



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:00 PM UTC

PDB ID : 4C0B / pdb_00004c0b
Title : Structure of wild-type Clp1p-Pcf11p (454 -563) complex
Authors : Fribourg, S.; Dupin, A.F.
Deposited on : 2013-08-01
Resolution : 2.77 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

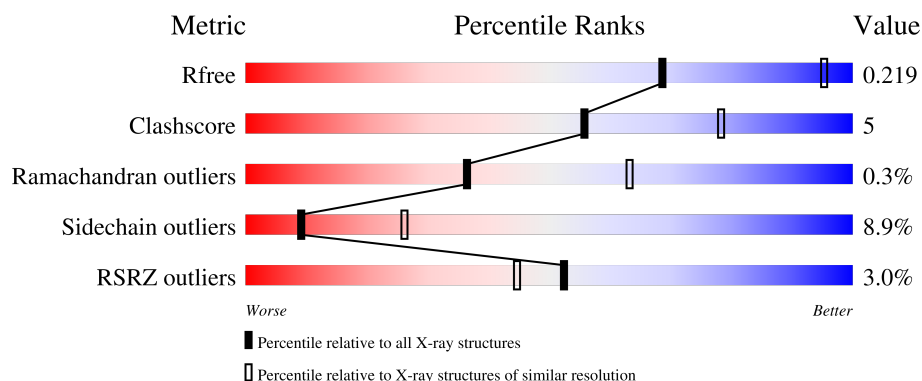
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	446	2% 77% 17% • •
1	B	446	0% 76% 17% • •
2	C	110	2% 21% • • 75%
2	D	110	10% 20% 11% • • 67%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7464 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 MRNA CLEAVAGE AND POLYADENYLATION FACTOR CLP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3410	2191	571	636	12			
1	B	430	Total	C	N	O	S	0	0	0
			3426	2201	574	639	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLN	-	expression tag	UNP Q08685
B	446	GLN	-	expression tag	UNP Q08685

- Molecule 2 is a protein called PCF11P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	0	0	0
			230	143	41	46			
2	D	36	Total	C	N	O	0	0	0
			290	177	51	62			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

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

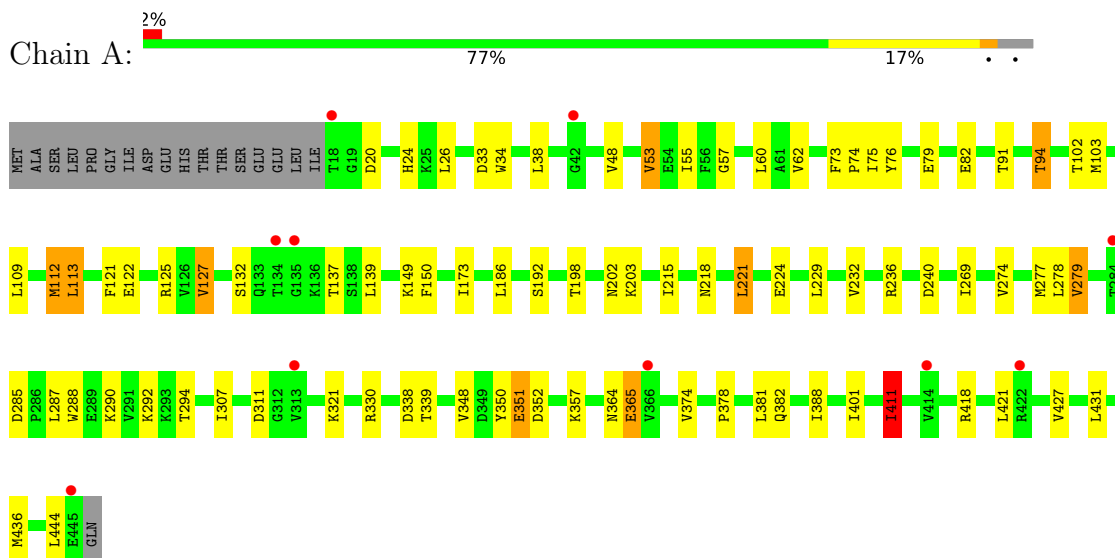
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	18	Total	O	0	0
			18	18		
5	C	1	Total	O	0	0
			1	1		
5	D	6	Total	O	0	0
			6	6		

