



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:25 PM UTC

PDB ID : 3U8X / pdb_00003u8x
Title : Crystal Structure of a chimera containing the N-terminal domain (residues 8-29) of drosophila Ciboulot and the C-terminal domain (residues 18-44) of bovine Thymosin-beta4, bound to G-actin-ATP
Authors : Renault, L.; Husson, C.; Carlier, M.F.; Didry, D.
Deposited on : 2011-10-17
Resolution : 2.00 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

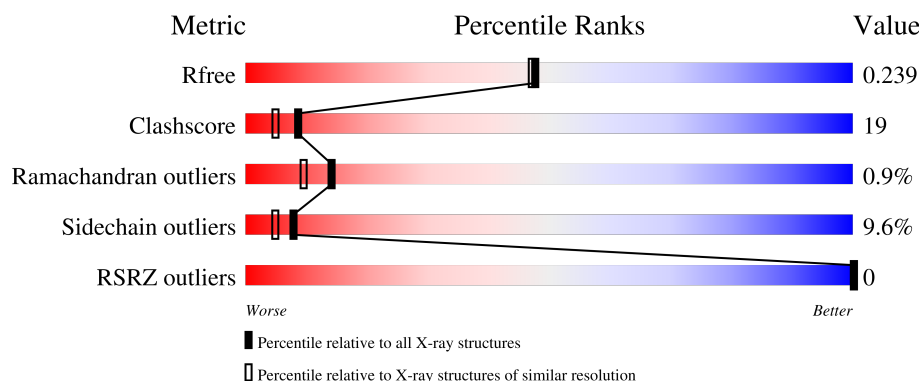
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	375	
1	C	375	
2	B	54	
2	D	54	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	C	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5990 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2794	1771	469	536	18			
1	C	357	Total	C	N	O	S	0	0	0
			2794	1771	469	536	18			

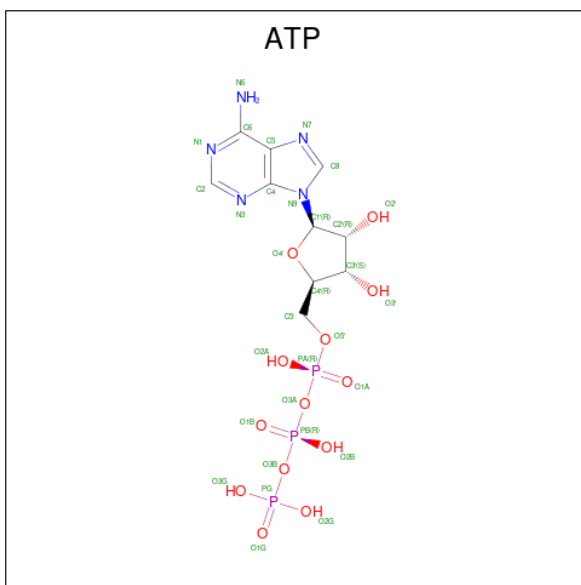
- Molecule 2 is a protein called Thymosin beta-4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	0	0	0
			169	107	30	32			
2	D	21	Total	C	N	O	0	0	0
			169	107	30	32			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	expression tag	UNP O97428
B	4	PRO	-	expression tag	UNP O97428
B	5	LEU	-	expression tag	UNP O97428
B	6	GLY	-	expression tag	UNP O97428
B	7	SER	-	expression tag	UNP O97428
D	3	GLY	-	expression tag	UNP O97428
D	4	PRO	-	expression tag	UNP O97428
D	5	LEU	-	expression tag	UNP O97428
D	6	GLY	-	expression tag	UNP O97428
D	7	SER	-	expression tag	UNP O97428

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



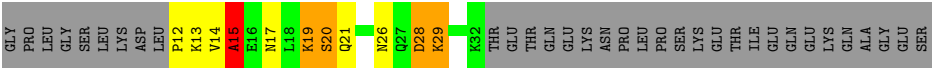
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0



● Molecule 2: Thymosin beta-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.01Å 75.33Å 128.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.00 19.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.70-2.00) 97.9 (19.70-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.238 0.192 , 0.239	Depositor DCC
R_{free} test set	4178 reflections (7.18%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 10.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -h,-k,l	Depositor
Outliers	0 of 58182 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: MG, 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	1.30	9/2855 (0.3%)	1.38	29/3872 (0.7%)
1	C	1.44	13/2855 (0.5%)	1.39	15/3872 (0.4%)
2	B	1.32	2/170 (1.2%)	1.35	1/223 (0.4%)
2	D	1.69	2/170 (1.2%)	1.61	1/223 (0.4%)
All	All	1.38	26/6050 (0.4%)	1.39	46/8190 (0.6%)

