



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 1TFW / pdb_00001tfw
Title : How CCA is added to the 3' end of immature tRNA without the use of an oligonucleotide template
Authors : Xiong, Y.; Steitz, T.A.
Deposited on : 2004-05-27
Resolution : 2.20 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

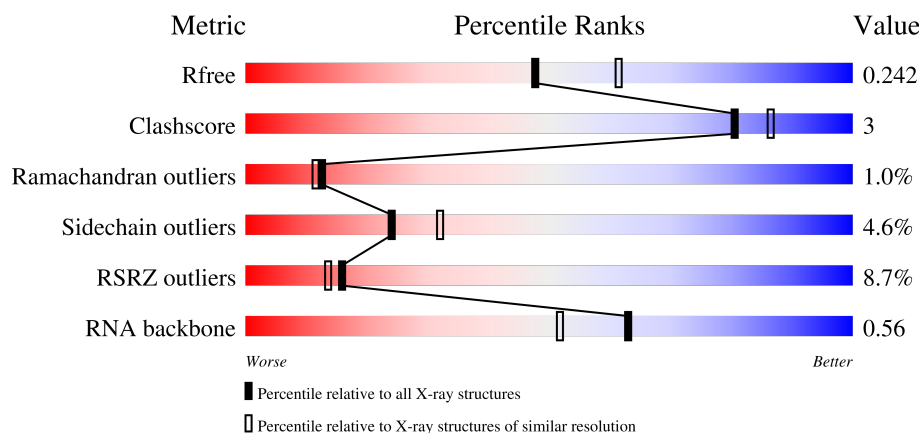
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	E	12	17% 75% 25%
2	G	13	15% 77% 15% 8%
2	H	13	23% 77% 23%
2	I	13	8% 77% 23%

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Mol	Chain	Length	Quality of chain
3	F	12	92% 8%
4	J	13	23% 62% 15% 15% 8%
5	A	437	8% 89% 9%
5	B	437	6% 92% 6%
5	C	437	6% 91% 8%
5	D	437	13% 92% 8%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17241 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 RNA chain called 5'-R(*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	12	Total	C	N	O	P	0	0	0
			253	114	47	81	11			

- Molecule 2 is a RNA chain called 5'-R(*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			
2	I	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			
2	G	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			

- Molecule 3 is a RNA chain called 5'-R(*GP*CP*GP*GP*AP*CP*CP*CP*GP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			253	114	48	80	11			

- Molecule 4 is a RNA chain called 5'-R(*CP*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			

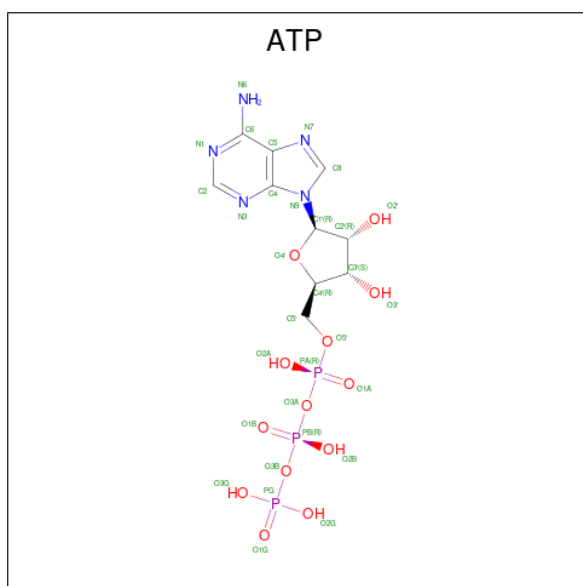
- Molecule 5 is a protein called tRNA nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	B	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	C	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	D	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

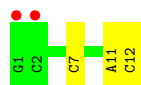


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	10	Total 10	O 10	0	0
8	H	14	Total 14	O 14	0	0
8	F	7	Total 7	O 7	0	0
8	I	7	Total 7	O 7	0	0
8	G	34	Total 34	O 34	0	0
8	J	41	Total 41	O 41	0	0
8	A	289	Total 289	O 289	0	0
8	B	211	Total 211	O 211	0	0
8	C	278	Total 278	O 278	0	0
8	D	168	Total 168	O 168	0	0

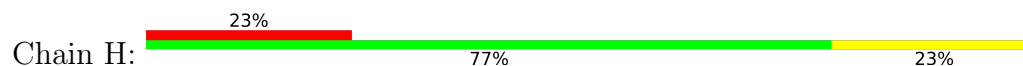
3 Residue-property plots

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.

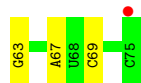
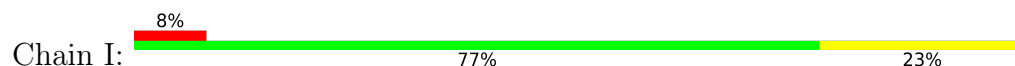
- Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*C)-3'



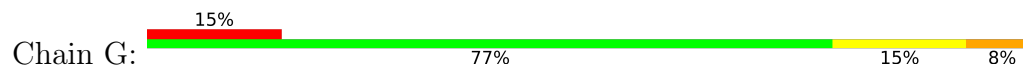
- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*CP*C)-3'



- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*CP*C)-3'



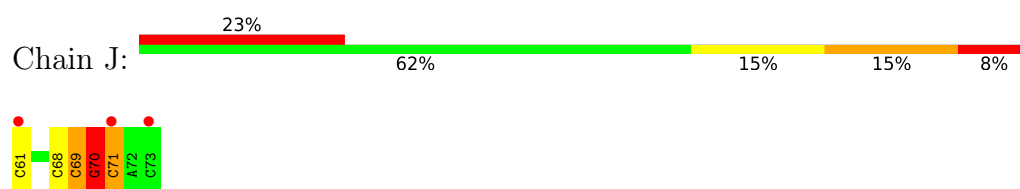
- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*CP*C)-3'