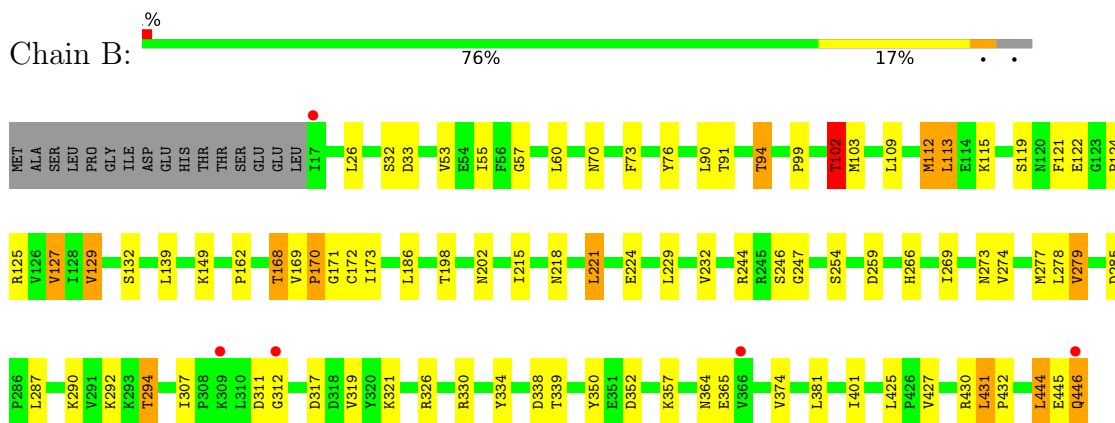
3 Residue-property plots [i](#)

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.

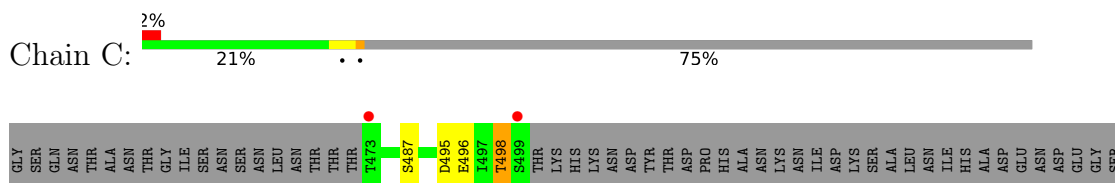
• Molecule 1: MRNA CLEAVAGE AND POLYADENYLATION FACTOR CLP1



• Molecule 1: MRNA CLEAVAGE AND POLYADENYLATION FACTOR CLP1



• Molecule 2: PCF11P



VAL
ASP
ASN
THR
LEU
GLY
SER
ASP
ARG
SER
ASN
GLU
LEU
GLU
ILE
ARG
GLY
LYS
TYR
VAL
VAL
VAL
PRO
GLU
THR
SER
GLN
ASP
MET
ALA
PHE
LYS

● Molecule 2: PCF11P



GLY
SER
GLN
ASN
THR
ALA
N460
N461
G462
N463
S464
N465
S466
N467
N468
N469
THR
THR
THR
THR
ARG
N475
N476
N477
N483
S487
D495
F496
N497
T498
S499
T500
LYS
HIS
LYS
ASN
ASP
TYR
THR
ASP
PRO
HIS
ALA
ASN
LYS
ASN
TLE
ASP
LYS
SER
ALA
LEU
ASN
TLE
HIS
ALA
ASP

GLU
ASN
ASP
GLU
GLY
SER
VAL
ASP
ASN
THR
LEU
GLY
SER
ASP
ARG
SER
ASN
GLU
LEU
GLU
ILE
ARG
GLY
LYS
TYR
VAL
VAL
VAL
PRO
GLU
THR
SER
GLN
ASP
MET
ALA
PHE
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.35Å 95.41Å 182.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.55 – 2.77 40.55 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.55-2.77) 99.5 (40.55-2.77)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.179 , 0.214 0.191 , 0.219	Depositor DCC
R_{free} test set	2018 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7464	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