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	ILE	CA-CB	7.58	1.63	1.54
1	A	257	CYS	CA-C	7.05	1.60	1.52
1	A	357	ILE	N-CA	6.94	1.54	1.46
2	B	14	VAL	CA-CB	6.87	1.63	1.54
2	D	15	ALA	N-CA	6.60	1.54	1.46
1	C	340	TRP	CA-C	6.58	1.61	1.52
1	A	159	VAL	CA-CB	6.44	1.62	1.55
2	D	20	SER	CA-C	-6.31	1.44	1.52
1	A	177	ARG	C-O	6.28	1.31	1.24
1	A	73	HIS	N-CA	5.94	1.53	1.46
1	C	310	ALA	CA-CB	5.93	1.62	1.53
1	A	278	THR	CA-CB	5.85	1.62	1.53
1	C	37	ARG	CA-C	5.70	1.57	1.52
1	A	263	GLN	C-O	-5.69	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	151	ILE	N-CA	5.65	1.53	1.46
1	C	299	MET	CA-C	-5.64	1.45	1.52
1	C	312	ARG	N-CA	5.54	1.53	1.46
1	C	162	ASN	CA-C	-5.52	1.46	1.52
1	C	212	ILE	CA-CB	5.49	1.60	1.54
1	C	335	ARG	CD-NE	-5.48	1.38	1.46
2	B	14	VAL	CA-C	5.32	1.59	1.52
1	A	310	ALA	CA-CB	5.26	1.61	1.53
1	C	230	ALA	CA-CB	5.24	1.61	1.53
1	C	295	ALA	CA-CB	5.17	1.62	1.53
1	C	72	GLU	CA-C	5.14	1.59	1.52
1	C	181	ALA	CA-CB	-5.09	1.50	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	GLU	N-CA-C	-11.40	94.17	110.24
1	A	257	CYS	CA-C-N	-9.03	110.43	120.45
1	A	257	CYS	C-N-CA	-9.03	110.43	120.45
1	A	171	LEU	CA-C-N	-8.50	110.89	119.56
1	A	171	LEU	C-N-CA	-8.50	110.89	119.56
1	C	257	CYS	CA-C-N	-8.20	111.70	120.47
1	C	257	CYS	C-N-CA	-8.20	111.70	120.47
2	D	15	ALA	N-CA-C	7.63	127.06	110.80
1	A	111	ASN	CA-C-N	7.42	127.47	119.90
1	A	111	ASN	C-N-CA	7.42	127.47	119.90
1	A	271	SER	N-CA-C	7.16	120.21	110.55
1	A	26	ALA	CA-C-N	-6.99	113.11	120.03
1	A	26	ALA	C-N-CA	-6.99	113.11	120.03
1	C	151	ILE	N-CA-C	-6.40	98.41	107.75
1	A	335	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	A	335	ARG	CG-CD-NE	-6.07	98.65	112.00
1	C	171	LEU	CB-CA-C	5.99	115.83	110.44
1	A	226	GLU	N-CA-C	5.96	117.86	111.36
1	A	62	ARG	N-CA-C	5.96	118.56	111.71
1	C	71	ILE	CB-CA-C	-5.91	104.26	112.36
1	A	128	ASN	N-CA-C	5.88	119.53	111.54
1	A	346	LEU	N-CA-C	-5.85	104.98	111.36
1	C	270	GLU	N-CA-C	5.79	120.19	113.18
1	A	218	TYR	CA-C-N	-5.79	115.50	122.90
1	A	218	TYR	C-N-CA	-5.79	115.50	122.90
1	A	260	THR	N-CA-C	5.73	119.08	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	VAL	CA-C-N	-5.65	114.15	120.14
1	C	163	VAL	C-N-CA	-5.65	114.15	120.14
1	A	37	ARG	CA-C-N	-5.60	114.19	119.85
1	A	37	ARG	C-N-CA	-5.60	114.19	119.85
2	B	16	GLU	N-CA-C	5.50	117.28	111.28
1	A	225	ASN	N-CA-C	-5.43	105.36	111.28
1	C	226	GLU	N-CA-C	-5.37	105.51	111.36
1	C	129	VAL	CA-C-N	5.34	124.85	119.19
1	C	129	VAL	C-N-CA	5.34	124.85	119.19
1	A	75	ILE	CA-C-N	-5.29	115.54	122.37
1	A	75	ILE	C-N-CA	-5.29	115.54	122.37
1	C	335	ARG	CG-CD-NE	-5.23	100.49	112.00
1	C	319	ALA	N-CA-C	-5.22	105.76	111.82
1	C	110	LEU	CB-CA-C	-5.21	104.20	111.80
1	A	278	THR	N-CA-C	-5.20	105.50	111.07
1	A	357	ILE	N-CA-CB	5.19	116.77	110.95
1	A	357	ILE	CB-CA-C	-5.15	105.05	111.08
1	C	139	VAL	N-CA-C	-5.06	105.49	111.00
1	A	192	ILE	CB-CA-C	-5.05	105.42	111.88
1	A	316	GLU	N-CA-C	5.01	116.44	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	GLU	Peptide

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	2794	0	2757	84	0
1	C	2794	0	2757	113	0
2	B	169	0	180	14	0
2	D	169	0	180	25	0
3	A	31	0	12	4	0
3	C	31	0	12	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	5990	0	5898	224	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 19.

