



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:07 PM EDT

PDB ID : 4A8Y
Title : Non-Catalytic Ions Direct the RNA-Dependent RNA Polymerase of Bacterial dsRNA virus phi6 from De Novo Initiation to Elongation
Authors : Wright, S.; Poranen, M.M.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2011-11-21
Resolution : 3.41 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

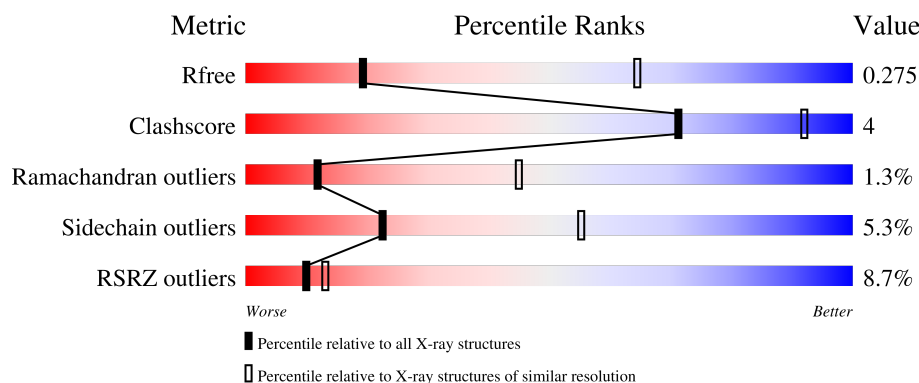
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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	665	<div> <div>6%</div> <div>91%</div> <div>8%</div> </div>
1	B	665	<div> <div>12%</div> <div>87%</div> <div>11%</div> </div>
1	C	665	<div> <div>7%</div> <div>81%</div> <div>12%</div> </div>
2	F	14	<div> <div>14%</div> <div>7%</div> <div>7%</div> <div>86%</div> </div>
2	G	14	<div> <div>21%</div> <div>14%</div> <div>7%</div> <div>79%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	14	<div><div></div><div></div><div></div><div></div></div> <div>7%14%21%57%</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15867 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	C	640	Total	C	N	O	S	0	0	0
			5080	3227	879	943	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	SEE REMARK 999	UNP P11124
A	634	GLN	GLU	engineered mutation	UNP P11124
B	456	MET	ILE	SEE REMARK 999	UNP P11124
B	634	GLN	GLU	engineered mutation	UNP P11124
C	456	MET	ILE	SEE REMARK 999	UNP P11124
C	634	GLN	GLU	engineered mutation	UNP P11124

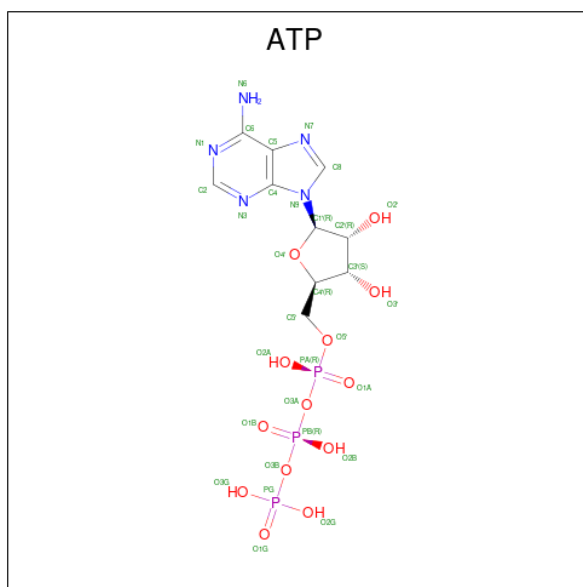
- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*AP*AP*GP*CP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
2	G	3	Total	C	N	O	P	0	0	0
			60	29	13	16	2			
2	H	6	Total	C	N	O	P	0	0	0
			118	59	16	38	5			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

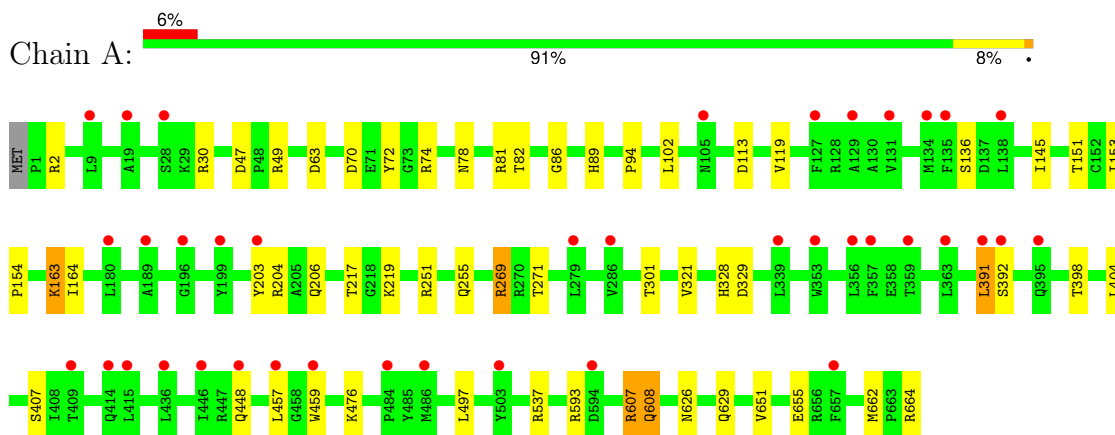


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 13 10 3	0	0
4	B	1	Total O P 13 10 3	0	0
4	C	1	Total O P 13 10 3	0	0

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.

