206:ARG:HA	1.93	0.51
1:E:304:THR:HG22	1:E:304:THR:O	2.09	0.51
1:E:190:MET:HE1	1:E:206:ARG:HA	1.92	0.51
1:C:267:ILE:HG22	1:C:267:ILE:O	2.09	0.51
1:E:5:THR:O	1:E:101:HIS:ND1	2.43	0.51
1:E:267:ILE:O	1:E:267:ILE:HG22	2.10	0.51
1:A:190:MET:HE1	1:A:206:ARG:HA	1.93	0.50
1:A:44:MET:HG3	1:B:168:GLY:HA2	1.93	0.50
1:A:5:THR:O	1:A:101:HIS:ND1	2.44	0.50
1:C:190:MET:HE1	1:C:206:ARG:HA	1.94	0.50
1:C:317:ILE:HG22	1:C:327:ILE:HD13	1.93	0.50
1:D:5:THR:O	1:D:101:HIS:ND1	2.42	0.50
1:A:219:VAL:HG22	1:A:258:PRO:HB2	1.93	0.50
1:C:5:THR:O	1:C:101:HIS:ND1	2.44	0.50
1:A:142:LEU:CD2	1:A:165:ILE:HG21	2.42	0.50
1:B:236:LEU:O	1:B:254:ARG:NH2	2.45	0.50
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.93	0.49
1:C:332:PRO:O	1:C:335:ARG:HB3	2.12	0.49
1:A:236:LEU:O	1:A:254:ARG:NH2	2.45	0.49
1:B:317:ILE:HG22	1:B:327:ILE:HD13	1.93	0.49
1:D:313:MET:O	1:D:317:ILE:HD12	2.13	0.49
1:A:169:TYR:HA	1:C:42:GLY:CA	2.43	0.49
1:B:219:VAL:HG22	1:B:258:PRO:HB2	1.95	0.49
1:B:253:GLU:HA	1:B:256:ARG:HG2	1.95	0.49
1:D:219:VAL:HG22	1:D:258:PRO:HB2	1.95	0.49
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.95	0.49
1:B:142:LEU:CD2	1:B:165:ILE:HG21	2.43	0.49
1:D:236:LEU:O	1:D:254:ARG:NH2	2.45	0.49
1:C:236:LEU:O	1:C:254:ARG:NH2	2.46	0.49
1:C:313:MET:O	1:C:317:ILE:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:MET:HE1	1:D:206:ARG:HA	1.95	0.49
1:C:253:GLU:HA	1:C:256:ARG:HG2	1.95	0.49
1:C:59:GLN:NE2	1:C:207:GLU:OE1	2.45	0.49
1:E:205:GLU:HA	1:E:208:ILE:HD12	1.95	0.49
1:B:313:MET:O	1:B:317:ILE:HD12	2.13	0.48
1:E:332:PRO:O	1:E:335:ARG:HB3	2.13	0.48
1:B:205:GLU:HA	1:B:208:ILE:HD12	1.94	0.48
1:D:142:LEU:CD2	1:D:165:ILE:HG21	2.43	0.48
1:E:313:MET:O	1:E:317:ILE:HD12	2.13	0.48
1:E:236:LEU:O	1:E:254:ARG:NH2	2.46	0.48
1:A:313:MET:O	1:A:317:ILE:HD12	2.12	0.48
1:B:332:PRO:O	1:B:335:ARG:HB3	2.12	0.48
1:D:267:ILE:O	1:D:267:ILE:CG2	2.61	0.48
1:D:332:PRO:O	1:D:335:ARG:HB3	2.12	0.48
1:A:253:GLU:HA	1:A:256:ARG:HG2	1.96	0.48
1:D:253:GLU:HA	1:D:256:ARG:HG2	1.96	0.48
1:D:205:GLU:HA	1:D:208:ILE:HD12	1.95	0.48
1:A:332:PRO:O	1:A:335:ARG:HB3	2.13	0.48
1:D:59:GLN:NE2	1:D:207:GLU:OE1	2.47	0.47
1:E:317:ILE:HG22	1:E:327:ILE:HD13	1.94	0.47
