



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:36 am BST

PDB ID : 2Y5W
Title : Crystal structure of Drosophila melanogaster kinesin-1 motor domain dimer
Authors : Kaan, H.Y.K.; Hackney, D.D.; Kozielski, F.
Deposited on : 2011-01-18
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

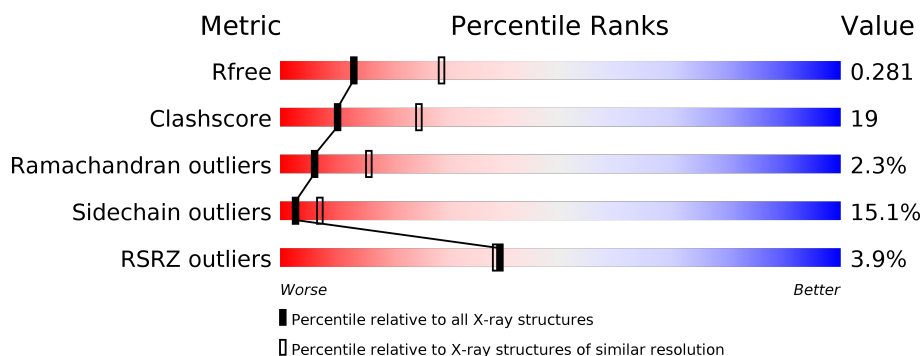
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	365	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>23%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	365	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>23%</div> <div>6%</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5388 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 KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2576	1620	440	507	9			
1	B	330	Total	C	N	O	S	0	2	0
			2576	1614	446	507	9			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

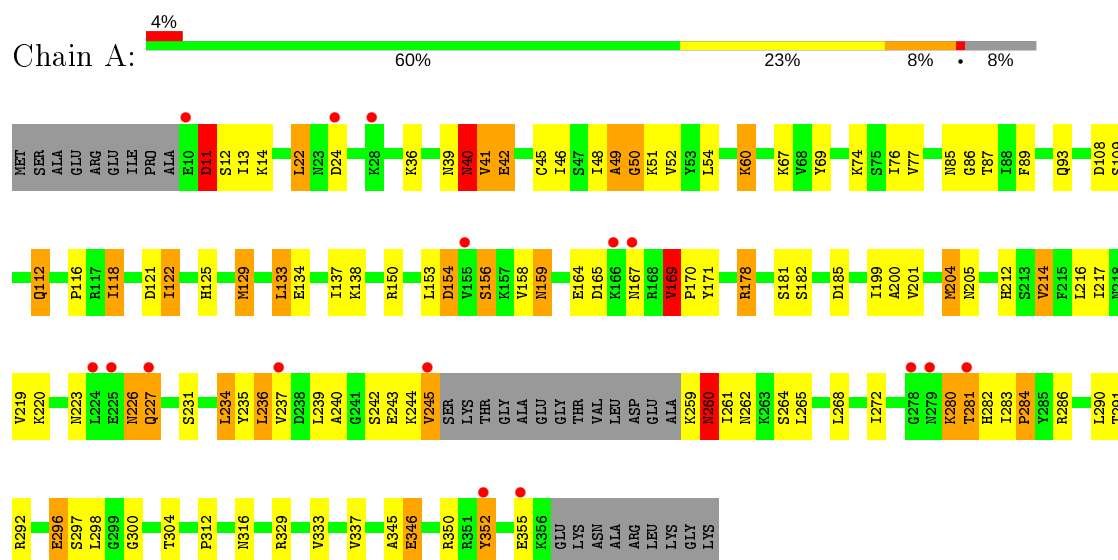
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total 82	O 82	0	0
4	B	98	Total 98	O 98	0	0

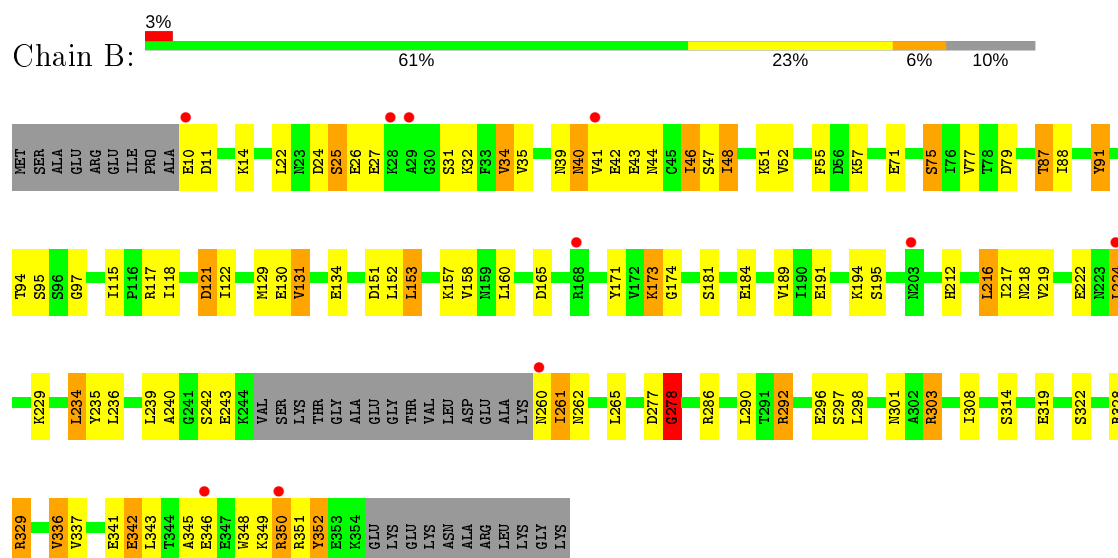
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: KINESIN HEAVY CHAIN



• Molecule 1: KINESIN HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.89Å 89.18Å 138.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.70 29.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.74-2.70) 99.9 (29.74-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.289 0.205 , 0.281	Depositor DCC
R_{free} test set	1346 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.60	0/2629	0.85	4/3559 (0.1%)
1	B	0.62	0/2622	0.86	2/3541 (0.1%)
All	All	0.61	0/5251	0.86	6/7100 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	169	VAL	C-N-CD	-6.37	106.59	120.60
