



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:20 PM UTC

PDB ID : 4A8F / pdb_00004a8f
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 : 3.30 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

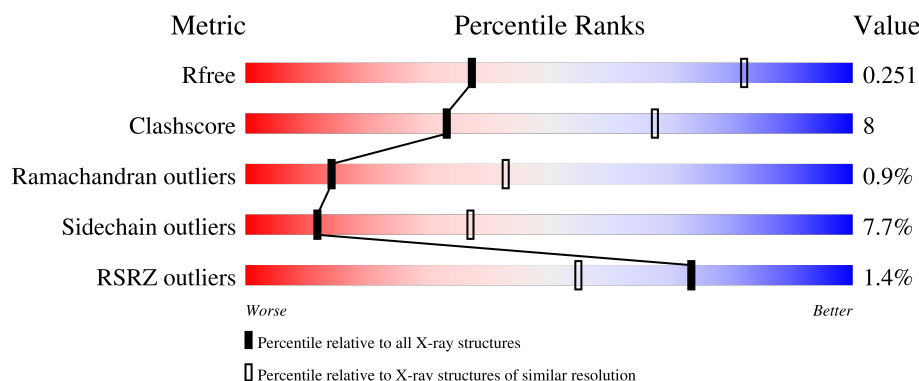
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	81% 16% .
1	B	665	74% 22% .
1	C	665	73% 21% ..
2	G	4	75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	1666	-	X	-	-
4	ATP	C	1666	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16048 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	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124

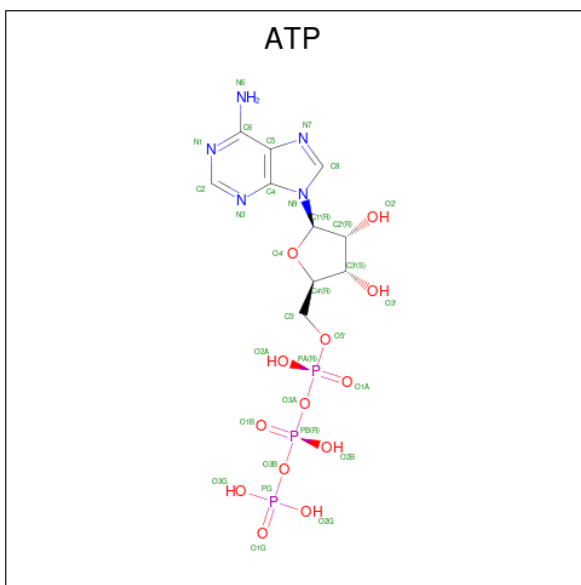
- Molecule 2 is a DNA chain called 5'-D(*DAP*GP*CP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	P	0	0	0
			81	39	18	21	3			

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

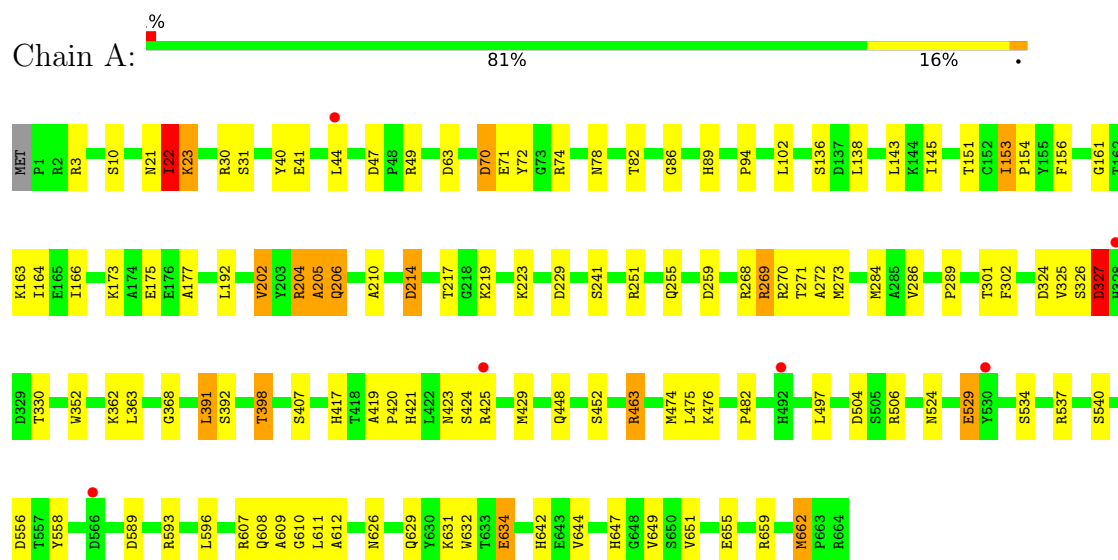


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	A	1	Total 13	O 10	P 3			0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

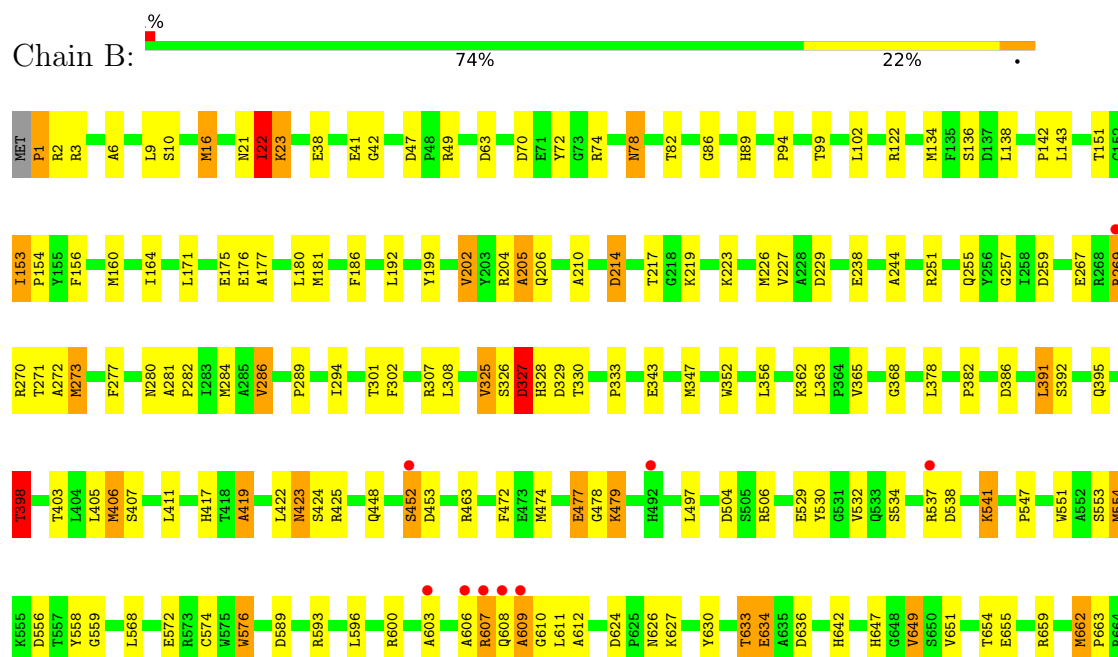
3 Residue-property plots

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.

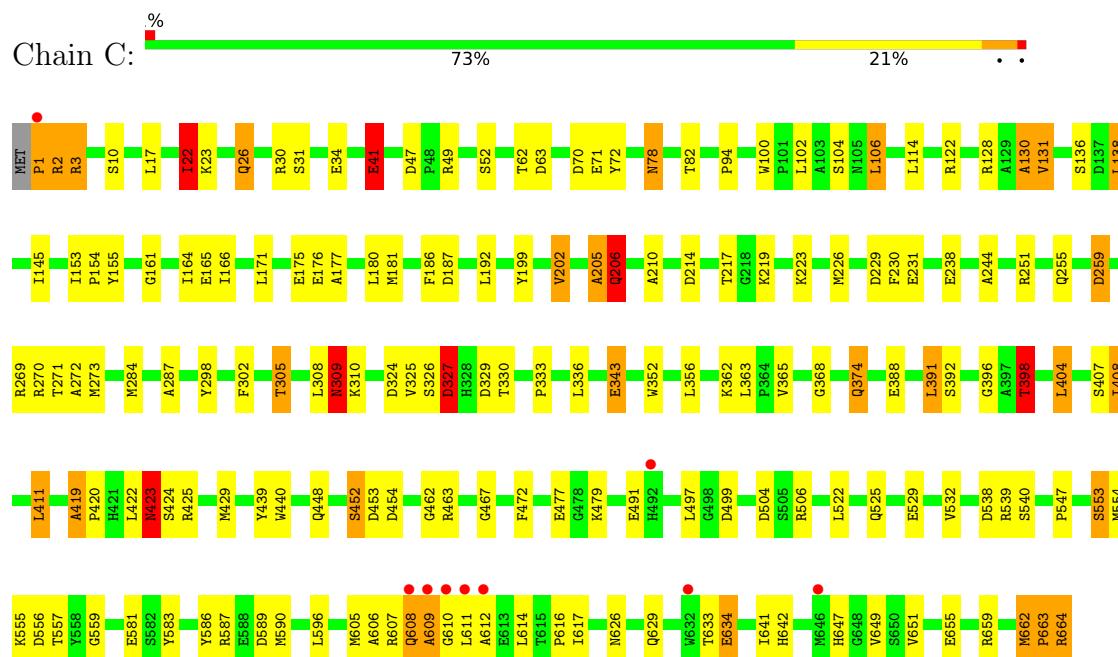
• Molecule 1: RNA-DIRECTED RNA POLYMERASE



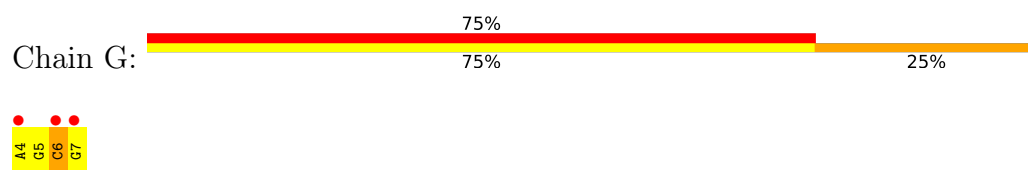
• Molecule 1: RNA-DIRECTED RNA POLYMERASE



● Molecule 1: RNA-DIRECTED RNA POLYMERASE



● Molecule 2: 5'-D(*DAP*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	105.92Å 91.77Å 140.46Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	46.01 – 3.30 46.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-3.30) 99.6 (46.01-3.30)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.243 , 0.290 0.202 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.944	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16048	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	6/5396 (0.1%)	1.38	28/7297 (0.4%)
1	B	1.16	11/5396 (0.2%)	1.51	58/7297 (0.8%)
1	C	1.21	19/5396 (0.4%)	1.54	61/7297 (0.8%)
2	G	0.64	0/91	1.78	3/139 (2.2%)
All	All	1.14	36/16279 (0.2%)	1.48	150/22030 (0.7%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	ALA	CA-C	9.73	1.64	1.53
1	B	16	MET	SD-CE	9.44	2.03	1.79
1	C	305	THR	CA-C	8.97	1.56	1.52
1	B	22	ILE	CG1-CD1	8.44	1.84	1.51
1	C	374	GLN	CA-C	7.58	1.61	1.52
1	A	22	ILE	CG1-CD1	7.18	1.79	1.51
1	A	429	MET	SD-CE	-6.77	1.62	1.79
1	A	153	ILE	CA-C	6.54	1.59	1.52
1	B	405	LEU	C-N	6.46	1.42	1.33
1	C	22	ILE	CG1-CD1	6.16	1.75	1.51
1	C	284	MET	SD-CE	6.09	1.94	1.79
1	C	429	MET	SD-CE	-6.02	1.64	1.79
1	C	423	ASN	C-N	6.01	1.42	1.34
1	C	114	LEU	C-N	5.81	1.41	1.33
1	C	411	LEU	CA-C	5.71	1.60	1.52
1	C	131	VAL	CA-CB	5.70	1.61	1.54
1	C	398	THR	CA-CB	-5.70	1.44	1.53
1	A	40	TYR	CA-C	-5.62	1.45	1.52
1	B	608	GLN	CA-C	5.61	1.59	1.52
1	C	554	MET	CA-C	5.61	1.60	1.52
1	C	287	ALA	CA-C	-5.58	1.45	1.52
1	C	187	ASP	CA-C	-5.45	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	ILE	CA-C	5.36	1.58	1.52
1	B	647	HIS	CA-C	5.36	1.59	1.52
1	C	398	THR	CA-C	-5.36	1.46	1.52
1	B	398	THR	CA-CB	-5.34	1.45	1.53
1	C	608	GLN	CA-C	5.30	1.58	1.52
1	C	522	LEU	CA-C	5.30	1.59	1.52
1	B	662	MET	C-N	5.30	1.40	1.33
1	A	398	THR	CA-C	-5.19	1.46	1.52
1	A	177	ALA	CA-C	5.14	1.59	1.52
1	B	273	MET	SD-CE	-5.14	1.66	1.79
1	C	408	ILE	CA-C	5.12	1.59	1.52
1	B	551	TRP	CA-C	-5.03	1.46	1.52
1	C	554	MET	SD-CE	-5.02	1.67	1.79
1	C	128	ARG	CA-C	5.00	1.59	1.52

