



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:06 PM UTC

PDB ID : 3A7H / pdb_00003a7h
Title : Human MST3 kinase in complex with ATP
Authors : Ko, T.P.; Jeng, W.Y.; Liu, C.I.; Lai, M.D.; Wang, A.H.J.
Deposited on : 2009-09-26
Resolution : 1.96 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

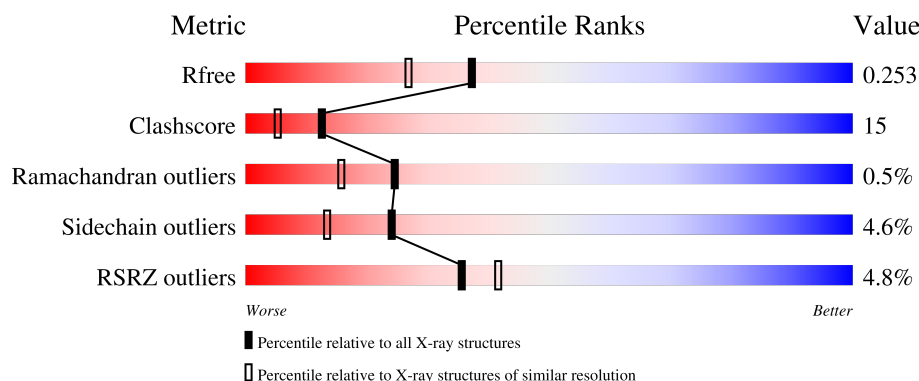
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	303	6% 62% 30% . .
1	B	303	4% 72% 20% . .

2 Entry composition [i](#)

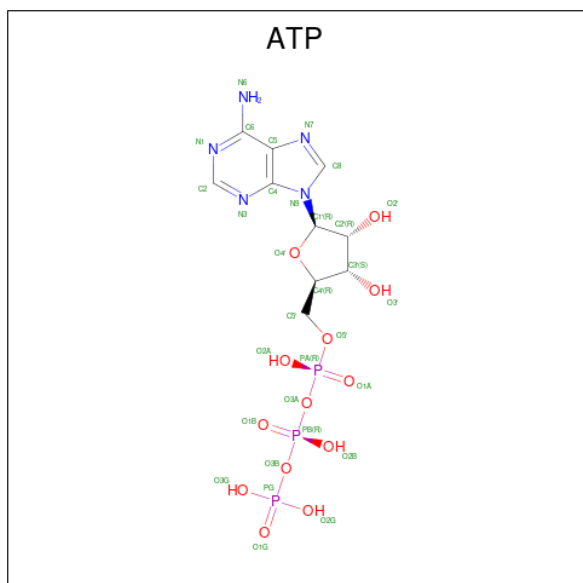
There are 3 unique types of molecules in this entry. The entry contains 5174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine/threonine kinase 24 (STE20 homolog, yeast).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	P	S	0	0	0
			2319	1490	382	440	1	6			
1	B	291	Total	C	N	O	P	S	0	0	0
			2325	1493	383	442	1	6			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

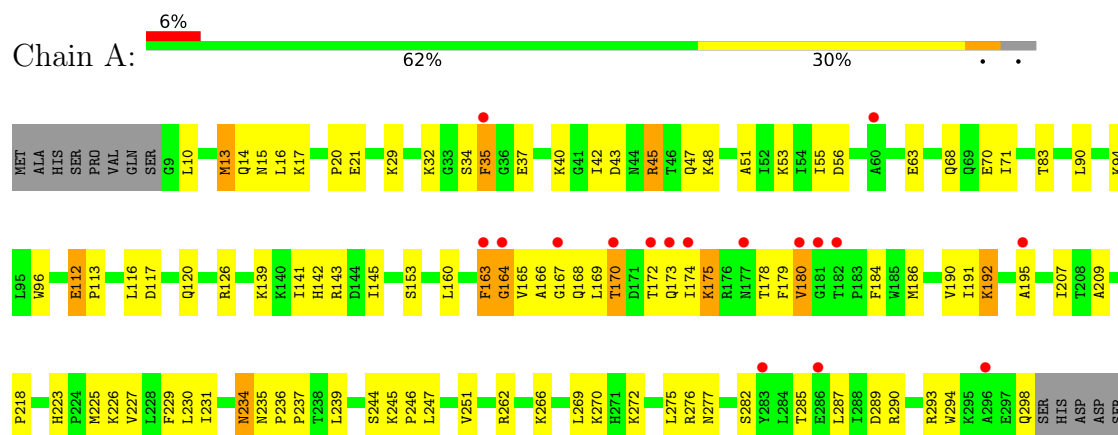
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total 247	O 247	0	0
3	B	229	Total 229	O 229	0	0