1	A	46	ILE	CB-CA-C	-6.25	99.11	111.60
1	B	224	LEU	CA-CB-CG	5.99	129.08	115.30
1	B	165	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	50	GLY	N-CA-C	-5.40	99.61	113.10
1	A	280	LYS	N-CA-C	5.28	125.26	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ASN	Peptide
1	B	278	GLY	Peptide

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	2576	0	2503	102	0
1	B	2576	0	2537	92	0
2	A	27	0	12	0	0
2	B	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	82	0	0	5	0
4	B	98	0	0	4	0
All	All	5388	0	5064	193	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 19.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:HA	1:A:41:VAL:HG22	1.18	1.17
1:B:39:ASN:HB2	1:B:40:ASN:O	1.48	1.09
1:B:39:ASN:HA	1:B:40:ASN:HB2	1.36	1.08
1:A:169:VAL:HB	1:A:170:PRO:C	1.82	1.00
1:B:40:ASN:HA	1:B:41:VAL:HB	1.39	1.00
1:A:212:HIS:HD2	1:A:240:ALA:H	1.11	0.97
1:B:40:ASN:HB3	1:B:43:GLU:H	1.26	0.97
1:A:165:ASP:OD2	1:A:169:VAL:HG13	1.65	0.96
1:A:40:ASN:HA	1:A:41:VAL:CG2	1.95	0.96
1:B:260:ASN:O	1:B:261:ILE:HG12	1.67	0.95
1:A:41:VAL:HG23	1:A:42:GLU:H	1.28	0.94
1:A:87[A]:THR:HG22	1:A:235:TYR:HB2	1.50	0.91
1:A:11:ASP:OD2	1:A:337:VAL:HG22	1.70	0.90
2:B:600:ADP:O2B	4:B:2093:HOH:O	1.88	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:CA	1:A:41:VAL:HG22	2.02	0.86
1:A:212:HIS:CD2	1:A:240:ALA:H	1.94	0.85
1:A:169:VAL:HG21	1:A:171:TYR:HD2	1.47	0.80
1:B:39:ASN:CA	1:B:40:ASN:HB2	2.11	0.79
1:B:87:THR:HG22	4:B:2064:HOH:O	1.82	0.79
1:A:281:THR:N	1:A:282:HIS:HA	1.97	0.77
1:A:87[B]:THR:HG21	1:A:297:SER:OG	1.85	0.76
1:B:292:ARG:HH11	1:B:292:ARG:HG2	1.51	0.75
1:A:41:VAL:CG2	1:A:42:GLU:H	2.00	0.73
1:B:39:ASN:HA	1:B:40:ASN:CB	2.16	0.73
1:A:259:LYS:O	1:A:260:ASN:HB2	1.87	0.72
1:A:169:VAL:HB	1:A:170:PRO:CA	2.20	0.71
1:B:343:LEU:HB2	1:B:348:TRP:NE1	2.06	0.71
