



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 4A8S / pdb_00004a8s
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 : 2.90 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:

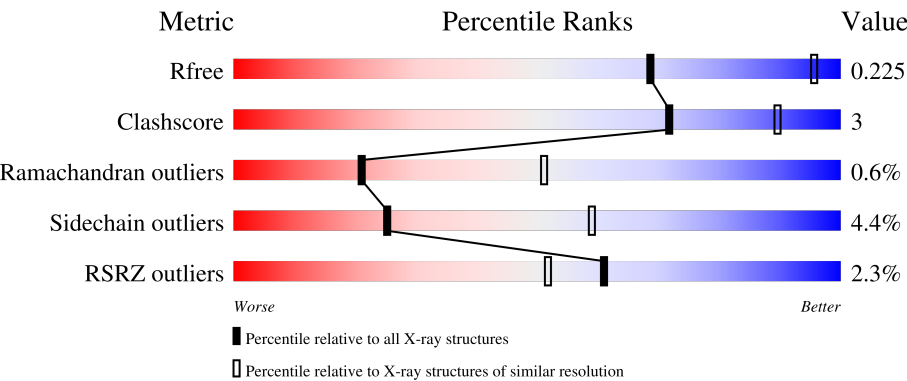
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	665	% 89%10%.
1	B	665	% 89%10%.
1	C	665	5% 82%13%. .
2	F	13	8% 15%8%77%
2	G	13	15% 31%69%

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Mol	Chain	Length	Quality of chain
2	H	13	8%8%15%31%54%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15955 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	646	Total	C	N	O	S	0	0	0
			5123	3255	887	949	32			

There are 6 discrepancies between the modelled and reference sequences:

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

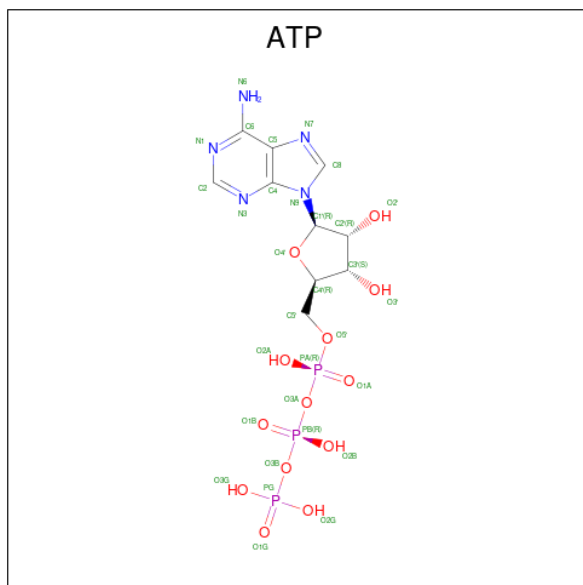
- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*AP*GP*CP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	P	0	0	0
			60	29	13	16	2			
2	G	4	Total	C	N	O	P	0	0	0
			81	39	18	21	3			
2	H	6	Total	C	N	O	P	0	0	0
			118	59	16	38	5			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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

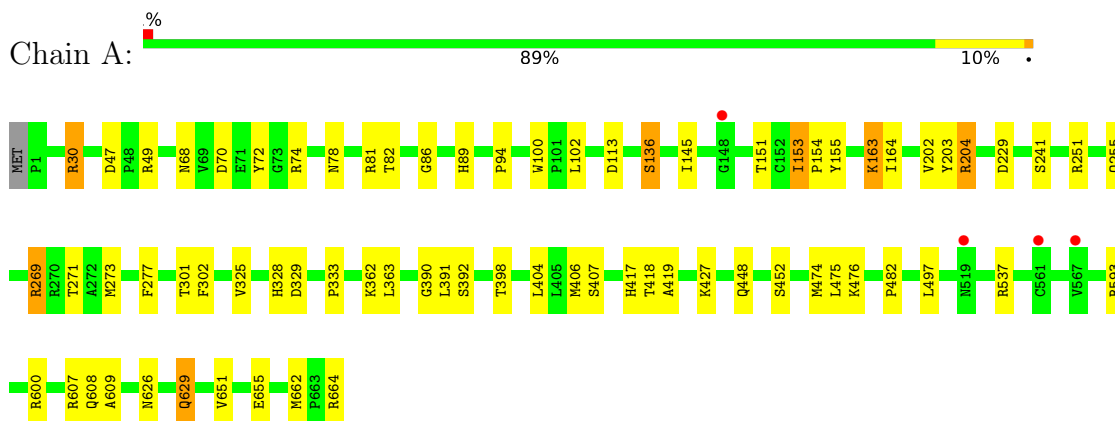
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0

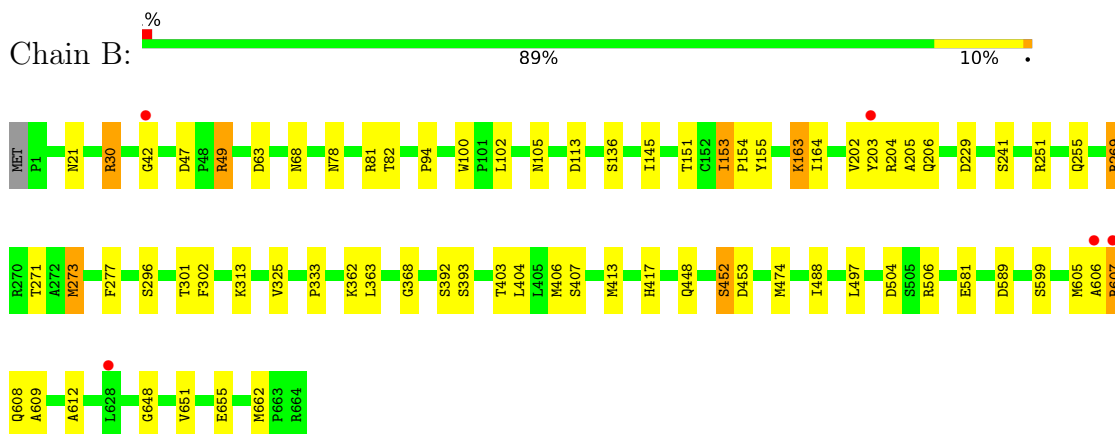
3 Residue-property plots

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.