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ASP	CA-CB-CG	10.75	123.35	112.60
1	C	327	ASP	CA-C-N	10.19	136.10	120.82
1	C	327	ASP	C-N-CA	10.19	136.10	120.82
1	C	581	GLU	CB-CG-CD	9.04	127.97	112.60
1	B	327	ASP	CA-C-N	8.90	134.17	120.82
1	B	327	ASP	C-N-CA	8.90	134.17	120.82
1	C	259	ASP	CA-CB-CG	8.90	121.50	112.60
1	C	41	GLU	CB-CG-CD	8.44	126.95	112.60
1	A	327	ASP	CA-C-N	8.08	134.04	121.19
1	A	327	ASP	C-N-CA	8.08	134.04	121.19
1	A	22	ILE	N-CA-C	7.84	117.94	110.42
2	G	5	DG	P-O3'-C3'	7.69	131.74	120.20
1	B	626	ASN	CA-CB-CG	7.47	120.07	112.60
1	C	259	ASP	CA-C-N	-7.43	114.39	122.85
1	C	259	ASP	C-N-CA	-7.43	114.39	122.85
1	C	1	PRO	CA-C-N	7.13	135.16	121.54
1	C	1	PRO	C-N-CA	7.13	135.16	121.54
1	C	589	ASP	CA-CB-CG	7.10	119.70	112.60
1	C	22	ILE	N-CA-C	6.94	117.09	110.42
1	C	302	PHE	N-CA-C	6.93	122.41	113.88
1	B	553	SER	CA-C-N	6.89	132.15	121.19
1	B	553	SER	C-N-CA	6.89	132.15	121.19
1	B	302	PHE	N-CA-C	6.89	122.35	113.88
1	B	554	MET	N-CA-C	6.88	122.64	111.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ASP	CA-CB-CG	6.79	119.39	112.60
1	C	363	LEU	N-CA-C	6.76	118.42	109.83
1	C	539	ARG	CA-C-N	6.73	130.20	120.38
1	C	539	ARG	C-N-CA	6.73	130.20	120.38
1	A	324	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	259	ASP	CA-C-N	6.52	127.03	122.60
1	B	259	ASP	C-N-CA	6.52	127.03	122.60
1	A	302	PHE	N-CA-C	6.50	121.88	113.88
1	C	663	PRO	CA-C-N	6.48	133.37	121.70
1	C	663	PRO	C-N-CA	6.48	133.37	121.70
1	A	556	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	205	ALA	N-CA-C	6.44	119.96	109.59
2	G	6	DC	N1-C1'-C2'	6.32	122.97	113.50
2	G	6	DC	P-O3'-C3'	6.32	129.67	120.20
1	B	423	ASN	CA-C-N	6.31	129.36	120.28
1	B	423	ASN	C-N-CA	6.31	129.36	120.28
1	B	547	PRO	CA-C-N	6.30	127.09	120.03
1	B	547	PRO	C-N-CA	6.30	127.09	120.03
1	B	1	PRO	CA-C-N	6.29	133.56	121.54
1	B	1	PRO	C-N-CA	6.29	133.56	121.54
1	B	229	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	176	GLU	CA-C-N	6.26	128.96	120.44
1	B	176	GLU	C-N-CA	6.26	128.96	120.44
1	A	21	ASN	CA-CB-CG	6.25	118.85	112.60
1	C	205	ALA	N-CA-C	6.22	119.60	109.59
1	B	363	LEU	N-CA-C	6.20	117.71	109.83
1	B	259	ASP	N-CA-CB	6.20	119.25	109.71
1	C	206	GLN	CA-C-N	6.18	130.58	120.63
1	C	206	GLN	C-N-CA	6.18	130.58	120.63
1	B	607	ARG	CA-C-N	6.14	129.63	120.17
1	B	607	ARG	C-N-CA	6.14	129.63	120.17
1	A	229	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	386	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	654	THR	CA-C-N	6.05	129.89	120.82
1	B	654	THR	C-N-CA	6.05	129.89	120.82
1	A	204	ARG	CA-C-N	-6.04	113.66	122.65
1	A	204	ARG	C-N-CA	-6.04	113.66	122.65
1	B	559	GLY	N-CA-C	5.98	121.08	113.24
1	B	477	GLU	CB-CG-CD	5.95	122.72	112.60
1	C	547	PRO	CA-C-N	5.95	126.70	120.03
1	C	547	PRO	C-N-CA	5.95	126.70	120.03
1	A	529	GLU	CB-CG-CD	5.93	122.68	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ILE	N-CA-C	5.89	116.08	110.42
1	C	22	ILE	CB-CA-C	5.89	119.51	111.97
1	B	21	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	78	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	136	SER	N-CA-C	5.80	123.16	110.80
1	C	166	ILE	CA-C-N	5.80	127.98	120.44
1	C	166	ILE	C-N-CA	5.80	127.98	120.44
1	B	419	ALA	N-CA-C	5.80	120.34	110.02
1	B	286	VAL	CA-C-N	5.79	128.36	120.54
1	B	286	VAL	C-N-CA	5.79	128.36	120.54
1	C	138	LEU	N-CA-C	5.79	118.97	109.76
1	A	649	VAL	N-CA-C	-5.74	101.40	109.21
1	B	663	PRO	CA-C-N	5.71	131.99	121.70
1	B	663	PRO	C-N-CA	5.71	131.99	121.70
1	A	214	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	396	GLY	N-CA-C	5.68	120.83	113.27
1	B	214	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	363	LEU	N-CA-C	5.67	117.03	109.83
1	B	333	PRO	N-CA-C	5.65	119.76	110.55
1	B	136	SER	N-CA-C	5.57	122.66	110.80
1	A	558	TYR	N-CA-C	5.55	120.21	113.38
1	C	114	LEU	CA-C-N	5.55	128.73	120.90
1	C	114	LEU	C-N-CA	5.55	128.73	120.90
1	A	205	ALA	N-CA-C	5.53	118.83	109.76
1	C	231	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	558	TYR	N-CA-C	5.53	120.18	113.38
1	A	173	LYS	N-CA-C	5.50	119.69	112.92
1	C	333	PRO	N-CA-C	5.50	119.52	110.55
1	C	462	GLY	CA-C-N	5.50	127.59	120.44
1	C	462	GLY	C-N-CA	5.50	127.59	120.44
1	B	22	ILE	CB-CA-C	5.48	118.99	111.97
1	C	467	GLY	CA-C-N	5.48	126.18	119.99
1	C	467	GLY	C-N-CA	5.48	126.18	119.99
1	A	70	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	259	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	186	PHE	N-CA-C	5.42	117.19	111.28
1	B	649	VAL	N-CA-C	-5.41	101.85	109.21
1	C	327	ASP	N-CA-CB	5.40	119.62	110.49
1	C	419	ALA	N-CA-C	5.39	118.43	108.94
1	B	633	THR	CA-C-N	5.38	127.74	120.38
1	B	633	THR	C-N-CA	5.38	127.74	120.38
1	B	406	MET	N-CA-C	5.37	116.81	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	GLU	CA-C-N	5.37	127.42	120.44
1	C	176	GLU	C-N-CA	5.37	127.42	120.44
1	C	309	ASN	CA-C-N	5.35	127.72	120.44
1	C	309	ASN	C-N-CA	5.35	127.72	120.44
1	B	277	PHE	N-CA-C	5.35	117.80	111.33
1	C	136	SER	N-CA-C	5.34	122.18	110.80
1	A	419	ALA	N-CA-C	5.32	118.30	109.79
1	C	62	THR	N-CA-C	-5.29	105.60	111.36
1	C	626	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	186	PHE	N-CA-C	5.27	117.11	111.36
1	B	603	ALA	CA-C-N	5.27	127.61	120.44
1	B	603	ALA	C-N-CA	5.27	127.61	120.44
1	C	649	VAL	N-CA-C	-5.27	102.04	109.21
1	C	165	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	3	ARG	N-CA-C	-5.23	101.17	109.96
1	C	130	ALA	CA-C-N	5.21	127.13	120.56
1	C	130	ALA	C-N-CA	5.21	127.13	120.56
1	C	155	TYR	N-CA-C	5.21	119.72	112.90
1	B	574	CYS	N-CA-C	5.18	117.83	111.82
1	B	138	LEU	N-CA-C	5.17	118.37	110.20
1	A	524	ASN	CA-CB-CG	5.17	117.77	112.60
1	C	70	ASP	N-CA-C	5.15	116.58	110.19
1	A	161	GLY	CA-C-N	5.14	127.17	120.28
1	A	161	GLY	C-N-CA	5.14	127.17	120.28
1	C	633	THR	CA-C-N	5.13	127.41	120.38
1	C	633	THR	C-N-CA	5.13	127.41	120.38
1	C	161	GLY	O-C-N	5.13	127.10	122.18
1	B	9	LEU	CA-C-N	5.10	127.36	120.38
1	B	9	LEU	C-N-CA	5.10	127.36	120.38
1	C	309	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	166	ILE	CA-C-N	5.09	127.05	120.44
1	A	166	ILE	C-N-CA	5.09	127.05	120.44
1	C	398	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	241	SER	N-CA-C	5.07	117.51	109.50
1	C	491	GLU	CB-CG-CD	5.04	121.17	112.60
1	C	100	TRP	N-CA-C	-5.04	103.30	109.65
1	B	479	LYS	CA-C-N	5.03	129.58	123.10
1	B	479	LYS	C-N-CA	5.03	129.58	123.10
1	C	454	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	478	GLY	CA-C-N	5.01	129.00	120.88
1	B	478	GLY	C-N-CA	5.01	129.00	120.88
1	B	78	ASN	CA-CB-CG	5.00	117.61	112.60

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	5165	58	0
1	B	5265	0	5165	84	0
1	C	5265	0	5165	94	0
2	G	81	0	46	8	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	44	0	11	3	0
4	B	62	0	24	9	0
4	C	62	0	24	24	0
All	All	16048	0	15600	247	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 8.