1:A:182:SER:O	1:A:185:ASP:HB2	1.91	0.71
1:B:329:ARG:HG2	1:B:329:ARG:HH11	1.54	0.70
1:B:87:THR:HG21	1:B:297:SER:OG	1.92	0.69
1:A:212:HIS:HD2	1:A:240:ALA:N	1.88	0.69
1:A:352:TYR:HB2	1:B:352:TYR:HB2	1.74	0.69
1:A:41:VAL:HG23	1:A:42:GLU:HG2	1.76	0.68
1:A:137:ILE:HD12	1:A:219:VAL:HG22	1.75	0.68
1:B:40:ASN:HA	1:B:41:VAL:CB	2.14	0.68
1:A:169:VAL:HG11	1:A:171:TYR:HB3	1.75	0.67
1:B:242:SER:HA	1:B:265:LEU:HD13	1.77	0.67
1:B:212:HIS:CD2	1:B:240:ALA:H	2.13	0.67
1:B:343:LEU:HB2	1:B:348:TRP:CD1	2.31	0.66
1:B:229:LYS:HB2	1:B:342:GLU:HB3	1.77	0.65
1:A:22:LEU:HD23	1:A:312:PRO:HG2	1.77	0.65
1:A:45:CYS:HB3	1:A:54:LEU:HD23	1.77	0.64
1:A:268:LEU:O	1:A:272:ILE:HG12	1.98	0.64
1:B:296:GLU:OE1	1:B:301:ASN:HB3	1.98	0.64
1:B:277:ASP:O	1:B:278:GLY:C	2.36	0.64
1:A:45:CYS:CB	1:A:54:LEU:HD23	2.28	0.63
1:B:260:ASN:O	1:B:261:ILE:CG1	2.45	0.63
1:A:87[B]:THR:HB	1:A:235:TYR:HB2	1.81	0.63
1:A:158:VAL:HG12	1:A:159:ASN:H	1.63	0.63
1:A:41:VAL:HG23	1:A:42:GLU:N	2.07	0.63
1:A:242:SER:HA	1:A:265:LEU:HD13	1.81	0.61
1:A:164:GLU:HA	1:A:169:VAL:HG23	1.83	0.61
1:A:11:ASP:OD2	1:A:337:VAL:CG2	2.47	0.61
1:A:244:LYS:O	1:A:245:VAL:HB	1.99	0.61
1:A:77:VAL:HG13	1:A:122:ILE:HG13	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:HB	1:A:170:PRO:O	2.02	0.60
1:B:242:SER:HA	1:B:265:LEU:CD1	2.30	0.60
1:A:108:ASP:O	1:A:112:GLN:HG2	2.02	0.60
1:A:216:LEU:HD12	1:A:217:ILE:N	2.17	0.59
1:B:171:TYR:CE1	1:B:173:LYS:HB2	2.37	0.59
1:A:296:GLU:HA	1:A:300:GLY:HA3	1.84	0.59
1:A:13:ILE:HD12	1:A:333:VAL:HB	1.86	0.57
1:A:212:HIS:HE1	1:A:264:SER:HB2	1.69	0.57
1:B:336:VAL:O	1:B:336:VAL:HG23	2.05	0.56
1:A:87[A]:THR:HG21	1:A:297:SER:OG	2.04	0.56
1:B:336:VAL:CG2	1:B:336:VAL:O	2.53	0.56
1:B:94:THR:O	1:B:95[B]:SER:OG	2.17	0.55
1:B:87:THR:HB	1:B:235:TYR:HB2	1.88	0.55