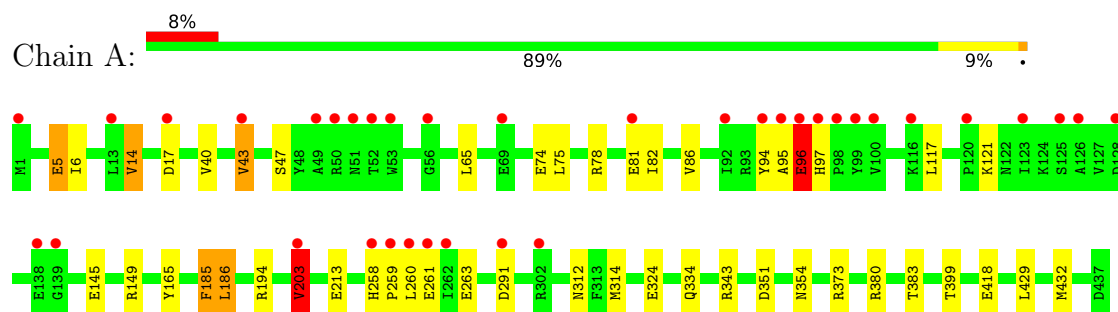
- Molecule 3: 5'-R(*GP*CP*GP*GP*AP*CP*CP*CP*GP*CP*AP*C)-3'



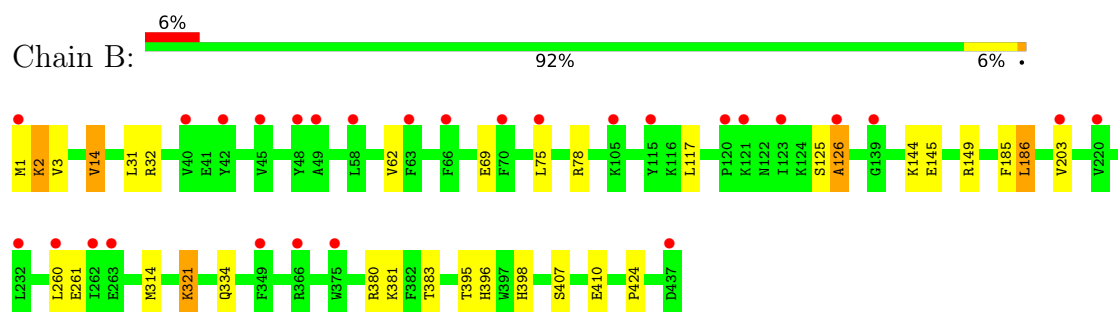
- Molecule 4: 5'-R(*CP*GP*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*C)-3'



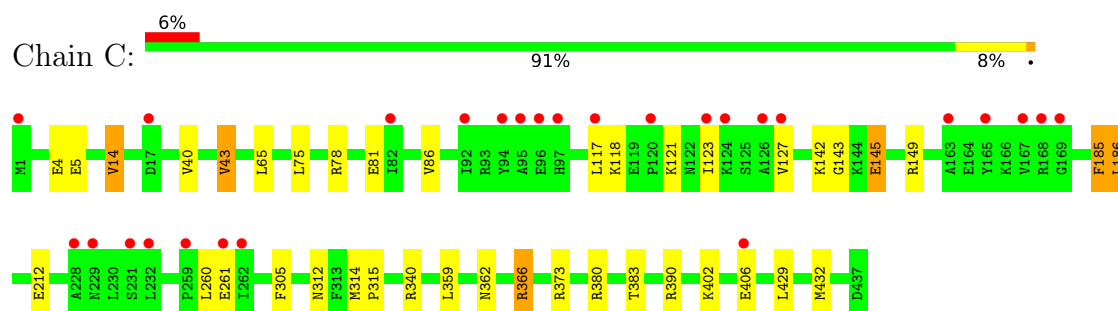
- Molecule 5: tRNA nucleotidyltransferase



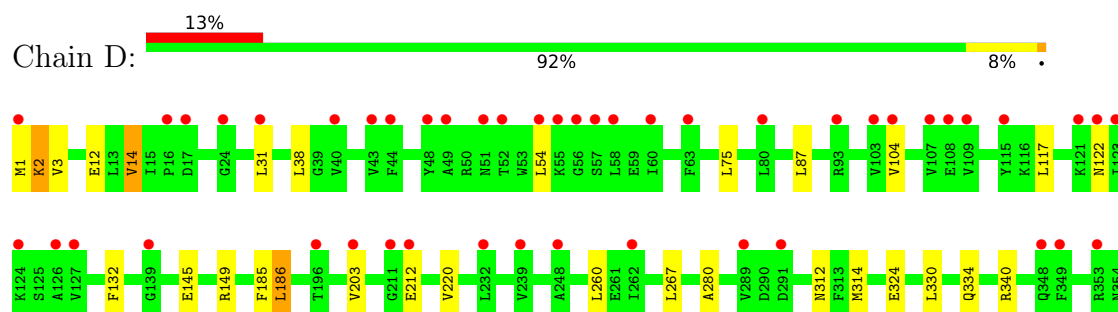
- Molecule 5: tRNA nucleotidyltransferase

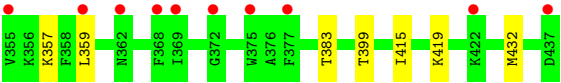


- Molecule 5: tRNA nucleotidyltransferase



- Molecule 5: tRNA nucleotidyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.64Å 84.77Å 135.81Å 90.00° 104.66° 90.00°	Depositor
Resolution (Å)	47.70 – 2.20 47.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.70-2.20) 99.0 (47.70-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.242 0.198 , 0.242	Depositor DCC
R_{free} test set	7348 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17241	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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, MG

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	E	0.52	0/282	0.92	0/438
2	G	0.95	1/304 (0.3%)	1.21	0/472
2	H	0.53	0/304	0.97	0/472
2	I	0.52	0/304	0.98	0/472
3	F	0.48	0/282	0.84	0/438
4	J	0.90	0/304	1.17	1/472 (0.2%)
5	A	0.70	0/3713	0.83	3/4987 (0.1%)
5	B	0.61	0/3713	0.74	0/4987
5	C	0.70	0/3713	0.80	1/4987 (0.0%)
5	D	0.58	0/3713	0.75	0/4987
All	All	0.65	1/16632 (0.0%)	0.81	5/22712 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	U	O3'-P	9.39	1.75	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	185	PHE	N-CA-C	-7.11	100.48	110.50
5	C	185	PHE	N-CA-C	-6.33	101.57	110.50
4	J	70	G	P-O3'-C3'	5.62	128.64	120.20
5	A	258	HIS	CA-C-N	5.06	126.17	119.84
5	A	258	HIS	C-N-CA	5.06	126.17	119.84

