



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:34 PM UTC

PDB ID : 3DWL / pdb_00003dwl
Title : Crystal Structure of Fission Yeast Arp2/3 Complex Lacking the Arp2 Subunit
Authors : Nolen, B.J.; Pollard, T.D.
Deposited on : 2008-07-22
Resolution : 3.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

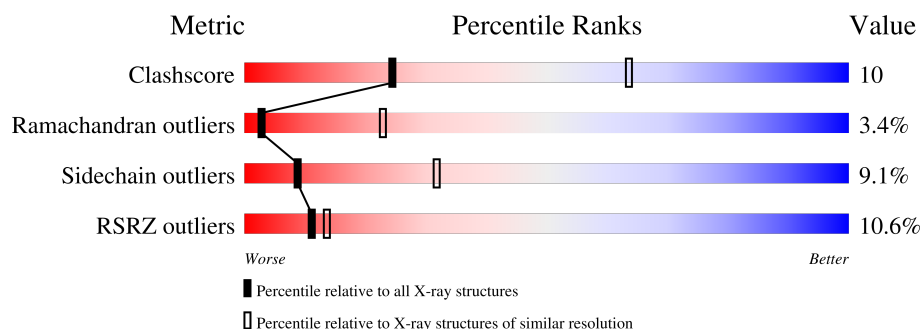
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	5% 62% 19% • 17%
1	B	427	6% 65% 16% • 17%
2	C	377	11% 64% 21% • 11%
2	H	377	18% 65% 21% • 11%
3	D	317	4% 64% 19% • 14%
3	I	317	6% 63% 21% • 14%
4	E	174	15% 27% 9% • 64%

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Mol	Chain	Length	Quality of chain
4	J	174	
5	F	168	
5	K	168	
6	G	152	
6	L	152	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	1	0	0
			2555	1617	432	496	10			
1	B	355	Total	C	N	O	S	1	0	0
			2556	1617	432	497	10			

- Molecule 2 is a protein called Actin-related protein 2/3 complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	336	Total	C	N	O	S	0	0	0
			2252	1413	402	432	5			
2	H	337	Total	C	N	O	S	0	0	0
			2262	1418	403	436	5			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2028	1302	350	368	8			
3	I	272	Total	C	N	O	S	0	0	0
			2028	1302	350	368	8			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	63	Total	C	N	O	S	0	0	0
			397	249	71	73	4			
4	J	63	Total	C	N	O	S	0	0	0
			397	249	71	73	4			

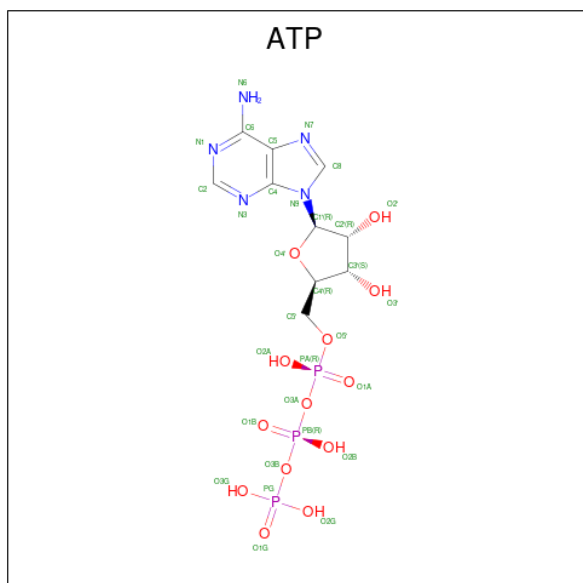
- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	166	Total	C	N	O	S	1	0	0
			1294	825	215	247	7			
5	K	166	Total	C	N	O	S	1	0	0
			1294	825	215	247	7			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	114	Total	C	N	O	S	0	0	0
			790	497	136	155	2			
6	L	114	Total	C	N	O	S	0	0	0
			790	497	136	155	2			

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

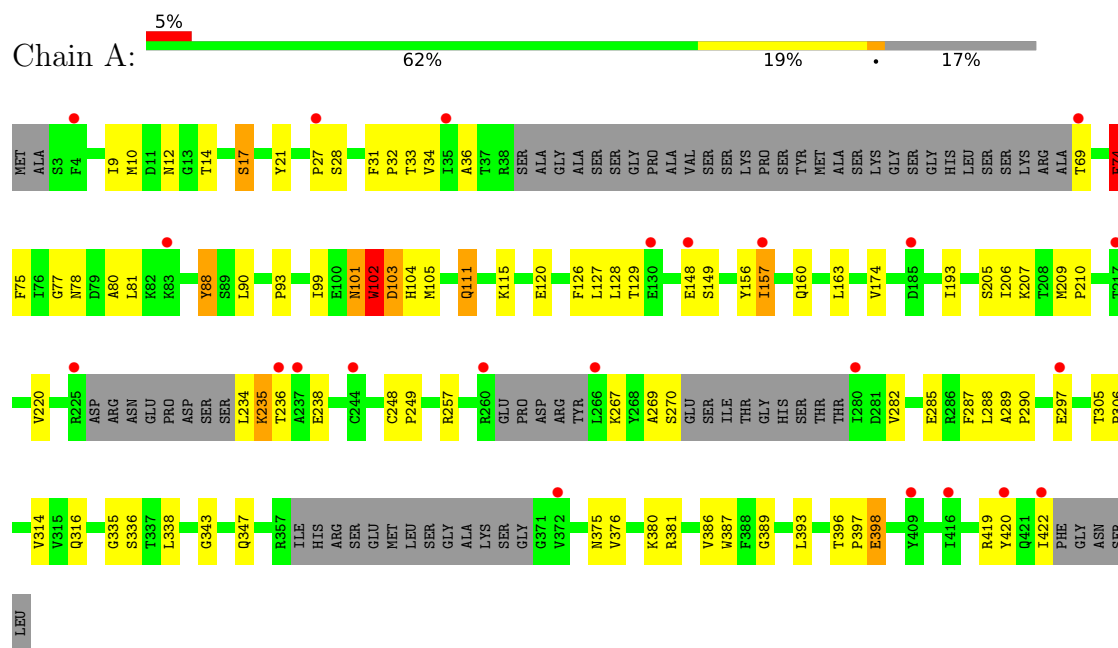


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

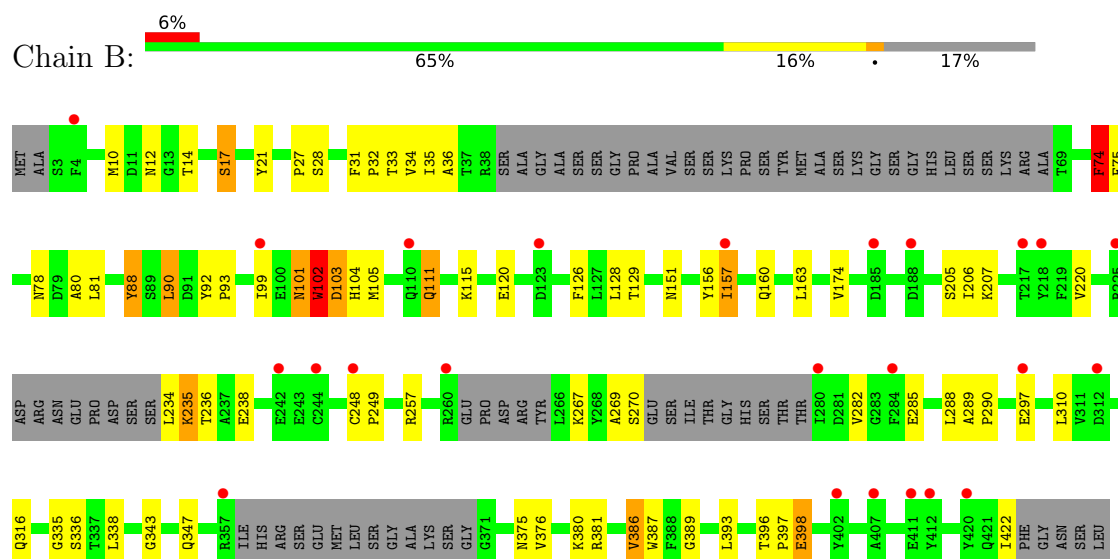
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