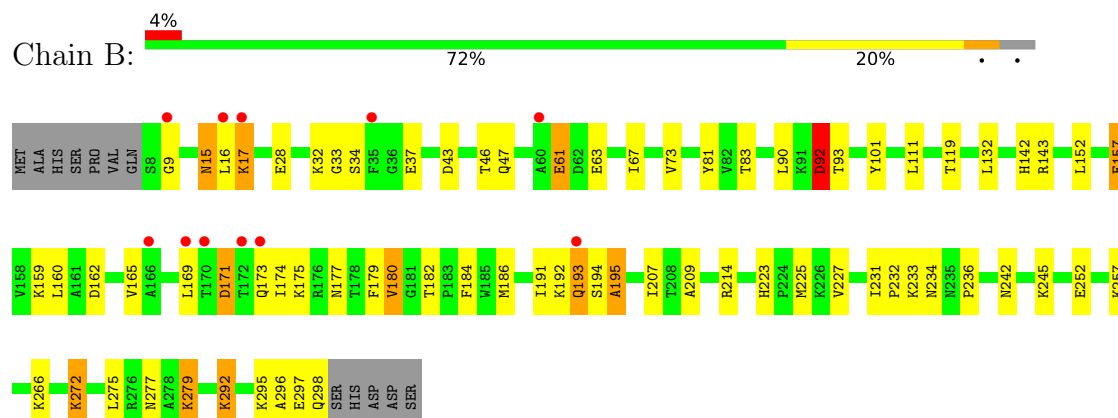
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine kinase 24 (STE20 homolog, yeast)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.68Å 95.19Å 61.48Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	20.00 – 1.96 20.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-1.96) 96.1 (20.00-1.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.252 0.204 , 0.253	Depositor DCC
R_{free} test set	2198 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 56.6	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	0.95	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: TPO, 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	1.07	5/2356 (0.2%)	1.22	15/3181 (0.5%)
1	B	1.07	1/2362 (0.0%)	1.18	15/3189 (0.5%)
All	All	1.07	6/4718 (0.1%)	1.20	30/6370 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ILE	CA-CB	6.57	1.57	1.54
1	B	73	VAL	CA-CB	6.36	1.62	1.54
1	A	251	VAL	CA-CB	6.26	1.62	1.54
1	A	145	ILE	CA-C	5.42	1.58	1.52
1	A	126	ARG	C-O	-5.38	1.18	1.24
1	A	209	ALA	CA-CB	5.29	1.61	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	GLU	N-CA-C	8.91	123.06	110.50
1	B	194	SER	N-CA-C	-8.28	99.37	110.55
1	A	262	ARG	CA-C-N	7.14	127.10	120.03
1	A	262	ARG	C-N-CA	7.14	127.10	120.03
1	A	112	GLU	CA-C-N	6.66	126.11	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLU	C-N-CA	6.66	126.11	118.85
1	B	233	LYS	N-CA-C	6.63	118.30	111.14
1	A	277	ASN	N-CA-C	6.55	121.94	113.88
1	A	163	PHE	O-C-N	6.41	128.95	122.03
1	B	43	ASP	N-CA-C	-6.41	99.45	109.25
1	B	171	ASP	N-CA-C	6.38	118.76	111.11
1	A	35	PHE	N-CA-C	6.33	117.84	111.07
1	B	92	ASP	CB-CA-C	-6.22	109.41	116.63
1	A	43	ASP	N-CA-C	-6.18	98.47	108.41
1	A	235	ASN	N-CA-C	-6.16	101.34	110.20
1	B	207	ILE	N-CA-C	-6.12	104.54	110.72
1	B	195	ALA	N-CA-C	-5.98	101.44	110.28
1	B	234	ASN	N-CA-C	5.90	118.51	110.55
1	A	40	LYS	N-CA-C	-5.84	99.73	109.24
1	B	9	GLY	N-CA-C	5.78	117.93	112.04
1	A	234	ASN	N-CA-C	5.72	118.08	110.53
1	A	163	PHE	N-CA-C	-5.59	104.82	111.03
1	A	51	ALA	N-CA-C	-5.56	100.64	109.76
1	B	209	ALA	N-CA-C	-5.42	105.29	111.14
1	B	182	THR	CA-C-N	5.34	126.52	119.84
1	B	182	THR	C-N-CA	5.34	126.52	119.84
1	A	153	SER	N-CA-C	-5.17	103.86	110.53
1	A	42	ILE	CB-CA-C	-5.14	102.58	110.50
1	B	111	LEU	N-CA-C	-5.12	106.54	112.89
1	B	162	ASP	N-CA-C	5.10	116.88	110.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	81	TYR	Sidechain

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	2319	0	2355	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2325	0	2360	66	0
2	A	27	0	12	0	0
2	B	27	0	12	3	0
3	A	247	0	0	7	0
3	B	229	0	0	10	0
All	All	5174	0	4739	144	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 15.