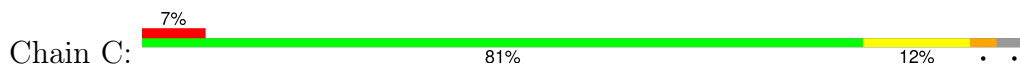
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

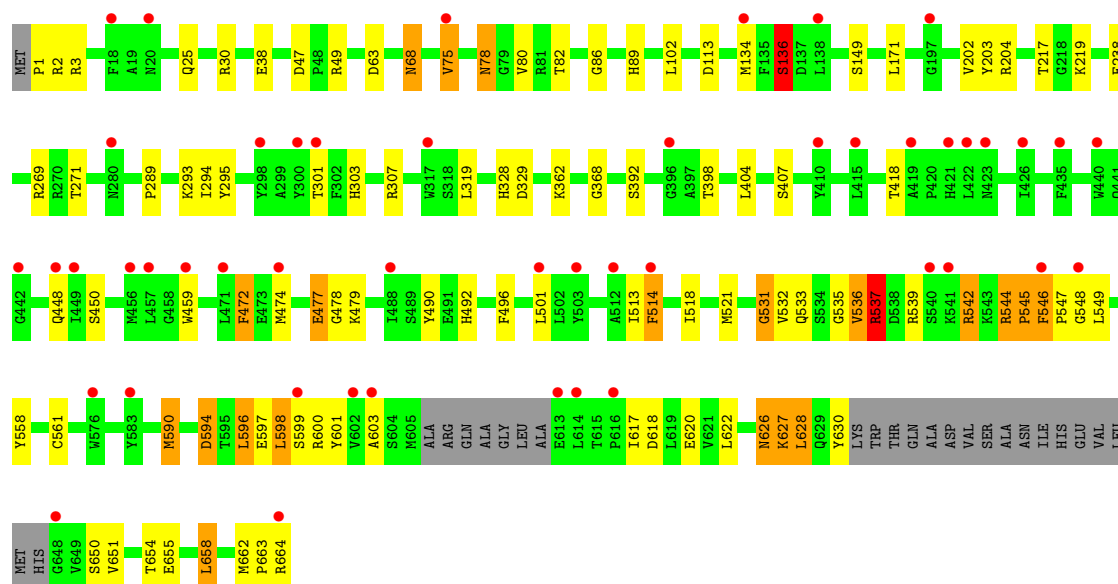


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE

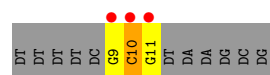




• Molecule 2: 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*AP*AP*GP*CP*GP)-3'



• Molecule 2: 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*AP*AP*GP*CP*GP)-3'



• Molecule 2: 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*AP*AP*GP*CP*GP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.76Å 89.29Å 140.99Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	67.61 – 3.41 67.61 – 3.41	Depositor EDS
% Data completeness (in resolution range)	87.0 (67.61-3.41) 86.9 (67.61-3.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.218 , 0.255 0.236 , 0.275	Depositor DCC
R_{free} test set	1551 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	1.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.1	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	0.91	EDS
Total number of atoms	15867	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.40	0/5396	0.63	1/7297 (0.0%)
1	B	0.42	0/5396	0.66	0/7297
1	C	0.42	0/5205	0.69	0/7034
2	F	1.11	0/42	1.70	1/63 (1.6%)
2	G	1.07	0/67	2.23	4/102 (3.9%)
2	H	1.46	0/129	2.57	13/195 (6.7%)
All	All	0.44	0/16235	0.72	19/21988 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	DT	P-O3'-C3'	9.19	130.73	119.70
2	F	8	DC	P-O3'-C3'	8.31	129.67	119.70
2	H	8	DC	C2-N1-C1'	7.74	127.31	118.80
2	H	7	DT	O4'-C1'-N1	7.63	113.34	108.00
2	H	6	DT	O4'-C1'-N1	7.62	113.33	108.00
2	H	8	DC	N1-C2-O2	7.49	123.40	118.90
2	G	10	DC	P-O3'-C3'	7.21	128.35	119.70
2	G	11	DG	C1'-O4'-C4'	-6.80	103.30	110.10
2	H	7	DT	P-O3'-C3'	6.68	127.72	119.70
2	G	11	DG	O4'-C1'-N9	6.65	112.65	108.00
2	H	8	DC	C5-C6-N1	6.14	124.07	121.00
2	G	9	DG	P-O3'-C3'	6.04	126.95	119.70
2	H	6	DT	P-O3'-C3'	5.90	126.78	119.70
2	H	8	DC	C6-N1-C2	-5.74	118.00	120.30
2	H	4	DT	N3-C2-O2	-5.38	119.07	122.30
1	A	206	GLN	N-CA-C	-5.32	96.64	111.00
2	H	5	DT	C4-C5-C7	5.24	122.14	119.00
2	H	8	DC	N3-C2-O2	-5.11	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	DC	C6-N1-C1'	-5.10	114.68	120.80

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	5265	0	5167	30	0
1	B	5265	0	5167	36	0
1	C	5080	0	4983	49	0
2	F	38	0	24	0	0
2	G	60	0	35	1	0
2	H	118	0	73	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	0	0	0
4	B	13	0	0	0	0
4	C	13	0	0	0	0
All	All	15867	0	15449	111	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 4.