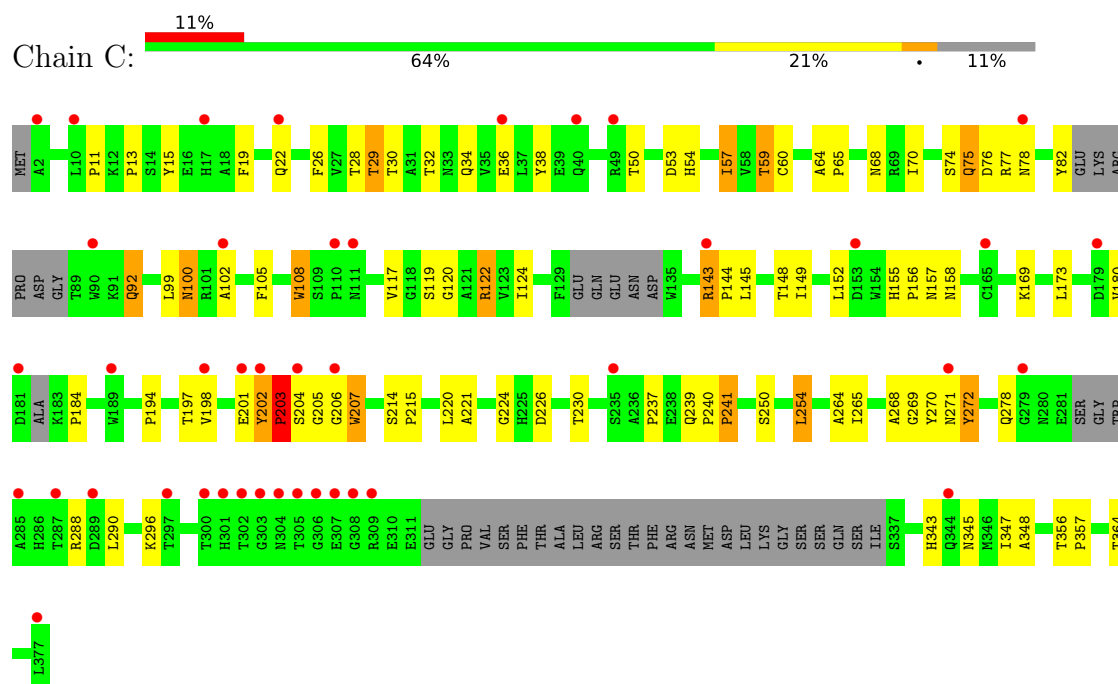
• Molecule 1: Actin-related protein 3



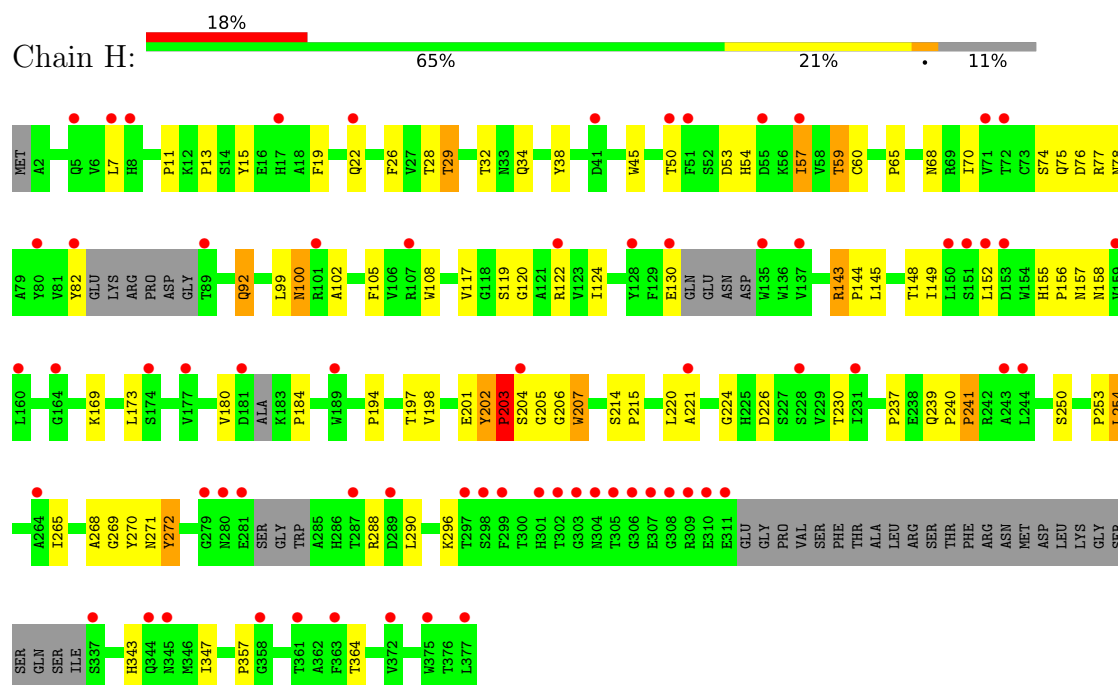
• Molecule 1: Actin-related protein 3



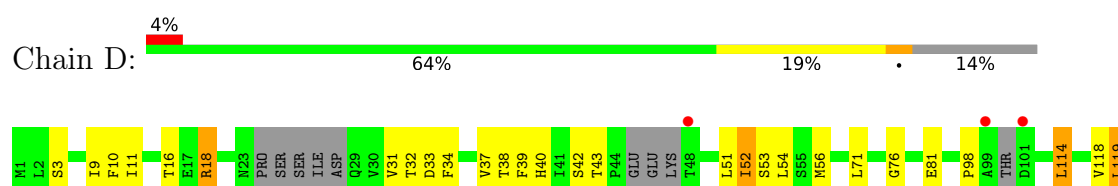
• Molecule 2: Actin-related protein 2/3 complex subunit 1

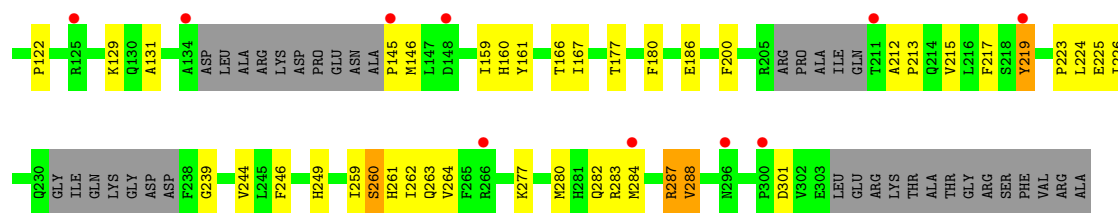


• Molecule 2: Actin-related protein 2/3 complex subunit 1

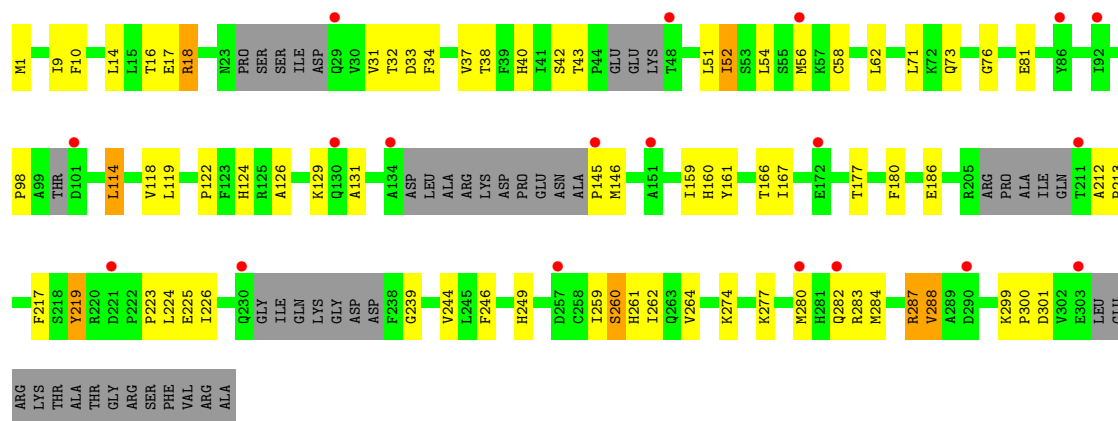


• Molecule 3: Actin-related protein 2/3 complex subunit 2

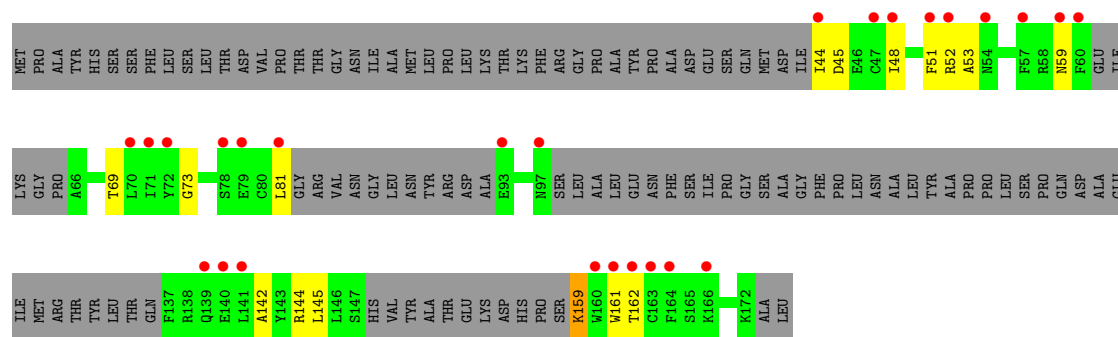




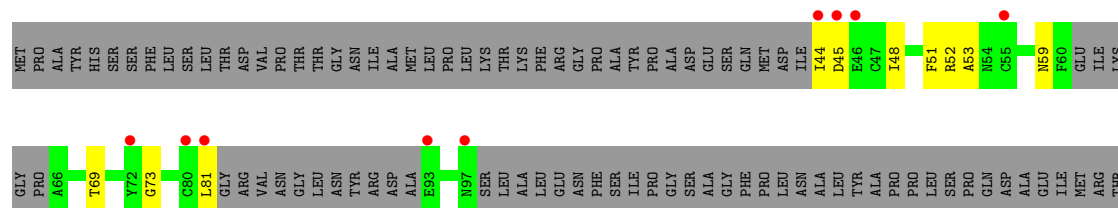
• Molecule 3: Actin-related protein 2/3 complex subunit 2

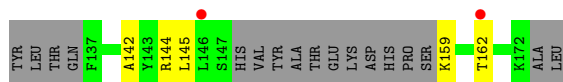


• Molecule 4: Actin-related protein 2/3 complex subunit 3

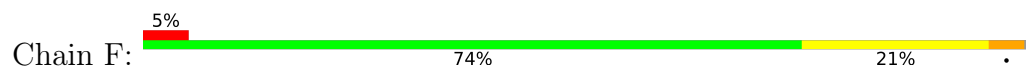


• Molecule 4: Actin-related protein 2/3 complex subunit 3

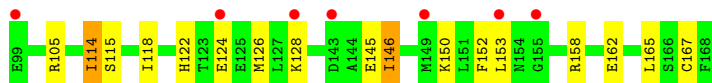
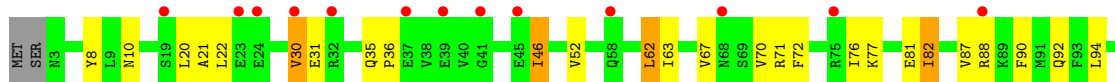
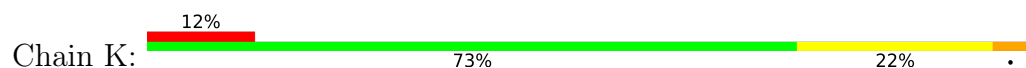




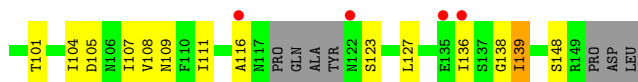
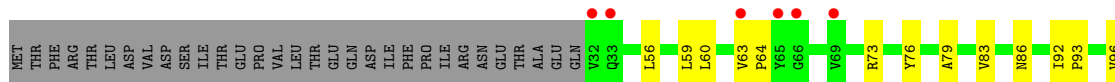
- Molecule 5: Actin-related protein 2/3 complex subunit 4



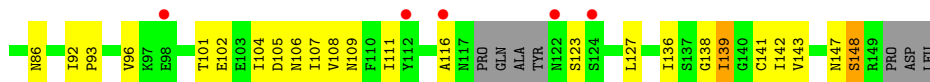
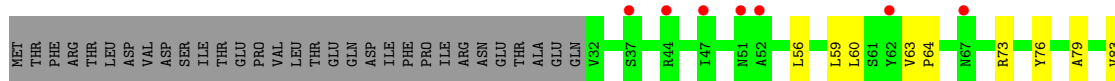
- Molecule 5: Actin-related protein 2/3 complex subunit 4



- Molecule 6: Actin-related protein 2/3 complex subunit 5



- Molecule 6: Actin-related protein 2/3 complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.97Å 218.97Å 315.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 3.78 29.00 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.00-3.78) 83.7 (29.00-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.324 , 0.344 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 96.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	18705	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	1/2610 (0.0%)	0.92	4/3567 (0.1%)
1	B	0.53	1/2611 (0.0%)	0.90	4/3569 (0.1%)
2	C	0.52	0/2300	0.89	8/3170 (0.3%)
2	H	0.50	1/2310 (0.0%)	0.89	8/3184 (0.3%)
3	D	0.48	0/2072	0.87	4/2816 (0.1%)
3	I	0.47	0/2072	0.88	4/2816 (0.1%)
4	E	0.44	0/399	0.81	0/540
4	J	0.46	0/399	0.82	0/540
5	F	0.44	0/1314	0.82	2/1777 (0.1%)
5	K	0.58	1/1314 (0.1%)	0.84	3/1777 (0.2%)
6	G	0.54	0/799	0.92	0/1097
6	L	0.51	0/799	0.92	0/1097
All	All	0.52	4/18999 (0.0%)	0.88	37/25950 (0.1%)