All (247) 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:22:ILE:CD1	1:C:22:ILE:CG1	1.75	1.62
1:A:22:ILE:CD1	1:A:22:ILE:CG1	1.79	1.59
1:B:22:ILE:CD1	1:B:22:ILE:CG1	1.84	1.54
4:C:1666:ATP:O4'	4:C:1666:ATP:C1'	1.64	1.45
1:B:16:MET:SD	1:B:16:MET:CE	2.03	1.45
4:C:1666:ATP:O4'	4:C:1666:ATP:C4'	1.63	1.44
4:C:1665:ATP:C8	4:C:1666:ATP:O2'	1.86	1.27
1:C:270:ARG:NH2	4:C:1666:ATP:H3'	1.60	1.15
1:A:608:GLN:HE22	1:B:593:ARG:HD3	1.12	1.09
1:C:270:ARG:HH22	4:C:1666:ATP:C3'	1.73	1.02
4:C:1665:ATP:N9	4:C:1666:ATP:O2'	1.94	1.01
1:C:419:ALA:HB1	1:C:422:LEU:HD12	1.42	0.98
1:B:1:PRO:HD3	1:B:238:GLU:HG3	1.48	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:ARG:N	1:C:664:ARG:HD3	1.83	0.94
4:C:1665:ATP:C8	4:C:1666:ATP:C2'	2.52	0.91
1:A:608:GLN:NE2	1:B:593:ARG:HD3	1.86	0.89
1:C:270:ARG:HH22	4:C:1666:ATP:C2'	1.89	0.84
1:B:541:LYS:HE2	2:G:4:DA:H3'	1.59	0.84
1:B:204:ARG:HE	2:G:7:DG:H21	1.27	0.81
1:B:651:VAL:O	1:B:655:GLU:HB2	1.81	0.80
1:C:270:ARG:HH22	4:C:1666:ATP:H2'	1.51	0.76
4:C:1665:ATP:H5'1	4:C:1666:ATP:O3'	1.87	0.75
1:A:270:ARG:HH22	4:A:1667:ATP:PA	2.09	0.74
1:B:391:LEU:HD22	1:B:398:THR:HG22	1.67	0.74
1:A:608:GLN:HE22	1:B:593:ARG:CD	1.97	0.74
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.37	0.72
1:C:343:GLU:OE1	1:C:343:GLU:HA	1.87	0.72
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.69	0.72
4:C:1665:ATP:O4'	4:C:1666:ATP:O3'	2.07	0.71
1:B:328:HIS:HB3	4:B:1666:ATP:O2'	1.90	0.71
1:C:1:PRO:HG2	1:C:238:GLU:HG3	1.73	0.71
1:C:391:LEU:HD22	1:C:398:THR:HG22	1.73	0.70
1:A:593:ARG:HG2	1:B:42:GLY:HA2	1.73	0.70
1:B:160:MET:HB3	2:G:4:DA:N1	2.07	0.70
1:C:525:GLN:NE2	1:C:583:TYR:OH	2.24	0.70
1:C:664:ARG:HD3	1:C:664:ARG:H	1.57	0.69
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.40	0.67
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.76	0.67
1:C:177:ALA:HA	1:C:180:LEU:HD12	1.75	0.67
4:C:1666:ATP:O4'	4:C:1666:ATP:C2'	2.42	0.67
4:C:1666:ATP:O4'	4:C:1666:ATP:C3'	2.42	0.66
1:C:22:ILE:CD1	1:C:22:ILE:HA	2.26	0.66
1:C:34:GLU:HG2	1:C:94:PRO:HD2	1.77	0.66
1:C:651:VAL:O	1:C:655:GLU:HB2	1.97	0.65
1:C:305:THR:H	1:C:309:ASN:ND2	1.94	0.65
1:C:106:LEU:HD21	1:C:388:GLU:HG3	1.80	0.64
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.45	0.64
1:C:617:ILE:H	1:C:617:ILE:HD12	1.63	0.63
1:B:22:ILE:CD1	1:B:22:ILE:HA	2.28	0.63
1:C:664:ARG:N	1:C:664:ARG:CD	2.60	0.63
1:A:22:ILE:CD1	1:A:22:ILE:HA	2.30	0.61
1:A:392:SER:O	1:A:398:THR:HG21	2.00	0.61
1:C:130:ALA:HB2	1:C:408:ILE:HD11	1.84	0.59
1:C:202:VAL:HG22	1:C:272:ALA:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:ARG:H	1:C:664:ARG:CD	2.16	0.59
4:C:1666:ATP:C4	4:C:1666:ATP:H5'2	2.38	0.59
1:C:538:ASP:OD1	1:C:540:SER:HB3	2.02	0.59
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.68	0.59
1:C:22:ILE:HG23	1:C:26:GLN:OE1	2.02	0.58
1:C:420:PRO:HA	1:C:423:ASN:HD21	1.68	0.58
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.04	0.58
1:C:1:PRO:HG2	1:C:238:GLU:CG	2.34	0.58
1:B:202:VAL:HG22	1:B:272:ALA:HB3	1.86	0.58
1:A:22:ILE:HA	1:A:22:ILE:HD13	1.86	0.57
1:A:651:VAL:O	1:A:655:GLU:HB2	2.05	0.57
1:B:554:MET:HE1	1:B:568:LEU:HD11	1.86	0.56
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.05	0.56
1:C:164:ILE:HD11	1:C:647:HIS:HD2	1.71	0.56
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.71	0.56
1:B:214:ASP:OD2	1:B:217:THR:HG22	2.06	0.55
1:B:453:ASP:OD2	4:B:1666:ATP:H1'	2.07	0.55
1:C:605:MET:HG2	1:C:609:ALA:HB3	1.87	0.55
1:B:554:MET:CE	1:B:568:LEU:HD11	2.36	0.55
1:A:206:GLN:HE21	1:A:268:ARG:HH11	1.55	0.55
1:C:270:ARG:HH12	4:C:1666:ATP:H5'2	1.72	0.55
1:C:270:ARG:HH21	4:C:1666:ATP:H3'	1.64	0.55
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.06	0.55
1:C:419:ALA:CB	1:C:422:LEU:HD12	2.27	0.55
1:C:22:ILE:HA	1:C:22:ILE:HD13	1.87	0.54
1:B:160:MET:HB3	2:G:4:DA:C2	2.42	0.54
1:C:270:ARG:NH2	4:C:1666:ATP:C2'	2.68	0.54
1:C:214:ASP:OD2	1:C:217:THR:HG22	2.07	0.54
1:A:202:VAL:HG22	1:A:272:ALA:HB3	1.88	0.54
1:C:270:ARG:NH2	4:C:1666:ATP:C3'	2.39	0.54
1:B:22:ILE:HA	1:B:22:ILE:HD13	1.89	0.53
1:B:1:PRO:CD	1:B:238:GLU:HG3	2.32	0.53
1:A:407:SER:HA	1:A:448:GLN:HE22	1.74	0.53
1:B:392:SER:O	1:B:398:THR:HG21	2.07	0.53
1:B:634:GLU:HG3	1:B:642:HIS:NE2	2.24	0.53
1:C:270:ARG:NH2	4:C:1666:ATP:H2'	2.21	0.53
1:A:164:ILE:HD11	1:A:647:HIS:HD2	1.74	0.52
1:B:181:MET:CE	1:B:356:LEU:HD23	2.39	0.52
1:B:452:SER:OG	4:B:1666:ATP:H2	1.92	0.52
1:A:420:PRO:HA	1:A:423:ASN:ND2	2.24	0.52
1:C:634:GLU:HG3	1:C:642:HIS:NE2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:HIS:HB3	4:B:1666:ATP:HO2'	1.75	0.52
1:C:34:GLU:CG	1:C:94:PRO:HD2	2.39	0.52
1:C:504:ASP:OD2	1:C:506:ARG:NH1	2.42	0.52
1:A:392:SER:O	1:A:398:THR:CG2	2.57	0.52
1:A:214:ASP:OD2	1:A:217:THR:HG22	2.10	0.51
1:B:210:ALA:HB3	1:B:223:LYS:HB2	1.91	0.51
1:A:151:THR:CG2	1:A:163:LYS:HG2	2.41	0.51
1:B:205:ALA:O	1:B:529:GLU:HG3	2.10	0.51
1:C:407:SER:HA	1:C:448:GLN:HE22	1.75	0.51
1:B:286:VAL:O	1:B:289:PRO:HD2	2.11	0.51
1:A:537:ARG:HD2	1:B:49:ARG:HG3	1.93	0.50
1:B:417:HIS:CE1	1:B:474:MET:HE1	2.46	0.50
1:A:273:MET:HE3	1:A:392:SER:HA	1.93	0.50
1:B:419:ALA:HB1	1:B:422:LEU:HD12	1.94	0.50
1:C:106:LEU:CD2	1:C:388:GLU:HG3	2.41	0.50
1:C:210:ALA:HB3	1:C:223:LYS:HB2	1.93	0.50
1:A:151:THR:HG22	1:A:163:LYS:HG2	1.94	0.50
1:B:273:MET:HE3	1:B:392:SER:HA	1.94	0.50
4:C:1665:ATP:C5'	4:C:1666:ATP:O3'	2.58	0.50
1:A:210:ALA:HB3	1:A:223:LYS:HB2	1.94	0.49
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.76	0.49
1:C:131:VAL:HG11	1:C:343:GLU:HB3	1.93	0.49
1:B:395:GLN:HB3	1:B:398:THR:HG23	1.93	0.49
1:C:206:GLN:HB2	1:C:270:ARG:HD2	1.93	0.49
1:C:273:MET:HE3	1:C:392:SER:HA	1.94	0.49
1:A:44:LEU:HD21	1:B:257:GLY:HA3	1.95	0.49
1:C:104:SER:OG	1:C:106:LEU:HD22	2.13	0.48
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.95	0.48
1:A:634:GLU:HG3	1:A:642:HIS:NE2	2.28	0.48
1:B:407:SER:HA	1:B:448:GLN:HE22	1.78	0.48
1:B:392:SER:O	1:B:398:THR:CG2	2.62	0.48
1:B:72:TYR:HB3	1:B:472:PHE:CZ	2.48	0.48
1:C:41:GLU:HG2	1:C:532:VAL:HG11	1.96	0.48
1:B:94:PRO:HB3	1:B:269:ARG:HG3	1.95	0.48
1:B:217:THR:HG23	1:B:219:LYS:HB2	1.96	0.48
1:C:1:PRO:CG	1:C:238:GLU:HG3	2.43	0.48
1:B:270:ARG:NH1	4:B:1666:ATP:H5'1	2.29	0.48
1:A:596:LEU:CD2	1:A:608:GLN:HG2	2.44	0.47
1:A:22:ILE:CD1	1:A:22:ILE:CB	2.82	0.47
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.49	0.47
1:A:23:LYS:HE2	1:A:156:PHE:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:VAL:HG21	1:B:406:MET:HE2	1.96	0.47
1:A:540:SER:HB2	1:A:644:VAL:O	2.14	0.47
1:B:204:ARG:HD2	1:B:530:TYR:OH	2.14	0.47
1:B:630:TYR:CE2	4:B:1665:ATP:H2'	2.50	0.47
1:A:504:ASP:OD2	1:A:506:ARG:NH1	2.47	0.47
1:C:420:PRO:O	1:C:423:ASN:ND2	2.48	0.47
1:C:138:LEU:HB2	1:C:662:MET:HE1	1.97	0.47
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.97	0.47
1:B:477:GLU:HB3	1:B:479:LYS:HG3	1.97	0.46
1:C:72:TYR:HD2	1:C:472:PHE:CZ	2.33	0.46
1:A:417:HIS:CE1	1:A:474:MET:HE1	2.50	0.46
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.97	0.46
4:C:1665:ATP:H5'1	4:C:1666:ATP:C3'	2.46	0.46
1:B:143:LEU:HD21	1:B:284:MET:HE2	1.97	0.46
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.98	0.46
1:B:38:GLU:HB3	1:B:532:VAL:HG22	1.96	0.46
1:B:624:ASP:HB3	1:B:627:LYS:HD2	1.97	0.46
1:C:555:LYS:C	1:C:557:THR:H	2.23	0.46
1:B:160:MET:O	1:B:164:ILE:HD12	2.16	0.46
1:C:72:TYR:HD2	1:C:472:PHE:CE2	2.34	0.46
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.97	0.46
1:C:452:SER:HB3	1:C:453:ASP:H	1.61	0.45
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.12	0.45
1:A:270:ARG:NH1	4:A:1666:ATP:H3'	2.32	0.45
1:A:301:THR:HG23	1:A:448:GLN:HG3	1.99	0.45
1:B:164:ILE:HG23	1:B:649:VAL:HG22	1.98	0.45
1:C:34:GLU:HG2	1:C:94:PRO:CD	2.46	0.45
1:B:572:GLU:O	1:B:576:TRP:HB2	2.16	0.45
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.51	0.45
1:C:586:TYR:CE2	1:C:590:MET:CE	2.99	0.45
1:C:26:GLN:HE21	1:C:26:GLN:HB2	1.58	0.45
1:B:504:ASP:OD2	1:B:506:ARG:NH1	2.49	0.45
1:B:610:GLY:C	1:B:612:ALA:H	2.25	0.45
1:C:411:LEU:HD22	1:C:439:TYR:CD2	2.51	0.45
1:C:477:GLU:HB3	1:C:479:LYS:HE3	1.97	0.45
1:A:204:ARG:NH2	1:A:626:ASN:HD21	2.15	0.45
1:B:286:VAL:C	1:B:289:PRO:HD2	2.42	0.45
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.52	0.45
1:A:270:ARG:NH2	4:A:1667:ATP:O1A	2.44	0.45
1:B:633:THR:HG22	1:B:636:ASP:OD2	2.17	0.45
1:C:217:THR:HG23	1:C:219:LYS:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ARG:HH11	1:C:255:GLN:NE2	2.08	0.45
1:A:143:LEU:HD21	1:A:284:MET:HE2	1.98	0.44
1:B:538:ASP:OD2	2:G:4:DA:H8	2.00	0.44
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.17	0.44
4:B:1665:ATP:O5'	4:B:1665:ATP:H8	2.00	0.44
1:C:663:PRO:C	1:C:664:ARG:HD3	2.39	0.44
1:A:205:ALA:O	1:A:529:GLU:HG3	2.17	0.44
4:C:1665:ATP:C4'	4:C:1666:ATP:O3'	2.65	0.44
1:C:610:GLY:C	1:C:612:ALA:H	2.26	0.44
1:A:217:THR:HG23	1:A:219:LYS:HB2	2.00	0.43
1:C:336:LEU:HD21	1:C:404:LEU:HD12	1.98	0.43
1:C:122:ARG:NH1	1:C:423:ASN:OD1	2.49	0.43
1:B:23:LYS:HE2	1:B:156:PHE:O	2.19	0.43
1:C:199:TYR:HB2	1:C:365:VAL:HG12	2.00	0.43
1:B:70:ASP:CG	1:B:74:ARG:HB2	2.43	0.43
1:A:475:LEU:HD21	1:A:482:PRO:HG3	2.01	0.43
1:C:3:ARG:O	1:C:3:ARG:HG3	2.13	0.43
1:C:205:ALA:O	1:C:529:GLU:HG3	2.19	0.43
1:A:421:HIS:CE1	1:A:463:ARG:HB2	2.54	0.42
1:B:329:ASP:OD2	4:B:1666:ATP:H2'	2.18	0.42
1:C:230:PHE:CD1	1:C:230:PHE:C	2.97	0.42
1:A:153:ILE:HA	1:A:154:PRO:HA	1.81	0.42
1:C:587:ARG:HA	1:C:587:ARG:HD2	1.81	0.42
1:C:22:ILE:CD1	1:C:22:ILE:CB	2.81	0.42
1:C:181:MET:SD	1:C:356:LEU:HD23	2.60	0.42
1:C:214:ASP:CG	1:C:217:THR:HG22	2.44	0.42
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.54	0.42
1:B:99:THR:HB	1:B:227:VAL:HG12	2.00	0.42
1:A:286:VAL:O	1:A:289:PRO:HD2	2.20	0.42
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.55	0.42
1:B:199:TYR:HB2	1:B:365:VAL:HG12	2.02	0.42
1:A:391:LEU:HD22	1:A:398:THR:HG22	2.02	0.42
1:B:122:ARG:NH1	1:B:423:ASN:HD21	2.17	0.42
1:B:153:ILE:HA	1:B:154:PRO:HA	1.80	0.42
1:C:596:LEU:CD2	1:C:608:GLN:HG2	2.50	0.42
1:A:138:LEU:HB2	1:A:662:MET:HE1	2.01	0.42
1:B:6:ALA:HA	1:B:378:LEU:O	2.20	0.42
1:B:452:SER:OG	4:B:1666:ATP:C2	2.73	0.42
1:B:538:ASP:OD2	2:G:4:DA:C8	2.73	0.42
1:C:22:ILE:CD1	1:C:22:ILE:CA	2.97	0.42
1:B:160:MET:HG3	1:B:164:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ALA:HB1	1:C:404:LEU:HD22	2.02	0.41
1:C:553:SER:HB3	1:C:616:PRO:HA	2.01	0.41
1:C:555:LYS:O	1:C:559:GLY:HA3	2.20	0.41
1:C:298:TYR:CD1	1:C:440:TRP:HB3	2.56	0.41
1:B:134:MET:HG2	1:B:294:ILE:HG21	2.01	0.41
1:B:343:GLU:O	1:B:347:MET:N	2.47	0.41
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.56	0.41
4:C:1666:ATP:C4	4:C:1666:ATP:C5'	3.04	0.41
1:B:226:MET:HE1	1:B:244:ALA:HB2	2.01	0.41
1:B:142:PRO:HD3	1:B:651:VAL:HB	2.01	0.41
2:G:6:DC:H1'	2:G:7:DG:OP1	2.20	0.41
1:A:217:THR:HG23	1:A:219:LYS:H	1.86	0.41
1:B:177:ALA:HA	1:B:180:LEU:HD12	2.02	0.41
2:G:7:DG:OP1	2:G:7:DG:H3'	2.20	0.41
1:B:86:GLY:O	1:B:89:HIS:CD2	2.73	0.41
1:B:378:LEU:HD21	1:B:382:PRO:HD3	2.03	0.41
1:C:305:THR:H	1:C:309:ASN:HD21	1.68	0.41
1:C:392:SER:O	1:C:398:THR:HG21	2.20	0.41
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.41
1:C:614:LEU:HD21	1:C:641:ILE:HD11	2.03	0.41
1:A:610:GLY:C	1:A:612:ALA:H	2.29	0.40
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.55	0.40
1:A:634:GLU:CB	1:A:642:HIS:NE2	2.84	0.40
1:B:214:ASP:CG	1:B:217:THR:HG22	2.46	0.40
1:C:226:MET:HE1	1:C:244:ALA:HB2	2.03	0.40
1:A:206:GLN:HE21	1:A:268:ARG:NH1	2.18	0.40
1:C:153:ILE:HA	1:C:154:PRO:HA	1.80	0.40
1:C:270:ARG:NH2	4:C:1666:ATP:H5'1	2.37	0.40
1:C:310:LYS:NZ	1:C:499:ASP:OD2	2.51	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%)	634 (96%)	23 (4%)	5 (1%)	16	45
1	B	662/665 (100%)	628 (95%)	28 (4%)	6 (1%)	14	43
1	C	662/665 (100%)	616 (93%)	40 (6%)	6 (1%)	14	43
All	All	1986/1995 (100%)	1878 (95%)	91 (5%)	17 (1%)	14	43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ARG
1	B	2	ARG
1	B	607	ARG
1	C	2	ARG
1	B	327	ASP
1	B	611	LEU
1	C	327	ASP
1	C	607	ARG
1	C	609	ALA
1	C	611	LEU
1	A	327	ASP
1	A	609	ALA
1	A	611	LEU
1	B	609	ALA
1	C	368	GLY
1	B	368	GLY
1	A	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%)	524 (94%)	33 (6%)	18	46
1	B	557/558 (100%)	513 (92%)	44 (8%)	11	36
1	C	557/558 (100%)	506 (91%)	51 (9%)	8	30
All	All	1671/1674 (100%)	1543 (92%)	128 (8%)	12	37