All (111) 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:600:ARG:HB3	1:C:601:TYR:HA	1.19	1.10
1:B:410:TYR:HB3	1:B:457:LEU:HD21	1.57	0.85
1:C:600:ARG:HB3	1:C:601:TYR:CA	2.11	0.75
1:B:39:THR:HB	1:B:43:LEU:HD13	1.71	0.71
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.37	0.71
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.40	0.70
1:A:321:VAL:HG22	1:A:457:LEU:HB2	1.77	0.66
1:B:235:THR:HB	1:B:238:GLU:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:LYS:HD3	1:B:497:LEU:HD21	1.78	0.65
1:A:321:VAL:CG2	1:A:457:LEU:HB2	2.28	0.64
1:C:535:GLY:HA2	1:C:536:VAL:HB	1.81	0.62
1:C:539:ARG:HB3	1:C:545:PRO:HB3	1.81	0.62
1:C:136:SER:OG	1:C:293:LYS:NZ	2.33	0.62
1:C:38:GLU:HB3	1:C:532:VAL:HG22	1.82	0.60
1:A:537:ARG:HD2	1:B:49:ARG:HG3	1.83	0.60
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.68	0.58
1:C:149:SER:HB2	2:H:6:DT:H3'	1.84	0.58
1:C:628:LEU:HG	2:H:8:DC:C2	2.39	0.57
1:C:600:ARG:CB	1:C:601:TYR:HA	2.09	0.56
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.86	0.56
1:A:392:SER:O	1:A:398:THR:HG21	2.06	0.55
1:C:539:ARG:HA	1:C:542:ARG:HG2	1.89	0.55
1:A:593:ARG:HG2	1:B:42:GLY:HA2	1.88	0.55
1:B:407:SER:HA	1:B:448:GLN:HE22	1.72	0.55
1:C:392:SER:O	1:C:398:THR:HG21	2.07	0.54
1:C:651:VAL:O	1:C:655:GLU:HB2	2.07	0.54
1:C:78:ASN:HD22	1:C:80:VAL:H	1.55	0.54
1:C:628:LEU:HD13	1:C:628:LEU:H	1.72	0.54
1:A:407:SER:HA	1:A:448:GLN:HE22	1.73	0.53
1:C:407:SER:HA	1:C:448:GLN:HE22	1.72	0.53
1:B:392:SER:O	1:B:398:THR:HG21	2.07	0.53
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.44	0.53
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.44	0.53
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.09	0.53
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.73	0.52
1:A:651:VAL:O	1:A:655:GLU:HB2	2.10	0.52
1:B:544:ARG:HB3	1:B:547:PRO:HG3	1.92	0.52
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.93	0.51
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.93	0.51
1:C:319:LEU:HB3	1:C:459:TRP:HB2	1.92	0.50
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.48	0.49
1:A:321:VAL:HG22	1:A:459:TRP:HZ3	1.76	0.49
1:B:317:TRP:CE3	1:B:458:GLY:HA3	2.48	0.49
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.47	0.49
1:B:651:VAL:O	1:B:655:GLU:HB2	2.12	0.48
1:C:490:TYR:CE2	1:C:492:HIS:HD2	2.32	0.48
1:B:610:GLY:C	1:B:612:ALA:H	2.18	0.48
1:C:202:VAL:HG21	2:H:5:DT:H5''	1.96	0.48
1:C:289:PRO:HG2	1:C:658:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:SER:O	1:A:398:THR:CG2	2.62	0.47
1:B:328:HIS:HD2	1:B:329:ASP:OD1	1.97	0.47
1:A:163:LYS:HE3	1:A:163:LYS:HB2	1.64	0.47
1:C:546:PHE:HE1	1:C:622:LEU:HB3	1.78	0.47
1:A:328:HIS:HD2	1:A:329:ASP:OD1	1.98	0.47
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.13	0.47
1:C:328:HIS:HD2	1:C:329:ASP:OD1	1.98	0.47
1:C:521:MET:HB2	1:C:558:TYR:CD1	2.50	0.47
1:A:119:VAL:O	1:C:25:GLN:HG3	2.15	0.46
1:C:392:SER:O	1:C:398:THR:CG2	2.63	0.46
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.97	0.46
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.14	0.46
1:C:628:LEU:HG	2:H:8:DC:N1	2.31	0.46
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.98	0.46
1:C:68:ASN:HB2	1:C:78:ASN:ND2	2.30	0.46
1:C:598:LEU:HA	1:C:599:SER:HA	1.68	0.46
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.12	0.45
1:A:608:GLN:HG3	1:B:593:ARG:HD3	1.97	0.45
1:C:477:GLU:CD	1:C:477:GLU:H	2.20	0.45
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.46	0.45
1:B:392:SER:O	1:B:398:THR:CG2	2.65	0.45
1:C:134:MET:HG2	1:C:294:ILE:HG21	1.98	0.45
1:C:450:SER:HA	1:C:496:PHE:HE1	1.82	0.45
1:A:217:THR:HG23	1:A:219:LYS:H	1.81	0.45
1:C:1:PRO:HG2	1:C:238:GLU:OE2	2.17	0.45
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.16	0.44
1:B:78:ASN:ND2	1:B:80:VAL:H	2.16	0.44
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.10	0.44
1:C:597:GLU:C	1:C:598:LEU:HD13	2.37	0.44
1:C:650:SER:O	1:C:654:THR:HG23	2.17	0.44
1:C:301:THR:HG23	1:C:448:GLN:HG3	1.99	0.44
1:A:153:ILE:HA	1:A:154:PRO:HA	1.86	0.44
1:B:217:THR:HG23	1:B:219:LYS:H	1.83	0.44
1:C:518:ILE:HB	1:C:561:CYS:SG	2.58	0.43
1:C:533:GLN:HB2	1:C:542:ARG:HD3	1.99	0.43
1:A:301:THR:HG23	1:A:448:GLN:HG3	2.00	0.43
1:B:153:ILE:HA	1:B:154:PRO:HA	1.85	0.43
1:C:204:ARG:HD3	2:H:6:DT:O4	2.18	0.43
1:B:317:TRP:CD2	1:B:458:GLY:HA3	2.53	0.43
1:C:217:THR:HG23	1:C:219:LYS:H	1.84	0.43
1:C:590:MET:O	1:C:594:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LEU:HD22	1:B:398:THR:HG22	2.01	0.42
1:C:319:LEU:HD11	1:C:472:PHE:CD2	2.55	0.42
1:A:86:GLY:O	1:A:89:HIS:HD2	2.03	0.41
1:B:319:LEU:O	1:B:458:GLY:HA2	2.20	0.41
1:C:531:GLY:O	1:C:544:ARG:NH1	2.47	0.41
1:B:475:LEU:HD21	1:B:482:PRO:HG3	2.03	0.41
1:B:624:ASP:HB3	1:B:627:LYS:HD2	2.02	0.41
1:A:391:LEU:HD22	1:A:398:THR:HG22	2.03	0.41
1:C:75:VAL:HG13	1:C:501:LEU:O	2.21	0.41
1:C:86:GLY:O	1:C:89:HIS:HD2	2.02	0.41
1:C:295:TYR:HB3	1:C:303:HIS:CD2	2.55	0.41
1:B:490:TYR:CE2	1:B:492:HIS:HD2	2.39	0.41
1:C:307:ARG:O	1:C:514:PHE:HB3	2.21	0.41
1:C:536:VAL:HG13	1:C:537:ARG:H	1.85	0.41
1:B:277:PHE:HD1	2:G:10:DC:H42	1.69	0.41
1:B:518:ILE:HB	1:B:561:CYS:SG	2.61	0.41
1:B:86:GLY:O	1:B:89:HIS:HD2	2.04	0.41
1:C:490:TYR:HE2	1:C:492:HIS:HD2	1.68	0.40
1:B:490:TYR:HE2	1:B:492:HIS:HD2	1.68	0.40
1:A:204:ARG:HH12	1:A:626:ASN:HD21	1.67	0.40
1:B:136:SER:OG	1:B:293:LYS:NZ	2.54	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	662/665 (100%)	642 (97%)	17 (3%)	3 (0%)	29	65
1	B	662/665 (100%)	628 (95%)	26 (4%)	8 (1%)	13	46
1	C	634/665 (95%)	587 (93%)	32 (5%)	15 (2%)	6	33
All	All	1958/1995 (98%)	1857 (95%)	75 (4%)	26 (1%)	12	45