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.95	0.47
1:C:205:GLU:HA	1:C:208:ILE:HD12	1.95	0.47
1:E:253:GLU:HA	1:E:256:ARG:HG2	1.96	0.47
1:A:59:GLN:NE2	1:A:207:GLU:OE1	2.48	0.47
1:C:219:VAL:HG22	1:C:258:PRO:HB2	1.96	0.47
1:C:295:ALA:O	1:C:328:LYS:O	2.32	0.47
1:A:295:ALA:O	1:A:328:LYS:O	2.32	0.47
1:D:36:GLY:HA3	1:D:65:LEU:HD13	1.97	0.47
1:E:217:CYS:HA	1:E:254:ARG:HG2	1.97	0.47
1:A:36:GLY:HA3	1:A:65:LEU:HD13	1.96	0.46
1:B:217:CYS:HA	1:B:254:ARG:HG2	1.97	0.46
1:B:36:GLY:HA3	1:B:65:LEU:HD13	1.97	0.46
1:C:53:TYR:HD2	1:C:65:LEU:HD21	1.80	0.46
1:E:36:GLY:HA3	1:E:65:LEU:HD13	1.97	0.46
1:B:295:ALA:O	1:B:328:LYS:O	2.33	0.46
1:D:295:ALA:O	1:D:328:LYS:O	2.33	0.46
1:B:59:GLN:NE2	1:B:207:GLU:OE1	2.49	0.46
1:B:190:MET:HE3	1:B:206:ARG:HG2	1.97	0.46
1:B:53:TYR:HD2	1:B:65:LEU:HD21	1.81	0.46
1:E:142:LEU:CD2	1:E:165:ILE:HG21	2.42	0.46
1:A:63:GLY:O	1:B:286:ASP:OD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ILE:O	1:C:267:ILE:CG2	2.63	0.46
1:C:36:GLY:HA3	1:C:65:LEU:HD13	1.96	0.46
1:A:267:ILE:CG2	1:A:267:ILE:O	2.64	0.46
1:C:217:CYS:HA	1:C:254:ARG:HG2	1.98	0.46
1:E:59:GLN:NE2	1:E:207:GLU:OE1	2.49	0.46
1:E:295:ALA:O	1:E:328:LYS:O	2.34	0.45
1:A:53:TYR:HD2	1:A:65:LEU:HD21	1.81	0.45
1:C:142:LEU:CD2	1:C:165:ILE:HG21	2.42	0.45
1:D:53:TYR:HD2	1:D:65:LEU:HD21	1.80	0.45
1:B:267:ILE:CG2	1:B:267:ILE:O	2.63	0.45
1:E:190:MET:HE3	1:E:206:ARG:HG2	1.99	0.45
1:E:53:TYR:HD2	1:E:65:LEU:HD21	1.82	0.45
2:F:155:UNK:HA	2:G:155:UNK:HA	1.98	0.45
1:C:107:GLU:OE2	1:C:116:ARG:NE	2.50	0.45
1:D:217:CYS:HA	1:D:254:ARG:HG2	1.98	0.45
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.98	0.45
1:A:217:CYS:HA	1:A:254:ARG:HG2	1.98	0.45
1:A:216:LEU:HD22	1:A:238:LYS:HD2	1.99	0.45
1:A:242:LEU:HD13	1:A:248:ILE:HG12	1.99	0.45
1:D:107:GLU:OE2	1:D:116:ARG:NE	2.50	0.45
1:D:287:ILE:HA	1:D:290:ARG:HD3	1.99	0.45
1:E:287:ILE:HA	1:E:290:ARG:HD3	1.99	0.45
1:E:294:TYR:HB2	1:E:325:MET:HE1	1.99	0.45
1:C:287:ILE:HA	1:C:290:ARG:HD3	1.98	0.45
1:D:135:ALA:HB1	1:D:140:LEU:HD11	1.99	0.44
1:E:267:ILE:O	1:E:267:ILE:CG2	2.64	0.44
1:E:242:LEU:HD13	1:E:248:ILE:HG12	1.98	0.44
1:B:216:LEU:HD22	1:B:238:LYS:HD2	1.99	0.44
1:E:135:ALA:HB1	1:E:140:LEU:HD11	1.99	0.44
1:B:107:GLU:OE2	1:B:116:ARG:NE	2.50	0.44