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	22	ILE
1	A	23	LYS
1	A	30	ARG
1	A	31	SER
1	A	41	GLU
1	A	63	ASP
1	A	71	GLU
1	A	78	ASN
1	A	82	THR
1	A	102	LEU
1	A	192	LEU
1	A	202	VAL
1	A	206	GLN
1	A	269	ARG
1	A	271	THR
1	A	325	VAL
1	A	326	SER
1	A	327	ASP
1	A	330	THR
1	A	362	LYS
1	A	391	LEU
1	A	424	SER
1	A	425	ARG
1	A	452	SER
1	A	463	ARG
1	A	497	LEU
1	A	534	SER
1	A	589	ASP
1	A	629	GLN
1	A	634	GLU
1	A	659	ARG
1	A	662	MET
1	B	3	ARG
1	B	10	SER
1	B	22	ILE
1	B	23	LYS
1	B	41	GLU
1	B	78	ASN
1	B	82	THR
1	B	102	LEU
1	B	151	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	171	LEU
1	B	192	LEU
1	B	202	VAL
1	B	206	GLN
1	B	267	GLU
1	B	269	ARG
1	B	271	THR
1	B	280	ASN
1	B	307	ARG
1	B	308	LEU
1	B	325	VAL
1	B	326	SER
1	B	327	ASP
1	B	330	THR
1	B	362	LYS
1	B	391	LEU
1	B	398	THR
1	B	403	THR
1	B	411	LEU
1	B	424	SER
1	B	425	ARG
1	B	452	SER
1	B	463	ARG
1	B	497	LEU
1	B	534	SER
1	B	537	ARG
1	B	541	LYS
1	B	556	ASP
1	B	576	TRP
1	B	589	ASP
1	B	596	LEU
1	B	600	ARG
1	B	634	GLU
1	B	659	ARG
1	B	662	MET
1	C	2	ARG
1	C	3	ARG
1	C	10	SER
1	C	17	LEU
1	C	22	ILE
1	C	23	LYS
1	C	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	30	ARG
1	C	31	SER
1	C	41	GLU
1	C	52	SER
1	C	63	ASP
1	C	71	GLU
1	C	78	ASN
1	C	82	THR
1	C	102	LEU
1	C	106	LEU
1	C	171	LEU
1	C	192	LEU
1	C	202	VAL
1	C	206	GLN
1	C	259	ASP
1	C	269	ARG
1	C	271	THR
1	C	308	LEU
1	C	309	ASN
1	C	324	ASP
1	C	325	VAL
1	C	326	SER
1	C	327	ASP
1	C	329	ASP
1	C	330	THR
1	C	343	GLU
1	C	362	LYS
1	C	374	GLN
1	C	391	LEU
1	C	398	THR
1	C	404	LEU
1	C	423	ASN
1	C	424	SER
1	C	425	ARG
1	C	452	SER
1	C	463	ARG
1	C	497	LEU
1	C	553	SER
1	C	556	ASP
1	C	629	GLN
1	C	634	GLU
1	C	659	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	662	MET
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	191	GLN
1	A	206	GLN
1	A	255	GLN
1	A	288	GLN
1	A	292	ASN
1	A	309	ASN
1	A	448	GLN
1	A	525	GLN
1	A	608	GLN
1	A	626	ASN
1	A	647	HIS
1	B	25	GLN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	91	ASN
1	B	191	GLN
1	B	255	GLN
1	B	280	ASN
1	B	309	ASN
1	B	423	ASN
1	B	448	GLN
1	B	492	HIS
1	B	519	ASN
1	B	608	GLN
1	B	647	HIS
1	C	64	HIS
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	191	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	255	GLN
1	C	280	ASN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	C	1666	-	32,33,33	6.94	24 (75%)	48,52,52	3.95	30 (62%)
4	ATP	A	1667	-	10,12,33	2.13	2 (20%)	17,20,52	2.06	5 (29%)
4	ATP	B	1665	-	32,33,33	2.04	5 (15%)	48,52,52	1.69	8 (16%)
4	ATP	C	1665	-	32,33,33	2.92	10 (31%)	48,52,52	2.96	19 (39%)
4	ATP	B	1666	-	32,33,33	1.73	7 (21%)	48,52,52	2.00	13 (27%)
4	ATP	A	1666	-	32,33,33	6.06	26 (81%)	48,52,52	2.55	19 (39%)