5.1 Standard geometry

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	0.82	0/3487	1.36	22/4744 (0.5%)
1	B	0.87	0/3503	1.40	23/4766 (0.5%)
2	C	0.84	0/235	1.22	0/317
2	D	1.16	1/294 (0.3%)	1.60	6/397 (1.5%)
All	All	0.86	1/7519 (0.0%)	1.39	51/10224 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	476	ASN	CA-C	5.58	1.59	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	CYS	N-CA-C	9.71	125.48	110.42
1	B	170	PRO	N-CA-C	9.01	125.81	113.65
1	B	246	SER	N-CA-C	-7.34	101.06	110.53
1	A	351	GLU	CB-CG-CD	7.08	124.64	112.60
1	B	338	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	186	LEU	N-CA-C	6.53	119.08	109.62
1	A	411	ILE	CB-CA-C	6.48	119.47	111.25
2	D	476	ASN	N-CA-C	6.41	120.24	108.58
1	B	186	LEU	N-CA-C	6.24	118.66	109.62
1	A	338	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	381	LEU	N-CA-C	6.08	121.75	113.97
2	D	461	THR	CA-C-N	6.07	126.71	119.98
2	D	461	THR	C-N-CA	6.07	126.71	119.98
1	B	33	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	33	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	246	SER	CA-C-N	-6.01	109.64	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	SER	C-N-CA	-6.01	109.64	121.41
1	B	350	TYR	CA-C-N	6.00	128.91	120.28
1	B	350	TYR	C-N-CA	6.00	128.91	120.28
1	B	244	ARG	CA-C-N	5.98	128.78	120.29
1	B	244	ARG	C-N-CA	5.98	128.78	120.29
1	A	350	TYR	CA-C-N	5.92	128.80	120.28
1	A	350	TYR	C-N-CA	5.92	128.80	120.28
2	D	465	ASN	N-CA-C	-5.86	100.16	109.59
1	B	121	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	418	ARG	N-CA-C	-5.66	100.95	109.79
1	B	173	ILE	N-CA-C	-5.63	100.37	108.53
1	B	352	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	150	PHE	CA-C-N	5.61	130.82	122.74
1	A	150	PHE	C-N-CA	5.61	130.82	122.74
1	A	73	PHE	N-CA-C	5.49	113.07	108.13
1	A	121	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	411	ILE	N-CA-CB	5.41	117.96	111.31
1	B	290	LYS	CA-C-N	5.38	127.83	120.46
1	B	290	LYS	C-N-CA	5.38	127.83	120.46
1	A	173	ILE	N-CA-C	-5.37	100.75	108.48
1	B	73	PHE	N-CA-C	5.23	112.84	108.13
1	A	34	TRP	N-CA-C	-5.23	99.25	108.20
1	A	290	LYS	CA-C-N	5.23	127.62	120.46
1	A	290	LYS	C-N-CA	5.23	127.62	120.46
1	B	70	ASN	N-CA-C	5.21	118.38	111.30
1	A	381	LEU	N-CA-C	5.17	120.45	113.72
1	A	427	VAL	N-CA-C	5.16	113.62	107.73
1	B	427	VAL	N-CA-C	5.15	113.61	107.73
2	D	497	ILE	CA-C-N	5.10	131.28	121.54
2	D	497	ILE	C-N-CA	5.10	131.28	121.54
1	B	171	GLY	N-CA-C	5.06	121.59	115.31
1	A	352	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	102	THR	OG1-CB-CG2	5.01	119.32	109.30
1	A	38	LEU	CA-C-N	5.01	126.95	120.44
1	A	38	LEU	C-N-CA	5.01	126.95	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3410	0	3443	34	0
1	B	3426	0	3461	34	0
2	C	230	0	212	1	0
2	D	290	0	264	6	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	19	0	0	0	0
5	B	18	0	0	0	0
5	C	1	0	0	0	0
5	D	6	0	0	0	0
All	All	7464	0	7404	70	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 5.