1:B:242:LEU:HD13	1:B:248:ILE:HG12	1.99	0.44
1:C:242:LEU:HD13	1:C:248:ILE:HG12	2.00	0.44
1:A:107:GLU:OE2	1:A:116:ARG:NE	2.50	0.44
1:C:135:ALA:HB1	1:C:140:LEU:HD11	1.99	0.44
1:B:135:ALA:HB1	1:B:140:LEU:HD11	2.00	0.44
1:D:294:TYR:HB2	1:D:325:MET:HE1	2.00	0.44
1:D:242:LEU:HD13	1:D:248:ILE:HG12	1.99	0.44
1:D:324:THR:HG21	1:E:241:GLU:OE2	2.17	0.44
1:A:287:ILE:HA	1:A:290:ARG:HD3	1.99	0.43
1:C:294:TYR:HB2	1:C:325:MET:HE1	2.00	0.43
1:A:286:ASP:OD2	1:C:63:GLY:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:GLU:OE2	1:E:116:ARG:NE	2.52	0.43
1:A:47:MET:O	1:A:48:GLY:C	2.57	0.43
1:A:42:GLY:CA	1:B:169:TYR:HA	2.46	0.43
1:B:287:ILE:HA	1:B:290:ARG:HD3	2.00	0.43
1:C:229:THR:HG23	1:C:236:LEU:HD11	2.00	0.43
1:E:47:MET:O	1:E:48:GLY:C	2.57	0.43
1:D:47:MET:O	1:D:48:GLY:C	2.57	0.43
1:B:230:ALA:HA	1:B:236:LEU:HD12	2.01	0.42
1:B:47:MET:O	1:B:48:GLY:C	2.57	0.42
1:E:229:THR:HG23	1:E:236:LEU:HD11	2.00	0.42
1:B:78:ASN:ND2	1:B:81:ASP:OD2	2.52	0.42
1:A:230:ALA:HA	1:A:236:LEU:HD12	2.00	0.42
1:C:216:LEU:HD22	1:C:238:LYS:HD2	2.01	0.42
1:C:78:ASN:ND2	1:C:81:ASP:OD2	2.52	0.42
1:D:78:ASN:ND2	1:D:81:ASP:OD2	2.53	0.42
1:E:230:ALA:HA	1:E:236:LEU:HD12	2.00	0.42
1:B:229:THR:HG23	1:B:236:LEU:HD11	2.01	0.42
1:C:47:MET:O	1:C:48:GLY:C	2.57	0.42
1:D:171:LEU:CD2	1:E:40:HIS:CD2	3.03	0.42
1:A:229:THR:HG23	1:A:236:LEU:HD11	2.01	0.42
1:E:78:ASN:ND2	1:E:81:ASP:OD2	2.53	0.42
1:C:190:MET:HE3	1:C:206:ARG:HG2	2.00	0.42
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.53	0.42
1:D:229:THR:HG23	1:D:236:LEU:HD11	2.00	0.42
1:D:230:ALA:HA	1:D:236:LEU:HD12	2.01	0.42
1:E:216:LEU:HD22	1:E:238:LYS:HD2	2.01	0.42
1:A:294:TYR:HB2	1:A:325:MET:HE1	2.02	0.41
1:C:302:GLY:HA3	3:C:401:ADP:O5'	2.21	0.41
1:D:216:LEU:HD22	1:D:238:LYS:HD2	2.01	0.41
1:A:160:THR:OG1	1:A:180:LEU:O	2.36	0.41
1:C:230:ALA:HA	1:C:236:LEU:HD12	2.01	0.41
1:D:302:GLY:HA3	3:D:401:ADP:O5'	2.19	0.41
1:A:302:GLY:HA3	3:A:401:ADP:O5'	2.21	0.41
1:D:257:CYS:CB	1:D:258:PRO:HD3	2.50	0.41
1:A:180:LEU:HG	1:A:269:MET:CE	2.51	0.41
1:E:187:ASP:O	1:E:190:MET:HB3	2.21	0.41
1:D:190:MET:HE3	1:D:206:ARG:HG2	2.02	0.41
1:A:257:CYS:CB	1:A:258:PRO:HD3	2.50	0.41
1:B:180:LEU:HG	1:B:269:MET:CE	2.51	0.41