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	E	253	0	133	0	0
2	G	273	0	144	4	0
2	H	273	0	144	2	0
2	I	273	0	144	1	0
3	F	253	0	134	0	0
4	J	273	0	144	9	0
5	A	3630	0	3633	29	0
5	B	3630	0	3633	20	0
5	C	3630	0	3633	24	0
5	D	3630	0	3633	18	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	31	0	12	0	0
7	D	31	0	12	0	0
8	A	289	0	0	2	0
8	B	211	0	0	0	0
8	C	278	0	0	3	0
8	D	168	0	0	2	0
8	E	10	0	0	0	0
8	F	7	0	0	0	0
8	G	34	0	0	0	0
8	H	14	0	0	0	0
8	I	7	0	0	1	0
8	J	41	0	0	0	0
All	All	17241	0	15399	81	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 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:12:A:H61	4:J:61:C:N4	1.54	1.05
2:G:12:A:N6	4:J:61:C:H42	1.58	1.01
5:A:314:MET:HE2	5:B:314:MET:CE	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:402:LYS:O	5:C:406:GLU:HG3	1.83	0.78
5:C:314:MET:HE2	5:D:314:MET:HE2	1.71	0.72
5:C:406:GLU:HB3	8:C:438:HOH:O	1.89	0.72
5:C:14:VAL:HG13	5:C:149:ARG:HB3	1.72	0.71
5:A:314:MET:HE2	5:B:314:MET:HE2	1.71	0.71
5:A:314:MET:CE	5:B:314:MET:CE	2.69	0.71
5:A:314:MET:CE	5:B:314:MET:HE3	2.23	0.69
5:C:314:MET:CE	5:D:314:MET:CE	2.71	0.68
5:C:314:MET:CE	5:D:314:MET:HE2	2.24	0.67
5:D:14:VAL:HG13	5:D:149:ARG:HB3	1.78	0.65
5:C:402:LYS:O	5:C:406:GLU:CG	2.46	0.64
5:C:314:MET:HE3	5:D:314:MET:CE	2.32	0.60
5:B:395:THR:HG22	5:B:396:HIS:CD2	2.37	0.59
5:A:185:PHE:O	5:A:186:LEU:CB	2.48	0.59
5:A:14:VAL:HG13	5:A:149:ARG:HB3	1.85	0.58
5:C:366:ARG:HH11	5:C:366:ARG:HG3	1.68	0.57
5:B:31:LEU:HD21	5:B:62:VAL:HG21	1.85	0.57
4:J:70:G:O2'	4:J:71:C:H4'	2.04	0.57
4:J:69:C:H4'	5:A:291:ASP:OD2	2.06	0.56
5:A:40:VAL:HG21	5:A:82:ILE:HD13	1.88	0.56
2:G:12:A:H61	4:J:61:C:H42	0.75	0.56
5:B:14:VAL:HG13	5:B:149:ARG:HB3	1.89	0.55
5:B:125:SER:O	5:B:126:ALA:HB2	2.10	0.52
5:C:185:PHE:O	5:C:186:LEU:CB	2.58	0.52
5:A:43:VAL:HG22	5:A:65:LEU:HD11	1.92	0.50
5:D:280:ALA:HB2	5:D:330:LEU:HD23	1.94	0.50
5:B:185:PHE:O	5:B:186:LEU:CB	2.59	0.50
5:C:390:ARG:NH1	8:C:697:HOH:O	2.44	0.50
5:D:203:VAL:HG23	8:D:1669:HOH:O	2.11	0.50
5:B:125:SER:O	5:B:126:ALA:CB	2.59	0.50
5:A:5:GLU:HG2	5:A:6:ILE:N	2.27	0.49
5:A:43:VAL:CG2	5:A:65:LEU:HD11	2.42	0.49
2:G:14:C:C5	5:C:127:VAL:HG22	2.49	0.48
5:A:78:ARG:NH1	5:A:81:GLU:OE1	2.46	0.48
5:A:380:ARG:HH22	5:B:334:GLN:NE2	2.12	0.48
5:A:95:ALA:O	5:A:96:GLU:CG	2.62	0.47
5:A:74:GLU:O	5:A:78:ARG:HG2	2.14	0.47
5:C:143:GLY:N	5:C:145:GLU:OE1	2.47	0.47
5:B:1:MET:O	5:B:2:LYS:CB	2.63	0.47
5:B:185:PHE:O	5:B:186:LEU:HB3	2.15	0.46
5:B:125:SER:OG	5:B:126:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:351:ASP:CG	5:A:354:ASN:HD22	2.22	0.46
5:D:340:ARG:HD2	8:D:1618:HOH:O	2.15	0.46
5:A:373:ARG:NH2	8:A:712:HOH:O	2.49	0.45
5:C:78:ARG:NH1	5:C:81:GLU:OE1	2.49	0.45
5:A:185:PHE:O	5:A:186:LEU:HB3	2.16	0.45
5:C:314:MET:CE	5:D:314:MET:HE3	2.46	0.45
2:I:63:G:H3'	8:I:424:HOH:O	2.17	0.45
5:D:185:PHE:O	5:D:186:LEU:HB3	2.17	0.45
5:C:43:VAL:HG22	5:C:65:LEU:HD11	1.97	0.45
2:H:68:U:H2'	2:H:69:C:C6	2.52	0.44
5:D:185:PHE:O	5:D:186:LEU:CB	2.63	0.44
5:A:429:LEU:HD23	5:A:432:MET:CE	2.47	0.44
5:A:96:GLU:CG	5:A:97:HIS:H	2.30	0.44
5:B:321:LYS:NZ	5:B:424:PRO:O	2.51	0.44
5:C:312:ASN:O	5:D:314:MET:HE1	2.19	0.43
5:B:407:SER:O	5:B:410:GLU:HG2	2.18	0.43
4:J:70:G:C2	5:A:95:ALA:HB3	2.53	0.43
5:C:185:PHE:O	5:C:186:LEU:HB3	2.19	0.43
5:C:305:PHE:CE1	5:C:315:PRO:HB2	2.53	0.43
5:D:1:MET:SD	5:D:2:LYS:N	2.91	0.43
4:J:68:C:O2'	5:A:291:ASP:CG	2.62	0.43
5:A:312:ASN:HB3	5:B:314:MET:HE1	2.00	0.43
5:C:429:LEU:HD23	5:C:432:MET:CE	2.48	0.43
5:A:95:ALA:O	5:A:96:GLU:HG2	2.19	0.42
5:A:334:GLN:NE2	5:B:380:ARG:HH22	2.17	0.42
5:C:366:ARG:HH11	5:C:366:ARG:CG	2.32	0.42
5:C:373:ARG:HD2	8:C:560:HOH:O	2.20	0.41
4:J:70:G:N2	5:A:95:ALA:HB3	2.36	0.41
2:H:65:G:OP1	5:B:398:HIS:HD2	2.03	0.41
4:J:68:C:H1'	5:A:165:TYR:CE1	2.56	0.41
5:C:380:ARG:HH22	5:D:334:GLN:NE2	2.18	0.41
5:D:132:PHE:CB	5:D:220:VAL:HG21	2.51	0.41
5:D:415:ILE:HG23	5:D:419:LYS:HD2	2.02	0.41
5:C:314:MET:HE1	5:D:312:ASN:O	2.21	0.40
5:A:380:ARG:HH12	5:B:334:GLN:HE21	1.69	0.40
5:A:203:VAL:CG1	8:A:551:HOH:O	2.69	0.40
5:D:14:VAL:HG22	5:D:54:LEU:HD11	2.03	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	
5	A	435/437 (100%)	418 (96%)	12 (3%)	5 (1%)	11	10
5	B	435/437 (100%)	414 (95%)	15 (3%)	6 (1%)	9	7
5	C	435/437 (100%)	420 (97%)	12 (3%)	3 (1%)	18	19
5	D	435/437 (100%)	414 (95%)	17 (4%)	4 (1%)	14	14
All	All	1740/1748 (100%)	1666 (96%)	56 (3%)	18 (1%)	12	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	96	GLU
5	B	2	LYS
5	A	186	LEU
5	A	203	VAL
5	B	126	ALA
5	B	186	LEU
5	B	261	GLU
5	C	117	LEU
5	C	121	LYS
5	C	186	LEU
5	D	2	LYS
5	D	117	LEU
5	D	186	LEU
5	A	259	PRO
5	B	117	LEU
5	A	117	LEU
5	B	3	VAL
5	D	3	VAL