All (70) 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:A:364:ASN:O	1:A:365:GLU:HB2	1.61	1.00
1:A:127:VAL:HG22	1:A:274:VAL:HG11	1.53	0.90
1:B:127:VAL:HG22	1:B:274:VAL:HG11	1.51	0.89
1:B:168:THR:HG23	2:D:483:TYR:OH	1.76	0.83
1:A:364:ASN:O	1:A:365:GLU:CB	2.36	0.74
1:B:364:ASN:O	1:B:365:GLU:HB2	1.87	0.73
1:B:278:LEU:HB3	1:B:307:ILE:HD11	1.70	0.73
1:A:278:LEU:HB3	1:A:307:ILE:HD11	1.70	0.72
2:D:463:ILE:HG12	2:D:464:SER:H	1.63	0.63
1:A:55:ILE:HD12	1:A:60:LEU:HD21	1.84	0.60
1:B:55:ILE:HD12	1:B:60:LEU:HD21	1.85	0.58
1:A:48:VAL:HG23	1:A:62:VAL:HA	1.84	0.58
1:B:326:ARG:NH2	1:B:444:LEU:O	2.36	0.58
1:A:378:PRO:O	1:A:382:GLN:HB2	2.04	0.58
1:A:57:GLY:O	1:A:149:LYS:NZ	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:HG22	1:B:169:VAL:H	1.71	0.55
1:B:91:THR:H	1:B:94:THR:HG22	1.72	0.54
1:B:162:PRO:O	1:B:170:PRO:O	2.25	0.54
1:B:57:GLY:O	1:B:149:LYS:NZ	2.34	0.54
1:B:278:LEU:HB3	1:B:307:ILE:CD1	2.38	0.54
1:B:102:THR:HG21	1:B:311:ASP:H	1.73	0.53
2:D:495:ASP:HA	2:D:498:THR:HB	1.90	0.53
1:B:312:GLY:HA3	3:B:1447:ATP:N6	2.24	0.53
1:A:125:ARG:NH2	1:B:122:GLU:OE2	2.42	0.53
1:B:218:ASN:CG	1:B:221:LEU:HB2	2.33	0.53
1:A:411:ILE:HD13	1:A:421:LEU:HD23	1.92	0.52
1:A:278:LEU:HB3	1:A:307:ILE:CD1	2.39	0.52
1:A:91:THR:H	1:A:94:THR:HG22	1.73	0.52
1:A:53:VAL:CG2	1:A:75:ILE:HG22	2.40	0.52
1:A:102:THR:HG21	1:A:311:ASP:H	1.75	0.51
2:C:495:ASP:HA	2:C:498:THR:HB	1.91	0.51
1:B:124:PRO:O	1:B:247:GLY:HA3	2.12	0.50
1:A:112:MET:HE3	1:A:113:LEU:HD13	1.93	0.50
1:B:125:ARG:HD2	1:B:273:ASN:O	2.12	0.49
1:A:236:ARG:NH1	1:A:240:ASP:OD2	2.45	0.49
1:A:357:LYS:HB2	1:A:374:VAL:HG22	1.94	0.49
1:B:112:MET:HE3	1:B:113:LEU:HD13	1.94	0.49
1:B:266:HIS:HE2	1:B:294:THR:HG22	1.78	0.49
1:A:279:VAL:CG1	1:A:288:TRP:HZ3	2.26	0.48
1:B:364:ASN:O	1:B:365:GLU:CB	2.57	0.48
1:A:122:GLU:OE2	1:B:125:ARG:NH2	2.46	0.48
1:B:357:LYS:HB2	1:B:374:VAL:HG22	1.94	0.48
1:A:127:VAL:HG22	1:A:274:VAL:CG1	2.36	0.47
1:B:168:THR:HG23	2:D:483:TYR:HH	1.73	0.47
1:B:127:VAL:CG2	1:B:274:VAL:HG11	2.35	0.47
1:A:218:ASN:CG	1:A:221:LEU:HB2	2.39	0.46
1:A:74:PRO:HG3	3:A:1446:ATP:C6	2.51	0.46
1:A:279:VAL:HG13	1:A:288:TRP:HZ3	1.81	0.45
1:B:127:VAL:HG22	1:B:274:VAL:CG1	2.34	0.45
1:B:198:THR:HG21	1:B:202:ASN:HD21	1.82	0.44
1:A:53:VAL:HG21	1:A:75:ILE:HG22	2.00	0.43
1:B:334:TYR:OH	2:D:468:LEU:HD23	2.19	0.43
1:A:388:ILE:HG12	1:A:436:MET:HE2	2.00	0.43
1:B:76:TYR:CZ	1:B:103:MET:HG3	2.53	0.43
1:A:76:TYR:CZ	1:A:103:MET:HG3	2.53	0.43
1:A:198:THR:HG21	1:A:202:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:HD11	1:B:277:MET:CE	2.48	0.42
1:A:269:ILE:HD11	1:A:277:MET:CE	2.48	0.42
1:A:53:VAL:HG22	1:A:75:ILE:HG22	2.00	0.42
1:B:129:VAL:HG12	1:B:279:VAL:HG13	2.02	0.42
1:B:431:LEU:HD22	1:B:432:PRO:HD2	2.02	0.41
1:A:279:VAL:HG13	1:A:288:TRP:CZ3	2.55	0.41
1:B:446:GLN:H	1:B:446:GLN:HG3	1.69	0.41
2:D:460:ASN:C	2:D:462:GLY:H	2.28	0.41
1:A:269:ILE:HA	1:A:274:VAL:HB	2.03	0.41
1:B:317:ASP:OD2	1:B:319:VAL:HB	2.20	0.41
1:B:32:SER:HA	1:B:99:PRO:HA	2.03	0.40
1:A:192:SER:HA	1:A:203:LYS:O	2.22	0.40
1:A:20:ASP:HB3	1:A:24:HIS:HE1	1.86	0.40
1:A:279:VAL:CG1	1:A:288:TRP:CZ3	3.05	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	426/446 (96%)	408 (96%)	18 (4%)	0	100	100
1	B	428/446 (96%)	407 (95%)	21 (5%)	0	100	100
2	C	25/110 (23%)	23 (92%)	1 (4%)	1 (4%)	2	7
2	D	32/110 (29%)	26 (81%)	4 (12%)	2 (6%)	1	2
All	All	911/1112 (82%)	864 (95%)	44 (5%)	3 (0%)	36	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	498	THR