All (144) 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:177:ASN:O	1:B:193:GLN:HG3	1.56	1.05
1:A:143:ARG:HD3	1:A:165:VAL:O	1.69	0.92
1:B:298:GLN:HA	3:B:411:HOH:O	1.70	0.90
1:B:192:LYS:HE2	3:B:394:HOH:O	1.75	0.86
1:A:223:HIS:HD2	1:A:225:MET:H	1.24	0.85
1:B:33:GLY:HA3	2:B:400:ATP:O1A	1.84	0.77
1:A:16:LEU:HD21	3:A:310:HOH:O	1.86	0.76
1:A:143:ARG:HD2	1:A:167:GLY:N	2.01	0.75
1:B:179:PHE:CE2	1:B:186:MET:HE1	2.22	0.75
1:B:15:ASN:HD22	1:B:17:LYS:H	1.33	0.75
1:A:53:LYS:HE2	1:A:55:ILE:HD11	1.69	0.73
2:B:400:ATP:H3'	3:B:434:HOH:O	1.87	0.73
1:B:17:LYS:HE3	1:B:17:LYS:HA	1.67	0.73
1:B:184:PHE:CE2	1:B:227:VAL:HG21	2.24	0.73
1:B:16:LEU:HD11	1:B:90:LEU:HB3	1.70	0.73
1:A:35:PHE:HB3	1:A:55:ILE:HD13	1.71	0.72
1:B:295:LYS:HG2	3:B:427:HOH:O	1.89	0.72
1:A:141:ILE:HD11	1:A:169:LEU:HD21	1.73	0.71
1:B:223:HIS:CD2	1:B:225:MET:H	2.10	0.70
1:B:179:PHE:HE2	1:B:186:MET:HE1	1.57	0.68
1:B:165:VAL:HB	1:B:180:VAL:HG21	1.76	0.68
1:B:296:ALA:O	1:B:297:GLU:HG3	1.94	0.68
1:A:282:SER:O	1:A:285:THR:HG23	1.93	0.68
1:A:223:HIS:CD2	1:A:225:MET:H	2.11	0.68
1:B:184:PHE:CD1	3:B:518:HOH:O	2.47	0.67
1:A:175:LYS:HG3	1:A:195:ALA:HB1	1.75	0.67
1:B:223:HIS:HD2	1:B:225:MET:H	1.42	0.66
1:B:32:LYS:O	1:B:32:LYS:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:O	1:B:143:ARG:HB2	1.97	0.64
1:A:270:LYS:HE2	3:A:541:HOH:O	1.97	0.64
1:A:175:LYS:N	1:A:175:LYS:HD3	2.14	0.63
1:B:193:GLN:HG2	1:B:193:GLN:O	2.00	0.62
1:A:21:GLU:HG3	1:A:96:TRP:CZ2	2.35	0.62
1:B:119:THR:HG21	1:B:279:LYS:HD3	1.81	0.62
1:A:163:PHE:HB3	1:A:166:ALA:HB2	1.83	0.61
1:B:15:ASN:ND2	1:B:17:LYS:H	1.96	0.61
1:B:177:ASN:HB3	1:B:193:GLN:CG	2.30	0.61
1:B:17:LYS:HA	1:B:17:LYS:CE	2.30	0.60
1:A:186:MET:HE3	1:A:190:VAL:HG12	1.83	0.60
1:B:119:THR:CG2	1:B:279:LYS:HD3	2.32	0.60
1:A:172:THR:O	1:A:173:GLN:HG3	2.00	0.60
1:B:143:ARG:HD3	1:B:165:VAL:O	2.03	0.59
1:A:186:MET:HE2	1:A:191:ILE:HG13	1.85	0.57
1:B:277:ASN:ND2	3:B:338:HOH:O	2.35	0.57
1:A:143:ARG:NH1	1:A:178:TPO:O1P	2.37	0.57
1:A:113:PRO:HB2	1:A:290:ARG:NE	2.19	0.57
1:B:177:ASN:HB3	1:B:193:GLN:CD	2.30	0.57
1:A:175:LYS:HD3	1:A:175:LYS:H	1.70	0.56
1:B:15:ASN:HD22	1:B:15:ASN:C	2.13	0.56
1:A:10:LEU:O	1:A:13:MET:HB2	2.05	0.56
1:A:289:ASP:O	1:A:293:ARG:HG3	2.06	0.56
1:A:116:LEU:HD22	1:A:287:LEU:HD21	1.87	0.55
1:B:193:GLN:O	1:B:193:GLN:CG	2.53	0.55
1:A:117:ASP:OD2	1:A:120:GLN:HG3	2.06	0.55
3:A:332:HOH:O	1:B:242:ASN:HB2	2.07	0.55
1:A:16:LEU:CD2	3:A:310:HOH:O	2.49	0.54
1:A:163:PHE:O	1:A:165:VAL:N	2.31	0.54
1:B:223:HIS:CD2	1:B:225:MET:HB2	2.42	0.54
1:A:165:VAL:HB	1:A:180:VAL:HG11	1.90	0.54
1:A:175:LYS:CG	1:A:195:ALA:HB1	2.38	0.54
1:B:32:LYS:HD2	3:B:476:HOH:O	2.07	0.54
1:A:16:LEU:HD23	1:A:90:LEU:HB3	1.90	0.54
1:A:230:LEU:HD22	1:A:234:ASN:HD21	1.72	0.54
1:A:32:LYS:HG2	1:A:37:GLU:HG2	1.90	0.53
1:B:227:VAL:HG12	1:B:231:ILE:CD1	2.39	0.53
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.73	0.52
1:A:143:ARG:HH12	1:A:178:TPO:P	2.33	0.52
1:A:112:GLU:HB2	1:A:113:PRO:HD3	1.92	0.51
1:A:48:LYS:HG3	3:A:330:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:C	1:A:165:VAL:H	2.18	0.51
1:A:174:ILE:HG22	1:A:174:ILE:O	2.09	0.51
1:A:163:PHE:HB3	1:A:166:ALA:CB	2.40	0.51
1:A:174:ILE:O	1:A:174:ILE:CG2	2.58	0.51
1:A:272:LYS:HD2	1:A:276:ARG:NH1	2.25	0.51