All (224) 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:C:14:SER:HB2	3:C:501:ATP:O2G	1.34	1.21
1:C:14:SER:N	3:C:501:ATP:O1G	1.74	1.20
1:A:88:HIS:CD2	1:A:92:ASN:HD22	1.62	1.16
1:C:14:SER:CB	3:C:501:ATP:O2G	2.00	1.10
1:C:193:LEU:HD22	1:C:248:ILE:HD11	1.33	1.08
2:D:26:ASN:O	2:D:29:LYS:HG3	1.58	1.03
1:C:351:THR:O	1:C:351:THR:HG22	1.56	1.02
1:C:167:GLU:HG2	1:C:167:GLU:O	1.66	0.95
1:C:14:SER:HB2	3:C:501:ATP:PG	2.07	0.93
2:D:26:ASN:OD1	2:D:28:ASP:HB2	1.71	0.89
1:C:352:PHE:HA	1:C:355:MET:HG3	1.56	0.88
1:C:297:ASN:HD22	1:C:329:ILE:HD12	1.40	0.87
2:D:15:ALA:HB1	2:D:19:LYS:HZ3	1.41	0.85
2:D:15:ALA:HB1	2:D:19:LYS:NZ	1.91	0.85
1:A:88:HIS:CD2	1:A:92:ASN:ND2	2.44	0.84
1:A:13:GLY:HA2	3:A:501:ATP:O1G	1.78	0.84
1:C:359:LYS:HB3	1:C:360:GLN:NE2	1.95	0.82
1:A:162:ASN:HD22	1:A:176:MET:HB2	1.43	0.80
2:D:15:ALA:CB	2:D:19:LYS:NZ	2.45	0.79
1:A:99:GLU:OE2	1:C:99:GLU:HG3	1.82	0.79
1:C:278:THR:HG21	1:C:317:ILE:HD11	1.65	0.79
1:C:214:GLU:HG2	3:C:501:ATP:C5	2.17	0.79
1:C:359:LYS:HB3	1:C:360:GLN:HE22	1.49	0.78
1:C:335:ARG:HA	1:C:338:SER:OG	1.84	0.78
1:C:349:LEU:HB3	2:D:21:GLN:NE2	1.99	0.77
1:A:57:GLU:HA	1:A:60:SER:HB2	1.67	0.76
1:A:14:SER:H	3:A:501:ATP:PG	2.10	0.75
1:C:12:ASN:HD21	1:C:86:TRP:HE1	1.34	0.75
1:C:88:HIS:HE1	1:C:93:GLU:OE2	1.69	0.75
1:A:353:GLN:NE2	1:A:356:TRP:HE1	1.83	0.75
1:C:54:VAL:HB	1:C:88:HIS:CD2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:VAL:HA	1:C:212:ILE:HD12	1.69	0.74
1:A:351:THR:HG21	2:B:18:LEU:N	2.02	0.74
1:C:355:MET:HE3	2:D:14:VAL:HG11	1.68	0.73
1:A:162:ASN:ND2	1:A:277:THR:HB	2.03	0.73
2:D:15:ALA:O	2:D:19:LYS:HD3	1.89	0.73
1:C:167:GLU:O	1:C:167:GLU:CG	2.37	0.72
1:A:162:ASN:HD21	1:A:277:THR:CB	2.01	0.72
1:C:364:GLU:OE1	1:C:364:GLU:HA	1.88	0.71
1:A:192:ILE:HG21	1:A:253:GLU:HG2	1.73	0.71
1:C:154:ASP:OD1	1:C:300:SER:HB2	1.91	0.70
1:A:56:ASP:O	1:A:59:GLN:HB2	1.91	0.69
2:D:26:ASN:CG	2:D:28:ASP:HB2	2.18	0.69
1:A:208:ILE:HG21	1:A:242:LEU:HD22	1.75	0.69
1:C:252:ASN:O	1:C:256:ARG:HG3	1.93	0.69
1:C:70:PRO:HB3	1:C:81:ASP:HB2	1.76	0.68
1:C:14:SER:HB3	3:C:501:ATP:O2G	1.93	0.68
2:D:15:ALA:CB	2:D:19:LYS:HZ2	2.08	0.66
1:C:238:LYS:O	1:C:249:THR:HG23	1.96	0.66
1:C:230:ALA:HB2	1:C:236:LEU:HD12	1.77	0.66
1:C:6:THR:O	1:C:101:HIS:HD2	1.79	0.66
2:D:15:ALA:CB	2:D:19:LYS:HZ3	2.07	0.66
2:D:15:ALA:HB2	2:D:19:LYS:HZ2	1.60	0.66
1:C:88:HIS:CE1	1:C:93:GLU:OE2	2.50	0.65
1:A:207:GLU:HA	1:A:207:GLU:OE2	1.97	0.65
1:C:78:ASN:CG	1:C:81:ASP:OD1	2.40	0.65
1:C:107:GLU:OE1	1:C:116:ARG:HG3	1.97	0.65
1:C:352:PHE:CA	1:C:355:MET:HG3	2.26	0.64
1:A:8:LEU:HD11	1:A:96:VAL:HG21	1.77	0.64
1:C:172:PRO:HA	1:C:175:ILE:HD12	1.80	0.63
1:C:33:SER:OG	1:C:71:ILE:HD12	1.99	0.63
1:A:162:ASN:HD21	1:A:277:THR:HB	1.62	0.63
1:C:201:VAL:O	1:C:202:THR:O	2.17	0.63
1:C:304:THR:O	1:C:335:ARG:NH1	2.34	0.61
1:C:188:TYR:CZ	1:C:192:ILE:HD11	2.35	0.61
1:A:104:LEU:HD12	1:A:133:TYR:HB3	1.83	0.61
1:C:59:GLN:O	1:C:62:ARG:HG3	2.01	0.60
1:A:132:MET:HE2	1:A:357:ILE:HD12	1.84	0.60
1:C:117:GLU:OE2	1:C:371:HIS:HE1	1.85	0.60
1:C:106:THR:HB	1:C:137:GLN:HG3	1.83	0.59
1:A:70:PRO:O	1:A:77:THR:HG22	2.02	0.59
1:A:190:MET:HE1	1:A:206:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HD22	1:A:329:ILE:CD1	2.16	0.59
1:C:132:MET:HE1	1:C:134:VAL:HG23	1.83	0.59
1:C:334:GLU:H	1:C:334:GLU:CD	2.10	0.59
2:B:14:VAL:HG12	2:B:14:VAL:O	2.03	0.59
1:C:247:VAL:HG12	1:C:247:VAL:O	2.01	0.58
1:A:6:THR:O	1:A:101:HIS:HD2	1.86	0.58
1:C:297:ASN:ND2	1:C:329:ILE:HD12	2.14	0.58
2:D:26:ASN:ND2	2:D:28:ASP:CB	2.67	0.58
1:C:304:THR:OG1	1:C:335:ARG:HD2	2.04	0.58
1:A:167:GLU:O	1:A:167:GLU:HG2	2.03	0.57
1:A:88:HIS:HD2	1:A:92:ASN:HD22	1.44	0.57
1:A:297:ASN:HD22	1:A:329:ILE:HD12	1.70	0.57
1:A:13:GLY:CA	3:A:501:ATP:O1G	2.49	0.57
1:C:252:ASN:HA	1:C:255:PHE:CE2	2.39	0.57
2:D:26:ASN:ND2	2:D:28:ASP:HB3	2.19	0.57
1:C:90:PHE:HB3	1:C:98:PRO:HD3	1.86	0.56
1:A:178:LEU:HD11	1:A:180:LEU:HD12	1.88	0.56
1:C:180:LEU:HD22	1:C:261:LEU:HD23	1.88	0.56
2:B:15:ALA:HB1	2:B:19:LYS:HZ3	1.71	0.55
1:C:198:TYR:CE2	1:C:248:ILE:HD12	2.41	0.55
1:C:198:TYR:CD2	1:C:248:ILE:HD12	2.41	0.55
2:D:26:ASN:HD21	2:D:28:ASP:CB	2.19	0.55
2:D:26:ASN:O	2:D:29:LYS:CG	2.47	0.55
1:A:167:GLU:HG3	2:B:19:LYS:HZ2	1.71	0.54
1:C:11:ASP:HA	1:C:106:THR:OG1	2.06	0.54
2:B:28:ASP:C	2:B:30:LEU:H	2.15	0.54
1:A:351:THR:HG21	2:B:18:LEU:CA	2.38	0.54
2:B:28:ASP:O	2:B:30:LEU:N	2.40	0.54
1:A:190:MET:HG3	1:A:209:VAL:HG21	1.90	0.53
1:A:360:GLN:CD	1:A:360:GLN:H	2.16	0.53
1:C:132:MET:CE	1:C:134:VAL:HG23	2.38	0.53
1:C:355:MET:HE3	2:D:14:VAL:CG1	2.37	0.52
1:C:352:PHE:C	1:C:355:MET:HG3	2.35	0.52
1:A:59:GLN:CA	1:A:59:GLN:OE1	2.58	0.52
1:A:82:MET:HE2	1:A:86:TRP:CE2	2.45	0.52
1:A:88:HIS:CE1	1:A:93:GLU:HG2	2.44	0.52
1:A:313:MET:O	1:A:317:ILE:HD12	2.10	0.52
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.57	0.52
1:C:70:PRO:HB3	1:C:81:ASP:CB	2.40	0.52
1:A:12:ASN:ND2	1:A:86:TRP:HE1	2.09	0.51
1:C:303:THR:HG22	1:C:303:THR:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:THR:HG21	1:C:317:ILE:CD1	2.38	0.51
1:C:282:ILE:O	1:C:285:CYS:HB2	2.09	0.51
1:C:71:ILE:O	1:C:71:ILE:HG22	2.11	0.51