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	C	1666	-	-	6/22/38/38	0/3/3/3
4	ATP	A	1667	-	-	2/12/12/38	-
4	ATP	B	1665	-	-	3/22/38/38	0/3/3/3
4	ATP	C	1665	-	-	5/22/38/38	0/3/3/3
4	ATP	B	1666	-	-	5/22/38/38	0/3/3/3
4	ATP	A	1666	-	-	8/22/38/38	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1666	ATP	PA-O3A	22.16	1.83	1.59
4	C	1666	ATP	PA-O3A	19.49	1.80	1.59
4	C	1666	ATP	PB-O3B	17.28	1.78	1.59
4	C	1666	ATP	PB-O3A	11.96	1.72	1.59
4	A	1666	ATP	PB-O3A	10.71	1.71	1.59
4	C	1666	ATP	O4'-C1'	9.69	1.64	1.42
4	A	1666	ATP	PA-O1A	8.66	1.80	1.50
4	C	1666	ATP	C4-N3	8.44	1.50	1.34
4	C	1666	ATP	O4'-C4'	8.35	1.63	1.45
4	A	1666	ATP	C2-N3	7.80	1.47	1.33
4	B	1665	ATP	PB-O3B	7.76	1.67	1.59
4	C	1665	ATP	C8-N9	7.53	1.50	1.37
4	C	1666	ATP	C5'-C4'	7.52	1.74	1.51
4	C	1666	ATP	C2-N1	7.31	1.46	1.33
4	C	1666	ATP	PB-O1B	6.69	1.74	1.50
4	C	1665	ATP	C5-C4	6.52	1.50	1.39
4	A	1666	ATP	C4-N3	6.45	1.46	1.34
4	C	1666	ATP	PG-O2G	6.34	1.78	1.54
4	C	1665	ATP	C1'-N9	6.21	1.63	1.46
4	C	1666	ATP	PG-O1G	6.00	1.69	1.50
4	A	1666	ATP	O4'-C1'	5.92	1.55	1.42
4	C	1665	ATP	O4'-C1'	5.75	1.55	1.42
4	C	1666	ATP	PA-O1A	5.73	1.70	1.50
4	C	1665	ATP	PB-O3B	5.67	1.65	1.59
4	A	1666	ATP	PG-O1G	5.63	1.68	1.50
4	A	1666	ATP	O4'-C4'	5.61	1.57	1.45
4	C	1666	ATP	C5-N7	5.44	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1666	ATP	C5-C6	5.35	1.55	1.41
4	A	1666	ATP	PB-O1B	5.27	1.69	1.50
4	B	1666	ATP	C4-N9	5.23	1.48	1.37
4	A	1666	ATP	C6-N1	5.18	1.50	1.35
4	A	1666	ATP	C4-N9	5.12	1.48	1.37
4	C	1666	ATP	O3'-C3'	4.99	1.55	1.43
4	A	1667	ATP	PB-O3B	4.92	1.64	1.59
4	A	1666	ATP	C2'-C3'	4.86	1.66	1.53
4	A	1666	ATP	PA-O5'	4.80	1.78	1.59
4	C	1666	ATP	C2'-C3'	4.78	1.66	1.53
4	A	1666	ATP	PB-O3B	4.75	1.64	1.59
4	C	1666	ATP	C6-N1	4.64	1.48	1.35
4	B	1665	ATP	O4'-C1'	4.48	1.52	1.42
4	C	1666	ATP	C8-N7	4.24	1.39	1.31
4	C	1665	ATP	C2-N1	4.20	1.41	1.33
4	A	1666	ATP	C5-C4	4.18	1.46	1.39
4	C	1666	ATP	C6-N6	4.06	1.44	1.34
4	A	1666	ATP	C5-C6	3.97	1.52	1.41
4	A	1666	ATP	C2'-C1'	3.87	1.65	1.53
4	A	1666	ATP	O3'-C3'	3.87	1.52	1.43
4	A	1666	ATP	C2-N1	3.71	1.40	1.33
4	C	1666	ATP	PA-O2A	3.57	1.71	1.55
4	A	1666	ATP	C6-N6	3.32	1.42	1.34
4	C	1666	ATP	C3'-C4'	-3.24	1.44	1.53
4	A	1666	ATP	PG-O2G	3.23	1.66	1.54
4	C	1666	ATP	PA-O5'	3.15	1.71	1.59
4	A	1667	ATP	PA-O5'	3.14	1.66	1.54
4	B	1666	ATP	C5-C6	3.13	1.49	1.41
4	C	1665	ATP	O4'-C4'	3.03	1.51	1.45
4	B	1665	ATP	PA-O3A	-2.97	1.56	1.59
4	B	1666	ATP	O4'-C1'	2.95	1.48	1.42
4	C	1665	ATP	C5'-C4'	2.79	1.59	1.51
4	A	1666	ATP	O2'-C2'	2.78	1.49	1.43
4	A	1666	ATP	C3'-C4'	2.74	1.59	1.53
4	B	1666	ATP	C5-C4	2.73	1.44	1.39
4	C	1666	ATP	C5-C4	2.72	1.43	1.39
4	B	1665	ATP	C2-N3	2.71	1.38	1.33
4	B	1666	ATP	C1'-N9	2.63	1.53	1.46
4	C	1666	ATP	C8-N9	2.62	1.42	1.37
4	B	1666	ATP	C2-N3	2.50	1.38	1.33
4	A	1666	ATP	C5-N7	2.49	1.43	1.39
4	B	1666	ATP	C6-N6	2.48	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1665	ATP	PB-O1B	2.40	1.59	1.50
4	A	1666	ATP	C8-N7	2.31	1.36	1.31
4	C	1665	ATP	PA-O3A	2.23	1.61	1.59
4	A	1666	ATP	PB-O2B	2.21	1.65	1.55
4	C	1665	ATP	C6-N6	2.03	1.39	1.34

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1665	ATP	O4'-C1'-N9	9.96	127.22	108.09
4	C	1665	ATP	C4-N9-C8	-9.00	96.28	105.74
4	C	1666	ATP	O4'-C1'-N9	7.76	123.00	108.09
4	C	1666	ATP	C2'-C1'-N9	-7.66	94.28	113.30
4	C	1666	ATP	O3'-C3'-C4'	-7.60	89.25	111.08
4	C	1666	ATP	O4'-C4'-C5'	7.32	132.79	109.33
4	C	1665	ATP	N9-C8-N7	6.91	123.75	113.94
4	C	1666	ATP	C4-N9-C8	6.54	112.61	105.74
4	C	1666	ATP	O5'-PA-O1A	-6.36	83.74	108.94
4	C	1666	ATP	O2'-C2'-C1'	-5.95	89.63	110.10
4	C	1666	ATP	C3'-C2'-C1'	5.72	112.28	101.46
4	C	1666	ATP	C4-N9-C1'	-5.66	113.39	126.63
4	C	1666	ATP	O2B-PB-O3A	5.63	122.48	107.27
4	C	1666	ATP	O3'-C3'-C2'	5.46	129.31	111.82
4	B	1666	ATP	C5-C4-N3	-5.45	119.21	126.72
4	A	1666	ATP	C5-N7-C8	5.32	111.82	103.45
4	B	1665	ATP	O2'-C2'-C1'	4.92	127.03	110.10
4	A	1666	ATP	O4'-C4'-C3'	4.90	114.88	105.15
4	A	1666	ATP	C3'-C2'-C1'	4.85	110.64	101.46
4	A	1667	ATP	O2A-PA-O3A	4.81	120.77	104.64
4	C	1666	ATP	C5'-C4'-C3'	-4.73	98.20	115.21
4	A	1666	ATP	C4-C5-N7	-4.63	105.29	110.58
4	C	1665	ATP	C3'-C2'-C1'	4.62	110.20	101.46
4	C	1666	ATP	O2A-PA-O3A	-4.48	95.17	107.27
4	C	1665	ATP	C5-N7-C8	-4.43	96.49	103.45
4	A	1666	ATP	N3-C4-N9	4.41	134.66	127.17
4	C	1666	ATP	O4'-C1'-C2'	-4.31	97.39	106.62
4	A	1666	ATP	C2'-C1'-N9	-4.30	102.62	113.30
4	C	1666	ATP	N3-C2-N1	-4.17	122.27	128.58
4	A	1666	ATP	C5-C4-N3	-4.16	120.98	126.72
4	C	1666	ATP	O2B-PB-O3B	4.12	118.42	107.27
4	C	1666	ATP	O2'-C2'-C3'	-4.08	98.73	111.82
4	C	1666	ATP	C6-C5-C4	-4.08	111.61	117.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1666	ATP	O2G-PG-O3B	-4.05	91.07	104.64
4	C	1665	ATP	C4-C5-N7	4.03	115.19	110.58
4	A	1666	ATP	C4-N9-C8	4.01	109.95	105.74
4	B	1666	ATP	N3-C4-N9	3.95	133.88	127.17
4	C	1665	ATP	O4'-C1'-C2'	-3.82	98.43	106.62
4	A	1666	ATP	N9-C8-N7	-3.80	108.55	113.94
4	A	1667	ATP	O2G-PG-O3B	3.80	117.37	104.64
4	C	1666	ATP	C4'-O4'-C1'	-3.79	101.11	109.47
4	C	1666	ATP	N9-C8-N7	-3.77	108.58	113.94
4	C	1665	ATP	O4'-C4'-C5'	3.72	121.24	109.33
4	B	1666	ATP	C4-N9-C1'	3.70	135.28	126.63
4	B	1665	ATP	O3'-C3'-C4'	3.64	121.55	111.08
4	C	1666	ATP	O3A-PA-O1A	3.59	121.51	110.70
4	B	1666	ATP	C2'-C1'-N9	3.58	122.20	113.30
4	C	1665	ATP	O2A-PA-O3A	3.57	116.93	107.27
4	A	1666	ATP	O4'-C4'-C5'	3.55	120.71	109.33
4	C	1666	ATP	O3G-PG-O3B	3.41	116.06	104.64
4	A	1666	ATP	O2B-PB-O3A	-3.39	98.12	107.27
4	B	1666	ATP	O2'-C2'-C3'	-3.37	101.01	111.82
4	C	1666	ATP	O3G-PG-O2G	3.32	120.23	107.80
4	A	1666	ATP	N6-C6-N1	3.28	125.69	118.38
4	B	1666	ATP	O3G-PG-O3B	3.18	115.31	104.64
4	B	1666	ATP	C5-N7-C8	3.17	108.43	103.45
4	C	1666	ATP	C2'-C3'-C4'	-3.16	96.49	102.61
4	B	1666	ATP	C2'-C3'-C4'	-3.12	96.58	102.61
4	A	1667	ATP	O2G-PG-O1G	-3.10	98.74	110.83
4	B	1665	ATP	O2G-PG-O3B	3.08	114.97	104.64
4	C	1666	ATP	C1'-N9-C8	3.08	133.93	127.09
4	C	1665	ATP	O2G-PG-O3B	3.05	114.87	104.64
4	C	1665	ATP	C4'-O4'-C1'	3.02	116.14	109.47
4	C	1665	ATP	O5'-C5'-C4'	2.97	119.09	108.99
4	B	1666	ATP	C4-C5-N7	-2.94	107.22	110.58
4	B	1666	ATP	O4'-C1'-N9	2.94	113.74	108.09
4	B	1665	ATP	C3'-C2'-C1'	2.90	106.95	101.46
4	A	1666	ATP	C1'-N9-C8	-2.89	120.69	127.09
4	B	1665	ATP	O3G-PG-O3B	2.88	114.29	104.64
4	C	1665	ATP	C1'-N9-C8	2.87	133.47	127.09
4	C	1666	ATP	C6-C5-N7	2.87	137.63	132.09
4	A	1666	ATP	C5-C6-N6	-2.87	116.17	123.29
4	A	1667	ATP	O2A-PA-O1A	-2.84	99.77	110.83
4	A	1666	ATP	O2A-PA-O1A	2.83	125.63	112.44
4	B	1665	ATP	C2'-C3'-C4'	2.81	108.03	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1666	ATP	O3A-PA-O1A	-2.77	102.36	110.70
4	B	1666	ATP	C1'-N9-C8	-2.70	121.11	127.09
4	B	1665	ATP	N3-C4-N9	2.54	131.49	127.17
4	C	1666	ATP	C5-C4-N9	-2.48	103.11	105.81
4	C	1665	ATP	O2A-PA-O1A	-2.35	101.52	112.44
4	B	1666	ATP	O3B-PB-O1B	-2.33	103.71	110.70
4	A	1667	ATP	O5'-PA-O1A	2.31	119.82	110.83
4	A	1666	ATP	C6-C5-C4	2.29	120.31	117.18
4	C	1665	ATP	O5'-PA-O1A	2.28	117.98	108.94
4	C	1665	ATP	O4'-C4'-C3'	-2.27	100.64	105.15
4	A	1666	ATP	O2'-C2'-C3'	2.26	119.07	111.82
4	C	1665	ATP	C2'-C3'-C4'	2.19	106.83	102.61
4	C	1665	ATP	C6-C5-N7	-2.16	127.93	132.09
4	A	1666	ATP	O3A-PB-O1B	2.16	117.19	110.70
4	C	1666	ATP	O2A-PA-O1A	2.15	122.43	112.44
4	B	1665	ATP	C4-N9-C1'	2.10	131.54	126.63
4	C	1666	ATP	O2B-PB-O1B	-2.07	102.84	112.44
4	B	1666	ATP	C4-N9-C8	-2.03	103.60	105.74
4	C	1665	ATP	O3A-PB-O1B	-2.01	104.67	110.70

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1666	ATP	C5'-O5'-PA-O1A
4	A	1666	ATP	C5'-O5'-PA-O2A
4	A	1666	ATP	C5'-O5'-PA-O3A
4	A	1666	ATP	C4'-C5'-O5'-PA
4	B	1666	ATP	C5'-O5'-PA-O2A
4	B	1666	ATP	C5'-O5'-PA-O3A
4	C	1665	ATP	PB-O3B-PG-O2G
4	C	1666	ATP	C4'-C5'-O5'-PA
4	C	1666	ATP	O4'-C1'-N9-C8
4	C	1666	ATP	O4'-C1'-N9-C4
4	C	1665	ATP	C3'-C4'-C5'-O5'
4	A	1666	ATP	O4'-C4'-C5'-O5'
4	C	1665	ATP	O4'-C4'-C5'-O5'
4	A	1666	ATP	O4'-C1'-N9-C4
4	A	1666	ATP	C3'-C4'-C5'-O5'
4	C	1666	ATP	C3'-C4'-C5'-O5'
4	B	1665	ATP	PB-O3B-PG-O3G
4	A	1666	ATP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