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	GLU
1	C	2	ARG
1	C	136	SER
1	C	536	VAL
1	C	537	ARG
1	A	607	ARG
1	B	136	SER
1	B	611	LEU
1	C	478	GLY
1	C	531	GLY
1	C	548	GLY
1	C	596	LEU
1	C	626	ASN
1	C	627	LYS
1	B	612	ALA
1	C	547	PRO
1	A	136	SER
1	B	2	ARG
1	B	609	ALA
1	C	545	PRO
1	A	2	ARG
1	B	41	GLU
1	C	603	ALA
1	C	663	PRO
1	C	368	GLY
1	B	368	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	557/558 (100%)	540 (97%)	17 (3%)	40	70
1	B	557/558 (100%)	526 (94%)	31 (6%)	21	53
1	C	539/558 (97%)	499 (93%)	40 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1653/1674 (99%)	1565 (95%)	88 (5%)	22 55

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	63	ASP
1	A	78	ASN
1	A	81	ARG
1	A	82	THR
1	A	102	LEU
1	A	113	ASP
1	A	163	LYS
1	A	269	ARG
1	A	391	LEU
1	A	404	LEU
1	A	497	LEU
1	A	607	ARG
1	A	608	GLN
1	A	629	GLN
1	A	662	MET
1	A	664	ARG
1	B	30	ARG
1	B	41	GLU
1	B	43	LEU
1	B	63	ASP
1	B	78	ASN
1	B	82	THR
1	B	99	THR
1	B	102	LEU
1	B	113	ASP
1	B	136	SER
1	B	269	ARG
1	B	307	ARG
1	B	391	LEU
1	B	395	GLN
1	B	404	LEU
1	B	450	SER
1	B	453	ASP
1	B	470	ARG
1	B	474	MET
1	B	476	LYS

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Mol	Chain	Res	Type
1	B	497	LEU
1	B	501	LEU
1	B	514	PHE
1	B	527	SER
1	B	534	SER
1	B	605	MET
1	B	607	ARG
1	B	628	LEU
1	B	647	HIS
1	B	662	MET
1	B	664	ARG
1	C	3	ARG
1	C	30	ARG
1	C	63	ASP
1	C	68	ASN
1	C	75	VAL
1	C	78	ASN
1	C	82	THR
1	C	102	LEU
1	C	113	ASP
1	C	136	SER
1	C	171	LEU
1	C	269	ARG
1	C	362	LYS
1	C	404	LEU
1	C	418	THR
1	C	472	PHE
1	C	474	MET
1	C	477	GLU
1	C	479	LYS
1	C	513	ILE
1	C	514	PHE
1	C	537	ARG
1	C	542	ARG
1	C	544	ARG
1	C	546	PHE
1	C	549	LEU
1	C	590	MET
1	C	594	ASP
1	C	596	LEU
1	C	598	LEU
1	C	617	ILE

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Mol	Chain	Res	Type
1	C	618	ASP
1	C	620	GLU
1	C	626	ASN
1	C	627	LYS
1	C	628	LEU
1	C	630	TYR
1	C	658	LEU
1	C	662	MET
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	255	GLN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	525	GLN
1	A	626	ASN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	91	ASN
1	B	255	GLN
1	B	309	ASN
1	B	328	HIS
1	B	448	GLN
1	B	492	HIS
1	B	525	GLN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	288	GLN
1	C	303	HIS
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN

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Mol	Chain	Res	Type
1	C	492	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
4	ATP	B	666	-	10,12,33	2.08	2 (20%)	17,20,52	1.16	2 (11%)
4	ATP	C	666	-	10,12,33	1.01	0	17,20,52	1.17	2 (11%)
4	ATP	A	666	-	10,12,33	1.01	0	17,20,52	0.89	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
4	ATP	B	666	-	-	1/12/12/38	-
4	ATP	C	666	-	-	0/12/12/38	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	666	-	-	2/12/12/38	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	666	ATP	PB-O3A	5.62	1.65	1.59
4	B	666	ATP	PB-O1B	2.14	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	666	ATP	O2B-PB-O3A	3.06	115.55	107.27
4	C	666	ATP	O2A-PA-O3A	2.96	114.56	104.64
4	B	666	ATP	O2A-PA-O3A	2.39	112.66	104.64
4	C	666	ATP	O2G-PG-O3B	2.03	111.43	104.64

There are no chirality outliers.