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Mol	Chain	Res	Type
2	D	498	THR
2	D	461	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	384/401 (96%)	352 (92%)	32 (8%)	10	29
1	B	386/401 (96%)	349 (90%)	37 (10%)	8	23
2	C	25/98 (26%)	23 (92%)	2 (8%)	11	31
2	D	33/98 (34%)	30 (91%)	3 (9%)	9	25
All	All	828/998 (83%)	754 (91%)	74 (9%)	9	26

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	53	VAL
1	A	79	GLU
1	A	82	GLU
1	A	94	THR
1	A	109	LEU
1	A	112	MET
1	A	113	LEU
1	A	127	VAL
1	A	132	SER
1	A	137	THR
1	A	139	LEU
1	A	215	ILE
1	A	221	LEU
1	A	224	GLU
1	A	229	LEU
1	A	232	VAL
1	A	279	VAL
1	A	285	ASP

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	292	LYS
1	A	294	THR
1	A	321	LYS
1	A	330	ARG
1	A	339	THR
1	A	348	VAL
1	A	351	GLU
1	A	365	GLU
1	A	401	ILE
1	A	411	ILE
1	A	431	LEU
1	A	444	LEU
1	B	26	LEU
1	B	53	VAL
1	B	90	LEU
1	B	94	THR
1	B	102	THR
1	B	109	LEU
1	B	112	MET
1	B	113	LEU
1	B	115	LYS
1	B	119	SER
1	B	127	VAL
1	B	129	VAL
1	B	132	SER
1	B	139	LEU
1	B	168	THR
1	B	215	ILE
1	B	221	LEU
1	B	224	GLU
1	B	229	LEU
1	B	232	VAL
1	B	254	SER
1	B	259	ASP
1	B	279	VAL
1	B	285	ASP
1	B	287	LEU
1	B	292	LYS
1	B	294	THR
1	B	321	LYS
1	B	330	ARG

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Mol	Chain	Res	Type
1	B	339	THR
1	B	401	ILE
1	B	425	LEU
1	B	430	ARG
1	B	431	LEU
1	B	444	LEU
1	B	445	GLU
1	B	446	GLN
2	C	487	SER
2	C	496	GLU
2	D	461	THR
2	D	477	ILE
2	D	487	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	49	ASN
1	A	70	ASN
1	A	202	ASN
1	A	242	GLN
1	A	302	ASN
1	B	70	ASN
1	B	202	ASN
1	B	238	HIS
1	B	242	GLN
1	B	257	GLN
2	C	476	ASN
2	C	481	ASN
2	D	469	ASN
2	D	481	ASN

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 [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	$\# Z > 2$
3	ATP	A	1446	4	32,33,33	2.17	2 (6%)	48,52,52	0.49	0
3	ATP	B	1447	4	32,33,33	2.16	2 (6%)	48,52,52	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1446	4	-	1/22/38/38	0/3/3/3
3	ATP	B	1447	4	-	1/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1446	ATP	PA-O3A	-8.47	1.50	1.59
3	B	1447	ATP	PB-O3B	-8.47	1.50	1.59
3	A	1446	ATP	PB-O3B	-8.35	1.50	1.59
3	B	1447	ATP	PA-O3A	-8.29	1.50	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