1:A:245:LYS:HB3	1:A:246:PRO:HD3	1.93	0.51
1:B:165:VAL:HB	1:B:180:VAL:CG2	2.40	0.51
1:B:186:MET:HE2	1:B:191:ILE:HG13	1.93	0.51
1:B:227:VAL:HG12	1:B:231:ILE:HD11	1.93	0.51
1:A:168:GLN:HG3	1:A:170:THR:HG23	1.92	0.51
1:A:47:GLN:HB3	1:B:245:LYS:HB2	1.93	0.50
1:B:236:PRO:HD3	1:B:257:LYS:HG2	1.93	0.50
1:B:63:GLU:H	1:B:63:GLU:CD	2.17	0.50
1:A:15:ASN:OD1	1:A:17:LYS:HB3	2.12	0.49
1:B:223:HIS:HD2	1:B:225:MET:N	2.09	0.49
1:A:56:ASP:OD2	1:A:94:LYS:HE3	2.11	0.49
1:B:63:GLU:O	1:B:67:ILE:HG13	2.11	0.49
1:A:20:PRO:HB2	1:A:96:TRP:CE3	2.47	0.49
1:A:230:LEU:HD22	1:A:234:ASN:ND2	2.28	0.49
1:A:142:HIS:O	1:A:143:ARG:HB2	2.13	0.49
1:B:83:THR:HG23	1:B:160:LEU:O	2.13	0.49
1:A:143:ARG:HD2	1:A:167:GLY:H	1.76	0.49
1:B:292:LYS:HE2	3:B:428:HOH:O	2.13	0.48
1:A:29:LYS:NZ	3:A:317:HOH:O	2.47	0.48
1:A:165:VAL:HB	1:A:180:VAL:CG1	2.44	0.48
1:A:13:MET:HE2	1:A:14:GLN:H	1.79	0.47
1:B:15:ASN:ND2	1:B:17:LYS:HB2	2.30	0.47
1:B:223:HIS:HD2	1:B:225:MET:HB2	1.79	0.47
1:B:101:TYR:OH	3:B:424:HOH:O	2.20	0.46
1:B:272:LYS:NZ	3:B:440:HOH:O	2.47	0.46
1:A:48:LYS:CG	3:A:330:HOH:O	2.64	0.46
1:B:175:LYS:CB	1:B:195:ALA:HB1	2.46	0.46
1:B:46:THR:O	1:B:47:GLN:HB2	2.16	0.45
1:A:10:LEU:HD11	1:A:71:ILE:HD12	1.96	0.45
1:A:83:THR:HG23	1:A:160:LEU:O	2.16	0.45
1:B:63:GLU:OE2	1:B:63:GLU:N	2.32	0.45
1:A:139:LYS:HA	1:A:139:LYS:HD3	1.80	0.44
1:A:10:LEU:HD11	1:A:71:ILE:HB	1.99	0.44
1:B:231:ILE:HB	1:B:232:PRO:HD3	1.99	0.44
1:A:45:ARG:HH11	1:A:45:ARG:HG3	1.83	0.44
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:N	1:A:175:LYS:CD	2.80	0.43
1:B:174:ILE:O	1:B:175:LYS:HG2	2.19	0.43
1:A:207:ILE:HG23	1:A:218:PRO:HD2	2.01	0.43
1:A:163:PHE:N	1:A:163:PHE:CD2	2.86	0.43
1:B:119:THR:HG23	1:B:277:ASN:O	2.19	0.43
1:A:10:LEU:HB3	1:A:13:MET:HG3	2.01	0.43
1:A:294:TRP:O	1:A:298:GLN:HG2	2.19	0.42
1:B:15:ASN:HD22	1:B:16:LEU:N	2.17	0.42
1:B:184:PHE:HE2	1:B:227:VAL:HG21	1.79	0.42
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.76	0.42
1:A:13:MET:HE2	1:A:14:GLN:N	2.34	0.42
1:A:184:PHE:CE2	1:A:227:VAL:HG21	2.54	0.42
1:B:61:GLU:N	1:B:63:GLU:OE2	2.34	0.42
1:A:266:LYS:O	1:A:269:LEU:HB2	2.20	0.42
1:A:245:LYS:N	1:A:246:PRO:CD	2.83	0.42
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.74	0.41
1:A:244:SER:HB2	1:A:246:PRO:HD2	2.02	0.41
1:A:239:LEU:CD2	1:A:247:LEU:HG	2.50	0.41
1:A:163:PHE:C	1:A:165:VAL:N	2.77	0.41
1:B:92:ASP:HB3	1:B:93:THR:H	1.57	0.41
1:A:63:GLU:N	1:A:63:GLU:CD	2.78	0.41
1:A:112:GLU:CB	1:A:113:PRO:HD3	2.49	0.41
1:A:178:TPO:HG23	1:A:180:VAL:HG23	2.03	0.41
1:B:33:GLY:HA3	2:B:400:ATP:PA	2.61	0.41
1:B:142:HIS:O	1:B:143:ARG:CB	2.63	0.41
1:B:169:LEU:HD22	1:B:174:ILE:O	2.20	0.41
1:A:226:LYS:HA	1:A:229:PHE:CE2	2.56	0.40
1:B:152:LEU:HA	1:B:157:GLU:O	2.21	0.40
1:B:179:PHE:CD2	1:B:186:MET:HE1	2.55	0.40
1:A:70:GLU:HB2	1:A:164:GLY:HA2	2.04	0.40
1:A:236:PRO:HA	1:A:237:PRO:HD3	1.96	0.40
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.89	0.40
1:B:296:ALA:C	1:B:297:GLU:HG3	2.46	0.40
1:A:179:PHE:CE1	1:A:186:MET:HE1	2.57	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	287/303 (95%)	273 (95%)	13 (4%)	1 (0%)	36	28
1	B	288/303 (95%)	269 (93%)	17 (6%)	2 (1%)	18	10
All	All	575/606 (95%)	542 (94%)	30 (5%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	GLY
1	B	61	GLU
1	B	193	GLN