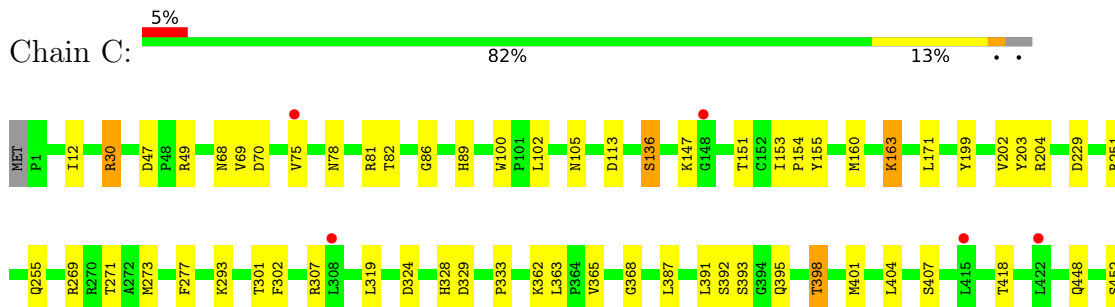
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

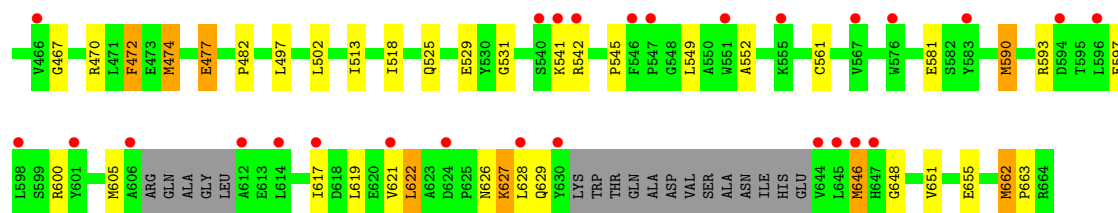


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE

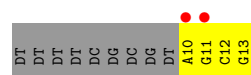




- Molecule 2: 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*AP*GP*CP*GP)-3'



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



- Molecule 2: 5'-D(*TP*TP*TP*TP*CP*GP*CP*GP*TP*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	107.51Å 91.71Å 142.08Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	33.49 – 2.90 33.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.49-2.90) 90.0 (33.49-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.216 , 0.250 (Not available) , 0.225	Depositor DCC
R_{free} test set	2743 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15955	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: 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	A	0.76	1/5396 (0.0%)	1.23	14/7297 (0.2%)
1	B	0.79	2/5396 (0.0%)	1.33	20/7297 (0.3%)
1	C	0.79	0/5249	1.35	25/7094 (0.4%)
2	F	0.59	0/67	1.48	1/102 (1.0%)
2	G	0.57	0/91	1.48	2/139 (1.4%)
2	H	0.65	0/130	1.94	6/199 (3.0%)
All	All	0.78	3/16329 (0.0%)	1.31	68/22128 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	273	MET	SD-CE	-6.59	1.63	1.79
1	A	273	MET	SD-CE	-6.03	1.64	1.79
1	B	296	SER	CA-C	5.48	1.56	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	DT	P-O3'-C3'	8.48	132.92	120.20
2	H	3	DT	P-O3'-C3'	8.47	132.91	120.20
1	C	302	PHE	N-CA-C	7.68	122.78	113.41
1	B	302	PHE	N-CA-C	7.20	122.19	113.41
1	A	302	PHE	N-CA-C	6.69	122.11	113.88
1	C	648	GLY	N-CA-C	6.60	120.77	111.14
1	C	628	LEU	N-CA-C	-6.58	105.64	113.21
1	B	100	TRP	N-CA-C	-6.56	101.52	109.72
2	H	1	DT	O4'-C1'-N1	6.55	118.22	108.40
1	C	105	ASN	CA-CB-CG	6.52	119.12	112.60
1	C	646	MET	N-CA-C	6.37	119.65	108.75
1	B	155	TYR	N-CA-C	6.18	120.02	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	TRP	N-CA-C	-6.16	102.02	109.72
1	C	474	MET	N-CA-C	-6.14	106.76	114.56
1	B	229	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	206	GLN	CA-C-N	6.12	129.31	120.38
1	B	206	GLN	C-N-CA	6.12	129.31	120.38
1	C	229	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	153	ILE	N-CA-C	6.04	115.55	108.96
1	B	205	ALA	N-CA-C	6.02	118.22	108.41
1	C	155	TYR	N-CA-C	6.02	119.81	112.23
2	G	13	DG	O5'-C5'-C4'	6.02	119.83	110.80
1	C	277	PHE	N-CA-C	6.01	118.60	111.33
1	C	100	TRP	N-CA-C	-5.96	102.27	109.72
1	A	155	TYR	N-CA-C	5.94	119.71	112.23
1	C	663	PRO	CA-C-N	5.93	132.38	121.70
1	C	663	PRO	C-N-CA	5.93	132.38	121.70
1	B	153	ILE	N-CA-C	5.93	115.42	108.96
1	A	277	PHE	N-CA-C	5.85	118.41	111.33
1	B	277	PHE	N-CA-C	5.83	118.38	111.33
1	B	313	LYS	CA-C-N	5.83	128.69	120.42
1	B	313	LYS	C-N-CA	5.83	128.69	120.42
1	A	229	ASP	CA-CB-CG	5.79	118.39	112.60
2	F	8	DG	P-O5'-C5'	5.76	128.64	120.00
1	B	648	GLY	N-CA-C	5.75	119.54	111.14
2	G	12	DC	P-O3'-C3'	5.72	128.78	120.20
1	C	590	MET	CA-C-N	5.67	127.88	120.28
1	C	590	MET	C-N-CA	5.67	127.88	120.28
1	C	363	LEU	N-CA-C	5.64	116.80	109.64
1	C	627	LYS	N-CA-C	-5.56	106.33	113.23
1	B	363	LEU	N-CA-C	5.55	116.88	109.83
1	C	593	ARG	CA-C-N	5.49	128.09	120.29
1	C	593	ARG	C-N-CA	5.49	128.09	120.29
1	A	363	LEU	N-CA-C	5.48	116.60	109.64
2	H	4	DT	P-O5'-C5'	5.47	128.21	120.00
1	C	541	LYS	CA-C-N	5.47	128.48	120.71
1	C	541	LYS	C-N-CA	5.47	128.48	120.71
1	B	241	SER	N-CA-C	5.44	118.33	109.24
1	B	105	ASN	CA-CB-CG	5.41	118.01	112.60
2	H	5	DC	N1-C1'-C2'	5.37	121.55	113.50
1	A	609	ALA	N-CA-C	5.29	117.05	111.28
1	A	419	ALA	N-CA-C	5.28	118.24	109.79
1	B	589	ASP	CA-C-N	5.27	127.34	120.28
1	B	589	ASP	C-N-CA	5.27	127.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	ASP	CA-C-N	5.25	129.00	120.60
1	C	70	ASP	C-N-CA	5.25	129.00	120.60
1	B	333	PRO	N-CA-C	5.23	119.07	110.55
2	H	3	DT	C2'-C3'-O3'	5.19	119.29	111.50
1	A	333	PRO	N-CA-C	5.16	118.96	110.55
1	B	21	ASN	CA-CB-CG	5.16	117.75	112.60
1	C	333	PRO	N-CA-C	5.13	118.92	110.55
1	C	68	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	136	SER	N-CA-C	5.10	121.67	110.80
1	A	390	GLY	N-CA-C	-5.10	105.18	111.45
1	C	662	MET	N-CA-C	5.08	116.91	109.84
1	B	68	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	68	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	241	SER	N-CA-C	5.04	117.46	109.50