1:C:242:LEU:O	1:C:243:PRO:C	2.54	0.51
1:A:133:TYR:OH	1:A:355:MET:HE2	2.11	0.51
1:C:202:THR:HG22	1:C:203:THR:N	2.26	0.51
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.93	0.51
1:A:358:THR:OG1	1:A:361:GLU:HG2	2.11	0.51
1:A:192:ILE:CG2	1:A:253:GLU:HG2	2.42	0.50
1:C:172:PRO:HA	1:C:175:ILE:CD1	2.41	0.50
1:C:153:LEU:HB3	1:C:299:MET:CE	2.41	0.50
1:A:358:THR:OG1	1:A:361:GLU:CG	2.59	0.50
1:A:6:THR:O	1:A:101:HIS:CD2	2.65	0.50
1:C:12:ASN:ND2	1:C:86:TRP:HE1	2.07	0.50
1:C:262:PHE:N	1:C:262:PHE:CD2	2.80	0.49
1:C:272:ALA:HB1	1:C:276:GLU:HB2	1.94	0.49
2:D:26:ASN:HD21	2:D:28:ASP:HB3	1.76	0.49
1:A:60:SER:O	1:A:61:LYS:HG3	2.12	0.49
1:A:71:ILE:C	1:A:72:GLU:O	2.49	0.49
1:C:202:THR:HG22	1:C:203:THR:H	1.77	0.49
2:D:15:ALA:HB2	2:D:19:LYS:NZ	2.21	0.49
2:B:15:ALA:HB1	2:B:19:LYS:NZ	2.28	0.48
1:A:191:LYS:HG2	1:A:195:GLU:OE1	2.14	0.48
1:A:261:LEU:HB3	1:A:274:ILE:HD13	1.95	0.48
1:C:132:MET:HE1	1:C:134:VAL:CG2	2.43	0.48
1:C:76:ILE:HD12	1:C:119:MET:HE2	1.96	0.48
2:D:26:ASN:ND2	2:D:28:ASP:HB2	2.29	0.48
1:A:313:MET:HG3	1:A:317:ILE:CD1	2.44	0.47
1:A:353:GLN:HE22	1:A:356:TRP:HE1	1.61	0.47
1:C:202:THR:HG22	1:C:204:ALA:H	1.79	0.47
1:C:13:GLY:C	3:C:501:ATP:O1G	2.51	0.47
1:A:34:ILE:HG13	1:A:34:ILE:O	2.15	0.47
1:A:222:ASP:HB3	1:A:225:ASN:HB2	1.97	0.47
1:C:360:GLN:CD	1:C:360:GLN:H	2.23	0.47
1:A:338:SER:O	1:A:339:VAL:C	2.54	0.46
1:C:6:THR:O	1:C:101:HIS:CD2	2.63	0.46
1:A:88:HIS:HD2	1:A:92:ASN:ND2	2.06	0.46
1:A:215:LYS:HA	1:A:215:LYS:HD3	1.80	0.46
1:A:358:THR:O	1:A:361:GLU:HB2	2.16	0.46
1:A:167:GLU:CG	2:B:19:LYS:HZ2	2.28	0.46
1:C:113:LYS:O	1:C:117:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:ALA:O	2:D:19:LYS:CD	2.62	0.46
1:C:117:GLU:OE2	1:C:371:HIS:CE1	2.67	0.45
1:C:131:ALA:HA	1:C:357:ILE:O	2.16	0.45
2:B:19:LYS:HG2	2:B:23:GLU:OE2	2.17	0.45
1:C:214:GLU:HG2	3:C:501:ATP:C4	2.51	0.45
1:A:57:GLU:O	1:A:60:SER:N	2.49	0.45
1:C:178:LEU:HD21	1:C:180:LEU:HD13	1.98	0.45
1:A:259:GLU:O	1:A:259:GLU:HG3	2.17	0.45
1:A:299:MET:HE1	1:A:313:MET:HE3	1.98	0.45
1:A:213:LYS:HA	1:A:217:CYS:SG	2.57	0.45
1:A:353:GLN:NE2	1:A:356:TRP:NE1	2.60	0.44
1:C:214:GLU:HG2	3:C:501:ATP:C6	2.51	0.44
1:C:314:GLN:HE21	1:C:329:ILE:HG12	1.82	0.44
2:B:16:GLU:H	2:B:16:GLU:HG2	1.66	0.44
1:A:330:ILE:HD12	1:A:330:ILE:N	2.33	0.44
1:A:15:GLY:O	1:A:32:PRO:HA	2.17	0.44
1:A:353:GLN:HE21	1:A:356:TRP:HE1	1.61	0.44
1:A:113:LYS:HB3	1:A:371:HIS:NE2	2.31	0.44
1:C:200:PHE:HD1	1:C:205:GLU:HB3	1.83	0.44
1:C:237:GLU:O	1:C:238:LYS:HD3	2.17	0.44
1:C:351:THR:O	1:C:351:THR:CG2	2.36	0.44
1:C:102:PRO:HA	1:C:131:ALA:O	2.18	0.44
1:C:317:ILE:HG21	1:C:317:ILE:HD13	1.65	0.44
1:A:171:LEU:O	1:A:172:PRO:C	2.58	0.43
1:A:360:GLN:CD	1:A:360:GLN:N	2.76	0.43
1:C:201:VAL:C	1:C:202:THR:O	2.62	0.43
1:C:295:ALA:O	1:C:328:LYS:HB3	2.19	0.43
1:C:190:MET:HE2	1:C:190:MET:HB2	1.77	0.43
1:A:59:GLN:OE1	1:A:59:GLN:N	2.51	0.43
1:C:357:ILE:HG23	1:C:369:ILE:HD13	2.01	0.43
1:A:120:THR:HG23	1:A:132:MET:SD	2.59	0.43
1:C:161:HIS:CE1	1:C:177:ARG:HG3	2.54	0.43
1:C:210:ARG:NH1	1:C:214:GLU:OE2	2.52	0.43
1:A:349:LEU:HD13	2:B:21:GLN:HB2	2.01	0.43
1:C:140:LEU:O	1:C:342:GLY:HA3	2.19	0.43
1:A:182:GLY:O	1:A:213:LYS:NZ	2.51	0.43
1:C:297:ASN:HD22	1:C:329:ILE:CD1	2.21	0.43
1:A:162:ASN:ND2	1:A:277:THR:CB	2.67	0.42
1:A:40:HIS:O	1:A:41:GLN:HB3	2.19	0.42
1:C:274:ILE:HG13	1:C:313:MET:HE1	2.02	0.42
1:C:349:LEU:HB3	2:D:21:GLN:HE22	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:NH2	1:A:179:ASP:OD2	2.49	0.42
1:C:59:GLN:C	1:C:61:LYS:H	2.28	0.42
1:C:85:ILE:O	1:C:88:HIS:HB3	2.20	0.42
1:A:360:GLN:O	1:A:364:GLU:HG2	2.20	0.42
1:A:21:PHE:CD2	1:A:21:PHE:N	2.87	0.42
1:C:355:MET:HE2	1:C:355:MET:HB3	1.77	0.42
2:D:26:ASN:CG	2:D:28:ASP:CB	2.91	0.42
1:C:360:GLN:CD	1:C:360:GLN:N	2.78	0.42
2:D:15:ALA:HB1	2:D:19:LYS:HD3	2.02	0.41
1:A:351:THR:HB	2:B:21:GLN:OE1	2.20	0.41
2:B:14:VAL:O	2:B:14:VAL:CG1	2.68	0.41
1:C:153:LEU:HD21	1:C:274:ILE:HD12	2.01	0.41
1:A:166:TYR:O	1:A:167:GLU:C	2.63	0.41
1:C:303:THR:O	1:C:303:THR:CG2	2.68	0.41
1:A:157:ASP:OD1	3:A:501:ATP:O3'	2.26	0.41
1:C:153:LEU:HB3	1:C:299:MET:HE1	2.02	0.41
1:A:210:ARG:O	1:A:214:GLU:HG3	2.21	0.41
1:C:351:THR:H	2:D:21:GLN:HE22	1.68	0.41
1:C:352:PHE:HA	1:C:355:MET:CG	2.41	0.41
1:C:250:ILE:HB	1:C:253:GLU:HB2	2.03	0.41
1:A:75:ILE:HD13	1:A:108:ALA:HB3	2.02	0.41
1:C:137:GLN:HG2	1:C:339:VAL:HG11	2.02	0.41
1:C:352:PHE:O	1:C:355:MET:HG3	2.20	0.41
1:C:75:ILE:HG23	1:C:75:ILE:HD12	1.81	0.41
1:C:145:SER:HB2	1:C:147:ARG:NH1	2.36	0.41
1:A:193:LEU:HD13	1:A:248:ILE:CD1	2.51	0.40
1:A:192:ILE:HG21	1:A:253:GLU:CG	2.49	0.40
1:C:111:ASN:HD21	1:C:119:MET:HE1	1.87	0.40
1:C:144:ALA:C	1:C:146:GLY:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	353/375 (94%)	339 (96%)	13 (4%)	1 (0%)	36	35
1	C	353/375 (94%)	328 (93%)	22 (6%)	3 (1%)	16	11
2	B	19/54 (35%)	15 (79%)	2 (10%)	2 (10%)	0	0
2	D	19/54 (35%)	17 (90%)	1 (5%)	1 (5%)	1	0
All	All	744/858 (87%)	699 (94%)	38 (5%)	7 (1%)	14	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	LYS
1	C	202	THR
2	D	15	ALA
2	B	29	LYS
1	A	202	THR
1	C	201	VAL
1	C	60	SER