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	A	0	1
1	B	0	1
5	F	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	TYR	C-O	17.62	1.46	1.24
5	K	167	CYS	C-O	-14.76	1.05	1.24
1	B	88	TYR	C-O	12.90	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	130	GLU	C-O	5.24	1.34	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TYR	CA-C-O	-19.02	93.31	120.51
1	B	88	TYR	O-C-N	-14.41	103.42	122.59
1	B	88	TYR	CA-C-O	-12.97	101.97	120.51
1	A	88	TYR	O-C-N	-9.72	109.67	122.59
3	D	213	PRO	N-CA-CB	8.13	110.55	103.31
2	H	237	PRO	N-CA-CB	8.09	110.37	103.17
2	C	237	PRO	N-CA-CB	7.91	110.21	103.17
3	I	213	PRO	N-CA-CB	7.87	110.31	103.31
5	K	167	CYS	O-C-N	7.80	131.35	122.22
1	B	396	THR	CA-C-N	7.67	129.43	119.84
1	B	396	THR	C-N-CA	7.67	129.43	119.84
3	D	98	PRO	N-CA-CB	7.34	110.29	103.39
1	A	396	THR	CA-C-N	7.32	128.99	119.84
1	A	396	THR	C-N-CA	7.32	128.99	119.84
2	C	240	PRO	N-CA-CB	7.32	110.18	103.08
2	H	240	PRO	N-CA-CB	7.26	110.13	103.08
3	I	98	PRO	N-CA-CB	7.13	110.09	103.39
2	C	241	PRO	N-CA-CB	7.12	110.72	103.25
5	K	167	CYS	CA-C-O	-7.00	112.18	120.10
2	H	241	PRO	N-CA-CB	6.97	110.57	103.25
2	H	357	PRO	N-CA-CB	6.90	110.49	103.25
2	C	357	PRO	N-CA-CB	6.79	110.38	103.25
3	I	145	PRO	N-CA-CB	6.58	110.24	103.00
2	C	184	PRO	N-CA-CB	6.51	110.59	103.23
2	H	11	PRO	N-CA-CB	6.51	110.19	103.23
2	C	11	PRO	N-CA-CB	6.50	110.19	103.23
2	H	184	PRO	N-CA-CB	6.49	110.56	103.23
3	D	145	PRO	N-CA-CB	6.47	110.11	103.00
2	C	203	PRO	N-CA-CB	6.42	109.99	103.25
2	H	203	PRO	N-CA-CB	6.36	109.93	103.25
2	H	13	PRO	N-CA-CB	6.31	109.88	103.25
2	C	13	PRO	N-CA-CB	6.22	109.78	103.25
5	F	167	CYS	CA-C-O	-6.13	113.17	120.10
5	F	153	LEU	N-CA-C	-5.58	106.60	113.41
3	D	219	TYR	N-CA-C	5.45	117.92	111.33
3	I	219	TYR	N-CA-C	5.42	117.88	111.33
5	K	153	LEU	N-CA-C	-5.17	106.66	113.12

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TYR	Mainchain
1	B	88	TYR	Mainchain
5	F	167	CYS	Mainchain

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	2555	0	2244	50	0
1	B	2556	0	2244	47	0
2	C	2252	0	1845	46	0
2	H	2262	0	1851	41	0
3	D	2028	0	1774	42	0
3	I	2028	0	1774	46	0
4	E	397	0	275	5	0
4	J	397	0	275	4	0
5	F	1294	0	1260	29	0
5	K	1294	0	1260	28	0
6	G	790	0	717	17	0
6	L	790	0	717	20	0
7	A	31	0	12	0	0
7	B	31	0	12	0	0
All	All	18705	0	16260	346	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 10.