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	35	0
1	B	5265	0	5167	35	0
1	C	5123	0	5029	36	0
2	F	60	0	35	7	0
2	G	81	0	46	4	0
2	H	118	0	72	5	0
3	A	2	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
5	C	1	0	0	0	0
All	All	15955	0	15516	105	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 (105) 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:B:393:SER:HB2	2:G:11:DG:H21	1.36	0.91
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.22	0.75
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.40	0.70
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.39	0.69
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.37	0.69
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.62	0.64
1:C:467:GLY:HA2	1:C:470:ARG:HE	1.62	0.64
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.32	0.64
1:A:392:SER:O	1:A:398:THR:HG21	1.98	0.64
1:C:474:MET:HE1	1:C:482:PRO:HB3	1.80	0.62
1:C:30:ARG:HD2	2:H:1:DT:H5"	1.82	0.62
1:C:391:LEU:HG	1:C:398:THR:HG22	1.84	0.60
1:A:537:ARG:HD2	1:B:49:ARG:HG3	1.84	0.59
1:A:30:ARG:HD2	2:F:6:DG:N2	2.17	0.59
1:B:151:THR:HG22	1:B:163:LYS:HG3	1.84	0.59
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.84	0.58
1:B:599:SER:HB3	1:B:605:MET:HE2	1.86	0.57
1:C:477:GLU:CD	1:C:477:GLU:H	2.13	0.57
1:B:393:SER:HB2	2:G:11:DG:N2	2.14	0.56
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.06	0.56
1:C:151:THR:HG22	1:C:163:LYS:HG3	1.87	0.56
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.42	0.55
1:C:273:MET:HE3	1:C:392:SER:HA	1.89	0.54
1:B:393:SER:CB	2:G:11:DG:H21	2.16	0.54
2:H:3:DT:H2"	2:H:4:DT:H5'	1.88	0.54
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.08	0.52
1:B:273:MET:HE3	1:B:392:SER:HA	1.91	0.52
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.91	0.52
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.92	0.52
1:A:392:SER:O	1:A:398:THR:CG2	2.58	0.51
1:A:651:VAL:O	1:A:655:GLU:HB2	2.12	0.50
1:C:651:VAL:O	1:C:655:GLU:HB2	2.11	0.50
1:B:651:VAL:O	1:B:655:GLU:HB2	2.11	0.50
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.11	0.50
1:B:417:HIS:CE1	1:B:474:MET:HE1	2.46	0.50
1:B:413:MET:CE	1:B:488:ILE:HG13	2.42	0.49
1:B:203:TYR:HB3	1:B:269:ARG:HD2	1.94	0.49
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.94	0.49
1:C:86:GLY:O	1:C:89:HIS:CD2	2.66	0.49
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.48	0.48
1:A:629:GLN:HG2	2:F:8:DG:C5	2.48	0.48
1:A:417:HIS:CE1	1:A:474:MET:HE1	2.48	0.48
1:B:407:SER:HA	1:B:448:GLN:HE22	1.79	0.48
1:C:136:SER:OG	1:C:293:LYS:NZ	2.47	0.48
1:C:407:SER:HA	1:C:448:GLN:HE22	1.79	0.48
1:B:504:ASP:OD2	1:B:506:ARG:NH1	2.47	0.47
1:A:407:SER:HA	1:A:448:GLN:HE22	1.79	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.47
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.45	0.47
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.97	0.47
1:C:549:LEU:HD22	1:C:619:LEU:HD22	1.96	0.47
1:A:30:ARG:HD2	2:F:6:DG:H21	1.78	0.46
1:C:621:VAL:HG22	1:C:627:LYS:HB2	1.97	0.46
1:C:629:GLN:NE2	2:H:4:DT:C4	2.84	0.46
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.96	0.46
1:C:395:GLN:HB3	1:C:398:THR:HG23	1.98	0.46
1:C:477:GLU:CD	1:C:477:GLU:N	2.73	0.46
2:H:4:DT:H2''	2:H:5:DC:O4'	2.16	0.46
1:A:204:ARG:CZ	2:F:7:DC:H41	2.27	0.45
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.13	0.45
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.17	0.44
1:C:301:THR:HG23	1:C:448:GLN:HG3	1.98	0.44
1:A:204:ARG:HD3	2:F:7:DC:N4	2.33	0.43
1:C:199:TYR:HB2	1:C:365:VAL:HG12	2.00	0.43
1:A:475:LEU:HD21	1:A:482:PRO:HG3	2.00	0.43
1:C:319:LEU:HD11	1:C:472:PHE:CD2	2.53	0.43
1:A:593:ARG:HG2	1:B:42:GLY:HA2	2.00	0.43
1:A:301:THR:HG23	1:A:448:GLN:HG3	2.01	0.43
1:A:600:ARG:HH12	1:B:581:GLU:CG	2.32	0.43
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.02	0.43
1:B:30:ARG:HD2	2:G:10:DA:H2	1.84	0.43
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.12	0.43
1:C:518:ILE:HB	1:C:561:CYS:SG	2.58	0.43
1:C:626:ASN:O	1:C:629:GLN:HB3	2.19	0.43
1:B:151:THR:CG2	1:B:163:LYS:HG3	2.49	0.43
1:B:606:ALA:C	1:B:608:GLN:H	2.25	0.43
1:C:328:HIS:HD2	1:C:329:ASP:OD1	2.02	0.43
2:H:1:DT:H1'	2:H:2:DT:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:HE3	1:C:12:ILE:HG21	2.01	0.42
1:A:204:ARG:HH12	1:A:626:ASN:HD21	1.66	0.42
1:A:325:VAL:HG21	1:A:406:MET:HE2	2.01	0.42
1:C:147:LYS:HG2	1:C:160:MET:HE3	2.02	0.42
1:C:151:THR:CG2	1:C:163:LYS:HG3	2.50	0.42
1:C:251:ARG:HH11	1:C:255:GLN:NE2	2.13	0.42
1:B:163:LYS:HE3	1:B:163:LYS:HB2	1.81	0.42
1:B:413:MET:HE1	1:B:488:ILE:HG13	2.02	0.42
1:C:69:VAL:HG22	1:C:75:VAL:HG22	2.01	0.42
1:A:86:GLY:O	1:A:89:HIS:HD2	2.03	0.41
1:A:204:ARG:NE	2:F:7:DC:H41	2.17	0.41
1:C:549:LEU:HD13	1:C:622:LEU:HD23	2.03	0.41
1:A:153:ILE:HA	1:A:154:PRO:HA	1.89	0.41
1:B:452:SER:HB3	1:B:453:ASP:H	1.67	0.41
1:B:413:MET:HE2	1:B:488:ILE:HG13	2.02	0.41
1:C:391:LEU:HD11	1:C:401:MET:HB2	2.02	0.41
1:A:151:THR:CG2	1:A:163:LYS:HG3	2.49	0.41
1:B:153:ILE:HA	1:B:154:PRO:HA	1.88	0.41
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.87	0.40
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.85	0.40
1:B:606:ALA:C	1:B:608:GLN:N	2.80	0.40
1:C:153:ILE:HA	1:C:154:PRO:HA	1.88	0.40
1:C:204:ARG:HD2	1:C:529:GLU:OE2	2.21	0.40
1:B:94:PRO:HB3	1:B:269:ARG:HG3	2.02	0.40
1:B:325:VAL:HG21	1:B:406:MET:HE2	2.03	0.40
1:A:204:ARG:HD3	2:F:7:DC:C5	2.56	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	662/665 (100%)	642 (97%)	18 (3%)	2 (0%)	36	65
1	B	662/665 (100%)	633 (96%)	25 (4%)	4 (1%)	21	51
1	C	640/665 (96%)	606 (95%)	28 (4%)	6 (1%)	14	41
All	All	1964/1995 (98%)	1881 (96%)	71 (4%)	12 (1%)	21	51