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	303/318 (95%)	275 (91%)	28 (9%)	8	5
1	C	303/318 (95%)	280 (92%)	23 (8%)	12	9
2	B	19/48 (40%)	15 (79%)	4 (21%)	1	0
2	D	19/48 (40%)	12 (63%)	7 (37%)	0	0
All	All	644/732 (88%)	582 (90%)	62 (10%)	8	5

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	39	ARG
1	A	59	GLN
1	A	60	SER

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Mol	Chain	Res	Type
1	A	66	THR
1	A	67	LEU
1	A	71	ILE
1	A	80	ASP
1	A	112	PRO
1	A	113	LYS
1	A	115	ASN
1	A	132	MET
1	A	151	ILE
1	A	180	LEU
1	A	190	MET
1	A	191	LYS
1	A	195	GLU
1	A	202	THR
1	A	207	GLU
1	A	215	LYS
1	A	244	ASP
1	A	247	VAL
1	A	248	ILE
1	A	289	ILE
1	A	299	MET
1	A	334	GLU
1	A	360	GLN
1	A	368	SER
2	B	13	LYS
2	B	16	GLU
2	B	19	LYS
2	B	27	GLN
1	C	14	SER
1	C	34	ILE
1	C	37	ARG
1	C	52	SER
1	C	57	GLU
1	C	59	GLN
1	C	62	ARG
1	C	66	THR
1	C	67	LEU
1	C	80	ASP
1	C	100	GLU
1	C	132	MET
1	C	164	PRO
1	C	195	GLU