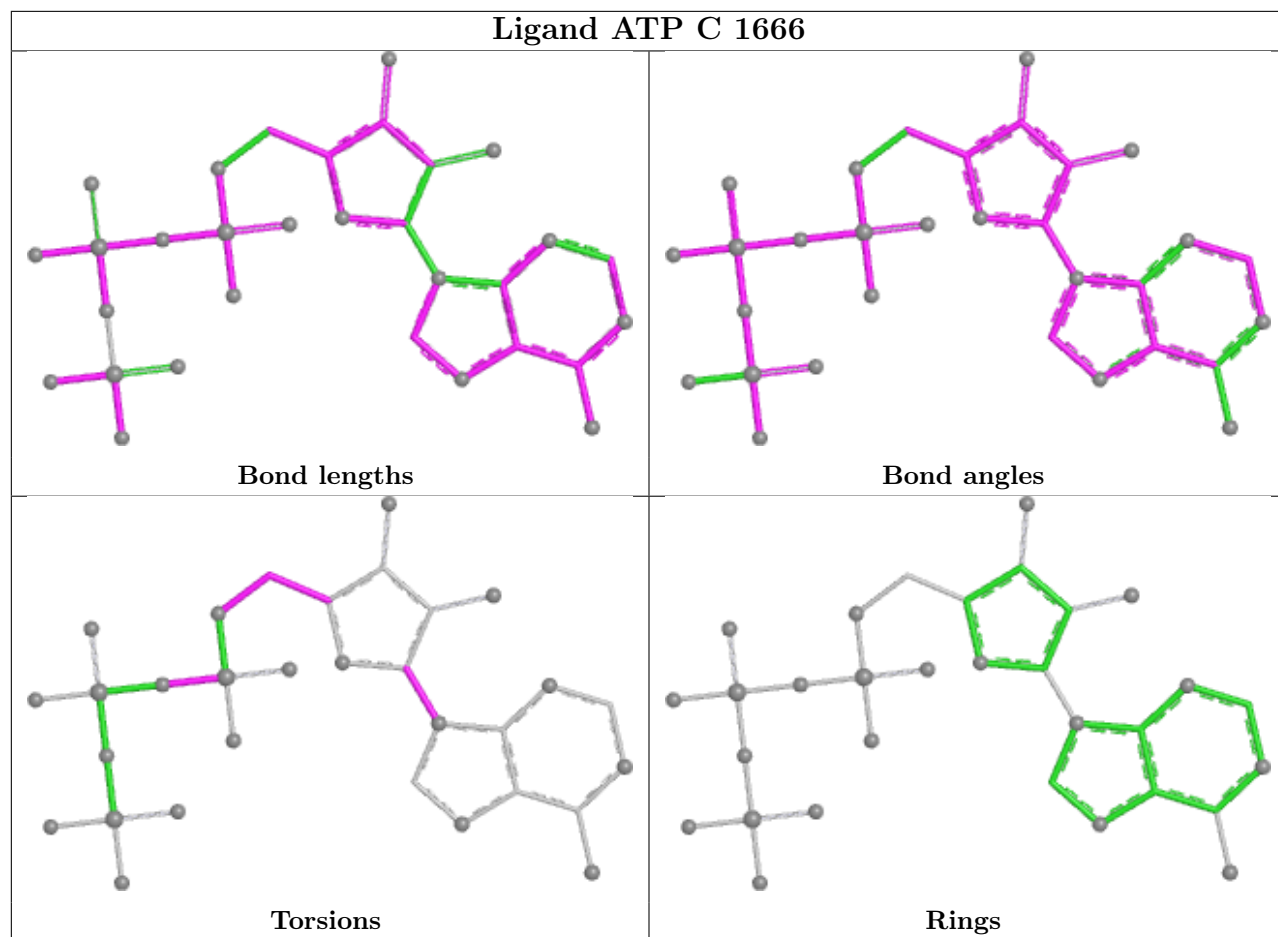
Mol	Chain	Res	Type	Atoms
4	B	1666	ATP	C5'-O5'-PA-O1A
4	B	1665	ATP	PA-O3A-PB-O2B
4	B	1666	ATP	C4'-C5'-O5'-PA
4	C	1665	ATP	PB-O3B-PG-O1G
4	A	1667	ATP	PB-O3A-PA-O2A
4	C	1665	ATP	PB-O3B-PG-O3G
4	B	1665	ATP	PA-O3A-PB-O1B
4	C	1666	ATP	O4'-C4'-C5'-O5'
4	A	1667	ATP	PG-O3B-PB-O2B
4	C	1666	ATP	PB-O3A-PA-O2A
4	B	1666	ATP	O4'-C4'-C5'-O5'

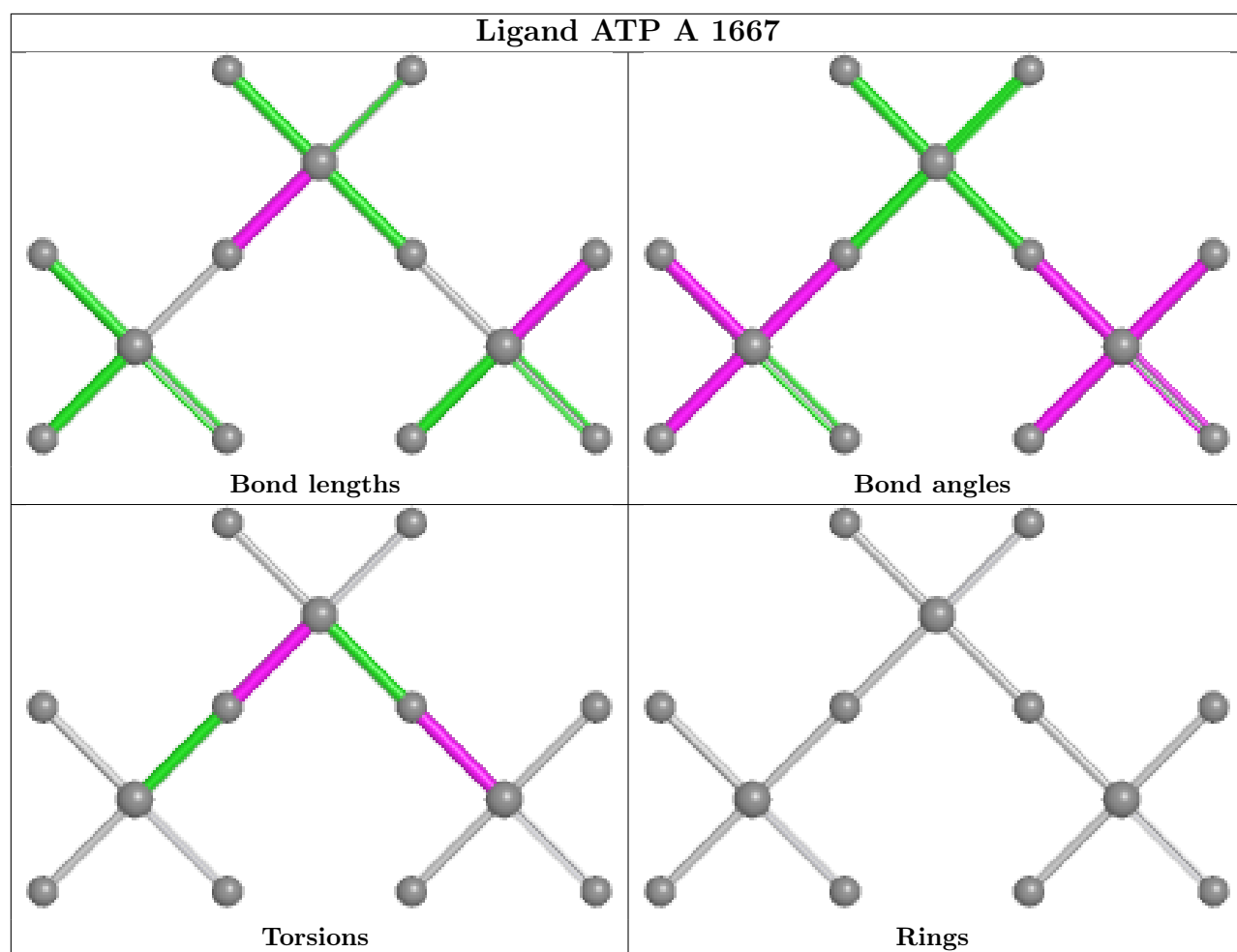
There are no ring outliers.

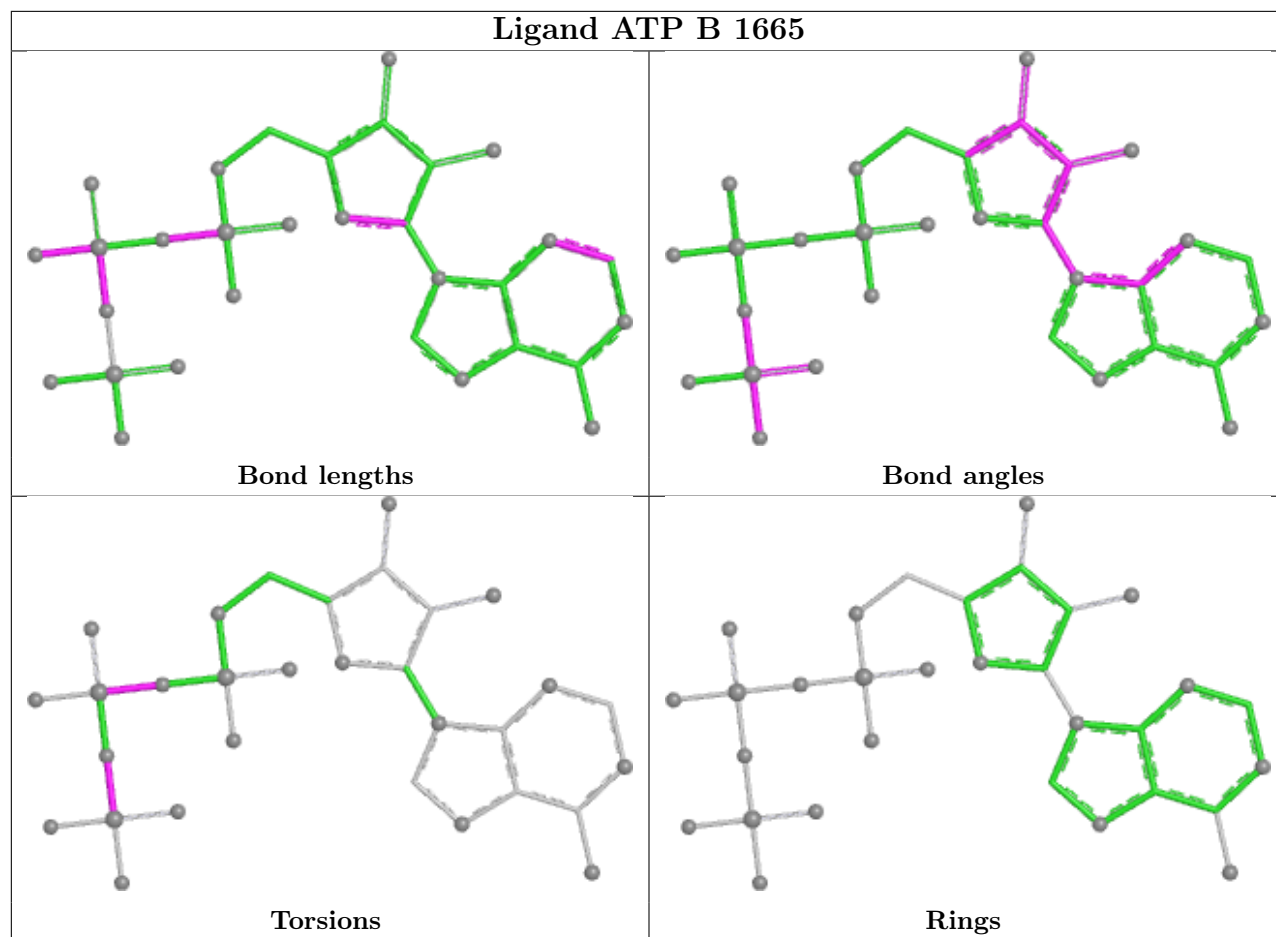
6 monomers are involved in 36 short contacts:

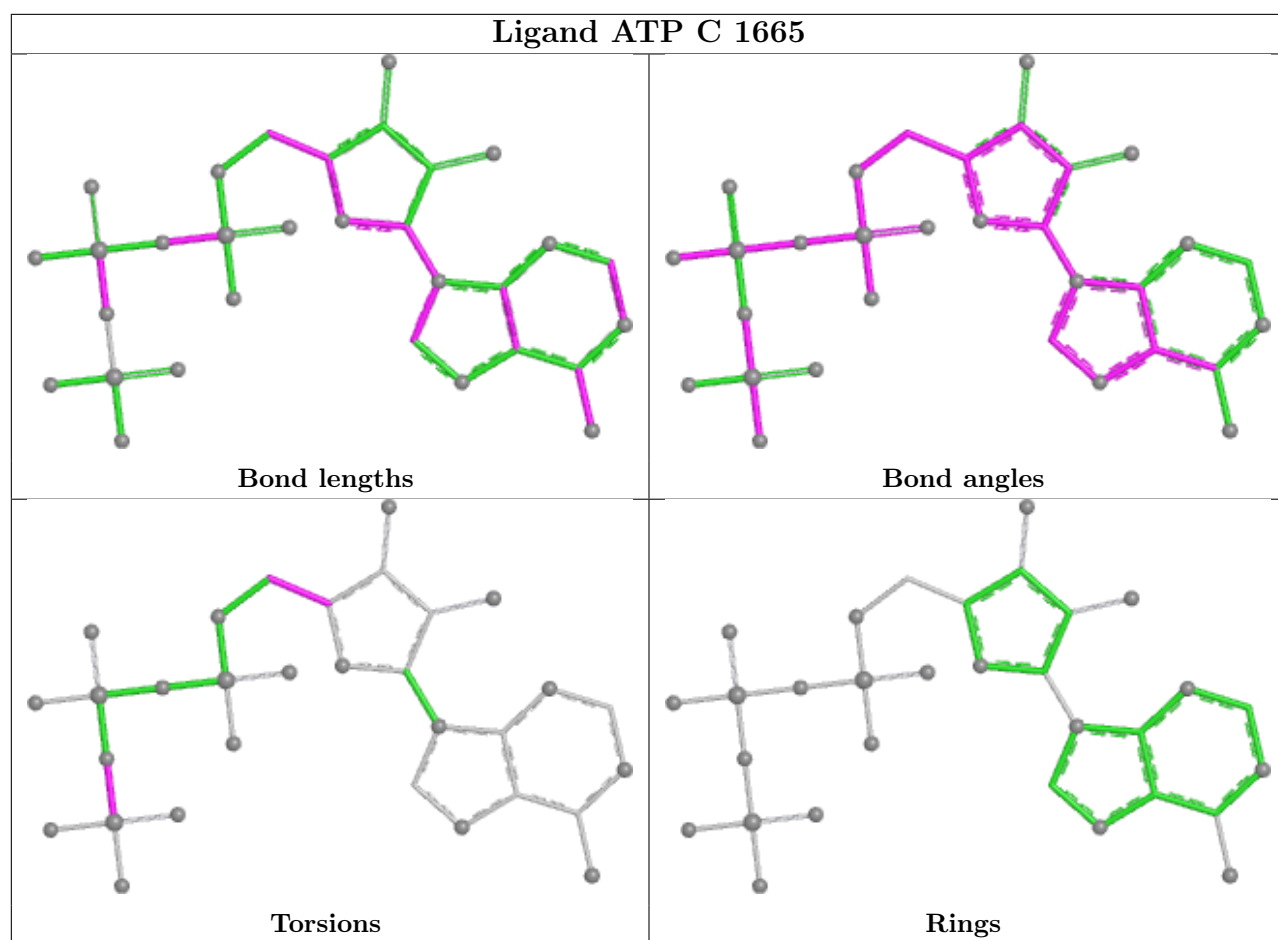
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1666	ATP	24	0
4	A	1667	ATP	2	0
4	B	1665	ATP	2	0
4	C	1665	ATP	8	0
4	B	1666	ATP	7	0
4	A	1666	ATP	1	0

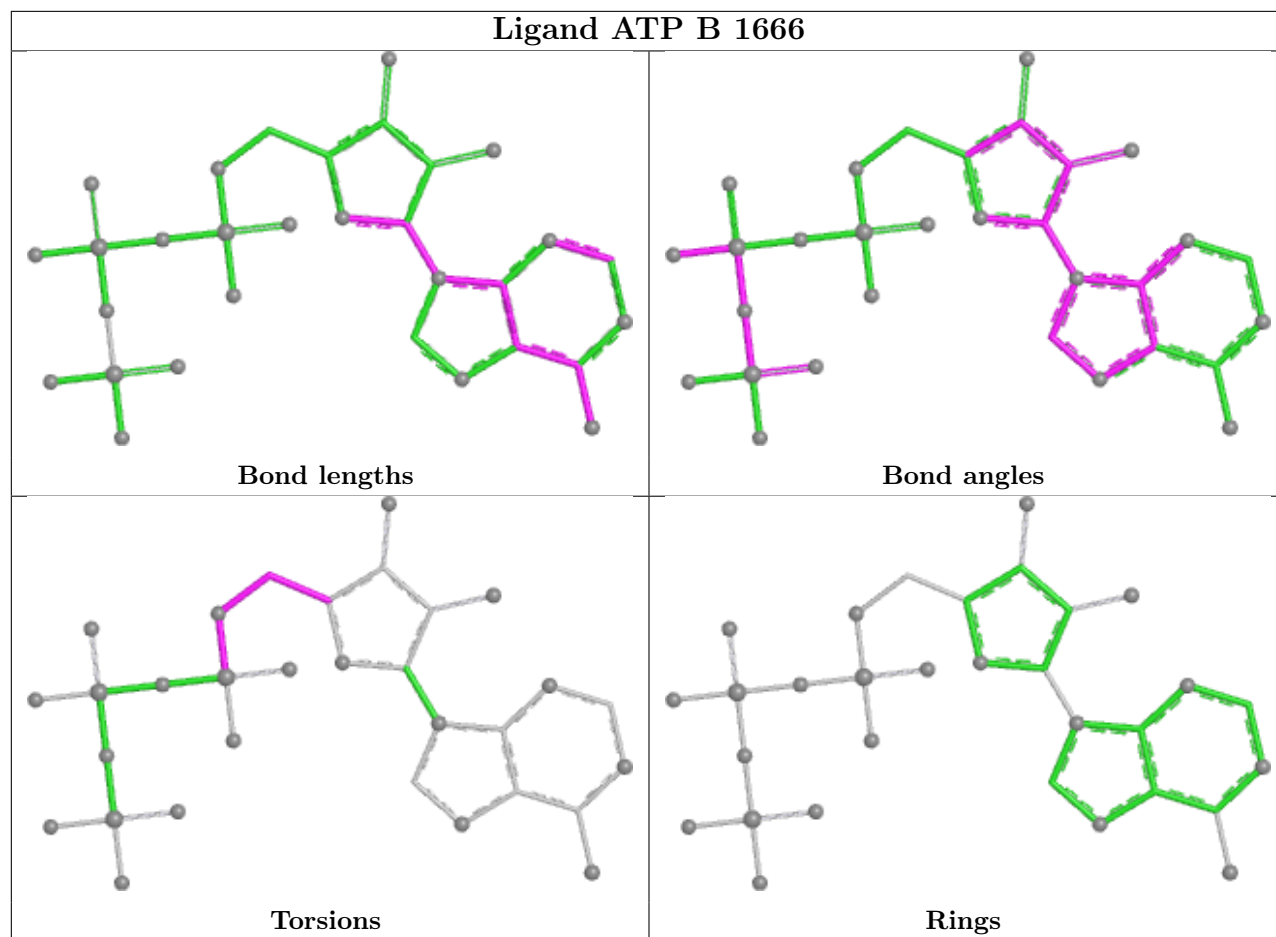
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

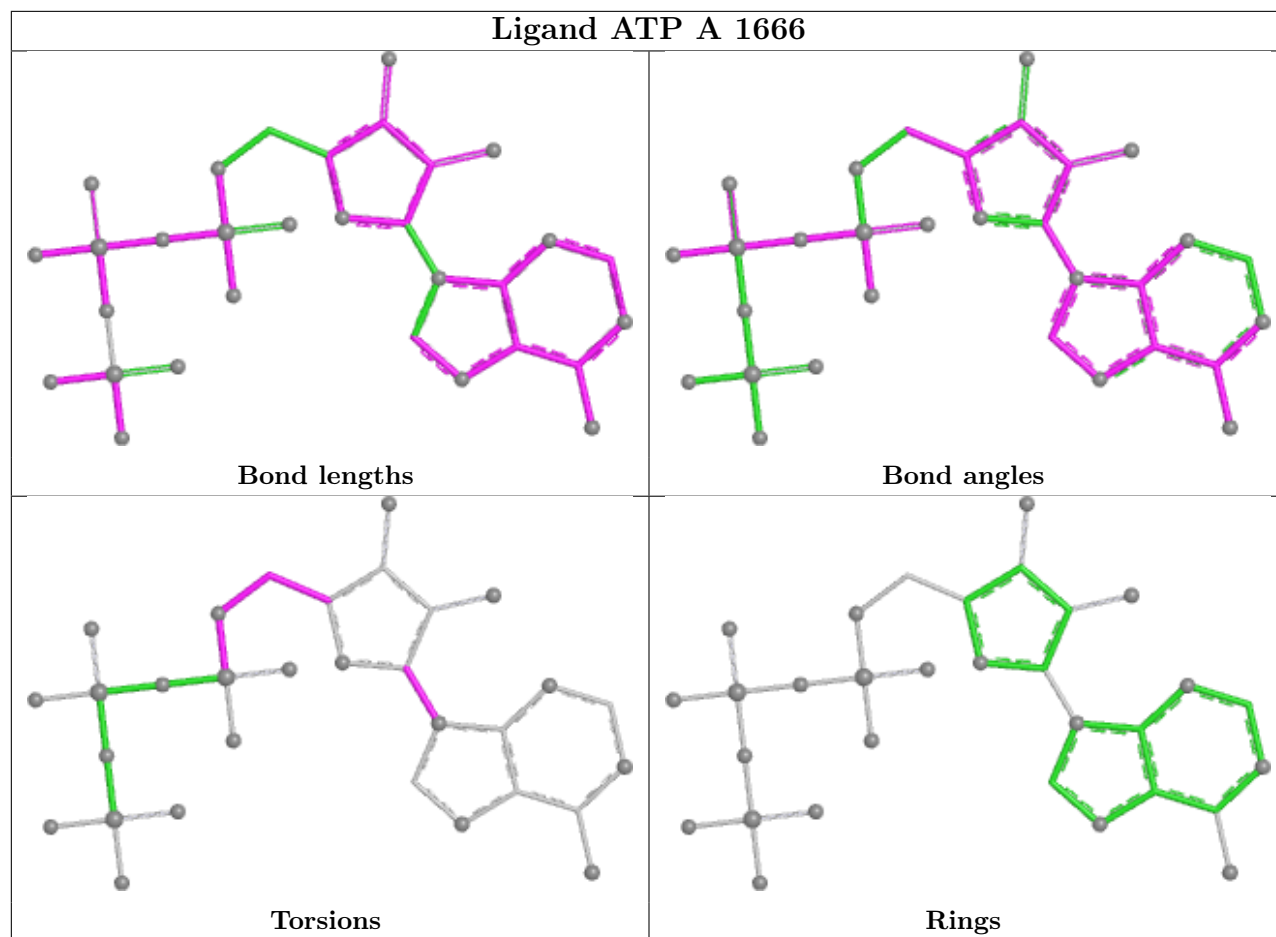












5.7 Other polymers [i](#)

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	664/665 (99%)	0.26	6 (0%) 81 65	41, 73, 109, 140	0
1	B	664/665 (99%)	0.21	9 (1%) 73 55	43, 69, 101, 149	0
1	C	664/665 (99%)	0.18	9 (1%) 73 55	38, 69, 104, 180	1 (0%)
2	G	4/4 (100%)	3.19	3 (75%) 0 0	171, 186, 187, 192	0
All	All	1996/1999 (99%)	0.22	27 (1%) 73 55	38, 70, 106, 192	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	7	DG	4.0
2	G	6	DC	3.8
2	G	4	DA	3.0
1	B	607	ARG	2.7
1	B	606	ALA	2.6
1	B	608	GLN	2.5
1	C	492	HIS	2.5
1	A	44	LEU	2.4
1	C	609	ALA	2.4
1	C	610	GLY	2.4
1	B	269	ARG	2.3
1	C	612	ALA	2.3
1	A	492	HIS	2.3
1	A	530	TYR	2.2
1	C	608	GLN	2.2
1	A	425	ARG	2.2
1	A	328	HIS	2.2
1	B	452	SER	2.2
1	B	609	ALA	2.1
1	C	1	PRO	2.1
1	C	632	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	492	HIS	2.1
1	C	611	LEU	2.1
1	C	646	MET	2.0
1	B	603	ALA	2.0
1	B	537	ARG	2.0
1	A	566	ASP	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](#)