All (346) 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)
3:D:177:THR:HG22	3:D:244:VAL:HG12	1.58	0.86
1:B:21:TYR:CE1	3:I:32:THR:HG22	2.13	0.83
3:I:177:THR:HG22	3:I:244:VAL:HG12	1.59	0.83
1:B:31:PHE:HB2	1:B:32:PRO:HD2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:ARG:CG	3:D:18:ARG:HH11	1.94	0.81
1:A:21:TYR:CE1	3:D:32:THR:HG22	2.16	0.81
1:A:31:PHE:HB2	1:A:32:PRO:HD2	1.63	0.80
3:I:18:ARG:CG	3:I:18:ARG:HH11	1.95	0.79
2:H:254:LEU:HA	2:H:269:GLY:HA3	1.68	0.74
5:F:8:TYR:HA	6:G:127:LEU:HD21	1.70	0.73
2:H:143:ARG:CB	2:H:144:PRO:HD3	2.18	0.73
2:H:144:PRO:HG2	2:H:198:VAL:CG2	2.18	0.73
2:C:144:PRO:HG2	2:C:198:VAL:CG2	2.18	0.73
3:D:71:LEU:HD11	3:D:118:VAL:HG12	1.70	0.73
1:B:10:MET:HE3	1:B:128:LEU:HD21	1.70	0.73
2:C:32:THR:HA	2:C:57:ILE:HG22	1.72	0.72
2:C:143:ARG:CB	2:C:144:PRO:HD3	2.20	0.71
2:H:32:THR:HA	2:H:57:ILE:HG22	1.72	0.71
2:C:254:LEU:HA	2:C:269:GLY:HA3	1.73	0.70
3:I:71:LEU:HD11	3:I:118:VAL:HG12	1.74	0.70
3:D:259:ILE:C	3:D:261:HIS:H	2.02	0.68
5:K:8:TYR:HA	6:L:127:LEU:HD21	1.76	0.68
5:F:87:VAL:HG12	5:F:146:ILE:HG12	1.76	0.68
2:C:143:ARG:HB2	2:C:144:PRO:HD3	1.76	0.68
5:K:87:VAL:HG12	5:K:146:ILE:HG12	1.75	0.68
2:H:143:ARG:HB2	2:H:144:PRO:HD3	1.74	0.68
3:I:259:ILE:C	3:I:261:HIS:H	2.03	0.67
1:A:10:MET:HE3	1:A:128:LEU:HD21	1.78	0.66
1:A:102:TRP:CD1	1:A:103:ASP:H	2.14	0.65
2:C:144:PRO:HG2	2:C:198:VAL:HG21	1.79	0.65
1:B:102:TRP:CD1	1:B:103:ASP:H	2.14	0.65
2:C:74:SER:C	2:C:76:ASP:H	2.05	0.64
3:I:18:ARG:HH11	3:I:18:ARG:HG3	1.64	0.63
4:E:44:ILE:HG23	4:E:45:ASP:H	1.63	0.63
2:H:74:SER:C	2:H:76:ASP:H	2.06	0.63
5:F:88:ARG:O	5:F:92:GLN:HB2	1.99	0.63
2:H:144:PRO:HG2	2:H:198:VAL:HG21	1.79	0.62
6:G:139:ILE:HD12	6:G:139:ILE:H	1.64	0.62
6:L:96:VAL:HG23	6:L:104:ILE:HD12	1.82	0.61
6:G:96:VAL:HG23	6:G:104:ILE:HD12	1.81	0.61
2:C:100:ASN:H	2:C:100:ASN:HD22	1.46	0.61
4:J:48:ILE:HD11	4:J:145:LEU:HA	1.83	0.61
6:L:139:ILE:HD12	6:L:139:ILE:H	1.65	0.61
2:H:100:ASN:H	2:H:100:ASN:HD22	1.47	0.60
3:I:287:ARG:HH11	5:K:145:GLU:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:52:VAL:HG12	5:F:62:LEU:HB2	1.82	0.60
1:B:129:THR:HB	1:B:160:GLN:HG3	1.84	0.60
2:C:270:TYR:CD2	5:F:21:ALA:HB1	2.36	0.60
5:K:52:VAL:HG12	5:K:62:LEU:HB2	1.83	0.60
3:D:18:ARG:HH11	3:D:18:ARG:HG3	1.64	0.60
1:A:129:THR:HB	1:A:160:GLN:HG3	1.83	0.59
1:B:335:GLY:O	1:B:338:LEU:HB2	2.01	0.59
3:D:18:ARG:HH11	3:D:18:ARG:HG2	1.66	0.59
2:H:250:SER:HB2	6:L:138:GLY:HA3	1.84	0.59
1:B:111:GLN:O	1:B:115:LYS:HB2	2.03	0.59
6:G:96:VAL:HG23	6:G:104:ILE:CD1	2.33	0.59
3:D:122:PRO:HG2	3:D:159:ILE:HD11	1.84	0.58
3:D:287:ARG:HH11	5:F:145:GLU:HB2	1.68	0.58
2:H:270:TYR:CD2	5:K:21:ALA:HB1	2.39	0.58
6:L:104:ILE:HA	6:L:107:ILE:HG22	1.83	0.58
6:L:96:VAL:HG23	6:L:104:ILE:CD1	2.33	0.58
1:A:111:GLN:O	1:A:115:LYS:HB2	2.04	0.58
1:A:289:ALA:HB3	1:A:290:PRO:HD3	1.85	0.58
3:I:18:ARG:HH11	3:I:18:ARG:HG2	1.68	0.58
3:D:287:ARG:NH1	5:F:145:GLU:HB2	2.19	0.58
6:G:104:ILE:HA	6:G:107:ILE:HG22	1.84	0.58
6:G:59:LEU:O	6:G:76:TYR:OH	2.21	0.57
1:B:129:THR:HB	1:B:160:GLN:CG	2.35	0.57
3:I:40:HIS:CD2	3:I:42:SER:HB2	2.39	0.57
4:J:44:ILE:HG23	4:J:45:ASP:H	1.68	0.57
1:A:248:CYS:HB2	1:A:249:PRO:HD2	1.87	0.57
3:D:51:LEU:HG	3:D:52:ILE:H	1.69	0.57
4:E:48:ILE:HD11	4:E:145:LEU:HA	1.87	0.56
1:B:248:CYS:HB2	1:B:249:PRO:HD2	1.87	0.56
3:I:122:PRO:HG2	3:I:159:ILE:HD11	1.86	0.56
3:D:40:HIS:CD2	3:D:42:SER:HB2	2.40	0.56
2:H:119:SER:H	2:H:149:ILE:HD12	1.71	0.56
2:C:250:SER:HB2	6:G:138:GLY:HA3	1.87	0.56
5:K:88:ARG:O	5:K:92:GLN:HB2	2.05	0.55
1:A:129:THR:HB	1:A:160:GLN:CG	2.36	0.55
3:D:18:ARG:HG2	3:D:18:ARG:NH1	2.22	0.55
6:L:92:ILE:O	6:L:96:VAL:HG12	2.07	0.55
1:B:398:GLU:CD	1:B:398:GLU:H	2.15	0.55
3:I:51:LEU:HG	3:I:52:ILE:H	1.72	0.54
1:A:220:VAL:HG23	1:A:285:GLU:HB2	1.90	0.54
3:I:287:ARG:NH1	5:K:145:GLU:HB2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:63:VAL:HG12	6:L:76:TYR:OH	2.07	0.54
3:I:219:TYR:HA	3:I:239:GLY:HA2	1.90	0.54
1:B:220:VAL:HG23	1:B:285:GLU:HB2	1.90	0.54
6:G:108:VAL:HA	6:G:111:ILE:HD12	1.90	0.54
6:L:59:LEU:O	6:L:76:TYR:OH	2.23	0.54
6:G:92:ILE:O	6:G:96:VAL:HG12	2.08	0.53
3:I:18:ARG:CG	3:I:18:ARG:NH1	2.62	0.53
2:C:119:SER:H	2:C:149:ILE:HD12	1.74	0.53
1:B:269:ALA:O	1:B:270:SER:HB2	2.09	0.53
1:A:398:GLU:CD	1:A:398:GLU:H	2.17	0.53
2:H:19:PHE:CD2	2:H:26:PHE:HB3	2.44	0.53
6:G:63:VAL:HG12	6:G:76:TYR:OH	2.09	0.52
3:I:18:ARG:HG2	3:I:18:ARG:NH1	2.23	0.52
1:B:234:LEU:N	1:B:236:THR:HG1	2.06	0.52
2:H:124:ILE:HG13	2:H:145:LEU:HD21	1.92	0.52
3:D:219:TYR:HA	3:D:239:GLY:HA2	1.91	0.52
1:B:289:ALA:HB3	1:B:290:PRO:HD3	1.90	0.52
1:A:343:GLY:O	1:A:376:VAL:HG11	2.10	0.51
2:C:19:PHE:CD2	2:C:26:PHE:HB3	2.46	0.51
5:K:20:LEU:HD11	5:K:118:ILE:HG21	1.92	0.51
1:A:101:ASN:HB3	1:A:104:HIS:HB2	1.93	0.51
3:I:54:LEU:HD21	3:I:56:MET:HG3	1.93	0.51
3:D:18:ARG:CG	3:D:18:ARG:NH1	2.61	0.51
2:H:26:PHE:CE1	2:H:38:TYR:HB2	2.46	0.50
1:A:335:GLY:O	1:A:338:LEU:HB2	2.11	0.50
1:B:343:GLY:O	1:B:376:VAL:HG11	2.12	0.50
2:C:26:PHE:CE1	2:C:38:TYR:HB2	2.46	0.50
3:D:259:ILE:C	3:D:261:HIS:N	2.70	0.50
1:B:267:LYS:O	1:B:282:VAL:HB	2.12	0.50
2:C:224:GLY:C	2:C:226:ASP:H	2.21	0.49
3:I:33:ASP:OD1	3:I:34:PHE:N	2.40	0.49
2:C:169:LYS:HA	2:C:203:PRO:CB	2.42	0.49
2:H:155:HIS:C	2:H:157:ASN:H	2.21	0.49
6:L:56:LEU:O	6:L:60:LEU:HB2	2.12	0.49
1:A:269:ALA:O	1:A:270:SER:HB2	2.13	0.49
2:C:124:ILE:HG13	2:C:145:LEU:HD21	1.94	0.49
1:B:347:GLN:HB2	1:B:376:VAL:HG12	1.95	0.49
1:B:10:MET:HB2	1:B:128:LEU:CD2	2.43	0.49
2:H:169:LYS:HA	2:H:203:PRO:CB	2.42	0.49
3:D:54:LEU:HD21	3:D:56:MET:HG3	1.94	0.48
5:K:70:VAL:HG12	5:K:118:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:259:ILE:O	3:D:261:HIS:N	2.45	0.48
1:A:163:LEU:O	1:A:389:GLY:HA3	2.13	0.48
1:B:101:ASN:HB3	1:B:104:HIS:HB2	1.94	0.48
3:I:280:MET:O	3:I:284:MET:HB2	2.14	0.48
5:F:8:TYR:CA	6:G:127:LEU:HD21	2.41	0.48
5:F:70:VAL:HG12	5:F:118:ILE:HB	1.95	0.48
6:G:56:LEU:O	6:G:60:LEU:HB2	2.14	0.48
1:A:234:LEU:N	1:A:236:THR:HG1	2.11	0.48
3:D:51:LEU:HG	3:D:52:ILE:N	2.28	0.48
4:E:51:PHE:C	4:E:53:ALA:H	2.21	0.48
3:I:259:ILE:C	3:I:261:HIS:N	2.71	0.48
3:D:129:LYS:C	3:D:131:ALA:H	2.22	0.48
1:B:34:VAL:HG21	1:B:81:LEU:CD2	2.44	0.48
1:A:126:PHE:O	1:A:156:TYR:N	2.46	0.48
1:B:115:LYS:O	3:I:9:ILE:HD13	2.13	0.48
2:H:92:GLN:H	2:H:92:GLN:HE21	1.61	0.48
4:E:142:ALA:C	4:E:144:ARG:H	2.22	0.47
2:H:214:SER:HB2	2:H:215:PRO:HD2	1.96	0.47
3:I:129:LYS:C	3:I:131:ALA:H	2.21	0.47
4:J:51:PHE:C	4:J:53:ALA:H	2.22	0.47
1:A:34:VAL:HG21	1:A:81:LEU:CD2	2.44	0.47
2:C:214:SER:HB2	2:C:215:PRO:HD2	1.95	0.47
1:A:27:PRO:HG3	1:A:387:TRP:CD2	2.50	0.47
2:H:15:TYR:H	2:H:29:THR:HG23	1.80	0.47
3:I:37:VAL:HG22	3:I:56:MET:HG2	1.96	0.47
6:L:108:VAL:HA	6:L:111:ILE:HD12	1.96	0.47
6:G:64:PRO:HB2	6:G:73:ARG:HG2	1.97	0.47
3:I:259:ILE:O	3:I:261:HIS:N	2.47	0.47
2:C:271:ASN:O	5:F:128:LYS:NZ	2.48	0.47
2:H:268:ALA:HB1	2:H:347:ILE:HG13	1.96	0.47
5:K:87:VAL:CG1	5:K:146:ILE:HG12	2.44	0.47
2:C:155:HIS:C	2:C:157:ASN:H	2.21	0.47
5:K:114:ILE:HD13	5:K:115:SER:H	1.80	0.47
5:F:20:LEU:HD11	5:F:118:ILE:HG21	1.96	0.47
1:A:74:PHE:CZ	1:A:111:GLN:HG3	2.50	0.46
4:J:142:ALA:C	4:J:144:ARG:H	2.23	0.46
1:A:347:GLN:HB2	1:A:376:VAL:HG12	1.97	0.46
2:C:343:HIS:CD2	2:C:347:ILE:HD11	2.50	0.46
2:C:155:HIS:O	2:C:157:ASN:N	2.46	0.46
3:D:180:PHE:HZ	3:D:262:ILE:O	1.98	0.46
1:B:157:ILE:HD13	1:B:157:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:288:VAL:HG13	5:K:94:LEU:HD22	1.96	0.46
2:C:70:ILE:HG12	2:C:82:TYR:HB2	1.97	0.46
1:B:163:LEU:O	1:B:389:GLY:HA3	2.15	0.46
6:L:64:PRO:HB2	6:L:73:ARG:HG2	1.97	0.46