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	252/264 (96%)	244 (97%)	8 (3%)	34	25
1	B	253/264 (96%)	238 (94%)	15 (6%)	18	7
All	All	505/528 (96%)	482 (95%)	23 (5%)	24	13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	34	SER
1	A	45	ARG

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	170	THR
1	A	175	LYS
1	A	180	VAL
1	A	192	LYS
1	B	15	ASN
1	B	17	LYS
1	B	34	SER
1	B	37	GLU
1	B	92	ASP
1	B	157	GLU
1	B	159	LYS
1	B	171	ASP
1	B	173	GLN
1	B	180	VAL
1	B	252	GLU
1	B	266	LYS
1	B	272	LYS
1	B	279	LYS
1	B	292	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	173	GLN
1	A	177	ASN
1	A	193	GLN
1	A	223	HIS
1	A	234	ASN
1	A	277	ASN
1	B	15	ASN
1	B	223	HIS
1	B	277	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	TPO	B	178	1	8,10,11	0.77	0	10,14,16	0.69	0
1	TPO	A	178	1	8,10,11	0.97	0	10,14,16	0.84	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
1	TPO	B	178	1	-	1/9/11/13	-
1	TPO	A	178	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	178	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	178	TPO	3	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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
2	ATP	A	400	-	28,29,33	1.83	9 (32%)	43,45,52	1.98	13 (30%)
2	ATP	B	400	-	28,29,33	2.11	11 (39%)	43,45,52	1.70	11 (25%)