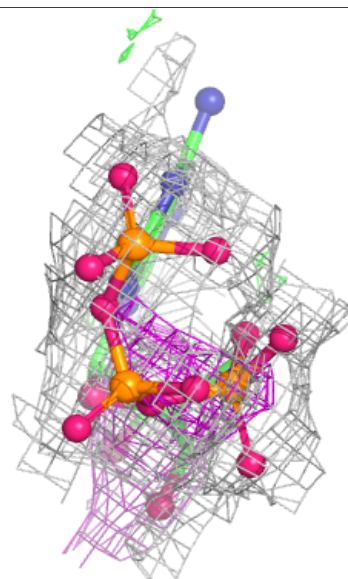
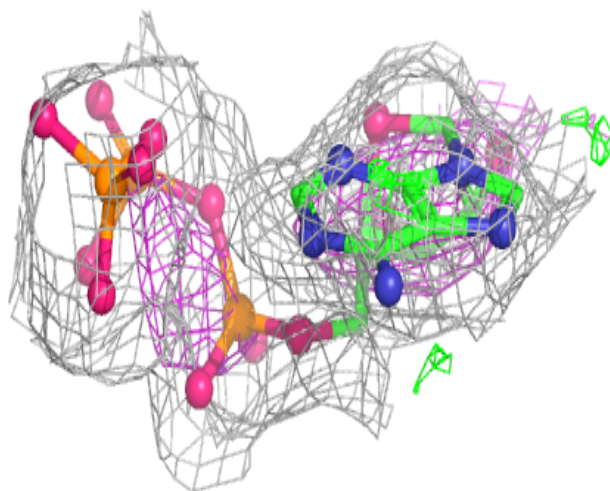
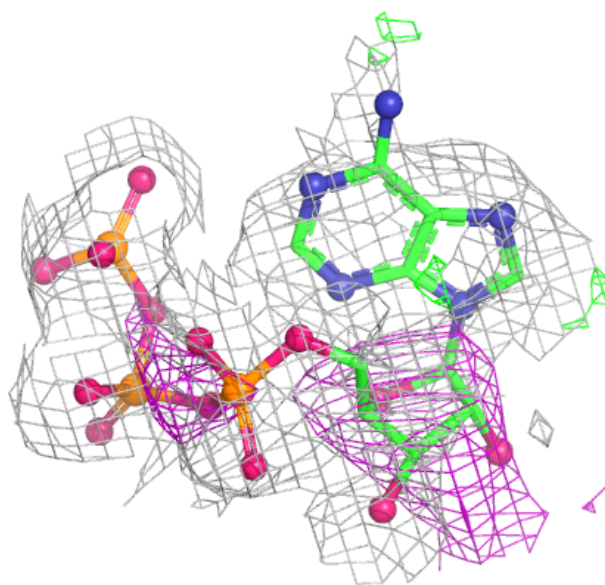
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ATP	C	1666	31/31	0.39	0.16	94,106,122,125	0
4	ATP	A	1666	31/31	0.43	0.17	89,104,131,133	0
4	ATP	A	1667	13/31	0.48	0.12	167,171,179,180	0
3	MG	A	1665[B]	1/1	0.61	0.32	57,57,57,57	1
4	ATP	B	1666	31/31	0.61	0.15	170,172,179,180	0
3	MG	A	1665[A]	1/1	0.61	0.32	29,29,29,29	1
4	ATP	B	1665	31/31	0.64	0.16	172,174,191,193	0
4	ATP	C	1665	31/31	0.65	0.16	176,178,179,181	0
3	MG	B	1667	1/1	0.81	0.14	49,49,49,49	0
3	MG	C	1667	1/1	0.92	0.12	56,56,56,56	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.

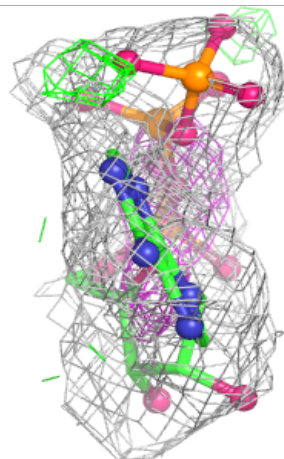
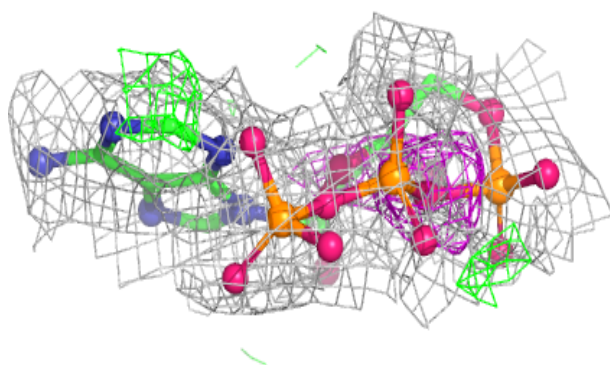
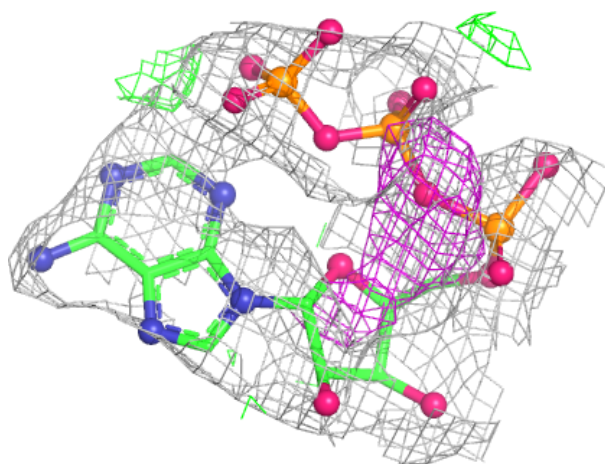
Electron density around ATP C 1666:

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



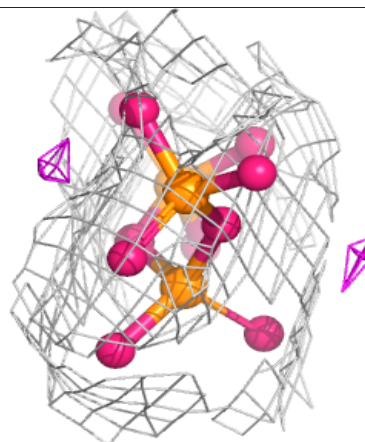
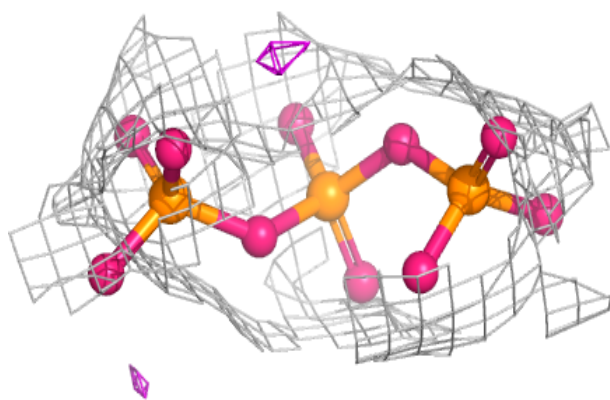
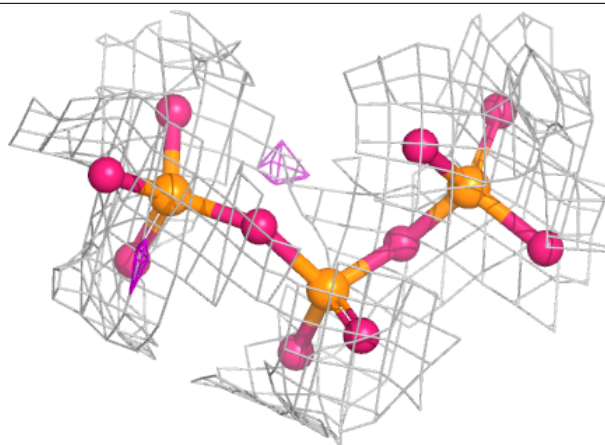
Electron density around ATP A 1666:

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

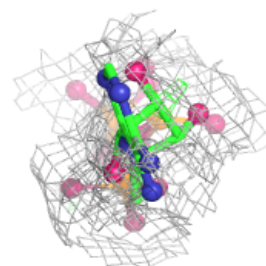
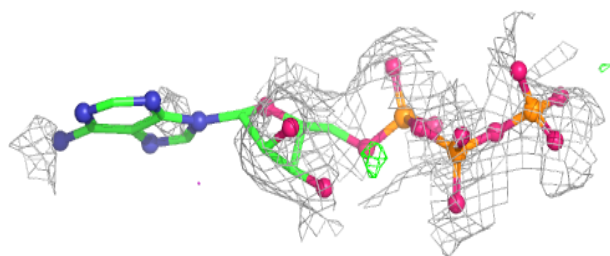
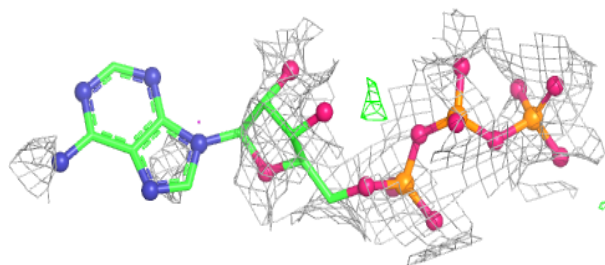


Electron density around ATP A 1667:

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

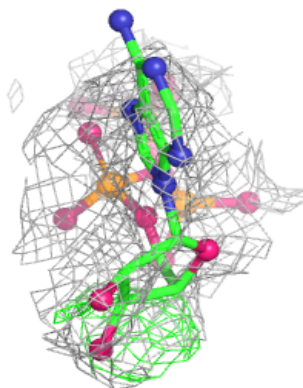
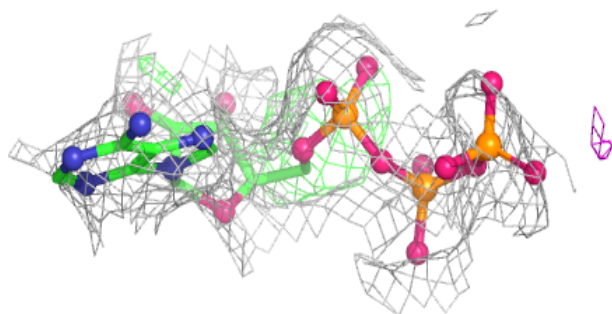
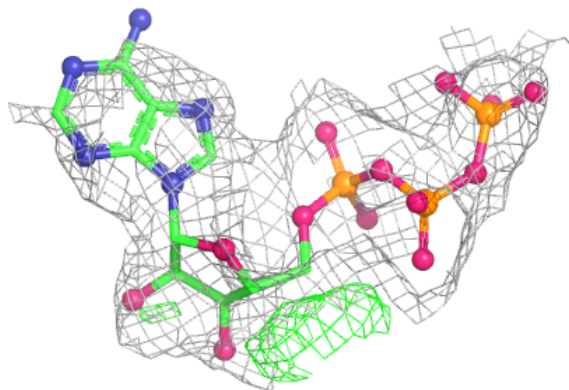
**Electron density around ATP B 1666:**

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

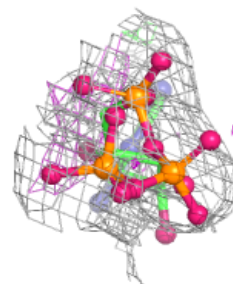
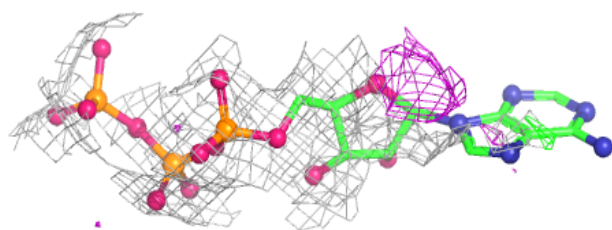
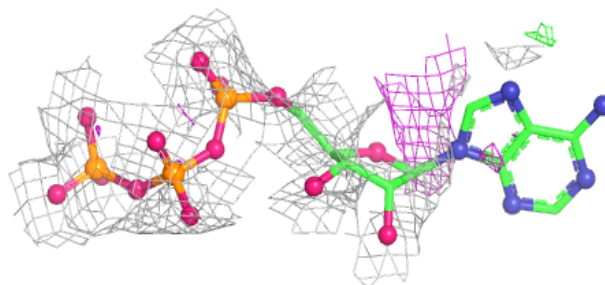


Electron density around ATP B 1665:

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

**Electron density around ATP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.