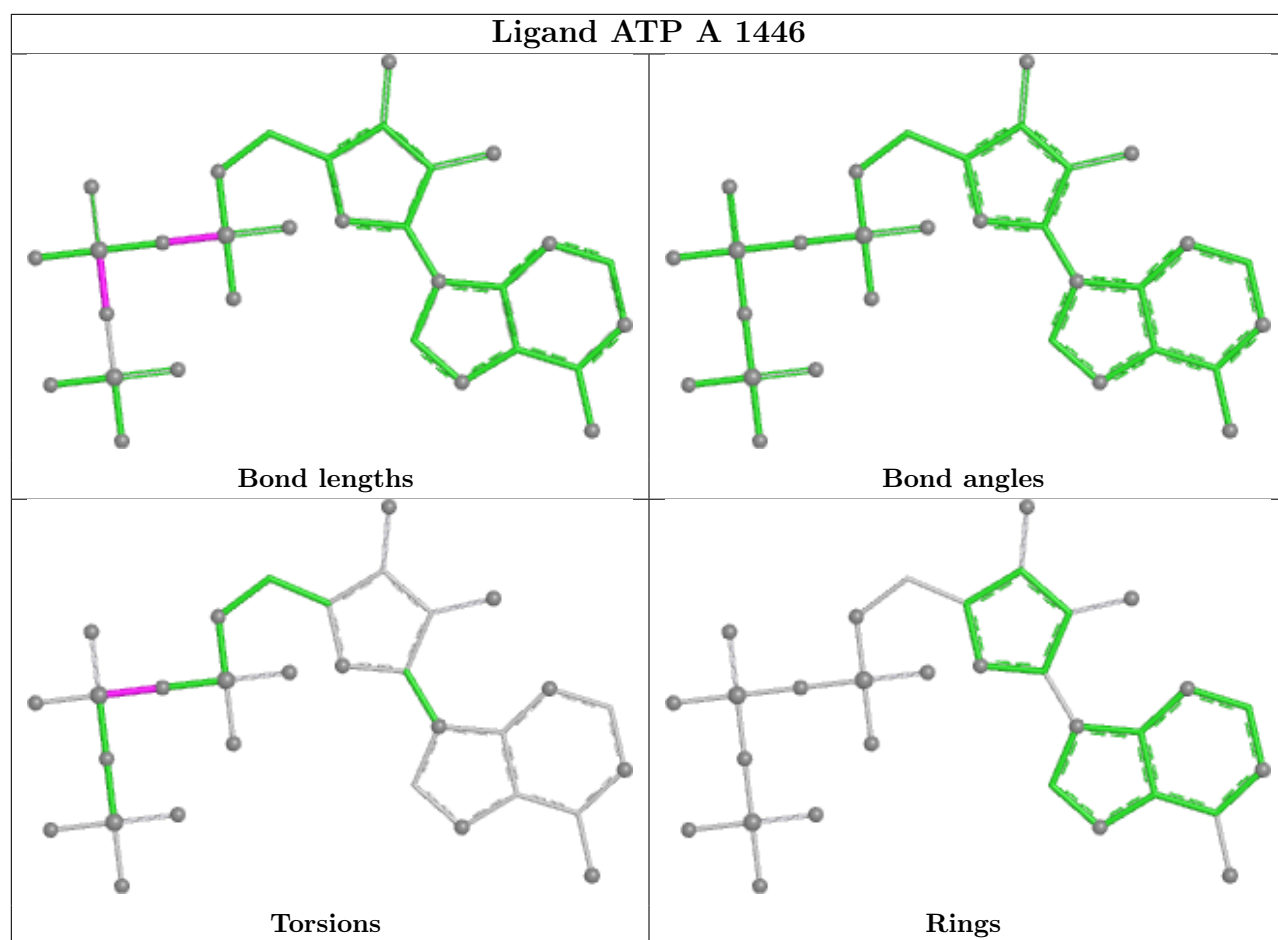
Mol	Chain	Res	Type	Atoms
3	B	1447	ATP	PA-O3A-PB-O2B
3	A	1446	ATP	PA-O3A-PB-O2B