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	136	SER
1	A	607	ARG
1	B	607	ARG
1	B	136	SER
1	C	368	GLY
1	A	136	SER
1	B	368	GLY
1	C	393	SER
1	C	552	ALA
1	B	612	ALA
1	C	545	PRO
1	C	531	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%)	537 (96%)	20 (4%)	31	65
1	B	557/558 (100%)	538 (97%)	19 (3%)	32	66
1	C	543/558 (97%)	509 (94%)	34 (6%)	16	45
All	All	1657/1674 (99%)	1584 (96%)	73 (4%)	25	59

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG

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Mol	Chain	Res	Type
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	202	VAL
1	A	204	ARG
1	A	269	ARG
1	A	362	LYS
1	A	391	LEU
1	A	404	LEU
1	A	418	THR
1	A	452	SER
1	A	497	LEU
1	A	608	GLN
1	A	629	GLN
1	A	662	MET
1	A	664	ARG
1	B	30	ARG
1	B	49	ARG
1	B	63	ASP
1	B	78	ASN
1	B	81	ARG
1	B	82	THR
1	B	102	LEU
1	B	113	ASP
1	B	163	LYS
1	B	202	VAL
1	B	204	ARG
1	B	269	ARG
1	B	362	LYS
1	B	403	THR
1	B	404	LEU
1	B	452	SER
1	B	497	LEU
1	B	607	ARG
1	B	662	MET
1	C	30	ARG
1	C	78	ASN
1	C	81	ARG
1	C	82	THR