1:B:234:LEU:HD23	1:B:234:LEU:C	2.27	0.55
1:B:350:ARG:C	1:B:352:TYR:H	2.09	0.55
1:B:349:LYS:O	1:B:352:TYR:HB3	2.07	0.54
1:B:234:LEU:CD2	1:B:236:LEU:CD2	2.86	0.54
1:B:39:ASN:HB2	1:B:40:ASN:C	2.23	0.53
1:A:158:VAL:HG12	1:A:159:ASN:N	2.24	0.53
1:A:41:VAL:CG2	1:A:42:GLU:HG2	2.39	0.53
1:A:169:VAL:HG23	1:A:170:PRO:HA	1.91	0.53
1:B:157:LYS:HB3	1:B:160:LEU:HD11	1.91	0.53
1:A:178:ARG:HH11	1:A:178:ARG:HG2	1.73	0.53
1:B:46:ILE:HG22	1:B:48:ILE:CD1	2.39	0.53
1:A:154:ASP:OD1	1:A:156:SER:HB3	2.10	0.52
1:B:329:ARG:NH1	1:B:329:ARG:HG2	2.23	0.52
1:B:217:ILE:HG22	1:B:219:VAL:HG23	1.93	0.51
1:B:261:ILE:HG13	1:B:262:ASN:H	1.75	0.51
1:B:115:ILE:O	1:B:118:ILE:HB	2.10	0.51
1:B:40:ASN:HB3	1:B:42:GLU:H	1.75	0.51
1:B:97:GLY:HA2	2:B:600:ADP:O2A	2.11	0.51
1:A:169:VAL:HG21	1:A:171:TYR:CD2	2.37	0.51
1:B:243:GLU:O	1:B:261:ILE:HG22	2.10	0.51
1:A:13:ILE:HG12	1:A:304:THR:HB	1.93	0.51
1:A:220:LYS:HD3	1:A:231:SER:HB3	1.92	0.50
1:B:234:LEU:CD2	1:B:236:LEU:HD21	2.42	0.50
1:B:34:VAL:HG21	1:B:314:SER:HB3	1.93	0.50
1:A:261:ILE:HG13	1:A:262:ASN:N	2.27	0.50
1:A:281:THR:H	1:A:282:HIS:HA	1.75	0.50
1:A:345:ALA:HA	1:B:345:ALA:HA	1.94	0.50
1:B:157:LYS:HD3	1:B:174:GLY:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:HB3	4:A:2055:HOH:O	2.12	0.49
1:B:46:ILE:CG2	1:B:48:ILE:HD11	2.42	0.49
1:A:214:VAL:HB	1:A:237:VAL:HG22	1.95	0.49
1:A:50:GLY:HA2	4:A:2009:HOH:O	2.13	0.49
1:A:69:TYR:HE1	1:A:118:ILE:HG12	1.76	0.49
1:B:40:ASN:CA	1:B:41:VAL:HB	2.27	0.49
1:B:47:SER:C	1:B:48:ILE:HD13	2.33	0.49
1:B:46:ILE:HG22	1:B:48:ILE:HD13	1.94	0.48
1:B:46:ILE:CD1	1:B:55:PHE:HE2	2.26	0.48
1:B:234:LEU:HD21	1:B:236:LEU:HD21	1.94	0.48
1:A:212:HIS:HE1	1:A:264:SER:CB	2.26	0.48
1:A:280:LYS:N	1:A:281:THR:HB	2.28	0.48
1:A:41:VAL:CG2	1:A:42:GLU:N	2.71	0.48