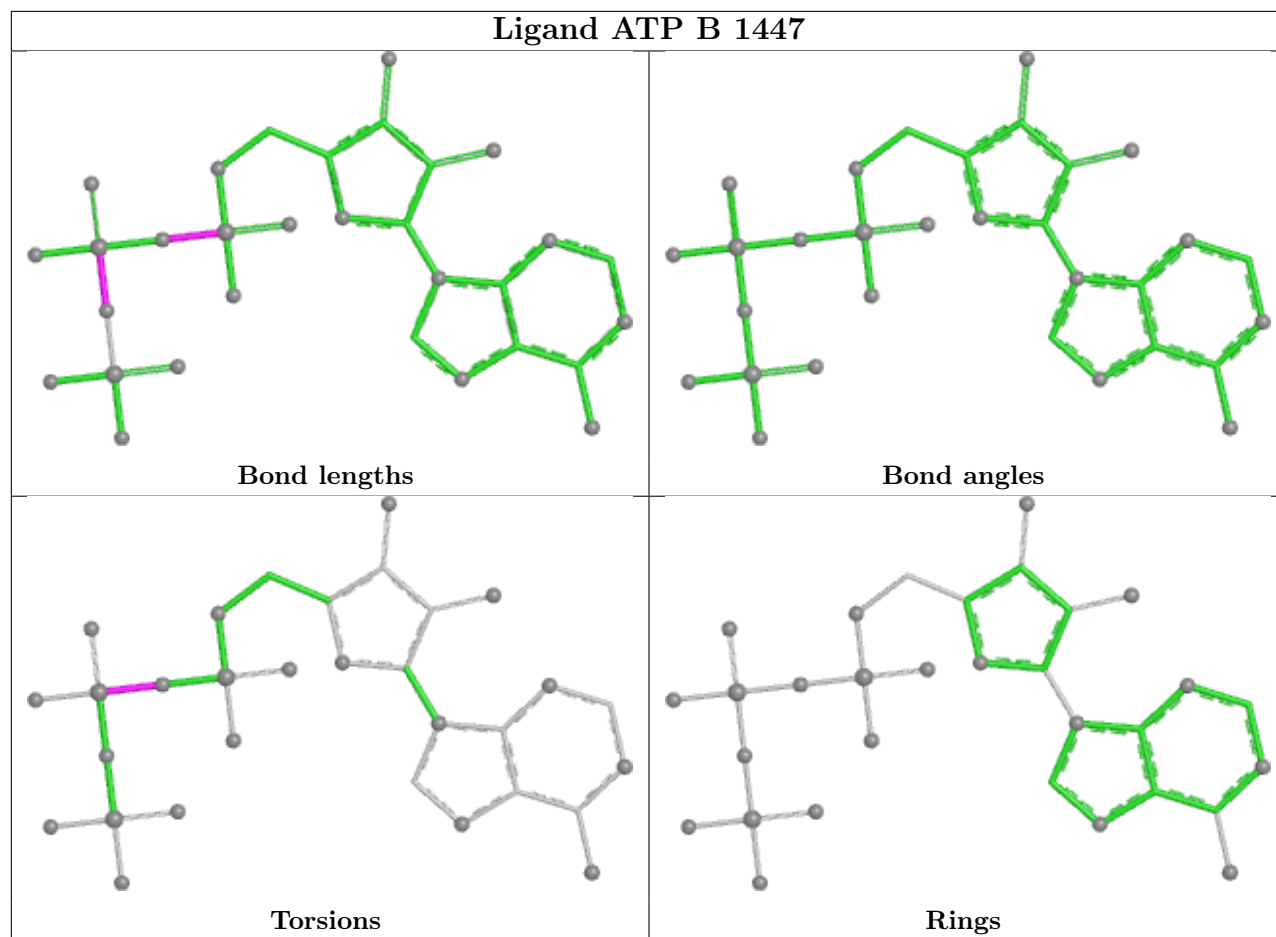
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1446	ATP	1	0
3	B	1447	ATP	1	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.