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Mol	Chain	Res	Type
1	C	102	LEU
1	C	113	ASP
1	C	163	LYS
1	C	171	LEU
1	C	202	VAL
1	C	269	ARG
1	C	307	ARG
1	C	324	ASP
1	C	362	LYS
1	C	387	LEU
1	C	398	THR
1	C	404	LEU
1	C	418	THR
1	C	452	SER
1	C	472	PHE
1	C	477	GLU
1	C	497	LEU
1	C	502	LEU
1	C	513	ILE
1	C	525	GLN
1	C	542	ARG
1	C	581	GLU
1	C	590	MET
1	C	597	GLU
1	C	600	ARG
1	C	605	MET
1	C	617	ILE
1	C	622	LEU
1	C	646	MET
1	C	662	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
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	519	ASN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	626	ASN
1	A	642	HIS
1	B	25	GLN
1	B	78	ASN
1	B	89	HIS
1	B	91	ASN
1	B	255	GLN
1	B	309	ASN
1	B	448	GLN
1	B	492	HIS
1	B	519	ASN
1	B	525	GLN
1	B	629	GLN
1	B	642	HIS
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	105	ASN
1	C	255	GLN
1	C	303	HIS
1	C	309	ASN
1	C	328	HIS
1	C	441	GLN
1	C	443	HIS
1	C	448	GLN
1	C	492	HIS
1	C	519	ASN
1	C	525	GLN
1	C	647	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 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	1666	-	10,12,33	1.40	1 (10%)	17,20,52	1.10	1 (5%)
4	ATP	A	1666	3	10,12,33	1.09	1 (10%)	17,20,52	0.98	0
4	ATP	C	1665	-	10,12,33	1.04	1 (10%)	17,20,52	1.06	1 (5%)

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	1666	-	-	1/12/12/38	-
4	ATP	A	1666	3	-	0/12/12/38	-
4	ATP	C	1665	-	-	0/12/12/38	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1666	ATP	PB-O3A	2.51	1.62	1.59
4	A	1666	ATP	PA-O5'	2.05	1.62	1.54
4	C	1665	ATP	PA-O5'	2.02	1.62	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1666	ATP	O2A-PA-O3A	3.26	115.55	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1665	ATP	O2G-PG-O3B	2.34	112.49	104.64

There are no chirality outliers.

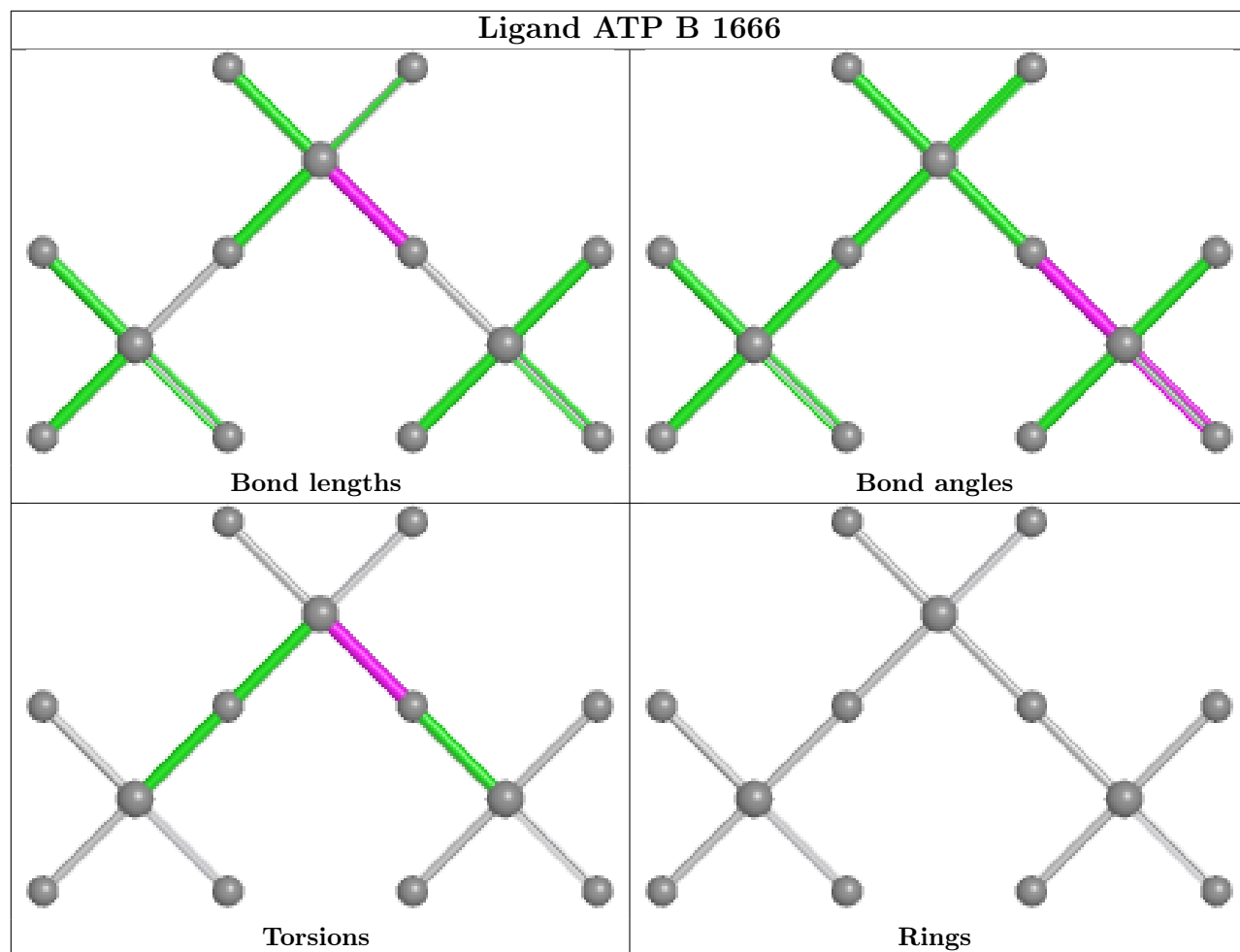
All (1) torsion outliers are listed below:

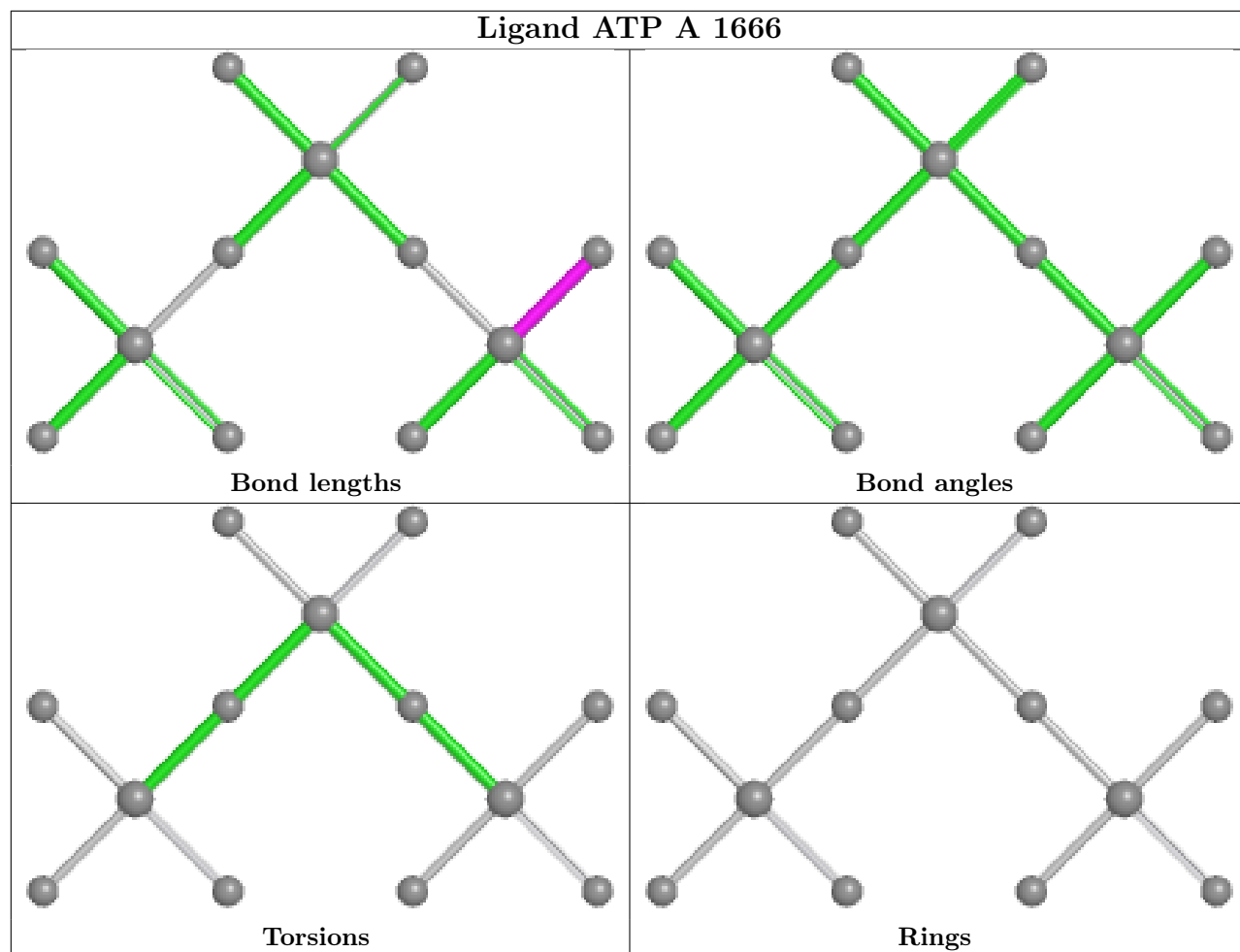
Mol	Chain	Res	Type	Atoms
4	B	1666	ATP	PA-O3A-PB-O2B