1:B:24:ASP:C	1:B:26:GLU:N	2.64	0.48
1:A:216:LEU:HD12	1:A:217:ILE:H	1.75	0.48
1:B:40:ASN:CB	1:B:42:GLU:H	2.26	0.48
1:A:280:LYS:H	1:A:281:THR:HB	1.79	0.48
1:A:281:THR:N	1:A:282:HIS:CA	2.74	0.48
1:B:292:ARG:NH1	1:B:292:ARG:HG2	2.23	0.48
1:B:319:GLU:HA	1:B:319:GLU:OE1	2.14	0.47
1:A:201:VAL:HG11	1:A:204:MET:HE3	1.96	0.47
1:A:39:ASN:HA	1:A:40:ASN:O	2.13	0.47
1:A:199:ILE:O	1:A:200:ALA:HB3	2.14	0.47
1:A:178:ARG:HG2	1:A:178:ARG:NH1	2.30	0.47
1:B:24:ASP:O	1:B:25:SER:C	2.53	0.47
1:A:244:LYS:O	1:A:245:VAL:CB	2.62	0.47
1:B:329:ARG:NE	4:B:2090:HOH:O	2.47	0.47
1:B:234:LEU:CD2	1:B:236:LEU:HD22	2.45	0.47
1:B:91:TYR:C	1:B:91:TYR:CD1	2.88	0.47
1:A:45:CYS:HB2	1:A:54:LEU:HD23	1.97	0.47
1:B:212:HIS:HD2	1:B:239:LEU:HA	1.80	0.47
1:A:129:MET:HG2	1:A:133:LEU:CD2	2.45	0.46
1:B:277:ASP:O	1:B:278:GLY:O	2.33	0.46
1:A:121:ASP:OD1	1:A:125:HIS:CD2	2.69	0.46
1:A:226:ASN:O	1:A:227:GLN:HG2	2.16	0.46
1:B:194:LYS:HB3	1:B:194:LYS:HE2	1.65	0.46
1:B:46:ILE:HG21	1:B:48:ILE:HD11	1.97	0.46
1:A:243:GLU:HG3	1:A:245:VAL:HG12	1.98	0.46
1:A:169:VAL:CB	1:A:170:PRO:CA	2.92	0.45
1:B:44:ASN:HB2	1:B:55:PHE:O	2.16	0.45
1:A:286:ARG:HB2	4:A:2067:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:HA	1:A:41:VAL:CB	2.46	0.45
1:B:153:LEU:HD11	1:B:189:VAL:HG13	1.97	0.45
1:B:24:ASP:HA	1:B:27:GLU:OE1	2.17	0.45
1:B:350:ARG:O	1:B:352:TYR:N	2.50	0.45
1:A:112:GLN:HB2	1:A:116:PRO:HG2	1.99	0.45
1:A:89:PHE:HB3	1:A:237:VAL:HB	1.98	0.45
1:A:296:GLU:HG3	4:A:2068:HOH:O	2.17	0.45
1:B:303:ARG:HH11	1:B:337:VAL:HG11	1.81	0.45
1:B:46:ILE:HD13	1:B:55:PHE:HE2	1.82	0.45
1:A:346:GLU:CD	1:A:346:GLU:H	2.19	0.44
1:A:165:ASP:CG	1:A:169:VAL:HG22	2.37	0.44
1:A:86:GLY:O	1:A:234:LEU:HD22	2.18	0.44
1:B:34:VAL:CG2	1:B:314:SER:HB3	2.48	0.44
1:B:75:SER:HB2	1:B:79:ASP:OD2	2.18	0.44