1:A:267:LYS:O	1:A:282:VAL:HB	2.16	0.46
3:D:280:MET:O	3:D:284:MET:HB2	2.15	0.46
2:H:269:GLY:C	2:H:271:ASN:H	2.24	0.46
2:C:30:THR:HG23	2:C:36:GLU:HG2	1.98	0.46
5:F:150:LYS:C	5:F:152:PHE:H	2.23	0.46
2:C:201:GLU:O	2:C:202:TYR:C	2.59	0.45
2:C:59:THR:HB	2:C:60:CYS:H	1.59	0.45
2:C:92:GLN:H	2:C:92:GLN:HE21	1.63	0.45
2:C:76:ASP:O	2:C:77:ARG:HB2	2.17	0.45
3:D:244:VAL:HG23	3:D:244:VAL:O	2.17	0.45
2:H:105:PHE:O	2:H:117:VAL:HA	2.16	0.45
2:H:271:ASN:O	5:K:128:LYS:NZ	2.49	0.45
5:K:150:LYS:C	5:K:152:PHE:H	2.24	0.45
2:C:120:GLY:HA2	2:C:148:THR:HG23	1.98	0.45
2:C:32:THR:HG23	2:C:34:GLN:H	1.82	0.45
1:B:31:PHE:HB2	1:B:32:PRO:CD	2.41	0.45
5:K:122:HIS:C	5:K:124:GLU:H	2.24	0.45
2:H:76:ASP:O	2:H:77:ARG:HB2	2.17	0.45
2:C:345:ASN:HA	5:F:128:LYS:HG2	1.99	0.45
3:I:244:VAL:HG23	3:I:244:VAL:O	2.17	0.45
3:I:160:HIS:HA	3:I:166:THR:HG22	1.98	0.45
3:D:54:LEU:HD13	3:D:114:LEU:HD12	1.98	0.44
5:F:71:ARG:HD2	5:F:105:ARG:NH1	2.32	0.44
5:F:158:ARG:O	5:F:162:GLU:HB2	2.18	0.44
1:B:21:TYR:CE2	3:I:31:VAL:HA	2.52	0.44
3:D:282:GLN:C	3:D:284:MET:H	2.25	0.44
1:B:27:PRO:HG3	1:B:387:TRP:CD2	2.52	0.44
2:H:28:THR:HB	2:H:29:THR:H	1.54	0.44
3:I:51:LEU:HG	3:I:52:ILE:N	2.30	0.44
1:B:126:PHE:O	1:B:156:TYR:N	2.48	0.44
1:B:347:GLN:NE2	1:B:375:ASN:HA	2.32	0.44
2:H:143:ARG:CB	2:H:144:PRO:CD	2.90	0.44
2:H:224:GLY:C	2:H:226:ASP:H	2.23	0.44
2:H:271:ASN:O	2:H:272:TYR:CB	2.65	0.44
2:C:271:ASN:O	2:C:272:TYR:CB	2.65	0.44
5:F:114:ILE:HD13	5:F:115:SER:H	1.81	0.44
2:H:70:ILE:HG12	2:H:82:TYR:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:221:ALA:HA	2:H:230:THR:O	2.17	0.44
1:A:10:MET:HB2	1:A:128:LEU:CD2	2.48	0.44
3:D:33:ASP:OD1	3:D:34:PHE:N	2.46	0.44
2:H:59:THR:HB	2:H:60:CYS:H	1.58	0.44
1:A:248:CYS:SG	1:A:287:PHE:HB2	2.57	0.44
2:C:75:GLN:HA	2:C:102:ALA:HB1	2.00	0.44
3:D:37:VAL:HG22	3:D:56:MET:HG2	1.99	0.44
3:D:246:PHE:H	3:D:249:HIS:HD2	1.65	0.44
5:F:87:VAL:HG23	5:F:88:ARG:N	2.32	0.44
5:F:87:VAL:CG1	5:F:146:ILE:HG12	2.46	0.44
1:B:32:PRO:HB2	1:B:34:VAL:HG13	1.99	0.44
1:B:93:PRO:HB2	1:B:105:MET:HE2	1.99	0.44
3:I:246:PHE:H	3:I:249:HIS:HD2	1.66	0.44
1:B:99:ILE:O	1:B:99:ILE:HG13	2.18	0.44
1:B:205:SER:O	1:B:207:LYS:N	2.51	0.44
2:H:253:PRO:HD3	6:L:143:VAL:HG11	1.99	0.44
1:A:21:TYR:CE2	3:D:31:VAL:HA	2.53	0.43
1:A:235:LYS:HD3	1:A:235:LYS:C	2.42	0.43
3:D:51:LEU:O	3:D:52:ILE:HB	2.19	0.43
1:A:347:GLN:NE2	1:A:375:ASN:HA	2.33	0.43
2:C:15:TYR:H	2:C:29:THR:HG23	1.83	0.43
3:D:122:PRO:CG	3:D:159:ILE:HD11	2.48	0.43
3:D:288:VAL:HG13	5:F:94:LEU:HD22	1.99	0.43
1:A:27:PRO:HG3	1:A:387:TRP:CG	2.54	0.43
1:A:28:SER:HB3	3:D:10:PHE:CE1	2.53	0.43
2:C:36:GLU:HB3	2:C:38:TYR:CE1	2.53	0.43
1:B:93:PRO:HA	1:B:101:ASN:HB2	2.00	0.43
3:I:122:PRO:CG	3:I:159:ILE:HD11	2.48	0.43
6:G:105:ASP:O	6:G:109:ASN:HB2	2.19	0.43
3:D:186:GLU:OE1	3:D:277:LYS:HE3	2.18	0.43
1:A:99:ILE:O	1:A:99:ILE:HG13	2.18	0.43
2:H:201:GLU:O	2:H:202:TYR:C	2.61	0.43
6:G:92:ILE:N	6:G:93:PRO:HD2	2.33	0.43
2:C:347:ILE:CG2	2:C:348:ALA:N	2.82	0.43
3:D:161:TYR:CE2	3:D:167:ILE:HG13	2.54	0.42
3:D:223:PRO:C	3:D:225:GLU:H	2.27	0.42
1:B:28:SER:HB3	3:I:10:PHE:CE1	2.54	0.42
1:B:101:ASN:HD22	1:B:101:ASN:HA	1.62	0.42
1:B:235:LYS:HD3	1:B:235:LYS:C	2.44	0.42
2:H:155:HIS:O	2:H:157:ASN:N	2.48	0.42
5:K:76:ILE:HG22	5:K:77:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PHE:HB2	1:A:32:PRO:CD	2.42	0.42
1:A:157:ILE:N	1:A:157:ILE:HD13	2.33	0.42
1:B:151:ASN:HD22	3:I:274:LYS:HE3	1.82	0.42
2:H:32:THR:HG23	2:H:34:GLN:H	1.83	0.42
1:A:205:SER:O	1:A:207:LYS:N	2.52	0.42
5:F:81:GLU:HG3	5:F:82:ILE:H	1.84	0.42
2:C:74:SER:C	2:C:76:ASP:N	2.73	0.42
1:B:12:ASN:HA	1:B:17:SER:OG	2.19	0.42
6:L:102:GLU:O	6:L:106:ASN:HB2	2.19	0.42
2:H:343:HIS:CD2	2:H:347:ILE:HD11	2.55	0.42
5:K:90:PHE:HE2	5:K:145:GLU:HG2	1.84	0.42
5:K:126:MET:HE2	5:K:126:MET:HB3	1.92	0.42
6:L:79:ALA:O	6:L:83:VAL:HG23	2.19	0.42
2:H:143:ARG:HB3	2:H:144:PRO:HD3	2.01	0.42
1:A:93:PRO:HA	1:A:101:ASN:HB2	2.00	0.42
1:A:93:PRO:HB2	1:A:105:MET:HE2	2.01	0.42
2:H:74:SER:C	2:H:76:ASP:N	2.74	0.42
3:I:54:LEU:HD13	3:I:114:LEU:HD12	2.01	0.42
1:A:282:VAL:HA	1:A:285:GLU:OE2	2.20	0.42
3:I:186:GLU:OE1	3:I:277:LYS:HE3	2.19	0.42
5:F:8:TYR:CD2	5:F:55:ARG:HD2	2.55	0.42
5:F:90:PHE:HE2	5:F:145:GLU:HG2	1.84	0.42
3:I:17:GLU:OE2	3:I:18:ARG:HG2	2.19	0.42
3:I:288:VAL:CG1	5:K:94:LEU:HD22	2.49	0.42
5:K:158:ARG:O	5:K:162:GLU:HB2	2.19	0.42
6:L:141:CYS:SG	6:L:142:ILE:N	2.93	0.42
3:D:39:PHE:HA	3:D:53:SER:O	2.20	0.42
3:I:161:TYR:CE2	3:I:167:ILE:HG13	2.55	0.42
6:L:92:ILE:N	6:L:93:PRO:HD2	2.35	0.42
6:L:147:ASN:O	6:L:148:SER:C	2.63	0.42
2:H:75:GLN:HA	2:H:102:ALA:HB1	2.02	0.41
6:L:105:ASP:O	6:L:109:ASN:HB2	2.20	0.41
2:C:105:PHE:O	2:C:117:VAL:HA	2.19	0.41
5:F:122:HIS:C	5:F:124:GLU:H	2.28	0.41
5:K:71:ARG:HD2	5:K:105:ARG:NH1	2.35	0.41
2:C:64:ALA:HB2	2:C:108:TRP:CE2	2.55	0.41
5:F:63:ILE:HG13	5:F:72:PHE:HD1	1.85	0.41
5:F:126:MET:HE2	5:F:126:MET:HB3	1.92	0.41
6:G:79:ALA:O	6:G:83:VAL:HG23	2.19	0.41
1:A:305:THR:HA	1:A:306:PRO:HD3	1.84	0.41
1:B:35:ILE:O	1:B:90:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:124:HIS:C	3:I:126:ALA:H	2.29	0.41
5:K:30:VAL:HG21	5:K:35:GLN:HE22	1.85	0.41
2:C:82:TYR:CE1	2:C:92:GLN:HB3	2.56	0.41
2:C:268:ALA:HB1	2:C:347:ILE:HG13	2.02	0.41
1:B:31:PHE:CB	1:B:32:PRO:HD2	2.40	0.41
1:B:36:ALA:HB2	1:B:80:ALA:HB1	2.02	0.41
1:B:92:TYR:HA	1:B:93:PRO:HD3	1.94	0.41
1:A:101:ASN:HD22	1:A:101:ASN:HA	1.61	0.41
3:D:10:PHE:O	3:D:11:ILE:C	2.64	0.41
1:B:74:PHE:N	1:B:74:PHE:CD2	2.89	0.41
3:I:40:HIS:HD2	3:I:42:SER:HB2	1.86	0.41
5:K:8:TYR:CA	6:L:127:LEU:HD21	2.49	0.41
5:F:46:ILE:HG23	5:F:67:VAL:HG12	2.02	0.41
3:I:180:PHE:HZ	3:I:262:ILE:O	2.03	0.41
5:K:63:ILE:HG13	5:K:72:PHE:HD1	1.86	0.41
1:A:32:PRO:O	1:A:77:GLY:HA2	2.21	0.41
1:A:69:THR:HA	5:F:156:ARG:NH2	2.36	0.41
1:A:101:ASN:C	1:A:102:TRP:CD1	2.99	0.41
1:A:193:ILE:HB	1:A:314:VAL:HG21	2.03	0.41
3:D:160:HIS:HA	3:D:166:THR:HG22	2.03	0.41
5:F:114:ILE:CD1	5:F:115:SER:H	2.33	0.41
3:I:58:CYS:O	3:I:62:LEU:HD12	2.20	0.41
3:I:282:GLN:C	3:I:284:MET:H	2.28	0.41
5:K:87:VAL:HG23	5:K:88:ARG:N	2.34	0.41
2:C:28:THR:HB	2:C:29:THR:H	1.55	0.41
4:E:159:LYS:C	4:E:161:TRP:H	2.29	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.94	0.41
3:I:51:LEU:O	3:I:52:ILE:HB	2.20	0.41
5:K:10:ASN:HD22	5:K:10:ASN:HA	1.66	0.41
5:K:81:GLU:HG3	5:K:82:ILE:H	1.86	0.41
1:A:12:ASN:HA	1:A:17:SER:OG	2.21	0.41
1:B:386:VAL:HG23	1:B:387:TRP:H	1.85	0.41
1:A:209:MET:HA	1:A:210:PRO:HD3	1.89	0.40
1:A:32:PRO:HB2	1:A:34:VAL:HG13	2.03	0.40
3:I:71:LEU:C	3:I:73:GLN:H	2.29	0.40
1:A:36:ALA:HB2	1:A:80:ALA:HB1	2.04	0.40
2:C:120:GLY:C	2:C:122:ARG:H	2.29	0.40
2:C:143:ARG:CB	2:C:144:PRO:CD	2.91	0.40
2:C:264:ALA:HA	2:C:278:GLN:HA	2.04	0.40
3:D:119:LEU:O	3:D:263:GLN:NE2	2.53	0.40
1:B:74:PHE:CZ	1:B:111:GLN:HG3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASN:C	1:B:102:TRP:CD1	2.99	0.40
1:A:9:ILE:HD12	1:A:127:LEU:HD22	2.03	0.40
2:C:269:GLY:C	2:C:271:ASN:H	2.28	0.40
5:F:30:VAL:HG21	5:F:35:GLN:HE22	1.86	0.40
6:G:107:ILE:O	6:G:111:ILE:HG13	2.21	0.40
2:H:7:LEU:HB3	2:H:45:TRP:HE1	1.86	0.40
3:I:223:PRO:C	3:I:225:GLU:H	2.29	0.40
3:I:299:LYS:HA	3:I:300:PRO:HD3	1.88	0.40
1:A:115:LYS:O	3:D:9:ILE:HD13	2.22	0.40
1:A:419:ARG:O	1:A:420:TYR:HB3	2.20	0.40
2:C:221:ALA:HA	2:C:230:THR:O	2.21	0.40
3:D:200:PHE:HD1	3:D:215:VAL:HG21	1.87	0.40
2:H:120:GLY:HA2	2:H:148:THR:HG23	2.02	0.40
5:K:46:ILE:HG23	5:K:67:VAL:HG12	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 X-ray entries followed by that with respect to entries of similar resolution.