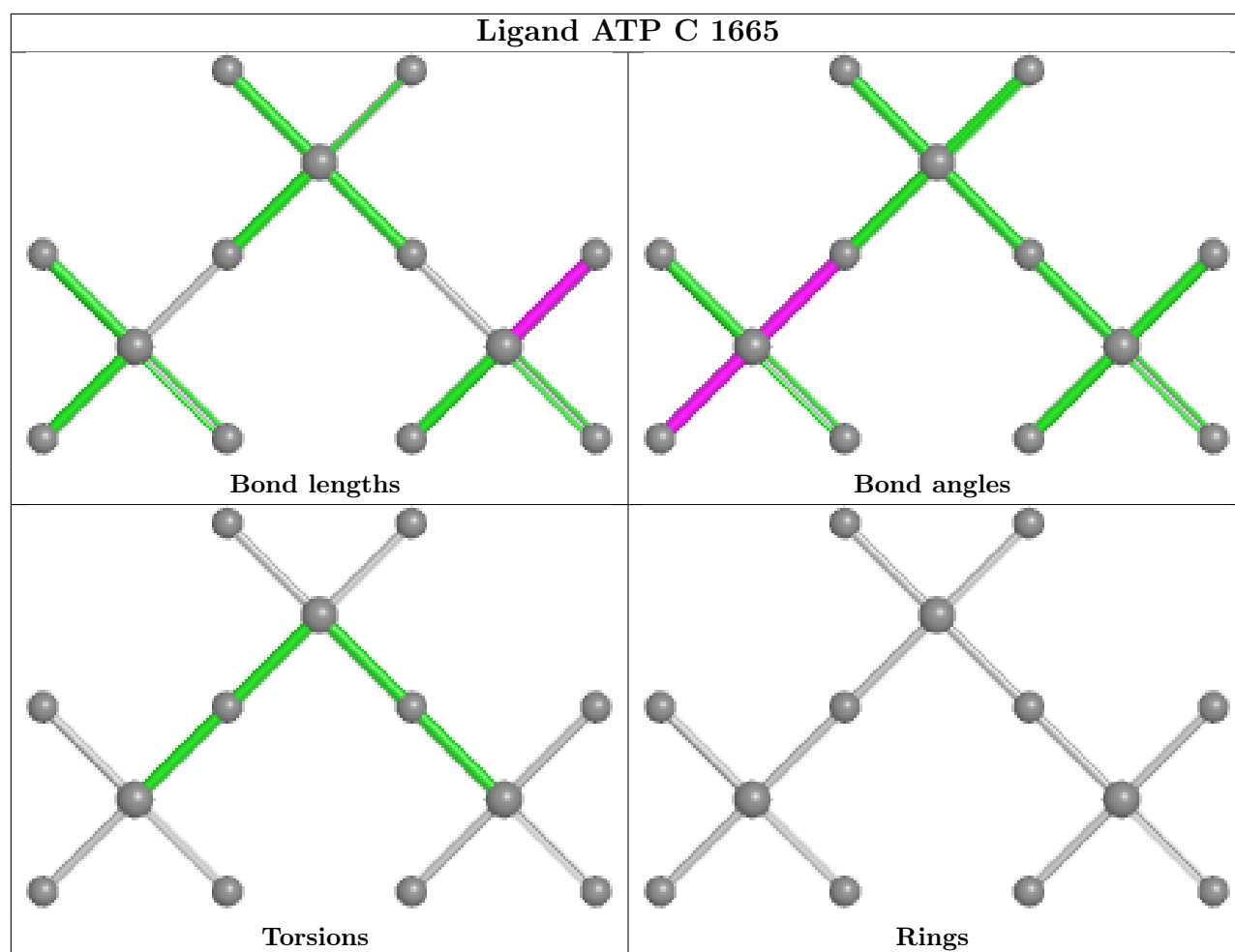
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	664/665 (99%)	0.07	4 (0%)	85 81	59, 83, 107, 136	0
1	B	664/665 (99%)	0.16	5 (0%)	82 77	69, 92, 124, 157	0
1	C	646/665 (97%)	0.45	32 (4%)	34 27	61, 105, 159, 217	0
2	F	3/13 (23%)	1.37	1 (33%)	1 1	108, 108, 112, 118	0
2	G	4/13 (30%)	2.11	2 (50%)	0 0	160, 166, 170, 181	0
2	H	6/13 (46%)	1.79	2 (33%)	1 1	121, 131, 141, 142	0
All	All	1987/2034 (97%)	0.23	46 (2%)	61 52	59, 90, 141, 217	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	630	TYR	4.3
1	C	546	PHE	3.5
2	G	10	DA	3.4
1	B	42	GLY	3.2
1	C	606	ALA	3.2
2	H	1	DT	3.1
1	B	606	ALA	3.1
1	C	567	VAL	3.0
1	C	541	LYS	3.0
1	C	628	LEU	3.0
1	A	567	VAL	3.0
1	C	540	SER	3.0
1	C	551	TRP	2.9
1	C	547	PRO	2.9
1	C	646	MET	2.9
1	C	594	ASP	2.8
1	C	645	LEU	2.8
1	C	601	TYR	2.7
1	B	607	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	466	VAL	2.7
1	C	576	TRP	2.6
1	C	612	ALA	2.6
1	C	621	VAL	2.6
1	C	596	LEU	2.5
1	C	617	ILE	2.5
1	B	203	TYR	2.5
1	C	598	LEU	2.5
1	B	628	LEU	2.4
1	C	422	LEU	2.4
1	C	75	VAL	2.4
1	C	644	VAL	2.4
1	A	148	GLY	2.4
1	C	308	LEU	2.3
1	C	614	LEU	2.3
1	C	583	TYR	2.3
1	C	148	GLY	2.3
2	G	11	DG	2.3
1	C	624	ASP	2.2
2	F	6	DG	2.2
1	C	647	HIS	2.1
1	C	415	LEU	2.1
1	C	542	ARG	2.1
1	C	555	LYS	2.1
2	H	4	DT	2.1
1	A	561	CYS	2.0
1	A	519	ASN	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.

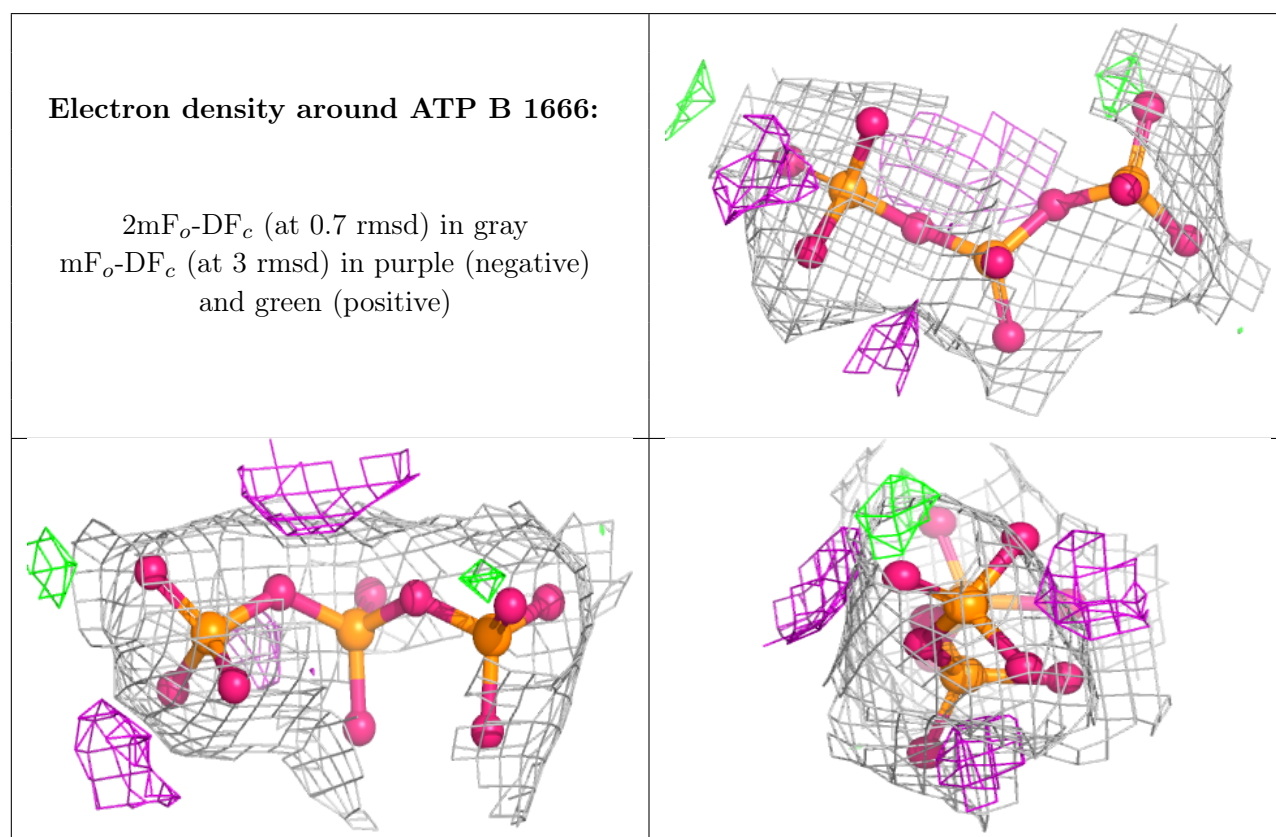
6.4 Ligands [i](#)

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.