1:A:350:ARG:C	1:A:352:TYR:N	2.72	0.43
1:B:151:ASP:C	1:B:151:ASP:OD1	2.57	0.43
1:B:329:ARG:CG	1:B:329:ARG:HH11	2.27	0.43
1:B:350:ARG:C	1:B:352:TYR:N	2.71	0.43
1:A:234:LEU:HD13	1:A:236:LEU:CD1	2.48	0.43
1:A:280:LYS:N	1:A:281:THR:CB	2.82	0.43
1:A:350:ARG:C	1:A:352:TYR:H	2.22	0.43
1:B:46:ILE:CD1	1:B:55:PHE:CE2	3.02	0.43
1:A:48:ILE:O	1:A:51:LYS:N	2.45	0.43
1:B:35:VAL:HG22	1:B:48:ILE:HD12	1.99	0.43
1:A:48:ILE:O	1:A:49:ALA:C	2.57	0.43
1:A:223:ASN:O	1:A:227:GLN:N	2.53	0.42
1:A:165:ASP:N	1:A:169:VAL:HG22	2.33	0.42
1:A:283:ILE:HA	1:A:284:PRO:HD2	1.63	0.42
1:B:117:ARG:O	1:B:121:ASP:HB2	2.20	0.42
1:B:216:LEU:HD22	1:B:217:ILE:N	2.34	0.42
1:B:22:LEU:HD23	1:B:27:GLU:HG3	2.00	0.42
1:A:42:GLU:HG2	1:A:42:GLU:H	1.42	0.42
1:A:133:LEU:HD12	1:A:223:ASN:HA	2.01	0.42
1:A:39:ASN:C	1:A:40:ASN:ND2	2.73	0.42
1:A:164:GLU:C	1:A:169:VAL:CG2	2.89	0.41
1:A:169:VAL:CG1	1:A:171:TYR:HB3	2.45	0.41
1:A:60:LYS:HZ2	1:A:60:LYS:HG3	1.73	0.41
1:B:91:TYR:O	1:B:308:ILE:HA	2.21	0.41
1:A:205:ASN:HD22	1:A:205:ASN:N	2.17	0.41
1:B:171:TYR:HE1	1:B:173:LYS:HB2	1.83	0.41
1:B:46:ILE:CG2	1:B:48:ILE:CD1	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:CG1	1:A:239:LEU:HD23	2.51	0.41
1:A:39:ASN:C	1:A:40:ASN:HD22	2.24	0.41
1:B:51:LYS:HB3	1:B:51:LYS:HE3	1.96	0.41
1:B:234:LEU:CD2	1:B:234:LEU:C	2.89	0.41
1:A:220:LYS:HZ3	1:A:231:SER:HB2	1.86	0.41
1:B:118:ILE:O	1:B:122:ILE:HG13	2.20	0.41
1:B:286:ARG:HA	1:B:292:ARG:HD2	2.02	0.41
1:B:52:VAL:O	1:B:328:ARG:NH2	2.54	0.41
1:B:88:ILE:HB	1:B:236:LEU:HD12	2.03	0.41
1:A:67[B]:LYS:HD2	4:A:2015:HOH:O	2.21	0.40
1:B:130:GLU:O	1:B:131:VAL:CB	2.69	0.40
1:B:46:ILE:HD12	1:B:46:ILE:N	2.36	0.40
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.79	0.40
1:A:93:GLN:HE22	1:A:316:ASN:HB3	1.87	0.40