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	343/427 (80%)	299 (87%)	36 (10%)	8 (2%)	5	29
1	B	343/427 (80%)	300 (88%)	37 (11%)	6 (2%)	7	33
2	C	324/377 (86%)	245 (76%)	56 (17%)	23 (7%)	1	12
2	H	325/377 (86%)	245 (75%)	59 (18%)	21 (6%)	1	13
3	D	258/317 (81%)	215 (83%)	35 (14%)	8 (3%)	3	24
3	I	258/317 (81%)	217 (84%)	33 (13%)	8 (3%)	3	24
4	E	53/174 (30%)	40 (76%)	11 (21%)	2 (4%)	2	20
4	J	53/174 (30%)	40 (76%)	11 (21%)	2 (4%)	2	20
5	F	164/168 (98%)	144 (88%)	18 (11%)	2 (1%)	10	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	164/168 (98%)	143 (87%)	19 (12%)	2 (1%)	10	39
6	G	110/152 (72%)	97 (88%)	11 (10%)	2 (2%)	6	32
6	L	110/152 (72%)	97 (88%)	11 (10%)	2 (2%)	6	32
All	All	2505/3230 (78%)	2082 (83%)	337 (14%)	86 (3%)	3	23

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	TRP
1	A	206	ILE
2	C	54	HIS
2	C	108	TRP
2	C	143	ARG
2	C	203	PRO
2	C	204	SER
2	C	272	TYR
2	C	296	LYS
1	B	102	TRP
1	B	206	ILE
2	H	54	HIS
2	H	143	ARG
2	H	203	PRO
2	H	204	SER
2	H	272	TYR
2	H	296	LYS
1	A	75	PHE
2	C	158	ASN
2	C	194	PRO
2	C	207	TRP
2	C	239	GLN
3	D	76	GLY
3	D	260	SER
6	G	116	ALA
1	B	75	PHE
2	H	108	TRP
2	H	194	PRO
2	H	207	TRP
2	H	239	GLN
2	H	288	ARG
3	I	76	GLY
3	I	260	SER

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Mol	Chain	Res	Type
6	L	116	ALA
2	C	50	THR
2	C	288	ARG
3	D	146	MET
3	D	224	LEU
6	G	148	SER
1	B	174	VAL
2	H	50	THR
2	H	158	ASN
3	I	146	MET
6	L	148	SER
1	A	174	VAL
2	C	180	VAL
2	C	202	TYR
2	C	290	LEU
4	E	52	ARG
5	F	31	GLU
2	H	180	VAL
2	H	202	TYR
2	H	290	LEU
3	I	224	LEU
5	K	31	GLU
1	A	74	PHE
1	A	397	PRO
2	C	241	PRO
3	D	212	ALA
3	D	226	ILE
3	D	283	ARG
1	B	74	PHE
1	B	397	PRO
2	H	241	PRO
3	I	226	ILE
3	I	283	ARG
4	J	52	ARG
1	A	148	GLU
1	A	149	SER
2	C	75	GLN
2	C	156	PRO
3	I	52	ILE
3	I	212	ALA
3	D	52	ILE
5	F	36	PRO

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Mol	Chain	Res	Type
2	H	156	PRO
4	J	73	GLY
2	C	65	PRO
2	C	205	GLY
2	C	206	GLY
4	E	73	GLY
2	H	65	PRO
2	H	206	GLY
5	K	36	PRO
2	C	356	THR
2	H	205	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	240/364 (66%)	215 (90%)	25 (10%)	7	26
1	B	240/364 (66%)	215 (90%)	25 (10%)	7	26
2	C	181/317 (57%)	162 (90%)	19 (10%)	6	26
2	H	182/317 (57%)	163 (90%)	19 (10%)	7	26
3	D	185/287 (64%)	171 (92%)	14 (8%)	12	37
3	I	185/287 (64%)	170 (92%)	15 (8%)	11	35
4	E	23/150 (15%)	18 (78%)	5 (22%)	1	6
4	J	23/150 (15%)	18 (78%)	5 (22%)	1	6
5	F	140/157 (89%)	132 (94%)	8 (6%)	18	44
5	K	140/157 (89%)	132 (94%)	8 (6%)	18	44
6	G	74/134 (55%)	69 (93%)	5 (7%)	14	40
6	L	74/134 (55%)	69 (93%)	5 (7%)	14	40
All	All	1687/2818 (60%)	1534 (91%)	153 (9%)	9	32

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	SER
1	A	33	THR
1	A	74	PHE
1	A	78	ASN
1	A	90	LEU
1	A	101	ASN
1	A	102	TRP
1	A	103	ASP
1	A	111	GLN
1	A	120	GLU
1	A	157	ILE
1	A	235	LYS
1	A	238	GLU
1	A	257	ARG
1	A	288	LEU
1	A	297	GLU
1	A	316	GLN
1	A	336	SER
1	A	380	LYS
1	A	381	ARG
1	A	386	VAL
1	A	393	LEU
1	A	398	GLU
1	A	422	ILE
2	C	22	GLN
2	C	29	THR
2	C	53	ASP
2	C	57	ILE
2	C	59	THR
2	C	68	ASN
2	C	78	ASN
2	C	92	GLN
2	C	99	LEU
2	C	100	ASN
2	C	122	ARG
2	C	152	LEU
2	C	173	LEU
2	C	197	THR
2	C	207	TRP
2	C	220	LEU
2	C	254	LEU
2	C	265	ILE

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Mol	Chain	Res	Type
2	C	364	THR
3	D	3	SER
3	D	16	THR
3	D	18	ARG
3	D	38	THR
3	D	43	THR
3	D	81	GLU
3	D	114	LEU
3	D	119	LEU
3	D	217	PHE
3	D	260	SER
3	D	264	VAL
3	D	287	ARG
3	D	288	VAL
3	D	301	ASP
4	E	59	ASN
4	E	69	THR
4	E	81	LEU
4	E	159	LYS
4	E	162	THR
5	F	22	LEU
5	F	30	VAL
5	F	46	ILE
5	F	62	LEU
5	F	82	ILE
5	F	114	ILE
5	F	146	ILE
5	F	165	LEU
6	G	86	ASN
6	G	101	THR
6	G	123	SER
6	G	136	ILE
6	G	139	ILE
1	B	14	THR
1	B	17	SER
1	B	33	THR
1	B	74	PHE
1	B	78	ASN
1	B	90	LEU
1	B	101	ASN
1	B	102	TRP
1	B	103	ASP

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Mol	Chain	Res	Type
1	B	111	GLN
1	B	120	GLU
1	B	157	ILE
1	B	235	LYS
1	B	238	GLU
1	B	257	ARG
1	B	288	LEU
1	B	297	GLU
1	B	316	GLN
1	B	336	SER
1	B	380	LYS
1	B	381	ARG
1	B	386	VAL
1	B	393	LEU
1	B	398	GLU
1	B	422	ILE
2	H	22	GLN
2	H	29	THR
2	H	53	ASP
2	H	57	ILE
2	H	59	THR
2	H	68	ASN
2	H	78	ASN
2	H	92	GLN
2	H	99	LEU
2	H	100	ASN
2	H	122	ARG
2	H	152	LEU
2	H	173	LEU
2	H	197	THR
2	H	207	TRP
2	H	220	LEU
2	H	254	LEU
2	H	265	ILE
2	H	364	THR
3	I	1	MET
3	I	14	LEU
3	I	16	THR
3	I	18	ARG
3	I	38	THR
3	I	43	THR
3	I	81	GLU

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Mol	Chain	Res	Type
3	I	114	LEU
3	I	119	LEU
3	I	217	PHE
3	I	260	SER
3	I	264	VAL
3	I	287	ARG
3	I	288	VAL
3	I	301	ASP
4	J	59	ASN
4	J	69	THR
4	J	81	LEU
4	J	159	LYS
4	J	162	THR
5	K	22	LEU
5	K	30	VAL
5	K	46	ILE
5	K	62	LEU
5	K	82	ILE
5	K	114	ILE
5	K	146	ILE
5	K	165	LEU
6	L	86	ASN
6	L	101	THR
6	L	123	SER
6	L	136	ILE
6	L	139	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	111	GLN
1	A	138	ASN
1	A	141	ASN
1	A	151	ASN
1	A	192	HIS
1	A	221	GLN
1	A	295	ASN
1	A	313	ASN
1	A	316	GLN
1	A	329	ASN
1	A	347	GLN

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Mol	Chain	Res	Type
1	A	375	ASN
1	A	379	HIS
1	A	382	GLN
1	A	395	GLN
2	C	92	GLN
2	C	100	ASN
2	C	196	ASN
3	D	80	HIS
3	D	249	HIS
3	D	253	GLN
3	D	254	ASN
3	D	267	ASN
5	F	10	ASN
5	F	58	GLN
5	F	120	ASN
6	G	86	ASN
1	B	101	ASN
1	B	111	GLN
1	B	138	ASN
1	B	141	ASN
1	B	151	ASN
1	B	192	HIS
1	B	221	GLN
1	B	295	ASN
1	B	316	GLN
1	B	329	ASN
1	B	347	GLN
1	B	375	ASN
1	B	379	HIS
1	B	395	GLN
2	H	68	ASN
2	H	78	ASN
2	H	92	GLN
2	H	100	ASN
2	H	196	ASN
3	I	80	HIS
3	I	249	HIS
3	I	253	GLN
3	I	254	ASN
3	I	263	GLN
3	I	267	ASN
3	I	296	ASN

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Mol	Chain	Res	Type
5	K	10	ASN
5	K	58	GLN
5	K	120	ASN
6	L	86	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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$
7	ATP	A	428	-	32,33,33	1.38	5 (15%)	48,52,52	1.72	10 (20%)
7	ATP	B	428	-	32,33,33	1.38	4 (12%)	48,52,52	1.81	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	A	428	-	-	4/22/38/38	0/3/3/3
7	ATP	B	428	-	-	5/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	428	ATP	C5-C4	4.85	1.47	1.39
7	A	428	ATP	C5-C4	4.69	1.47	1.39
7	B	428	ATP	C5-C6	2.96	1.49	1.41
7	A	428	ATP	C5-C6	2.74	1.48	1.41
7	B	428	ATP	C8-N7	2.40	1.36	1.31
7	A	428	ATP	C5-N7	-2.40	1.34	1.39
7	A	428	ATP	C8-N7	2.37	1.36	1.31
7	B	428	ATP	C5-N7	-2.15	1.35	1.39
7	A	428	ATP	C4-N9	-2.15	1.33	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	428	ATP	C5-C4-N3	-6.24	118.12	126.72
7	A	428	ATP	C5-C4-N3	-5.45	119.21	126.72
7	B	428	ATP	N3-C4-N9	4.80	135.33	127.17
7	A	428	ATP	N3-C4-N9	4.27	134.42	127.17
7	B	428	ATP	C2-N3-C4	3.92	121.42	111.83
7	B	428	ATP	C4-C5-N7	-3.76	106.29	110.58
7	A	428	ATP	C2-N3-C4	3.54	120.47	111.83
7	A	428	ATP	C4-C5-N7	-3.49	106.59	110.58
7	B	428	ATP	N3-C2-N1	-3.26	123.64	128.58
7	A	428	ATP	N3-C2-N1	-3.17	123.79	128.58
7	A	428	ATP	C4-N9-C8	2.77	108.65	105.74
7	B	428	ATP	C5-N7-C8	2.70	107.69	103.45
7	A	428	ATP	C5-N7-C8	2.52	107.41	103.45
7	B	428	ATP	C4-N9-C8	2.38	108.24	105.74
7	A	428	ATP	O4'-C1'-N9	2.27	112.44	108.09
7	A	428	ATP	C6-C5-N7	2.24	136.40	132.09
7	B	428	ATP	C6-C5-N7	2.23	136.39	132.09
7	B	428	ATP	O4'-C1'-N9	2.09	112.10	108.09
7	A	428	ATP	N9-C8-N7	-2.08	110.99	113.94

There are no chirality outliers.