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
2	ATP	A	400	-	-	7/16/32/38	0/3/3/3
2	ATP	B	400	-	-	5/16/32/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ATP	PA-O3A	4.75	1.64	1.59
2	B	400	ATP	PB-O3B	3.91	1.69	1.54
2	A	400	ATP	C1'-N9	3.75	1.56	1.46
2	B	400	ATP	C1'-N9	3.61	1.56	1.46
2	A	400	ATP	PB-O3B	3.44	1.67	1.54
2	B	400	ATP	C3'-C4'	3.34	1.61	1.53
2	B	400	ATP	O4'-C4'	-3.04	1.38	1.45
2	A	400	ATP	PB-O2B	-2.97	1.43	1.54
2	B	400	ATP	C4-N3	2.89	1.39	1.34
2	B	400	ATP	C8-N9	2.85	1.42	1.37
2	A	400	ATP	C4-N3	2.79	1.39	1.34
2	A	400	ATP	C8-N9	2.77	1.42	1.37
2	A	400	ATP	PA-O3A	2.69	1.62	1.59
2	B	400	ATP	PB-O2B	-2.59	1.45	1.54
2	A	400	ATP	O4'-C1'	2.57	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ATP	C2'-C1'	2.40	1.61	1.53
2	A	400	ATP	C2'-C1'	2.36	1.60	1.53
2	A	400	ATP	C3'-C4'	2.21	1.58	1.53
2	B	400	ATP	O4'-C1'	2.11	1.46	1.42
2	B	400	ATP	C5-C4	2.01	1.42	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	ATP	O3B-PB-O3A	-5.06	87.65	104.64
2	A	400	ATP	C2'-C3'-C4'	-4.44	94.03	102.61
2	B	400	ATP	O3B-PB-O3A	-3.93	91.44	104.64
2	A	400	ATP	O4'-C1'-C2'	-3.74	98.62	106.62
2	A	400	ATP	C4-N9-C8	-3.58	101.98	105.74
2	A	400	ATP	O3'-C3'-C2'	3.43	122.82	111.82
2	B	400	ATP	C2'-C3'-C4'	-3.26	96.31	102.61
2	A	400	ATP	O2B-PB-O1B	3.09	122.86	110.83
2	B	400	ATP	O3'-C3'-C2'	2.98	121.38	111.82
2	A	400	ATP	O4'-C4'-C5'	2.97	118.85	109.33
2	B	400	ATP	O2B-PB-O1B	2.83	121.86	110.83
2	B	400	ATP	O4'-C4'-C5'	2.80	118.31	109.33
2	B	400	ATP	C4-N9-C8	-2.71	102.90	105.74
2	B	400	ATP	N3-C2-N1	-2.65	124.56	128.58
2	B	400	ATP	O4'-C1'-N9	-2.55	103.19	108.09
2	A	400	ATP	N3-C2-N1	-2.49	124.82	128.58
2	A	400	ATP	N9-C8-N7	2.34	117.26	113.94
2	A	400	ATP	PA-O5'-C5'	2.30	134.55	121.35
2	B	400	ATP	PA-O5'-C5'	2.18	133.85	121.35
2	A	400	ATP	O2A-PA-O3A	2.10	112.95	107.27
2	A	400	ATP	O5'-C5'-C4'	-2.10	101.84	108.99
2	A	400	ATP	O5'-PA-O1A	2.06	117.08	108.94
2	B	400	ATP	O2A-PA-O3A	2.01	112.72	107.27
2	B	400	ATP	O3'-C3'-C4'	2.01	116.84	111.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	ATP	O4'-C4'-C5'-O5'
2	B	400	ATP	C5'-O5'-PA-O2A
2	B	400	ATP	O4'-C4'-C5'-O5'
2	B	400	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	400	ATP	C3'-C4'-C5'-O5'
2	A	400	ATP	PB-O3A-PA-O1A
2	A	400	ATP	C5'-O5'-PA-O1A
2	A	400	ATP	C5'-O5'-PA-O2A
2	A	400	ATP	C5'-O5'-PA-O3A
2	B	400	ATP	C5'-O5'-PA-O1A
2	B	400	ATP	C5'-O5'-PA-O3A
2	A	400	ATP	PB-O3A-PA-O2A

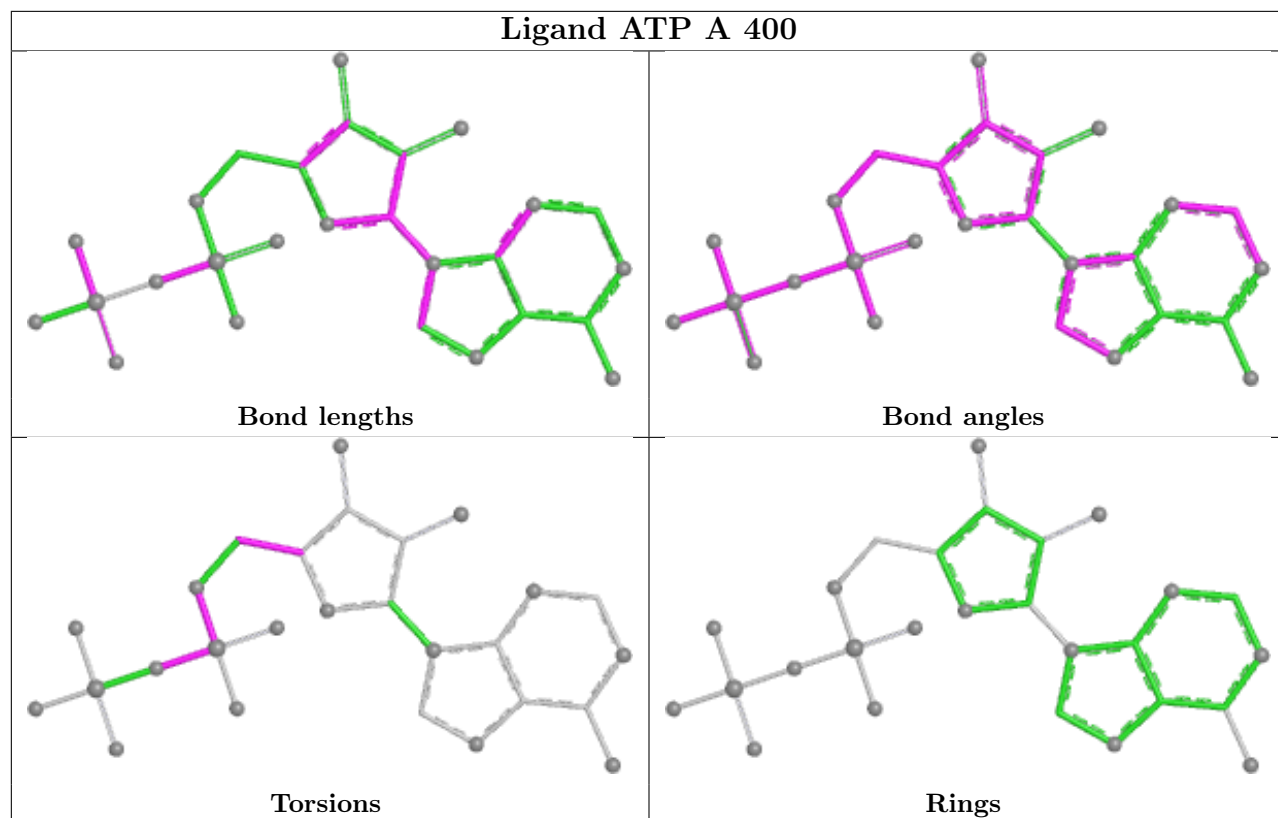
There are no ring outliers.