1:B:71:GLU:HB2	4:B:2017:HOH:O	2.22	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	334/365 (92%)	296 (89%)	28 (8%)	10 (3%)	4	10
1	B	328/365 (90%)	296 (90%)	27 (8%)	5 (2%)	10	26
All	All	662/730 (91%)	592 (89%)	55 (8%)	15 (2%)	6	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	169	VAL
1	A	260	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	261	ILE
1	B	278	GLY
1	A	49	ALA
1	A	41	VAL
1	A	167	ASN
1	B	131	VAL
1	B	351	ARG
1	A	159	ASN
1	B	40	ASN
1	A	40	ASN
1	A	109	SER
1	A	284	PRO

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	282/321 (88%)	238 (84%)	44 (16%)	2	7
1	B	287/321 (89%)	246 (86%)	41 (14%)	3	8
All	All	569/642 (89%)	484 (85%)	85 (15%)	3	7

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	12	SER
1	A	14	LYS
1	A	22	LEU
1	A	24	ASP
1	A	36	LYS
1	A	40	ASN
1	A	42	GLU
1	A	52	VAL
1	A	60	LYS
1	A	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	ILE
1	A	112	GLN
1	A	118	ILE
1	A	122	ILE
1	A	129	MET
1	A	133	LEU
1	A	134	GLU
1	A	138	LYS
1	A	150	ARG
1	A	153	LEU
1	A	154	ASP
1	A	156	SER
1	A	169	VAL
1	A	178	ARG
1	A	181	SER
1	A	204	MET
1	A	214	VAL
1	A	226	ASN
1	A	227	GLN
1	A	234	LEU
1	A	236	LEU
1	A	245	VAL
1	A	260	ASN
1	A	281	THR
1	A	290	LEU
1	A	291	THR
1	A	292	ARG
1	A	296	GLU
1	A	298	LEU
1	A	329	ARG
1	A	346	GLU
1	A	352	TYR
1	A	355	GLU
1	B	10	GLU
1	B	11	ASP
1	B	14	LYS
1	B	25	SER
1	B	31	SER
1	B	32	LYS
1	B	34	VAL
1	B	46	ILE
1	B	48	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	57	LYS
1	B	75	SER
1	B	77	VAL
1	B	87	THR
1	B	91	TYR
1	B	121	ASP
1	B	129	MET
1	B	134	GLU
1	B	153	LEU
1	B	158	VAL
1	B	173	LYS
1	B	181	SER
1	B	184	GLU
1	B	191	GLU
1	B	195	SER
1	B	216	LEU
1	B	218	ASN
1	B	222	GLU
1	B	224	LEU
1	B	234	LEU
1	B	290	LEU
1	B	292	ARG
1	B	298	LEU
1	B	303	ARG
1	B	322	SER
1	B	329	ARG
1	B	336	VAL