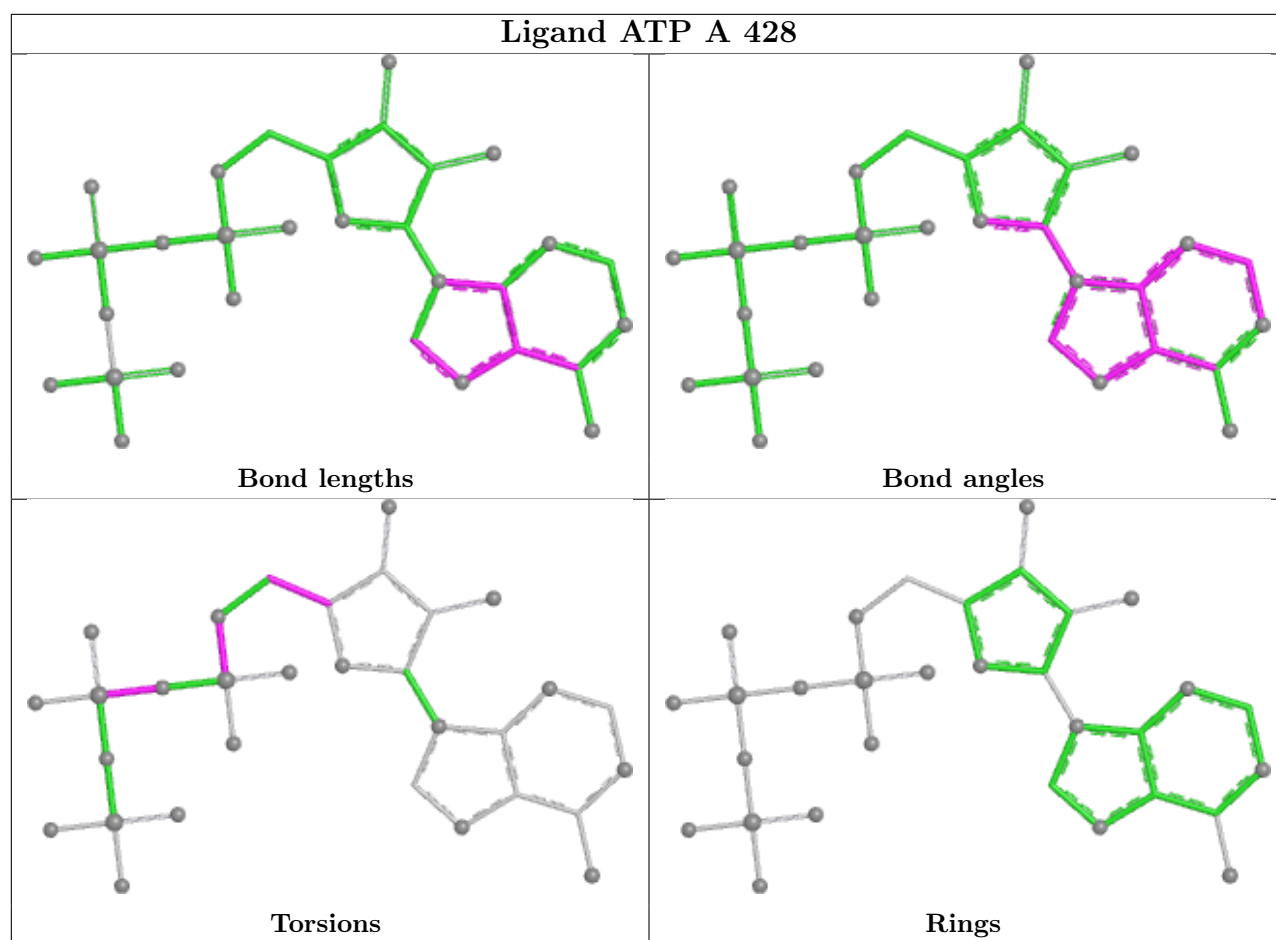
All (9) torsion outliers are listed below:

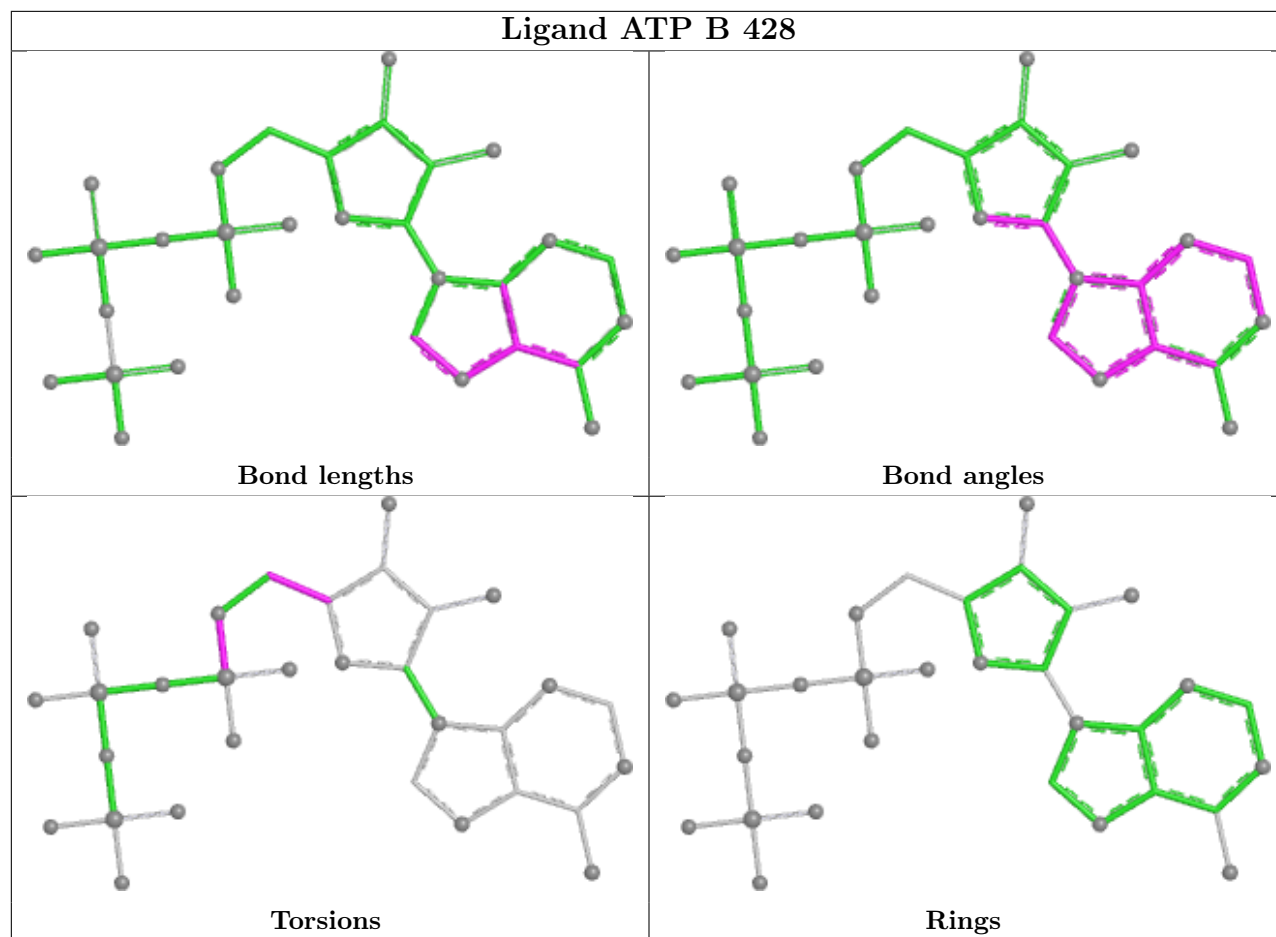
Mol	Chain	Res	Type	Atoms
7	B	428	ATP	C5'-O5'-PA-O2A
7	A	428	ATP	O4'-C4'-C5'-O5'
7	A	428	ATP	C3'-C4'-C5'-O5'
7	B	428	ATP	C3'-C4'-C5'-O5'
7	B	428	ATP	O4'-C4'-C5'-O5'
7	A	428	ATP	C5'-O5'-PA-O1A
7	B	428	ATP	C5'-O5'-PA-O1A
7	B	428	ATP	C5'-O5'-PA-O3A
7	A	428	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	355/427 (83%)	0.81	23 (6%)	25 21	62, 74, 88, 94	1 (0%)
1	B	355/427 (83%)	0.76	24 (6%)	23 20	62, 74, 88, 94	1 (0%)
2	C	336/377 (89%)	1.08	42 (12%)	8 11	65, 76, 86, 95	0
2	H	337/377 (89%)	1.33	68 (20%)	3 4	65, 76, 86, 95	0
3	D	272/317 (85%)	0.61	13 (4%)	35 26	65, 72, 86, 96	0
3	I	272/317 (85%)	0.78	19 (6%)	22 19	65, 72, 86, 96	0
4	E	63/174 (36%)	1.96	26 (41%)	0 1	66, 73, 83, 84	0
4	J	63/174 (36%)	1.24	11 (17%)	4 6	66, 73, 83, 84	0
5	F	166/168 (98%)	0.64	9 (5%)	31 24	55, 74, 84, 99	1 (0%)
5	K	166/168 (98%)	0.87	20 (12%)	9 12	55, 74, 84, 99	1 (0%)
6	G	114/152 (75%)	0.71	10 (8%)	15 16	66, 73, 82, 84	0
6	L	114/152 (75%)	1.09	12 (10%)	11 13	66, 73, 82, 84	0
All	All	2613/3230 (80%)	0.92	277 (10%)	11 13	55, 74, 86, 99	4 (0%)