1 monomer is involved in 3 short contacts:

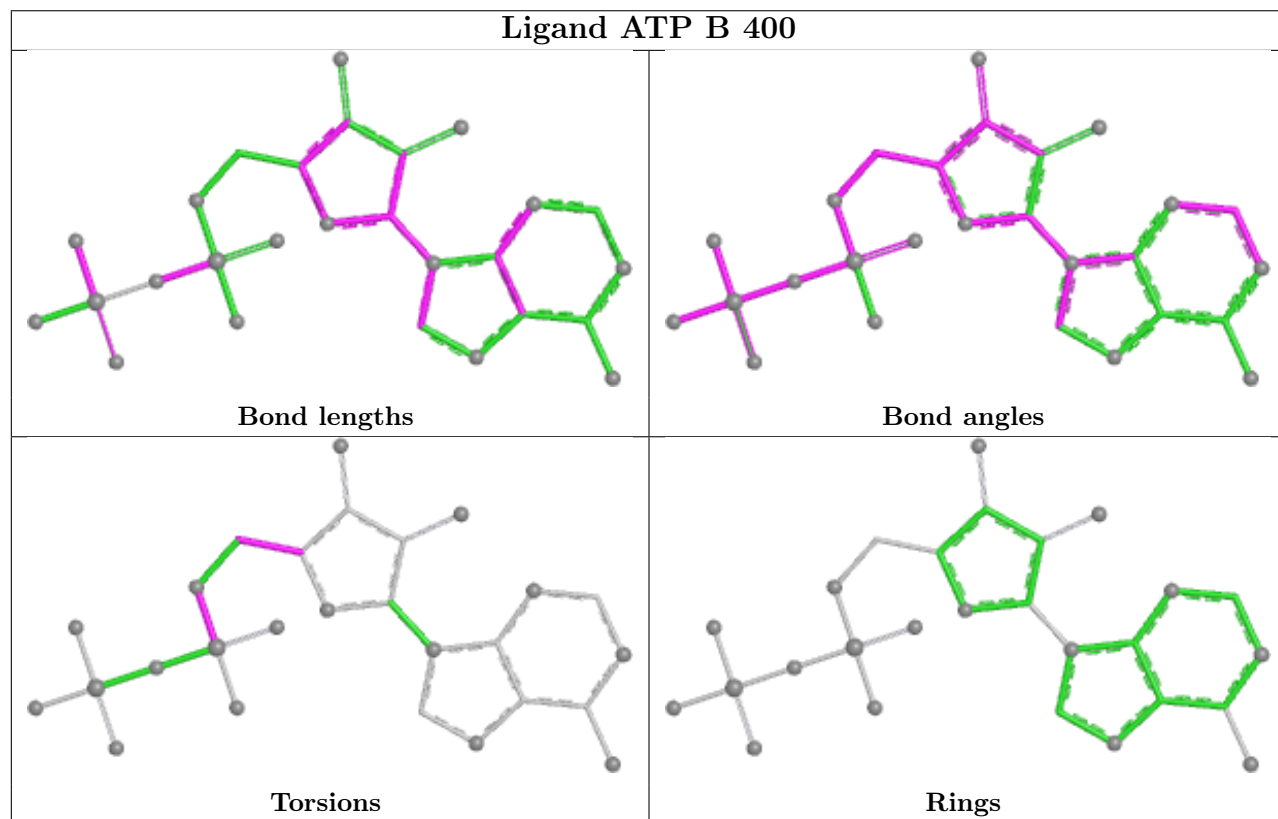
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ATP	3	0

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.