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	
5	A	387/387 (100%)	365 (94%)	22 (6%)	18	23
5	B	387/387 (100%)	375 (97%)	12 (3%)	35	48
5	C	387/387 (100%)	368 (95%)	19 (5%)	22	29
5	D	387/387 (100%)	369 (95%)	18 (5%)	23	31
All	All	1548/1548 (100%)	1477 (95%)	71 (5%)	24	32

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	5	GLU
5	A	14	VAL
5	A	17	ASP
5	A	43	VAL
5	A	47	SER
5	A	75	LEU
5	A	86	VAL
5	A	94	TYR
5	A	96	GLU
5	A	121	LYS
5	A	145	GLU
5	A	194	ARG
5	A	203	VAL
5	A	213	GLU
5	A	260	LEU
5	A	261	GLU
5	A	263	GLU
5	A	324	GLU
5	A	343	ARG
5	A	383	THR
5	A	399	THR
5	A	418	GLU
5	B	14	VAL
5	B	32	ARG

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Mol	Chain	Res	Type
5	B	69	GLU
5	B	75	LEU
5	B	78	ARG
5	B	144	LYS
5	B	145	GLU
5	B	203	VAL
5	B	260	LEU
5	B	321	LYS
5	B	381	LYS
5	B	383	THR
5	C	4	GLU
5	C	5	GLU
5	C	14	VAL
5	C	40	VAL
5	C	43	VAL
5	C	75	LEU
5	C	86	VAL
5	C	118	LYS
5	C	123	ILE
5	C	142	LYS
5	C	145	GLU
5	C	212	GLU
5	C	260	LEU
5	C	261	GLU
5	C	340	ARG
5	C	359	LEU
5	C	362	ASN
5	C	366	ARG
5	C	383	THR
5	D	12	GLU
5	D	14	VAL
5	D	31	LEU
5	D	38	LEU
5	D	75	LEU
5	D	87	LEU
5	D	104	VAL
5	D	122	ASN
5	D	145	GLU
5	D	212	GLU
5	D	260	LEU
5	D	267	LEU
5	D	324	GLU

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Mol	Chain	Res	Type
5	D	357	LYS
5	D	359	LEU
5	D	383	THR
5	D	399	THR
5	D	432	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	51	ASN
5	A	97	HIS
5	A	122	ASN
5	A	191	ASN
5	A	334	GLN
5	A	354	ASN
5	B	51	ASN
5	B	146	ASN
5	B	240	HIS
5	B	334	GLN
5	B	396	HIS
5	B	398	HIS
5	C	51	ASN
5	C	122	ASN
5	C	134	HIS
5	C	240	HIS
5	C	334	GLN
5	D	146	ASN
5	D	334	GLN
5	D	396	HIS
5	D	398	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	11/12 (91%)	3 (27%)	0
2	G	12/13 (92%)	1 (8%)	0
2	H	12/13 (92%)	0	0
2	I	12/13 (92%)	2 (16%)	0
3	F	11/12 (91%)	1 (9%)	0
4	J	12/13 (92%)	2 (16%)	1 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	70/76 (92%)	9 (12%)	1 (1%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	7	C
1	E	11	A
1	E	12	C
3	F	12	C
2	I	67	A
2	I	69	C
2	G	14	C
4	J	69	C
4	J	71	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	J	70	G

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](#)

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
7	ATP	D	1502	6	32,33,33	1.52	7 (21%)	48,52,52	1.80	11 (22%)
7	ATP	B	1501	6	32,33,33	1.75	7 (21%)	48,52,52	1.72	10 (20%)