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	304	ASN	8.2
4	E	161	TRP	7.4
2	C	301	HIS	6.3
1	B	225	ARG	6.2
2	H	301	HIS	5.8
2	H	287	THR	5.7
2	H	151	SER	5.5
2	H	303	GLY	5.4
4	J	46	GLU	5.2
2	H	181	ASP	4.8
6	G	66	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
4	E	51	PHE	4.7
2	C	17	HIS	4.6
2	H	306	GLY	4.4
2	H	305	THR	4.4
4	J	80	CYS	4.3
2	C	181	ASP	4.3
1	B	244	CYS	4.3
2	C	300	THR	4.2
5	K	39	GLU	4.2
1	A	225	ARG	4.2
2	H	308	GLY	4.2
2	C	287	THR	4.1
5	K	19	SER	4.0
1	A	237	ALA	4.0
2	C	302	THR	4.0
2	C	204	SER	3.9
2	C	308	GLY	3.9
2	H	17	HIS	3.9
2	H	152	LEU	3.9
4	E	44	ILE	3.8
5	F	99	GLU	3.8
3	I	211	THR	3.8
2	H	345	ASN	3.8
3	D	134	ALA	3.7
1	B	420	TYR	3.7
2	C	306	GLY	3.7
2	H	302	THR	3.7
3	I	101	ASP	3.6
2	C	297	THR	3.6
2	H	279	GLY	3.6
1	A	420	TYR	3.6
5	K	37	GLU	3.6
2	C	289	ASP	3.6
3	I	134	ALA	3.5
1	A	130	GLU	3.5
1	B	242	GLU	3.5
2	C	202	TYR	3.5
4	E	47	CYS	3.5
2	C	377	LEU	3.5
6	L	51	ASN	3.5
4	E	97	ASN	3.5
2	H	189	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	411	GLU	3.3
2	H	297	THR	3.3
3	I	221	ASP	3.3
6	L	37	SER	3.3
4	E	140	GLU	3.3
5	K	149	MET	3.3
1	B	188	ASP	3.3
2	H	128	TYR	3.3
6	L	122	ASN	3.2
1	B	297	GLU	3.2
2	H	299	PHE	3.2
3	I	303	GLU	3.2
4	J	44	ILE	3.2
2	C	143	ARG	3.2
2	H	281	GLU	3.2
1	A	280	ILE	3.2
6	L	52	ALA	3.2
4	E	54	ASN	3.1
2	H	164	GLY	3.1
3	I	48	THR	3.1
4	E	81	LEU	3.1
2	H	361	THR	3.1
4	E	141	LEU	3.1
2	H	135	TRP	3.1
1	B	412	TYR	3.1
2	C	235	SER	3.1
4	E	79	GLU	3.1
5	F	121	TYR	3.0
6	L	62	TYR	3.0
2	C	309	ARG	3.0
5	K	41	GLY	3.0
2	H	5	GLN	3.0
2	H	107	ARG	3.0
2	C	307	GLU	3.0
2	H	264	ALA	3.0
5	K	45	GLU	3.0
5	K	32	ARG	3.0
6	L	116	ALA	3.0
2	H	82	TYR	3.0
1	B	248	CYS	3.0
4	E	160	TRP	3.0
6	G	69	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	123	ASP	3.0
3	D	101	ASP	3.0
2	C	189	TRP	2.9
1	A	69	THR	2.9
2	H	231	ILE	2.9
4	J	97	ASN	2.9
1	A	297	GLU	2.9
2	H	7	LEU	2.9
2	H	375	TRP	2.9
5	K	58	GLN	2.9
2	H	298	SER	2.9
2	C	40	GLN	2.9
3	I	230	GLN	2.9
4	J	93	GLU	2.9
4	J	162	THR	2.8
6	G	65	TYR	2.8
2	C	304	ASN	2.8
2	H	159	VAL	2.8
2	H	160	LEU	2.8
4	E	162	THR	2.8
2	H	311	GLU	2.8
2	H	55	ASP	2.8
2	H	221	ALA	2.8
2	C	111	ASN	2.8
4	E	71	ILE	2.8
2	H	307	GLU	2.8
3	D	148	ASP	2.8
1	A	266	LEU	2.8
2	H	337	SER	2.8
4	E	166	LYS	2.8
5	F	133	ASP	2.7
4	E	163	CYS	2.7
3	D	300	PRO	2.7
5	F	148	GLU	2.7
3	I	145	PRO	2.7
1	A	148	GLU	2.7
6	G	122	ASN	2.7
3	D	125	ARG	2.7
4	E	57	PHE	2.7
5	K	99	GLU	2.7
6	L	47	ILE	2.7
2	H	280	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	49	ARG	2.6
4	E	139	GLN	2.6
1	A	244	CYS	2.6
2	C	285	ALA	2.6
2	H	344	GLN	2.6
5	K	88	ARG	2.6
2	C	305	THR	2.6
4	J	72	TYR	2.6
2	H	153	ASP	2.6
5	K	30	VAL	2.6
2	C	102	ALA	2.6
6	G	33	GLN	2.6
4	J	55	CYS	2.5
2	H	122	ARG	2.5
2	C	271	ASN	2.5
1	B	407	ALA	2.5
4	E	93	GLU	2.5
2	H	51	PHE	2.5
2	H	50	THR	2.5
4	J	45	ASP	2.5
4	E	52	ARG	2.5
4	E	78	SER	2.5
6	L	67	ASN	2.5
4	E	48	ILE	2.5
2	H	101	ARG	2.5
2	H	89	THR	2.5
1	A	372	VAL	2.5
4	E	72	TYR	2.5
6	G	135	GLU	2.5
2	C	179	ASP	2.5
2	C	198	VAL	2.5
1	A	409	TYR	2.5
2	H	8	HIS	2.4
1	A	422	ILE	2.4
5	F	58	GLN	2.4
2	C	153	ASP	2.4
2	H	41	ASP	2.4
5	K	23	GLU	2.4
2	H	358	GLY	2.4
2	H	377	LEU	2.4
2	H	57	ILE	2.4
3	I	56	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	145	PRO	2.4
5	F	29	ILE	2.4
3	I	172	GLU	2.4
2	C	344	GLN	2.4
2	C	90	TRP	2.4
3	I	282	GLN	2.3
2	H	363	PHE	2.3
5	K	155	GLY	2.3
2	H	71	VAL	2.3
2	H	80	TYR	2.3
3	I	257	ASP	2.3
2	C	36	GLU	2.3
2	H	174	SER	2.3
1	A	236	THR	2.3
2	C	22	GLN	2.3
2	H	22	GLN	2.3
6	L	98	GLU	2.3
1	A	157	ILE	2.3
4	E	70	LEU	2.3
2	H	204	SER	2.3
2	C	78	ASN	2.3
1	A	217	THR	2.3
3	D	48	THR	2.3
3	I	151	ALA	2.3
1	B	357	ARG	2.3
1	B	218	TYR	2.3
4	J	146	LEU	2.3
5	F	152	PHE	2.3
2	H	243	ALA	2.3
5	K	128	LYS	2.3
2	H	289	ASP	2.3
2	H	309	ARG	2.3
3	D	211	THR	2.2
1	B	157	ILE	2.2
2	C	165	CYS	2.2
2	C	110	PRO	2.2
1	B	185	ASP	2.2
1	A	185	ASP	2.2
1	A	83	LYS	2.2
4	E	164	PHE	2.2
4	E	59	ASN	2.2
5	K	68	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	280	MET	2.2
6	L	124	SER	2.2
1	B	260	ARG	2.2
1	B	402	TYR	2.2
5	K	153	LEU	2.2
6	L	44	ARG	2.2
6	L	112	TYR	2.2
1	B	99	ILE	2.2
1	B	4	PHE	2.2
2	C	10	LEU	2.2
4	J	81	LEU	2.2
1	A	35	ILE	2.1
3	I	86	TYR	2.1
6	G	63	VAL	2.1
1	A	27	PRO	2.1
2	H	130	GLU	2.1
3	D	296	ASN	2.1
4	E	60	PHE	2.1
2	C	206	GLY	2.1
2	H	310	GLU	2.1
3	D	266	ARG	2.1
3	I	130	GLN	2.1
2	C	303	GLY	2.1
2	C	201	GLU	2.1
6	G	116	ALA	2.1
1	B	110	GLN	2.1
2	H	244	LEU	2.1
3	I	290	ASP	2.1
1	B	217	THR	2.1
1	B	280	ILE	2.1
3	I	92	ILE	2.1
2	H	228	SER	2.1
1	B	284	PHE	2.1
3	I	29	GLN	2.1
1	B	312	ASP	2.1
5	K	75	ARG	2.1
2	H	372	VAL	2.1
2	C	279	GLY	2.0
2	H	72	THR	2.0
1	A	416	ILE	2.0
5	K	124	GLU	2.0
3	D	284	MET	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	219	TYR	2.0
6	G	136	ILE	2.0
5	F	23	GLU	2.0
5	F	162	GLU	2.0
5	K	24	GLU	2.0
2	H	150	LEU	2.0
2	H	137	VAL	2.0
1	A	260	ARG	2.0
1	A	4	PHE	2.0
2	C	2	ALA	2.0
3	D	99	ALA	2.0
5	K	143	ASP	2.0
2	H	177	VAL	2.0
6	G	32	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

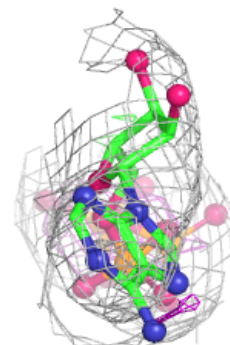
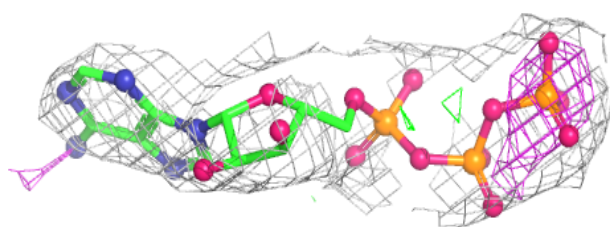
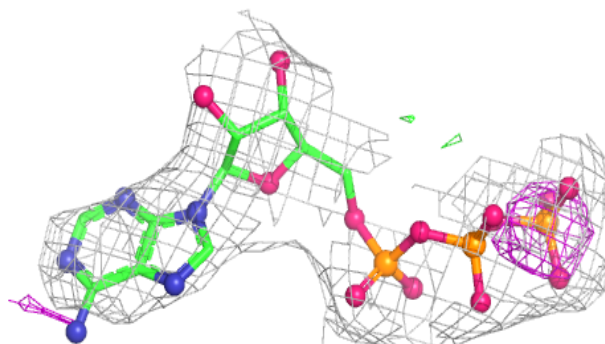
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ATP	B	428	31/31	0.84	0.16	102,102,108,108	0
7	ATP	A	428	31/31	0.87	0.13	97,98,106,106	0

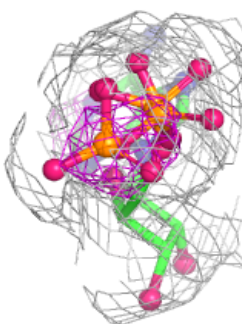
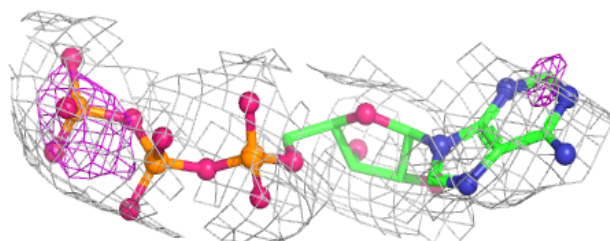
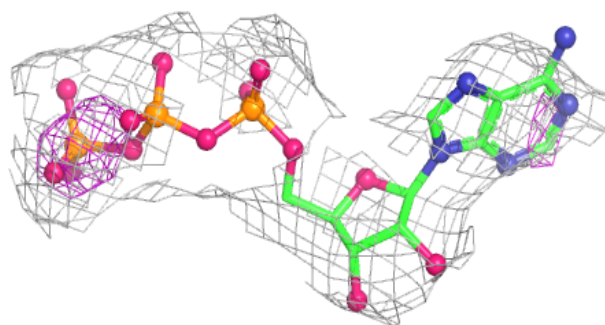
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP B 428:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP A 428:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.