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	428/446 (95%)	0.15	10 (2%) 61 53	35, 70, 117, 144	0
1	B	430/446 (96%)	-0.08	5 (1%) 76 70	33, 57, 93, 125	0
2	C	27/110 (24%)	0.22	2 (7%) 20 16	37, 54, 119, 128	0
2	D	36/110 (32%)	0.88	11 (30%) 1 1	35, 60, 122, 129	0
All	All	921/1112 (82%)	0.07	28 (3%) 52 45	33, 63, 111, 144	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	463	ILE	4.4
1	A	18	THR	4.2
2	D	500	THR	4.1
2	D	461	THR	4.0
1	B	446	GLN	3.8
2	D	469	ASN	3.8
2	D	466	SER	3.6
2	C	499	SER	3.5
2	D	475	LYS	3.4
1	B	366	VAL	3.4
1	B	17	ILE	3.3
2	C	473	THR	2.7
2	D	460	ASN	2.6
1	B	309	LYS	2.6
1	A	313	VAL	2.6
2	D	465	ASN	2.5
1	A	42	GLY	2.5
1	A	422	ARG	2.5
2	D	467	ASN	2.4
1	A	135	GLY	2.4
1	B	312	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	284	THR	2.3
2	D	464	SER	2.3
1	A	134	THR	2.3
2	D	476	ASN	2.3
1	A	414	VAL	2.2
1	A	445	GLU	2.1
1	A	366	VAL	2.1

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](#)

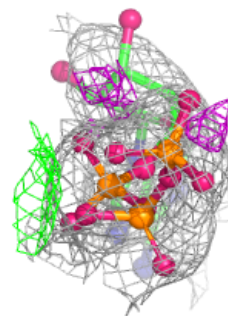
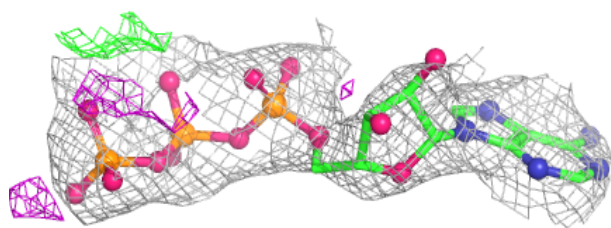
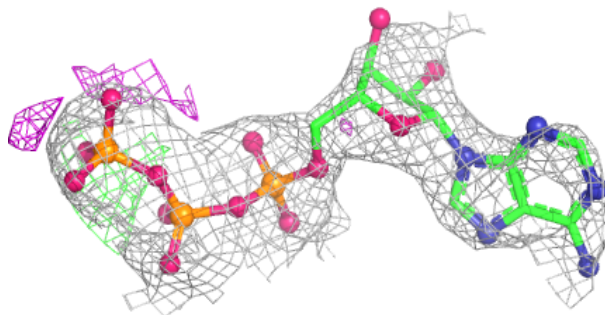
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	1447	1/1	0.87	0.20	67,67,67,67	0
4	MG	B	1448	1/1	0.87	0.27	66,66,66,66	0
3	ATP	A	1446	31/31	0.91	0.11	120,124,134,136	0
3	ATP	B	1447	31/31	0.92	0.12	103,110,117,118	0

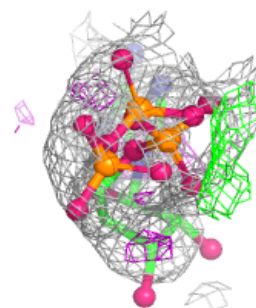
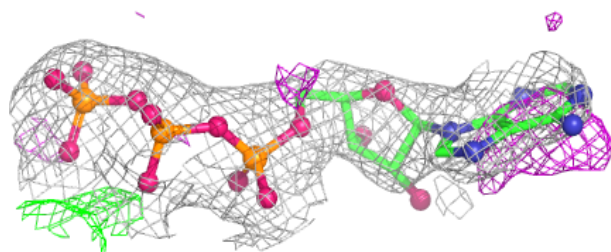
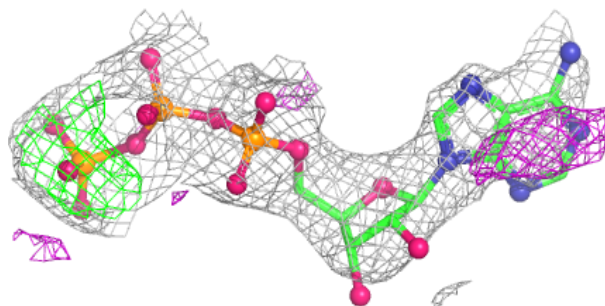
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 1446:

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

**Electron density around ATP B 1447:**

$2mF_o-DF_c$ (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.