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	D	1502	6	-	2/22/38/38	0/3/3/3
7	ATP	B	1501	6	-	3/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1501	ATP	C5-C4	5.03	1.48	1.39
7	D	1502	ATP	C5-C4	4.45	1.47	1.39
7	B	1501	ATP	PB-O3A	3.88	1.63	1.59
7	B	1501	ATP	PA-O3A	3.87	1.63	1.59
7	D	1502	ATP	PA-O3A	3.05	1.62	1.59
7	B	1501	ATP	PB-O3B	2.95	1.62	1.59
7	D	1502	ATP	PB-O3A	2.90	1.62	1.59
7	B	1501	ATP	C5-C6	2.83	1.48	1.41
7	D	1502	ATP	C5-C6	2.70	1.48	1.41
7	D	1502	ATP	PB-O3B	2.55	1.62	1.59
7	B	1501	ATP	C5-N7	-2.44	1.34	1.39
7	D	1502	ATP	C5-N7	-2.18	1.35	1.39
7	D	1502	ATP	C8-N7	2.16	1.35	1.31
7	B	1501	ATP	C8-N7	2.04	1.35	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1502	ATP	C5-C4-N3	-5.63	118.96	126.72
7	B	1501	ATP	C5-C4-N3	-5.46	119.20	126.72
7	D	1502	ATP	N3-C4-N9	4.64	135.06	127.17
7	B	1501	ATP	N3-C4-N9	4.55	134.91	127.17
7	D	1502	ATP	N3-C2-N1	-4.25	122.14	128.58
7	D	1502	ATP	C2-N3-C4	4.08	121.79	111.83
7	B	1501	ATP	N3-C2-N1	-3.72	122.96	128.58
7	B	1501	ATP	C2-N3-C4	3.71	120.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1502	ATP	C4-C5-N7	-3.13	107.01	110.58
7	B	1501	ATP	C4-C5-N7	-3.08	107.06	110.58
7	D	1502	ATP	C4-N9-C8	2.93	108.82	105.74
7	D	1502	ATP	C5-N7-C8	2.55	107.45	103.45
7	B	1501	ATP	C5-N7-C8	2.52	107.42	103.45
7	B	1501	ATP	C4-N9-C8	2.43	108.29	105.74
7	D	1502	ATP	N9-C8-N7	-2.25	110.74	113.94
7	D	1502	ATP	C6-C5-N7	2.22	136.38	132.09
7	D	1502	ATP	C2-N1-C6	2.22	122.37	118.73
7	B	1501	ATP	C2-N1-C6	2.18	122.31	118.73
7	B	1501	ATP	O4'-C1'-N9	2.13	112.18	108.09
7	D	1502	ATP	C2'-C1'-N9	-2.06	108.18	113.30
7	B	1501	ATP	C2'-C1'-N9	-2.06	108.20	113.30

There are no chirality outliers.

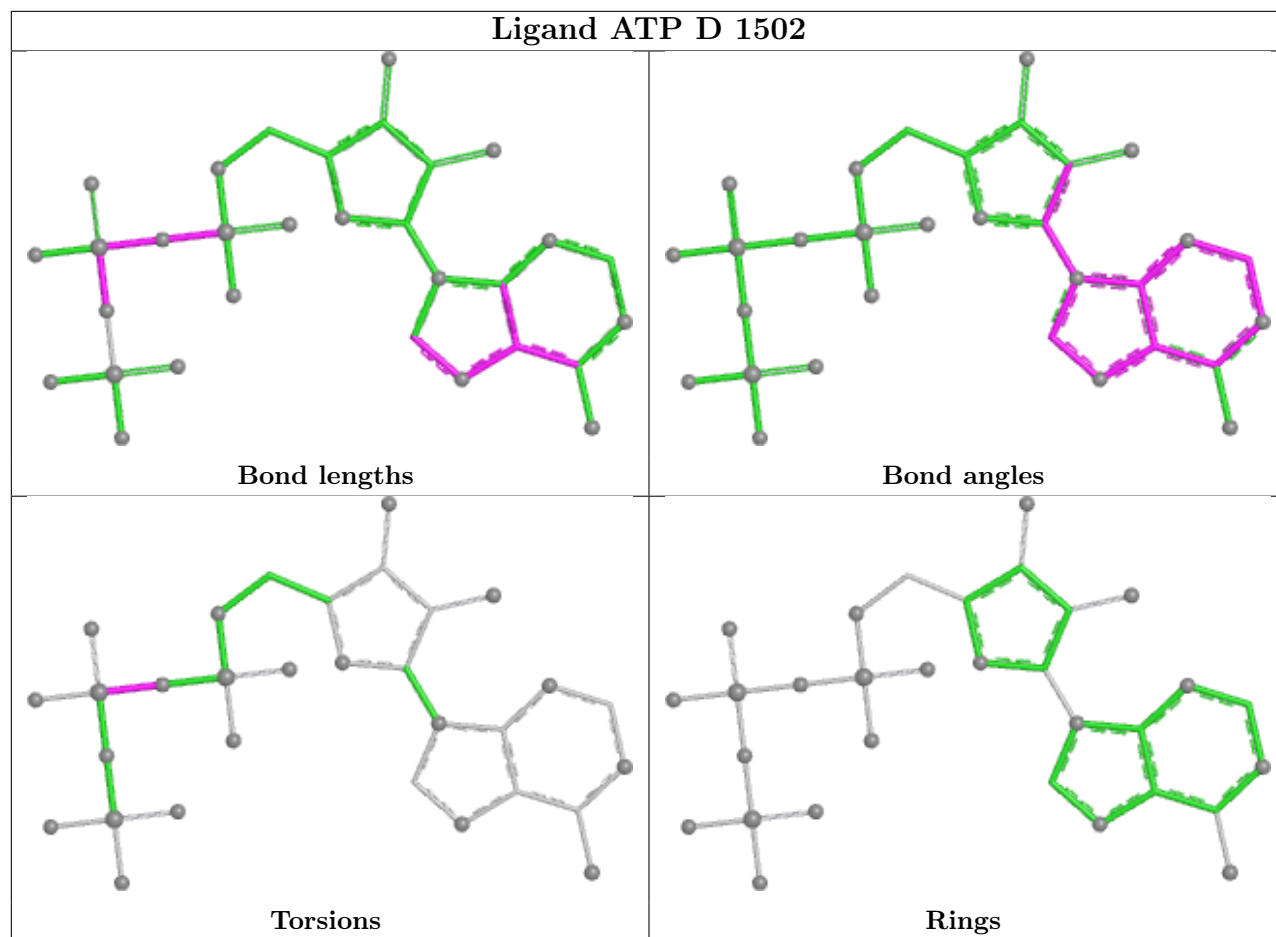
All (5) torsion outliers are listed below:

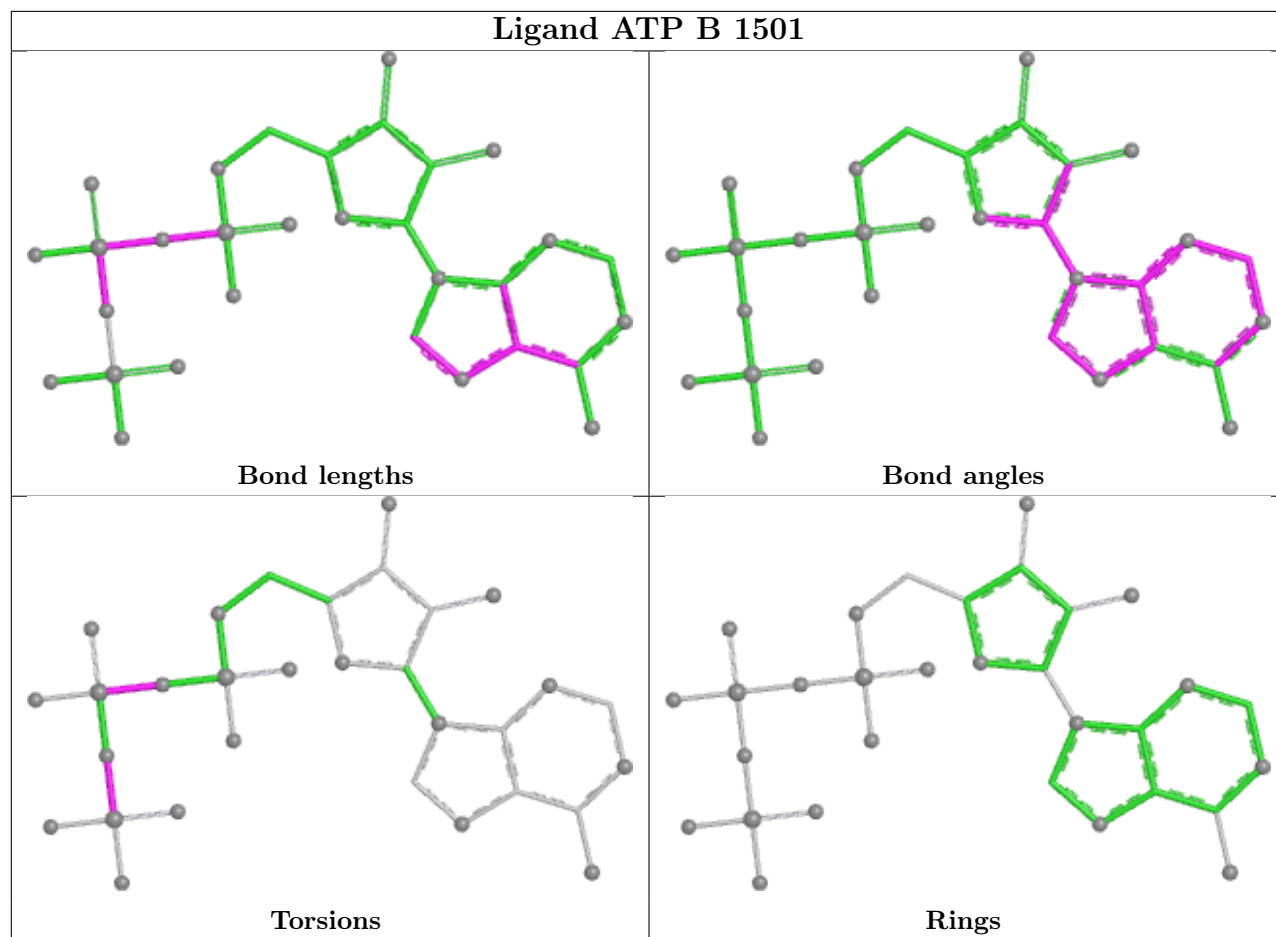
Mol	Chain	Res	Type	Atoms
7	B	1501	ATP	PB-O3B-PG-O3G
7	B	1501	ATP	PA-O3A-PB-O2B
7	D	1502	ATP	PA-O3A-PB-O2B
7	D	1502	ATP	PA-O3A-PB-O1B
7	B	1501	ATP	PB-O3B-PG-O1G