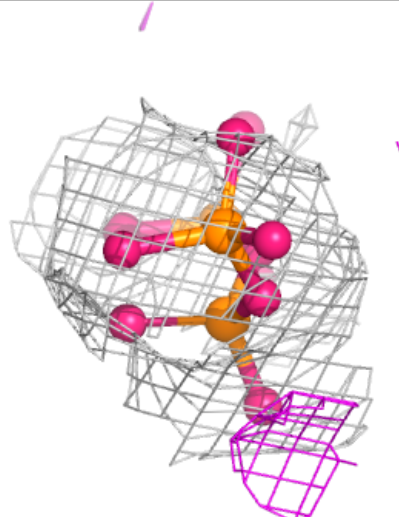
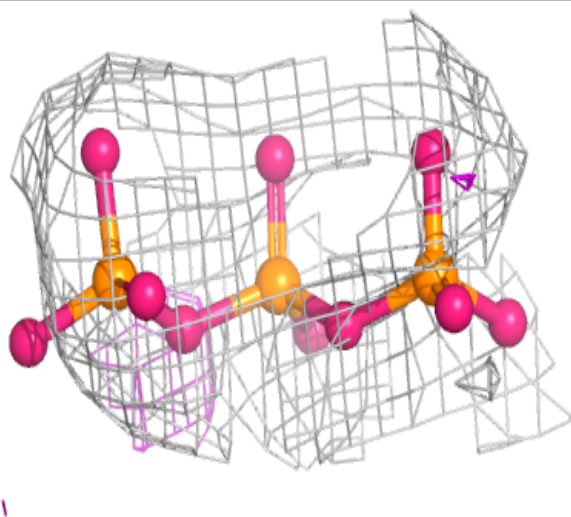
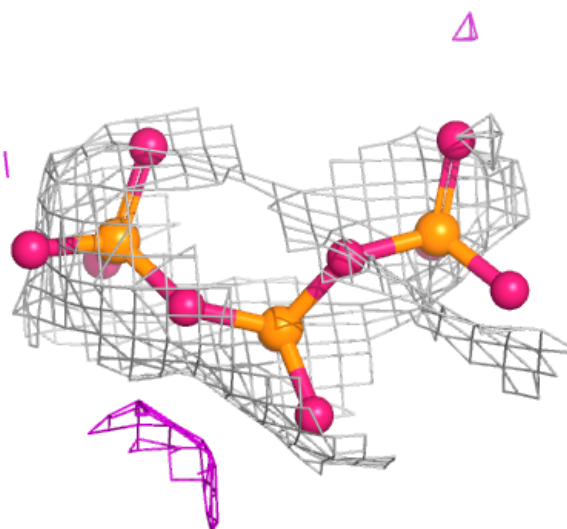
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	B	1666	13/31	0.55	0.11	154,159,164,165	0
4	ATP	C	1665	13/31	0.58	0.09	201,206,211,212	0
4	ATP	A	1666	13/31	0.60	0.12	180,184,185,186	0
3	MG	B	1665	1/1	0.92	0.11	71,71,71,71	0
3	MG	A	1665	1/1	0.92	0.13	72,72,72,72	0
3	MG	A	1667	1/1	0.93	0.08	69,69,69,69	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.



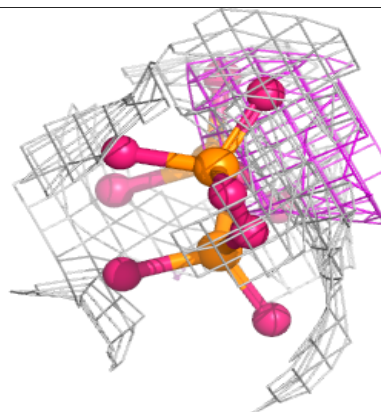
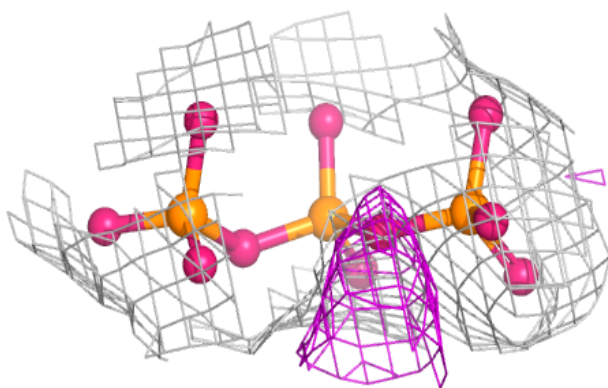
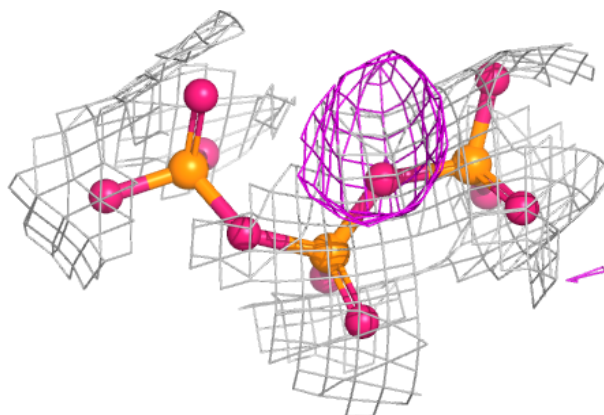
Electron density around ATP C 1665:

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



Electron density around ATP A 1666:

$2mF_o-DF_c$ (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.