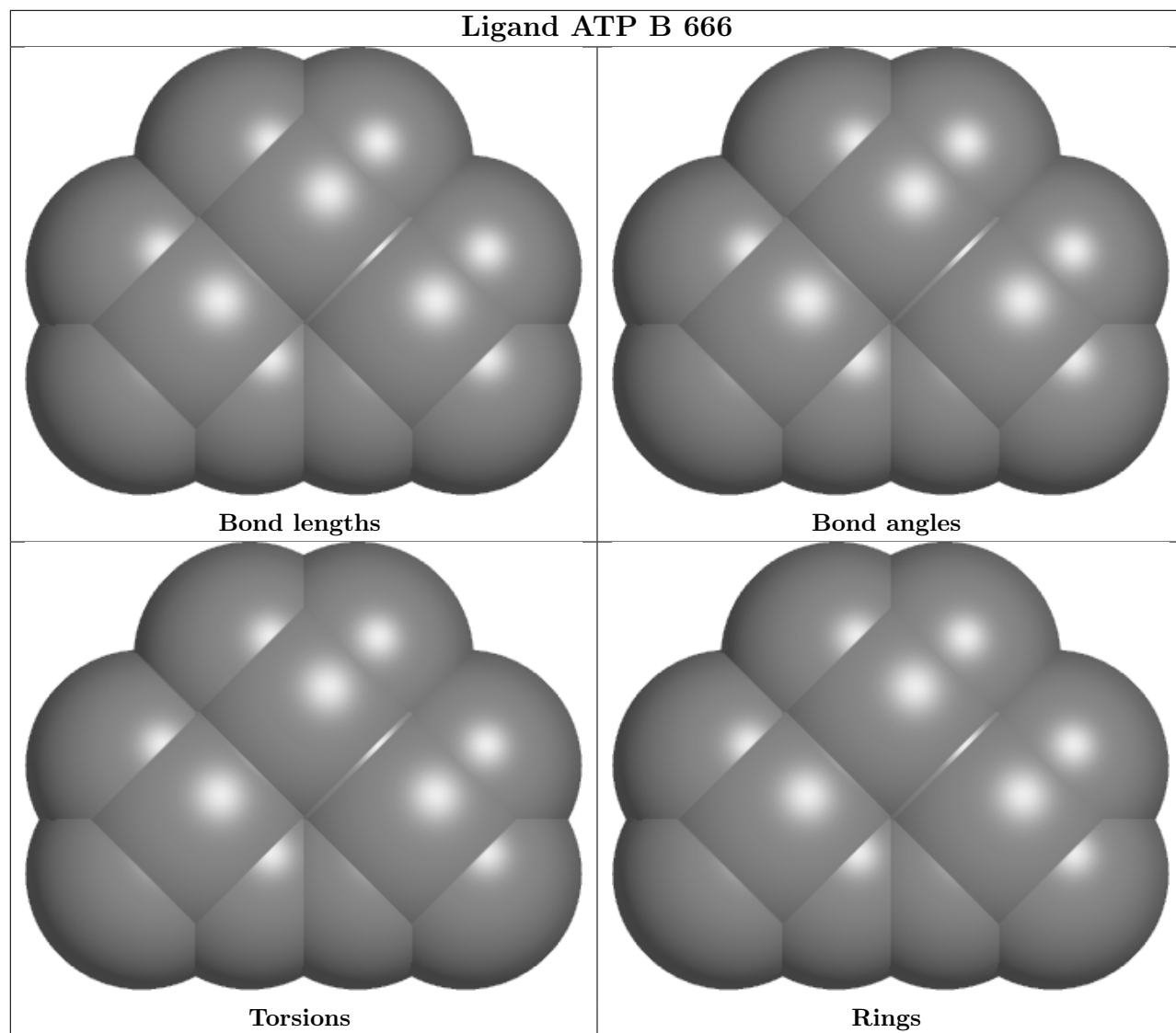
All (3) torsion outliers are listed below:

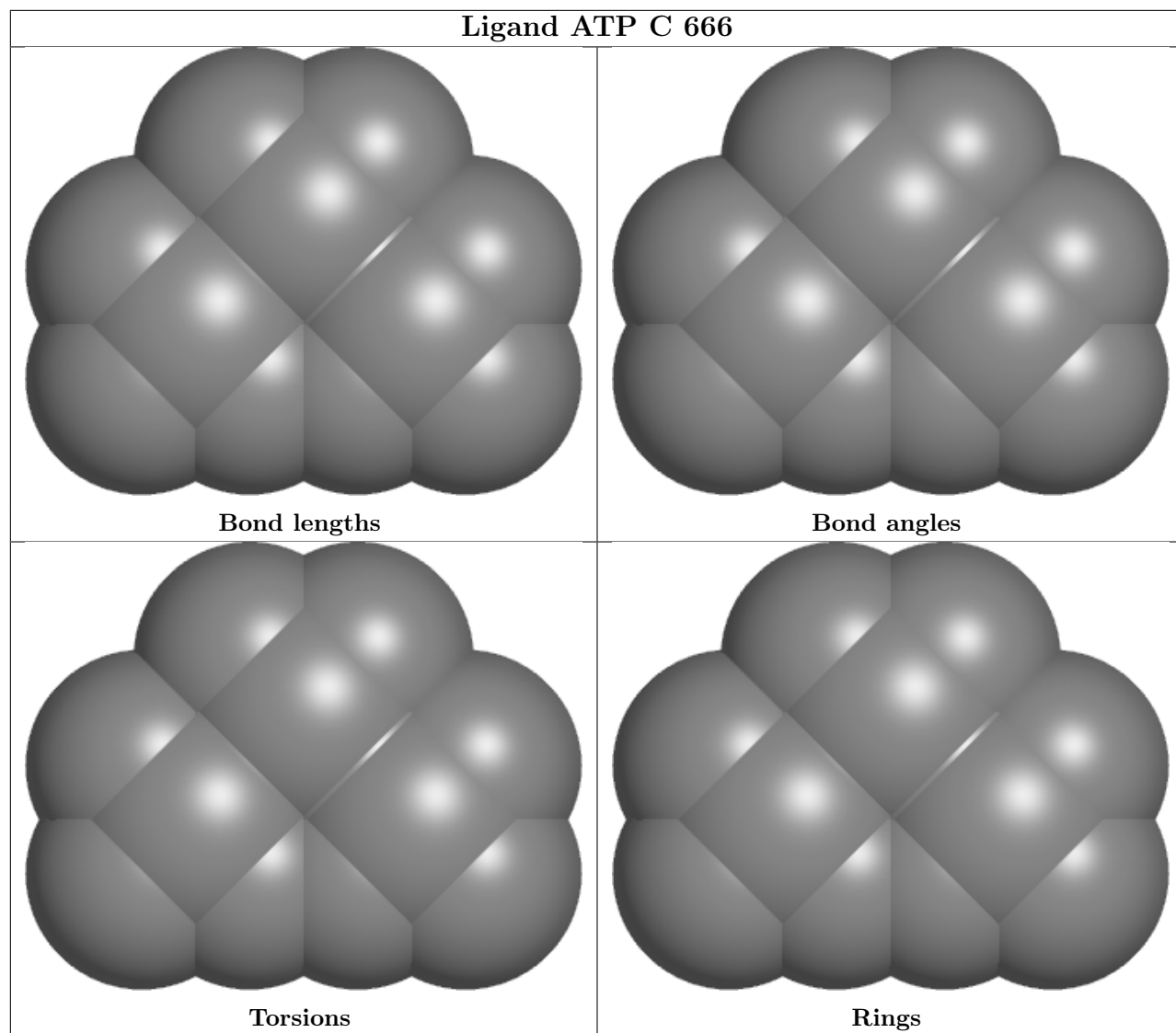
Mol	Chain	Res	Type	Atoms
4	A	666	ATP	PB-O3B-PG-O2G
4	B	666	ATP	PA-O3A-PB-O2B
4	A	666	ATP	PB-O3B-PG-O1G