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	E	12/12 (100%)	0.93	2 (16%) 4 3	46, 50, 65, 73	0
2	G	13/13 (100%)	0.85	2 (15%) 5 4	41, 48, 85, 98	0
2	H	13/13 (100%)	1.20	3 (23%) 2 1	43, 50, 58, 64	0
2	I	13/13 (100%)	0.84	1 (7%) 19 17	42, 49, 64, 65	0
3	F	12/12 (100%)	0.81	0 100 100	50, 54, 64, 72	0
4	J	13/13 (100%)	1.09	3 (23%) 2 1	26, 37, 99, 105	0
5	A	437/437 (100%)	0.86	36 (8%) 17 15	38, 48, 64, 76	0
5	B	437/437 (100%)	0.83	28 (6%) 25 22	37, 48, 58, 69	0
5	C	437/437 (100%)	0.89	27 (6%) 26 23	40, 48, 63, 75	0
5	D	437/437 (100%)	1.11	57 (13%) 7 5	40, 48, 57, 70	0
All	All	1824/1824 (100%)	0.92	159 (8%) 16 13	26, 48, 62, 105	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	123	ILE	5.5
5	A	94	TYR	5.1
5	C	123	ILE	4.9
5	C	95	ALA	4.6
5	A	1	MET	4.3
4	J	61	C	4.0
2	H	74	C	4.0
5	A	98	PRO	3.8
4	J	73	C	3.7
5	C	124	LYS	3.7
5	D	63	PHE	3.7
5	A	95	ALA	3.6
5	A	96	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	73	A	3.4
5	D	121	LYS	3.4
5	B	139	GLY	3.3
5	B	1	MET	3.3
5	D	123	ILE	3.2
5	C	406	GLU	3.2
5	D	40	VAL	3.2
2	H	75	C	3.1
5	D	359	LEU	3.1
5	A	97	HIS	3.0
5	D	368	PHE	3.0
5	C	167	VAL	3.0
5	A	43	VAL	3.0
5	A	49	ALA	2.9
5	D	55	LYS	2.9
5	C	92	ILE	2.9
5	C	120	PRO	2.9
5	B	49	ALA	2.9
2	G	2	G	2.9
5	D	31	LEU	2.9
5	C	1	MET	2.9
5	D	54	LEU	2.9
5	C	127	VAL	2.9
5	D	289	VAL	2.9
5	A	260	LEU	2.8
5	B	58	LEU	2.8
5	A	291	ASP	2.8
5	A	50	ARG	2.8
5	D	139	GLY	2.8
5	C	94	TYR	2.8
5	D	375	TRP	2.8
5	A	259	PRO	2.8
5	C	228	ALA	2.8
5	B	203	VAL	2.8
5	D	56	GLY	2.7
5	D	43	VAL	2.7
5	B	349	PHE	2.7
5	B	126	ALA	2.6
5	A	120	PRO	2.6
5	D	1	MET	2.6
5	C	259	PRO	2.6
5	B	260	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
5	D	51	ASN	2.6
5	B	70	PHE	2.6
5	D	349	PHE	2.6
5	A	203	VAL	2.6
5	B	220	VAL	2.5
5	C	165	TYR	2.5
5	C	168	ARG	2.5
5	A	52	THR	2.5
5	C	163	ALA	2.5
5	A	92	ILE	2.5
5	D	104	VAL	2.5
5	D	362	ASN	2.5
5	D	127	VAL	2.4
2	I	75	C	2.4
5	D	124	LYS	2.4
5	C	97	HIS	2.4
5	D	262	ILE	2.4
5	A	100	VAL	2.4
5	B	123	ILE	2.4
5	A	261	GLU	2.4
5	C	229	ASN	2.4
5	D	108	GLU	2.4
5	C	126	ALA	2.4
5	B	121	LYS	2.4
5	A	125	SER	2.4
5	A	262	ILE	2.4
5	C	82	ILE	2.4
5	C	262	ILE	2.4
5	A	258	HIS	2.4
5	B	375	TRP	2.4
5	B	115	TYR	2.3
5	D	49	ALA	2.3
5	D	57	SER	2.3
1	E	1	G	2.3
5	D	109	VAL	2.3
5	D	239	VAL	2.3
5	B	75	LEU	2.3
5	D	58	LEU	2.3
5	D	232	LEU	2.3
5	C	96	GLU	2.3
5	D	437	ASP	2.3
5	D	60	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
5	D	355	VAL	2.3
5	B	120	PRO	2.3
5	B	48	TYR	2.3
5	D	211	GLY	2.3
5	D	93	ARG	2.3
5	B	262	ILE	2.3
5	C	17	ASP	2.3
5	C	169	GLY	2.3
5	A	17	ASP	2.2
2	G	14	C	2.2
5	D	372	GLY	2.2
5	A	81	GLU	2.2
5	A	99	TYR	2.2
5	B	42	TYR	2.2
5	D	115	TYR	2.2
5	C	117	LEU	2.2
5	B	232	LEU	2.2
5	B	40	VAL	2.2
5	A	51	ASN	2.2
4	J	71	C	2.2
5	D	348	GLN	2.2
5	D	52	THR	2.2
5	A	53	TRP	2.2
5	C	232	LEU	2.2
5	B	66	PHE	2.2
5	A	69	GLU	2.2
5	A	138	GLU	2.2
5	A	56	GLY	2.2
5	D	48	TYR	2.1
5	D	291	ASP	2.1
5	A	116	LYS	2.1
5	B	105	LYS	2.1
5	D	44	PHE	2.1
5	D	196	THR	2.1
5	D	248	ALA	2.1
5	C	261	GLU	2.1
5	B	45	VAL	2.1
5	D	103	VAL	2.1
5	D	107	VAL	2.1
5	D	203	VAL	2.1
5	B	63	PHE	2.1
5	A	139	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
5	A	126	ALA	2.1
5	B	437	ASP	2.1
5	D	369	ILE	2.1
5	D	24	GLY	2.1
1	E	2	C	2.1
5	C	231	SER	2.1
5	D	126	ALA	2.1
5	D	212	GLU	2.1
5	A	13	LEU	2.1
5	D	80	LEU	2.1
5	A	128	ASP	2.1
5	D	17	ASP	2.1
5	D	122	ASN	2.1
5	D	16	PRO	2.1
5	D	377	PHE	2.1
5	D	353	ARG	2.1
5	B	366	ARG	2.0
5	D	422	LYS	2.0
5	B	263	GLU	2.0
5	A	302	ARG	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.