1:C:257:CYS:CB	1:C:258:PRO:HD3	2.51	0.41
1:E:365:ALA:HB1	1:E:369:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:O	1:B:190:MET:HB3	2.20	0.41
1:E:205:GLU:N	1:E:205:GLU:OE1	2.54	0.41
1:E:180:LEU:HG	1:E:269:MET:CE	2.51	0.40
1:D:180:LEU:HG	1:D:269:MET:CE	2.51	0.40
1:D:187:ASP:O	1:D:190:MET:HB3	2.22	0.40
1:B:205:GLU:N	1:B:205:GLU:OE1	2.55	0.40
1:C:187:ASP:O	1:C:190:MET:HB3	2.21	0.40
1:D:365:ALA:HB1	1:D:369:ILE:CG2	2.51	0.40
1:E:257:CYS:CB	1:E:258:PRO:HD3	2.51	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	364/375 (97%)	350 (96%)	12 (3%)	2 (0%)	34	77
1	B	364/375 (97%)	351 (96%)	11 (3%)	2 (0%)	34	77
1	C	364/375 (97%)	351 (96%)	11 (3%)	2 (0%)	34	77
1	D	364/375 (97%)	351 (96%)	11 (3%)	2 (0%)	34	77
1	E	364/375 (97%)	350 (96%)	12 (3%)	2 (0%)	34	77
All	All	1820/1875 (97%)	1753 (96%)	57 (3%)	10 (0%)	38	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLY
1	B	48	GLY
1	C	48	GLY
1	D	48	GLY
1	E	48	GLY

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Mol	Chain	Res	Type
1	A	6	THR
1	B	6	THR
1	C	6	THR
1	D	6	THR
1	E	6	THR

### 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	309/317 (98%)	306 (99%)	3 (1%)	82	93
1	B	309/317 (98%)	305 (99%)	4 (1%)	76	91
1	C	309/317 (98%)	306 (99%)	3 (1%)	82	93
1	D	309/317 (98%)	306 (99%)	3 (1%)	82	93
1	E	309/317 (98%)	306 (99%)	3 (1%)	82	93
All	All	1545/1585 (98%)	1529 (99%)	16 (1%)	83	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	186	THR
1	A	194	THR
1	B	10	CYS
1	B	165	ILE
1	B	186	THR
1	B	194	THR
1	C	10	CYS
1	C	186	THR
1	C	194	THR
1	D	10	CYS
1	D	186	THR
1	D	194	THR
1	E	10	CYS

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Mol	Chain	Res	Type
1	E	186	THR
1	E	194	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	88	HIS
1	A	92	ASN
1	A	115	ASN
1	B	88	HIS
1	B	92	ASN
1	B	115	ASN
1	C	12	ASN
1	C	88	HIS
1	C	92	ASN
1	C	115	ASN
1	D	12	ASN
1	D	88	HIS
1	D	92	ASN
1	D	115	ASN
1	E	40	HIS
1	E	88	HIS
1	E	92	ASN
1	E	115	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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
1	HIC	A	73	1	6,11,12	1.09	0	6,14,16	0.74	0
1	HIC	B	73	1	6,11,12	1.07	0	6,14,16	0.76	0
1	HIC	C	73	1	6,11,12	1.21	0	6,14,16	0.73	0