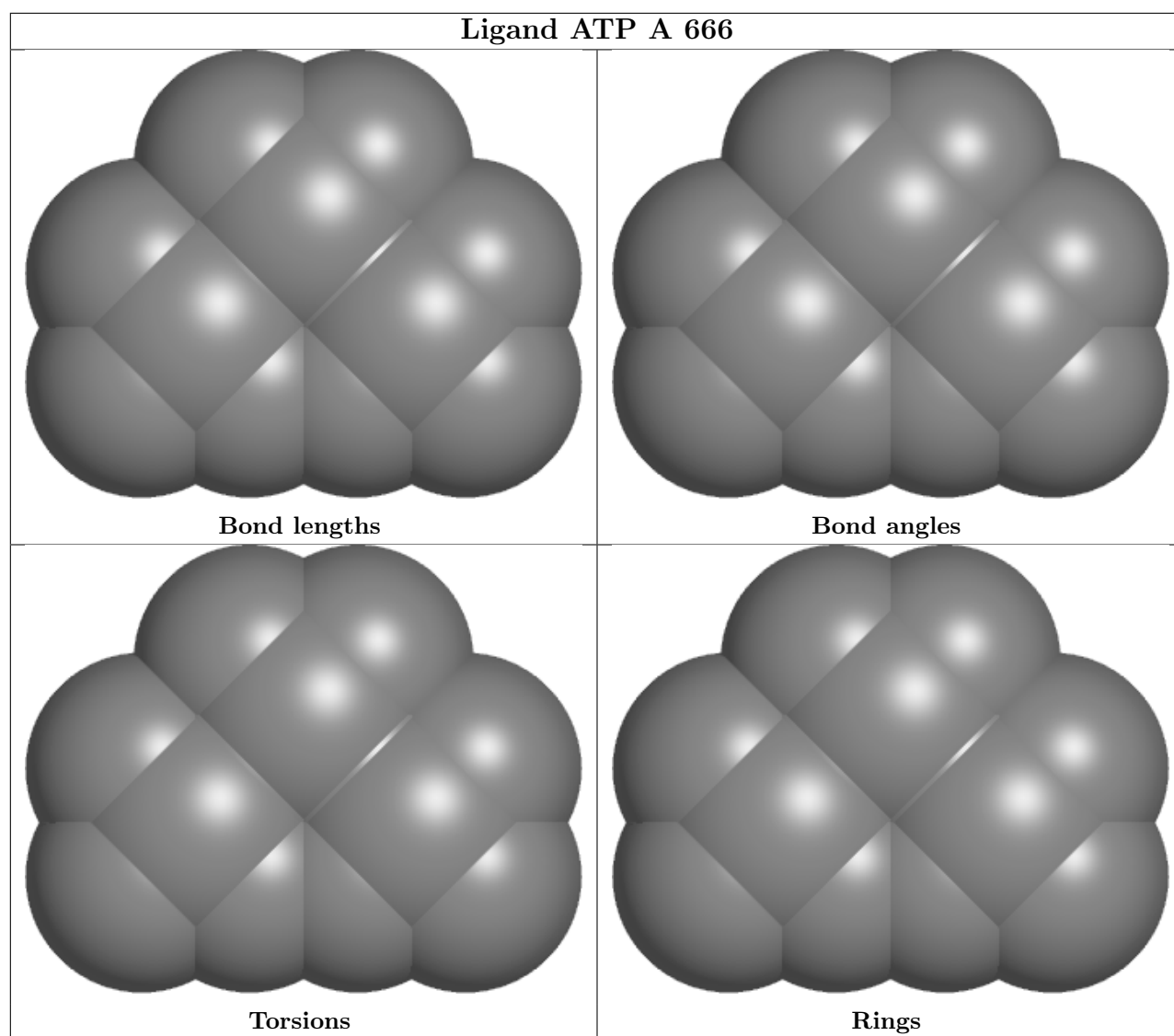
There are no ring outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	4:DT	O3'	5:DT	P	3.41