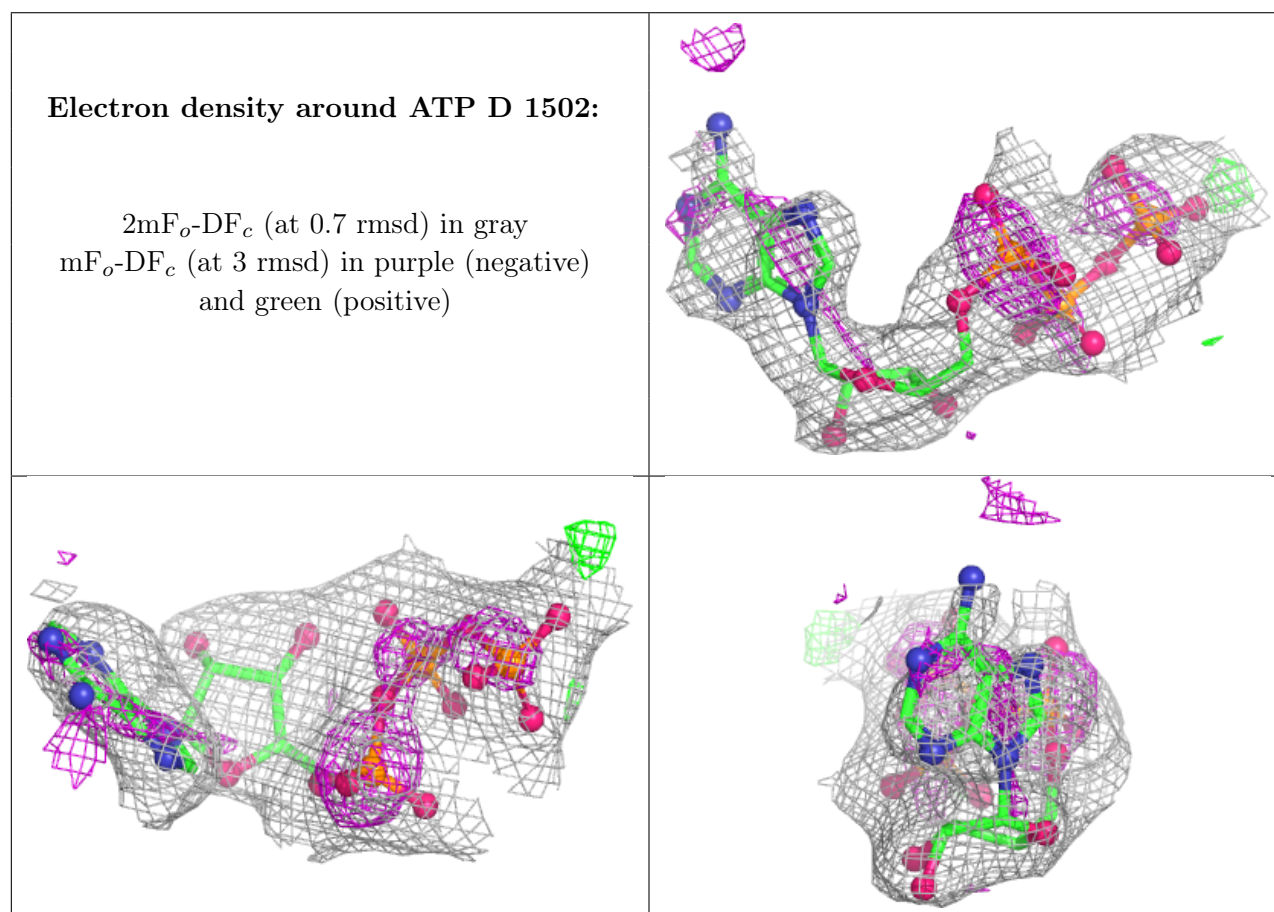
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ATP	D	1502	31/31	0.81	0.17	81,87,93,93	0
7	ATP	B	1501	31/31	0.83	0.17	63,71,73,77	0
6	MG	B	1601	1/1	0.88	0.10	73,73,73,73	0

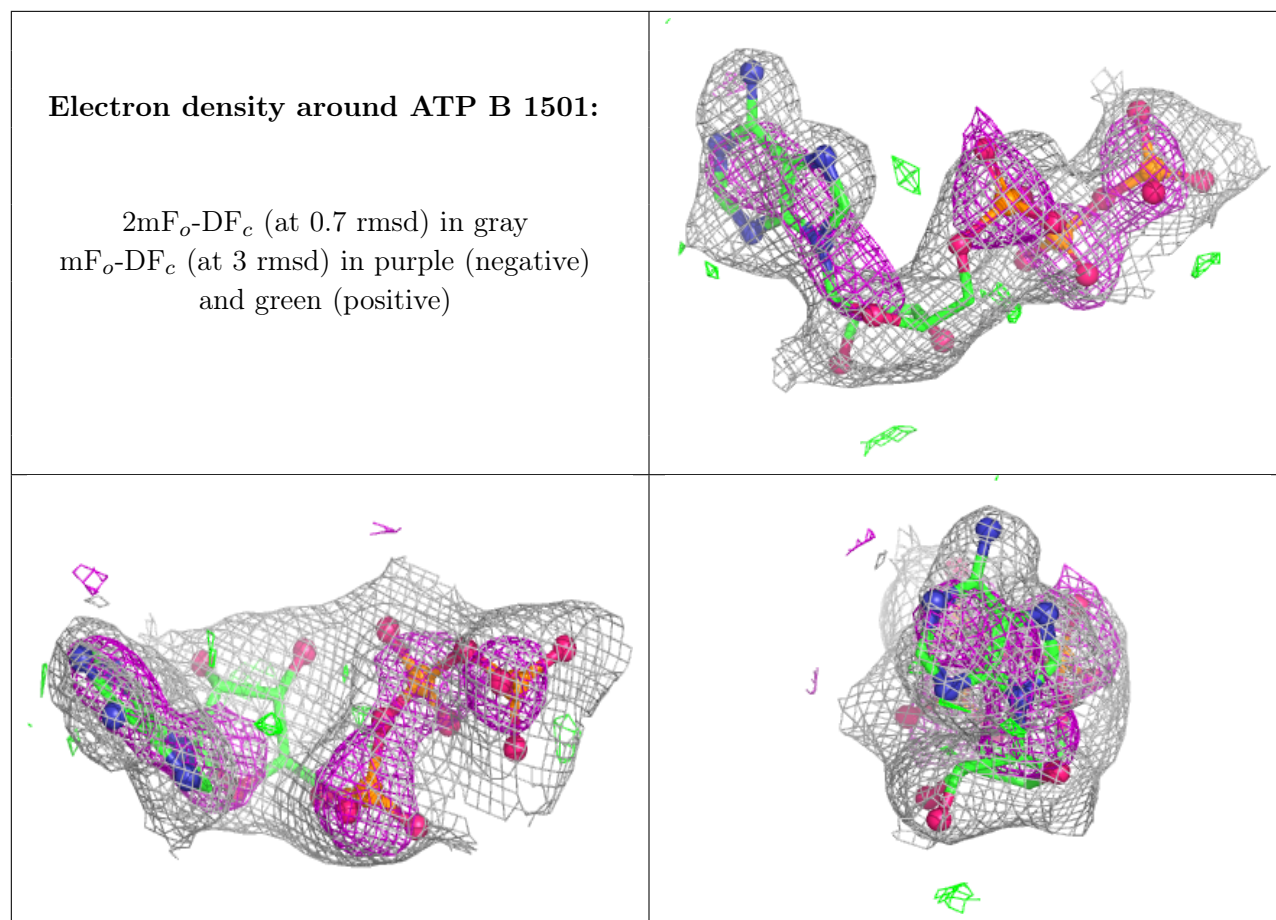
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	1602	1/1	0.95	0.09	68,68,68,68	0

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.





6.5 Other polymers ⓘ

There are no such residues in this entry.