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Mol	Chain	Res	Type
1	C	199	SER
1	C	201	VAL
1	C	208	ILE
1	C	243	PRO
1	C	271	SER
1	C	323	SER
1	C	353	GLN
1	C	364	GLU
1	C	368	SER
2	D	12	PRO
2	D	13	LYS
2	D	17	ASN
2	D	19	LYS
2	D	20	SER
2	D	28	ASP
2	D	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	73	HIS
1	A	88	HIS
1	A	92	ASN
1	A	101	HIS
1	A	162	ASN
1	A	246	GLN
1	A	297	ASN
1	A	314	GLN
1	A	353	GLN
1	C	12	ASN
1	C	88	HIS
1	C	101	HIS
1	C	111	ASN
1	C	161	HIS
1	C	162	ASN
1	C	297	ASN
1	C	314	GLN
1	C	360	GLN
1	C	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ATP	A	501	4	32,33,33	2.02	8 (25%)	48,52,52	1.94	15 (31%)
3	ATP	C	501	-	32,33,33	2.17	8 (25%)	48,52,52	2.21	15 (31%)

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	ATP	A	501	4	-	2/22/38/38	0/3/3/3
3	ATP	C	501	-	-	0/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	ATP	PB-O3A	7.23	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ATP	PB-O3A	5.48	1.65	1.59
3	C	501	ATP	PB-O3B	-5.25	1.53	1.59
3	A	501	ATP	C5-C4	4.99	1.48	1.39
3	A	501	ATP	PB-O3B	-4.09	1.55	1.59
3	C	501	ATP	C5-C4	3.36	1.45	1.39
3	C	501	ATP	C5-N7	-3.28	1.33	1.39
3	A	501	ATP	C4-N3	2.97	1.40	1.34
3	A	501	ATP	C8-N7	2.95	1.37	1.31
3	C	501	ATP	C8-N9	-2.77	1.32	1.37
3	C	501	ATP	C4-N9	-2.75	1.32	1.37
3	A	501	ATP	O4'-C1'	2.43	1.47	1.42
3	C	501	ATP	PG-O3G	2.43	1.63	1.54
3	C	501	ATP	C6-N6	2.39	1.40	1.34
3	A	501	ATP	C5-C6	2.32	1.47	1.41
3	A	501	ATP	PG-O3G	-2.16	1.46	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	ATP	O3G-PG-O2G	6.92	133.76	107.80
3	C	501	ATP	C4-N9-C8	5.11	111.10	105.74
3	C	501	ATP	N3-C4-N9	4.41	134.67	127.17
3	A	501	ATP	C4-N9-C8	4.33	110.29	105.74
3	C	501	ATP	O2G-PG-O3B	-4.27	90.30	104.64
3	A	501	ATP	O2A-PA-O3A	4.23	118.71	107.27
3	A	501	ATP	N3-C2-N1	-4.09	122.39	128.58
3	C	501	ATP	C5-C4-N3	-3.71	121.61	126.72
3	A	501	ATP	C5-C4-N3	-3.61	121.74	126.72
3	A	501	ATP	N3-C4-N9	3.60	133.29	127.17
3	C	501	ATP	O4'-C1'-C2'	-3.26	99.63	106.62
3	A	501	ATP	O2G-PG-O3B	3.20	115.36	104.64
3	A	501	ATP	C2-N1-C6	3.17	123.94	118.73
3	C	501	ATP	N3-C2-N1	-3.10	123.89	128.58
3	C	501	ATP	N6-C6-N1	2.94	124.93	118.38
3	C	501	ATP	N9-C8-N7	-2.89	109.84	113.94
3	A	501	ATP	C5'-C4'-C3'	-2.87	104.87	115.21
3	A	501	ATP	C6-C5-N7	2.75	137.38	132.09
3	A	501	ATP	C2-N3-C4	2.73	118.51	111.83
3	C	501	ATP	C2-N1-C6	2.54	122.91	118.73
3	C	501	ATP	O2B-PB-O1B	2.53	124.22	112.44
3	A	501	ATP	C2'-C1'-N9	-2.34	107.49	113.30
3	A	501	ATP	C4-C5-N7	-2.29	107.97	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ATP	O4'-C1'-N9	2.28	112.47	108.09
3	C	501	ATP	O3B-PG-O1G	-2.27	99.08	111.04
3	C	501	ATP	C2-N3-C4	2.24	117.31	111.83
3	A	501	ATP	O3A-PA-O1A	-2.16	104.20	110.70
3	C	501	ATP	O2A-PA-O5'	2.13	117.24	107.57
3	C	501	ATP	C5-N7-C8	2.05	106.68	103.45
3	A	501	ATP	C2'-C3'-C4'	2.04	106.56	102.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ATP	C3'-C4'-C5'-O5'
3	A	501	ATP	O4'-C4'-C5'-O5'