1	HIC	D	73	1	6,11,12	1.04	0	6,14,16	0.80	0
1	HIC	E	73	1	6,11,12	1.03	0	6,14,16	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1
1	HIC	B	73	1	-	0/4/6/8	0/1/1/1
1	HIC	C	73	1	-	0/4/6/8	0/1/1/1
1	HIC	D	73	1	-	0/4/6/8	0/1/1/1
1	HIC	E	73	1	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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
3	ADP	A	401	4	24,29,29	1.13	1 (4%)	23,45,45	1.79	4 (17%)
3	ADP	B	401	4	24,29,29	1.08	1 (4%)	23,45,45	1.79	4 (17%)
3	ADP	C	401	4	24,29,29	1.01	1 (4%)	23,45,45	1.81	4 (17%)
3	ADP	D	401	4	24,29,29	1.15	2 (8%)	23,45,45	1.73	4 (17%)
3	ADP	E	401	4	24,29,29	1.07	1 (4%)	23,45,45	1.87	4 (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
3	ADP	A	401	4	-	0/12/32/32	0/3/3/3
3	ADP	B	401	4	-	0/12/32/32	0/3/3/3
3	ADP	C	401	4	-	0/12/32/32	0/3/3/3
3	ADP	D	401	4	-	0/12/32/32	0/3/3/3
3	ADP	E	401	4	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	C2-N3	2.20	1.36	1.32
3	C	401	ADP	C5-C4	3.22	1.47	1.40
3	E	401	ADP	C5-C4	3.43	1.48	1.40
3	B	401	ADP	C5-C4	3.43	1.48	1.40
3	A	401	ADP	C5-C4	3.56	1.48	1.40
3	D	401	ADP	C5-C4	3.66	1.48	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	ADP	N3-C2-N1	-6.70	123.61	128.87
3	C	401	ADP	N3-C2-N1	-6.53	123.74	128.87
3	A	401	ADP	N3-C2-N1	-6.21	123.99	128.87
3	B	401	ADP	N3-C2-N1	-6.12	124.07	128.87
3	D	401	ADP	N3-C2-N1	-5.88	124.25	128.87
3	D	401	ADP	C1'-N9-C4	-2.66	123.84	126.81
3	A	401	ADP	C1'-N9-C4	-2.40	124.12	126.81
3	E	401	ADP	C1'-N9-C4	-2.33	124.21	126.81
3	B	401	ADP	C1'-N9-C4	-2.14	124.42	126.81
3	C	401	ADP	C1'-N9-C4	-2.12	124.44	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C4'-O4'-C1'	2.12	111.89	109.64
3	C	401	ADP	C4'-O4'-C1'	2.31	112.09	109.64
3	D	401	ADP	O3B-PB-O2B	2.35	116.07	107.44
3	E	401	ADP	C4'-O4'-C1'	2.40	112.18	109.64
3	A	401	ADP	C4'-O4'-C1'	2.41	112.20	109.64
3	A	401	ADP	O3B-PB-O2B	2.45	116.43	107.44
3	B	401	ADP	C4'-O4'-C1'	2.60	112.40	109.64
3	C	401	ADP	O3B-PB-O2B	2.64	117.12	107.44
3	E	401	ADP	O3B-PB-O2B	2.67	117.25	107.44
3	B	401	ADP	O3B-PB-O2B	2.68	117.29	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	1	0
3	C	401	ADP	1	0
3	D	401	ADP	1	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.