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	664/665 (99%)	0.56	39 (5%) 22 24	86, 113, 135, 158	1 (0%)
1	B	664/665 (99%)	0.75	80 (12%) 4 6	85, 113, 145, 174	1 (0%)
1	C	640/665 (96%)	0.67	48 (7%) 14 17	72, 119, 181, 235	1 (0%)
2	F	2/14 (14%)	3.74	2 (100%) 0 0	203, 203, 203, 207	0
2	G	3/14 (21%)	6.03	3 (100%) 0 0	203, 203, 205, 205	0
2	H	6/14 (42%)	0.86	0 100 100	148, 159, 161, 166	0
All	All	1979/2037 (97%)	0.67	172 (8%) 10 13	72, 114, 160, 235	3 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	9	DG	8.0
1	C	540	SER	7.8
1	C	541	LYS	6.6
2	G	10	DC	5.6
1	B	196	GLY	4.7
1	C	648	GLY	4.7
1	B	197	GLY	4.6
2	G	11	DG	4.5
1	C	457	LEU	4.3
1	C	514	PHE	4.3
1	B	319	LEU	4.2
2	F	8	DC	4.2
1	C	197	GLY	4.2
1	C	603	ALA	4.1
1	A	189	ALA	3.9
1	B	363	LEU	3.9
1	A	392	SER	3.8
1	B	194	GLN	3.7
1	C	448	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	3.6
1	B	317	TRP	3.5
1	B	283	ILE	3.4
1	C	459	TRP	3.4
1	B	642	HIS	3.4
1	C	599	SER	3.4
1	C	664	ARG	3.4
1	B	321	VAL	3.3
2	F	9	DG	3.3
1	B	361	LEU	3.2
1	C	138	LEU	3.2
1	B	514	PHE	3.2
1	B	143	LEU	3.1
1	B	409	THR	3.0
1	B	199	TYR	3.0
1	C	602	VAL	3.0
1	B	356	LEU	3.0
1	B	645	LEU	3.0
1	A	339	LEU	2.9
1	C	419	ALA	2.9
1	B	634	GLN	2.9
1	A	357	PHE	2.9
1	C	442	GLY	2.8
1	B	396	GLY	2.8
1	C	426	ILE	2.8
1	B	348	GLY	2.8
1	B	324	ASP	2.8
1	A	105	ASN	2.8
1	B	198	ALA	2.8
1	C	415	LEU	2.8
1	A	446	ILE	2.8
1	C	613	GLU	2.7
1	C	449	ILE	2.7
1	B	359	THR	2.7
1	B	168	GLU	2.7
1	B	410	TYR	2.7
1	B	422	LEU	2.7
1	B	181	MET	2.7
1	B	302	PHE	2.7
1	B	357	PHE	2.6
1	C	422	LEU	2.6
1	A	135	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	127	PHE	2.6
1	B	102	LEU	2.6
1	A	356	LEU	2.6
1	B	147	LYS	2.6
1	C	503	TYR	2.6
1	B	397	ALA	2.6
1	B	307	ARG	2.5
1	C	501	LEU	2.5
1	C	134	MET	2.5
1	C	614	LEU	2.5
1	B	640	ASN	2.5
1	C	396	GLY	2.5
1	A	459	TRP	2.5
1	A	9	LEU	2.5
1	B	608	GLN	2.5
1	B	426	ILE	2.5
1	A	353	TRP	2.4
1	B	125	LEU	2.4
1	A	127	PHE	2.4
1	C	456	MET	2.4
1	B	354	VAL	2.4
1	B	400	LEU	2.4
1	B	646	MET	2.4
1	A	129	ALA	2.4
1	C	616	PRO	2.4
1	B	144	LYS	2.4
1	B	341	CYS	2.4
1	B	294	ILE	2.4
1	C	20	ASN	2.4
1	A	203	TYR	2.4
1	B	447	ARG	2.4
1	B	440	TRP	2.4
1	B	404	LEU	2.4
1	B	303	HIS	2.4
1	C	440	TRP	2.4
1	B	134	MET	2.4
1	A	199	TYR	2.4
1	C	488	ILE	2.4
1	A	391	LEU	2.4
1	B	529	GLU	2.3
1	B	142	PRO	2.3
1	B	273	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLN	2.3
1	C	546	PHE	2.3
1	C	512	ALA	2.3
1	B	657	PHE	2.3
1	B	391	LEU	2.3
1	C	300	TYR	2.3
1	C	423	ASN	2.3
1	A	657	PHE	2.3
1	B	320	CYS	2.3
1	A	286	VAL	2.3
1	C	421	HIS	2.3
1	C	317	TRP	2.2
1	B	131	VAL	2.2
1	B	133	LEU	2.2
1	A	486	MET	2.2
1	B	277	PHE	2.2
1	A	180	LEU	2.2
1	C	576	TRP	2.2
1	A	279	LEU	2.2
1	B	622	LEU	2.2
1	B	328	HIS	2.2
1	B	661	VAL	2.2
1	A	196	GLY	2.2
1	B	366	TYR	2.2
1	A	415	LEU	2.2
1	A	457	LEU	2.2
1	A	594	ASP	2.2
1	B	344	LEU	2.2
1	A	409	THR	2.2
1	B	314	VAL	2.2
1	B	413	MET	2.2
1	C	280	ASN	2.2
1	B	335	TRP	2.1
1	B	19	ALA	2.1
1	B	401	MET	2.1
1	B	323	THR	2.1
1	B	439	TYR	2.1
1	B	435	PHE	2.1
1	B	446	ILE	2.1
1	B	203	TYR	2.1
1	B	448	GLN	2.1
1	C	298	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	37	ILE	2.1
1	B	411	LEU	2.1
1	B	282	PRO	2.1
1	C	548	GLY	2.1
1	A	131	VAL	2.1
1	A	436	LEU	2.1
1	A	28	SER	2.1
1	A	134	MET	2.1
1	C	471	LEU	2.0
1	A	138	LEU	2.0
1	A	359	THR	2.0
1	B	382	PRO	2.0
1	C	301	THR	2.0
1	B	163	LYS	2.0
1	C	18	PHE	2.0
1	C	435	PHE	2.0
1	A	414	GLN	2.0
1	C	75	VAL	2.0
1	C	410	TYR	2.0
1	C	583	TYR	2.0
1	C	474	MET	2.0
1	A	484	PRO	2.0
1	A	395	GLN	2.0
1	B	200	TYR	2.0
1	B	457	LEU	2.0
1	A	363	LEU	2.0
1	A	503	TYR	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 monosaccharides 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,