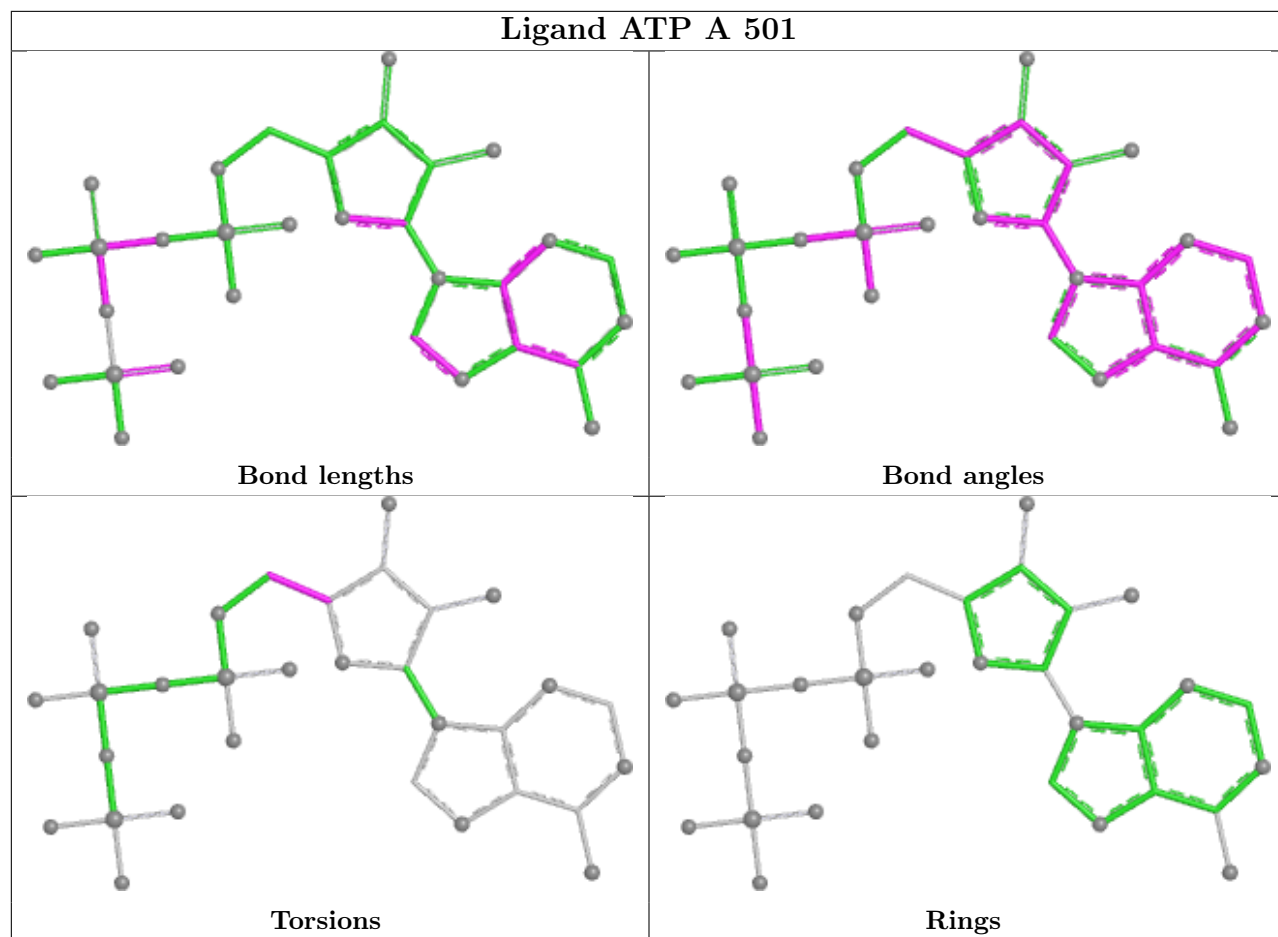
There are no ring outliers.

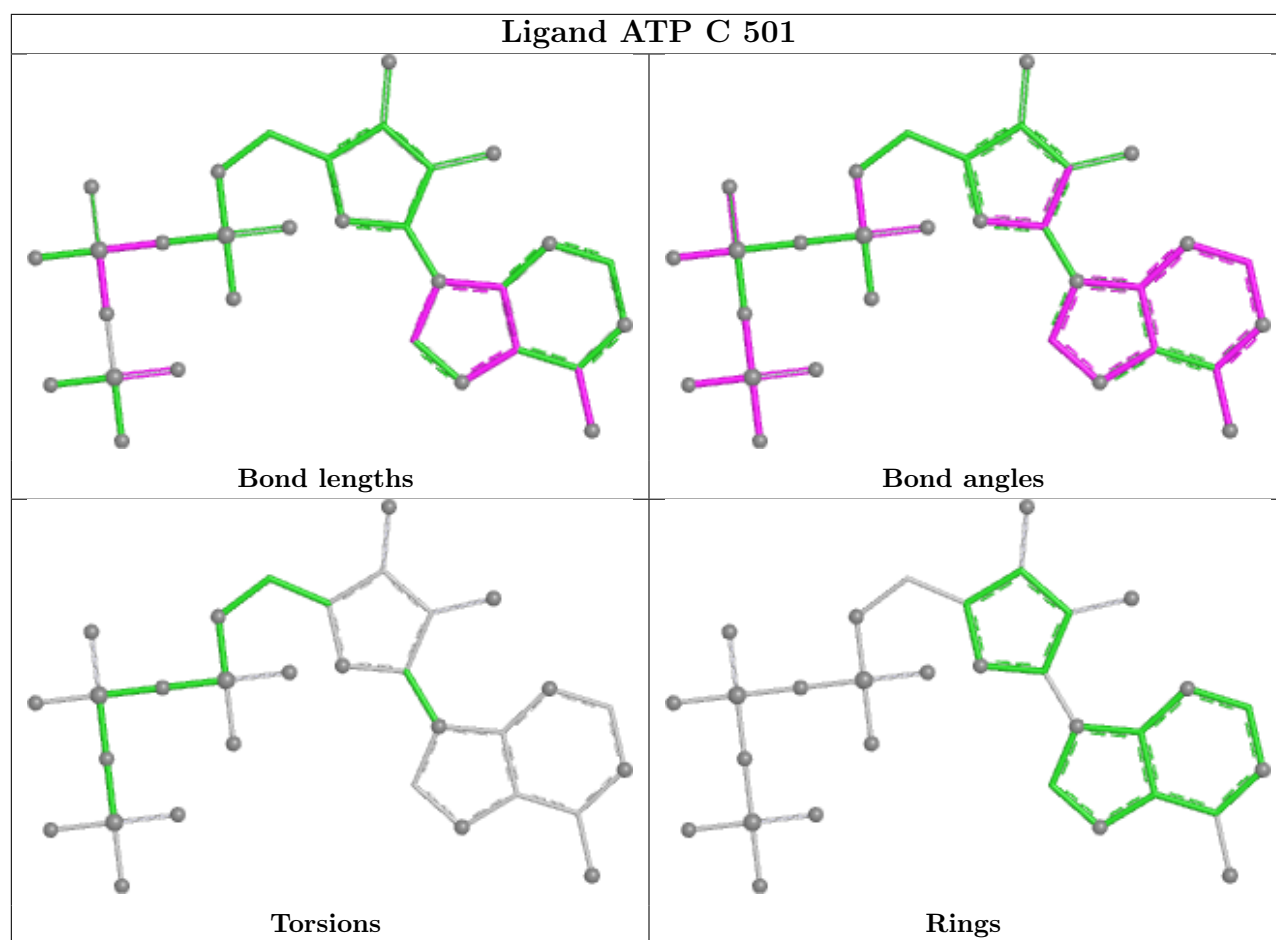
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ATP	4	0
3	C	501	ATP	9	0

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.