Ligand ATP A 400



Ligand ATP B 400



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	289/303 (95%)	0.32	17 (5%) 28 32	23, 40, 73, 97	0
1	B	290/303 (95%)	0.25	11 (3%) 44 50	25, 39, 71, 94	0
All	All	579/606 (95%)	0.28	28 (4%) 35 41	23, 40, 72, 97	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ILE	4.3
1	A	182	THR	4.2
1	A	167	GLY	3.7
1	B	9	GLY	3.7
1	B	166	ALA	3.5
1	B	60	ALA	3.2
1	B	35	PHE	3.1
1	B	169	LEU	3.0
1	A	60	ALA	3.0
1	A	35	PHE	2.9
1	A	170	THR	2.9
1	A	283	TYR	2.9
1	A	181	GLY	2.8
1	B	193	GLN	2.8
1	B	17	LYS	2.7
1	A	164	GLY	2.6
1	B	173	GLN	2.6
1	A	172	THR	2.6
1	A	163	PHE	2.5
1	A	195	ALA	2.5
1	B	16	LEU	2.5
1	A	173	GLN	2.4
1	B	172	THR	2.4
1	A	296	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	180	VAL	2.1
1	B	170	THR	2.0
1	A	286	GLU	2.0
1	A	177	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	B	178	11/12	0.80	0.15	60,65,67,68	0
1	TPO	A	178	11/12	0.81	0.16	66,73,77,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

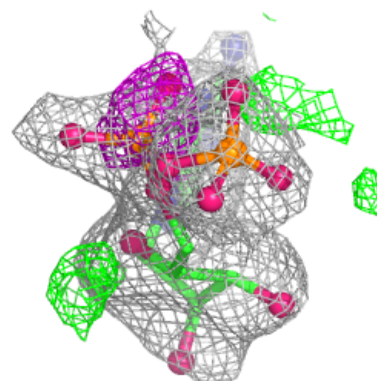
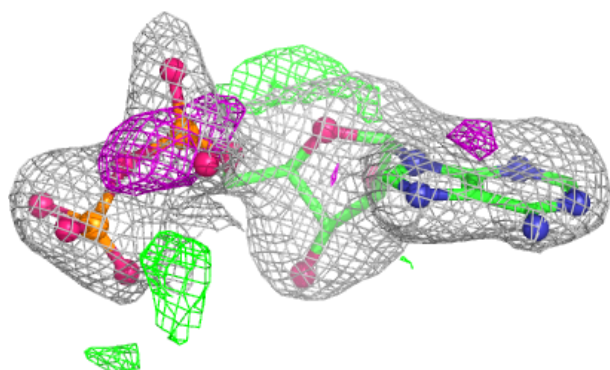
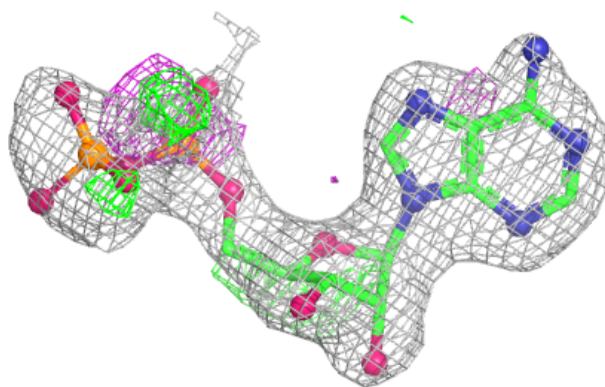
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	A	400	27/31	0.82	0.12	46,59,69,70	0
2	ATP	B	400	27/31	0.84	0.11	53,70,83,84	0

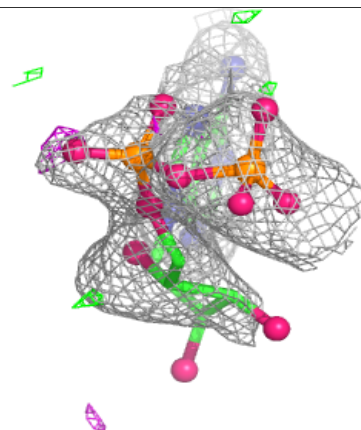
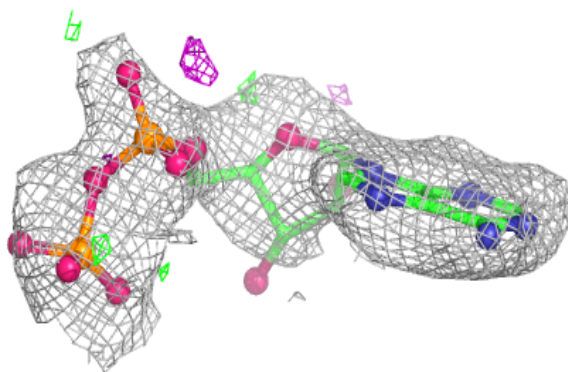
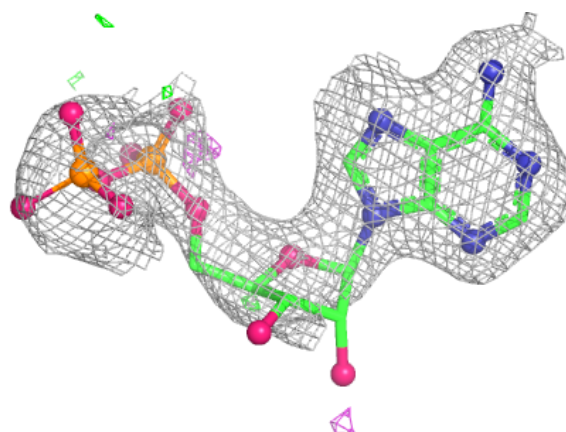
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 400:

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

**Electron density around ATP B 400:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.