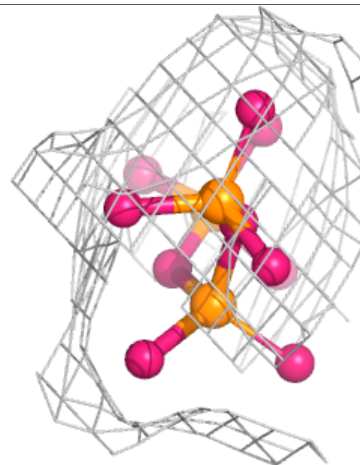
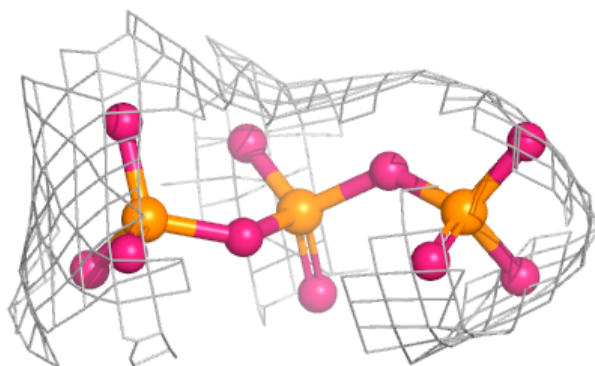
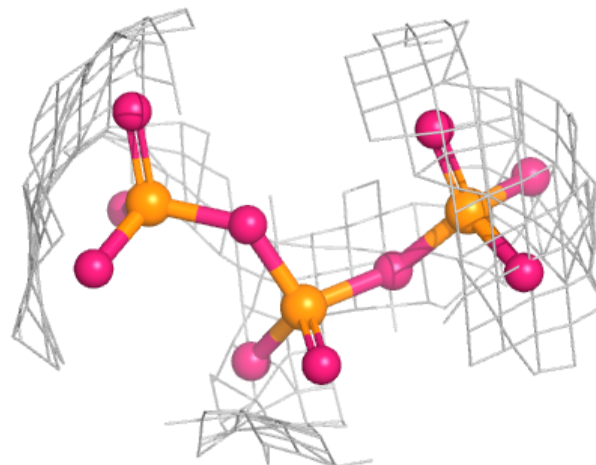
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ATP	C	666	13/31	0.73	0.34	213,216,219,220	0
4	ATP	B	666	13/31	0.75	0.23	164,168,169,170	0
4	ATP	A	666	13/31	0.79	0.21	184,190,195,196	0
3	MG	A	665	1/1	0.93	0.20	100,100,100,100	0
3	MG	B	665	1/1	0.97	0.13	84,84,84,84	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.

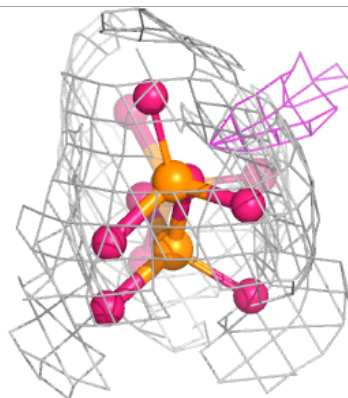
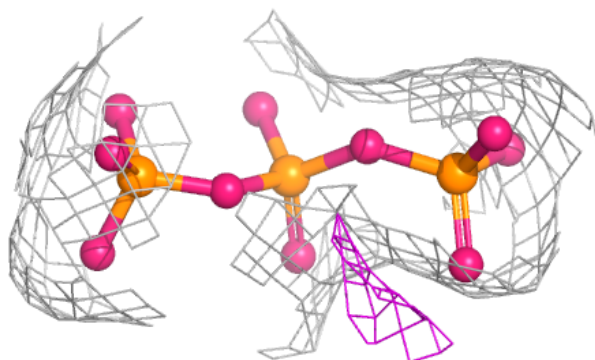
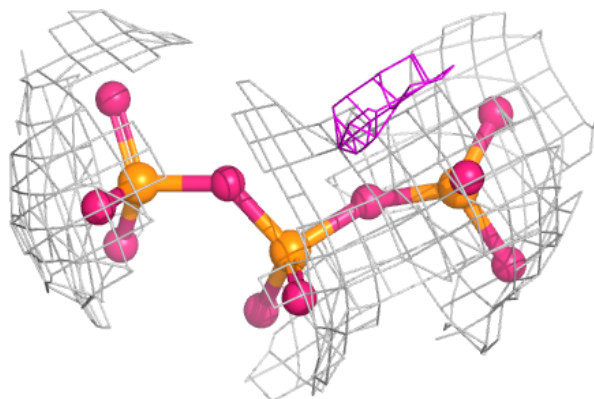
Electron density around ATP C 666:

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

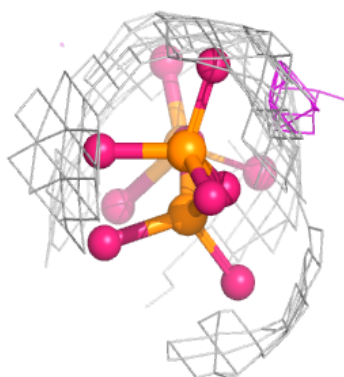
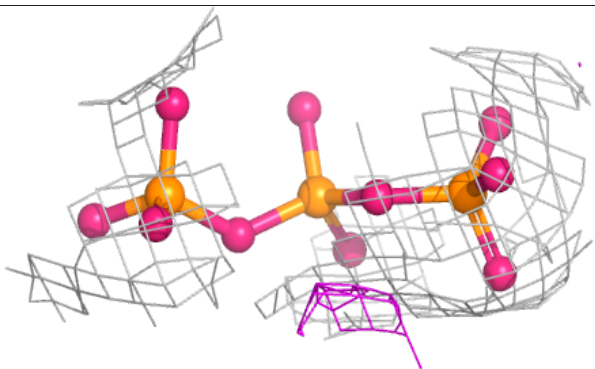
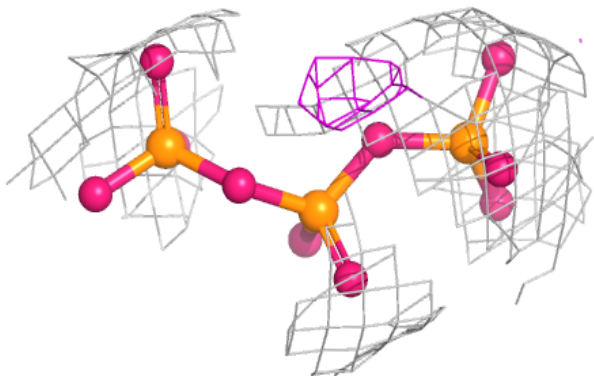


Electron density around ATP B 666:

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

**Electron density around ATP A 666:**

$2mF_o-DF_c$ (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.