Ligand ATP A 501





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	357/375 (95%)	-1.47	0 100 100	9, 26, 63, 94	0
1	C	357/375 (95%)	-1.64	0 100 100	2, 14, 35, 48	0
2	B	21/54 (38%)	-1.08	0 100 100	26, 44, 66, 89	0
2	D	21/54 (38%)	-1.56	0 100 100	11, 19, 28, 36	0
All	All	756/858 (88%)	-1.54	0 100 100	2, 20, 56, 94	0

There are no RSRZ outliers to report.

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](#)

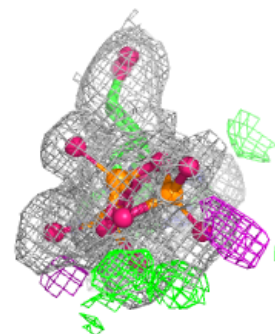
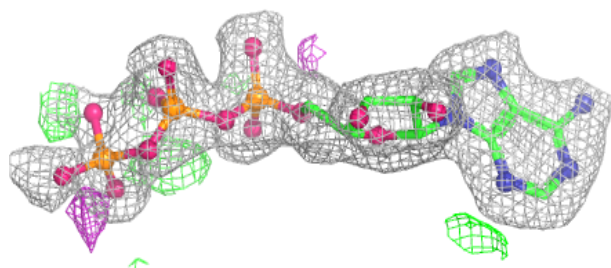
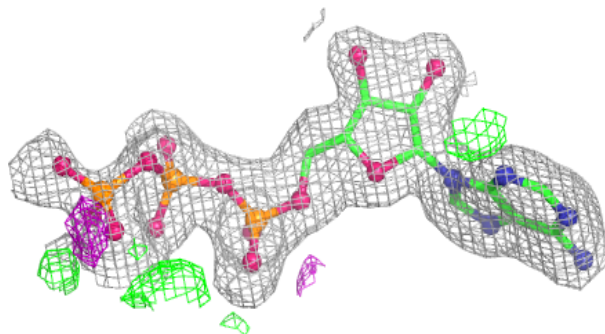
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

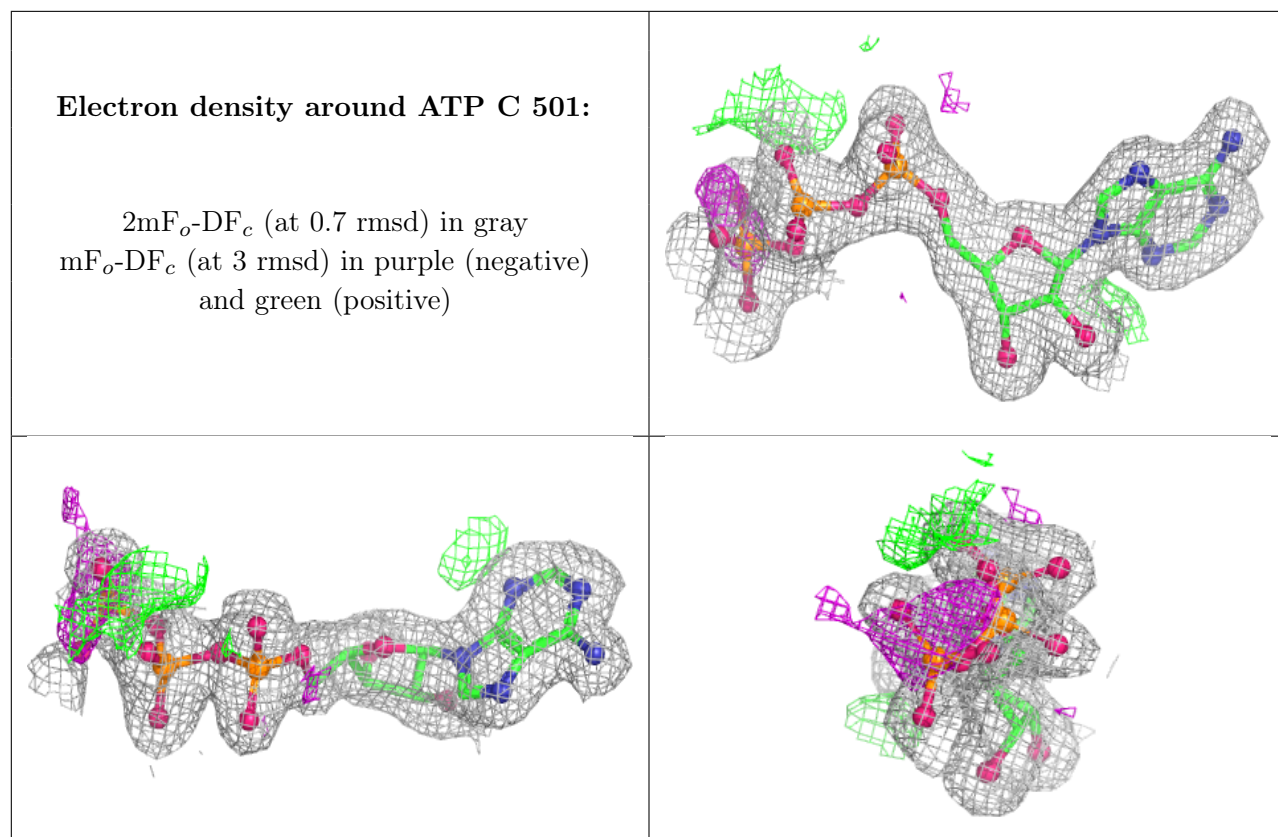
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATP	A	501	31/31	1.00	0.02	10,19,33,39	0
3	ATP	C	501	31/31	1.00	0.02	3,12,23,32	0
4	MG	A	502	1/1	1.00	0.02	10,10,10,10	0
4	MG	C	502	1/1	1.00	0.01	5,5,5,5	0

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 A 501:

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.