1	B	341	GLU
1	B	342	GLU
1	B	346	GLU
1	B	350	ARG
1	B	352	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	125	HIS
1	A	196	ASN
1	A	205	ASN
1	A	212	HIS
1	A	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	227	GLN
1	A	260	ASN
1	A	340	ASN
1	B	70	ASN
1	B	112	GLN
1	B	196	ASN
1	B	212	HIS
1	B	218	ASN
1	B	316	ASN
1	B	340	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	600	3	24,29,29	0.90	1 (4%)	29,45,45	1.60	4 (13%)
2	ADP	B	600	3	24,29,29	1.05	1 (4%)	29,45,45	1.56	6 (20%)

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	ADP	A	600	3	-	5/12/32/32	0/3/3/3
2	ADP	B	600	3	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ADP	C5-C4	3.10	1.49	1.40
2	A	600	ADP	C5-C4	2.51	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ADP	PA-O3A-PB	-4.39	117.76	132.83
2	A	600	ADP	C4-C5-N7	-3.92	105.31	109.40
2	B	600	ADP	N3-C2-N1	-3.53	123.17	128.68
2	B	600	ADP	O4'-C1'-C2'	-3.46	101.87	106.93
2	B	600	ADP	O3'-C3'-C2'	-2.87	102.53	111.82
2	B	600	ADP	C2-N1-C6	2.83	123.59	118.75
2	A	600	ADP	N3-C2-N1	-2.77	124.35	128.68
2	B	600	ADP	C4-C5-N7	-2.49	106.80	109.40
2	B	600	ADP	PA-O3A-PB	-2.32	124.86	132.83
2	A	600	ADP	O3A-PB-O1B	-2.29	98.49	111.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

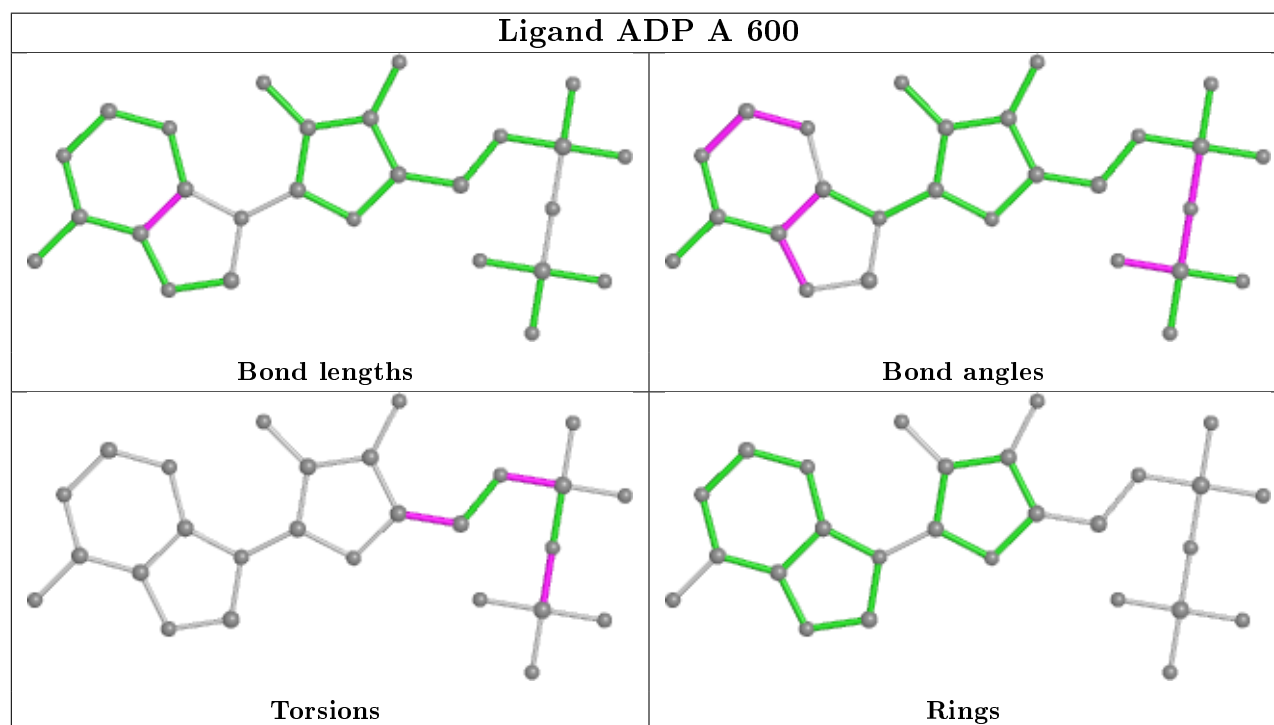
Mol	Chain	Res	Type	Atoms
2	A	600	ADP	PA-O3A-PB-O2B
2	A	600	ADP	C5'-O5'-PA-O1A
2	A	600	ADP	C5'-O5'-PA-O3A
2	B	600	ADP	PA-O3A-PB-O2B
2	A	600	ADP	O4'-C4'-C5'-O5'
2	A	600	ADP	PA-O3A-PB-O3B
2	B	600	ADP	PA-O3A-PB-O3B

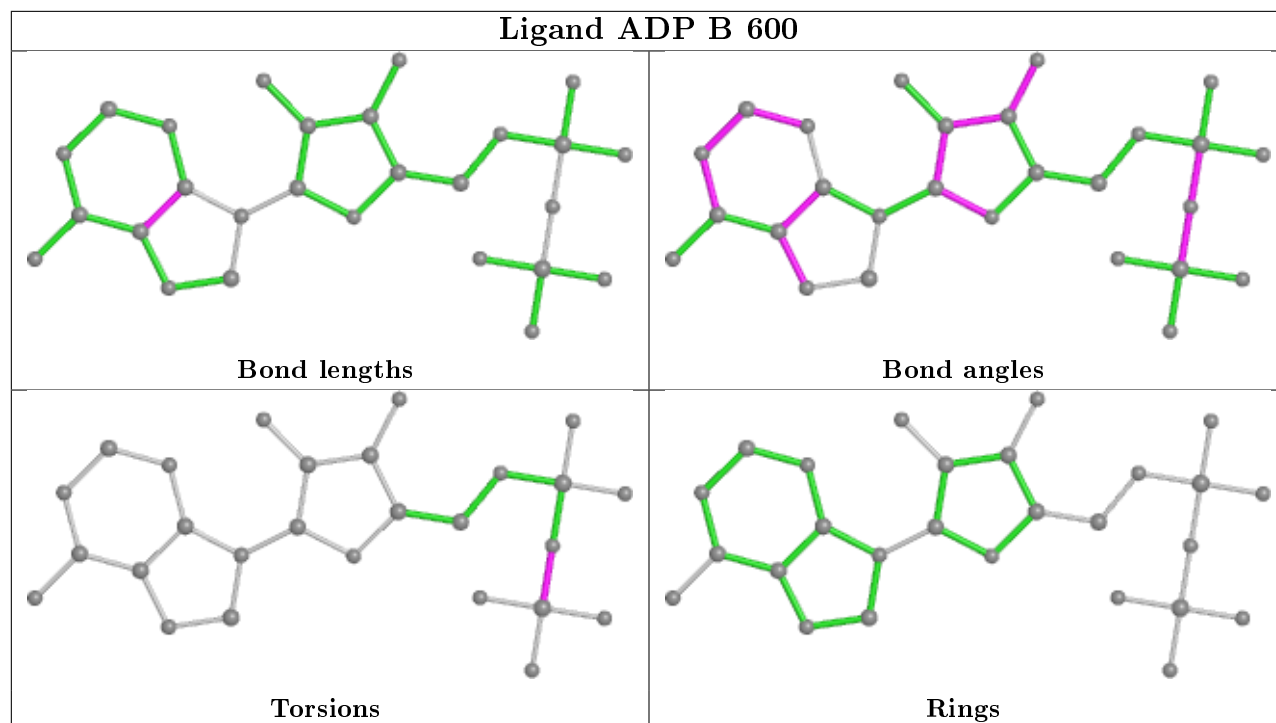
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	ADP	2	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	334/365 (91%)	0.04	16 (4%) 30 28	18, 43, 73, 100	0
1	B	330/365 (90%)	-0.21	10 (3%) 50 51	14, 35, 64, 96	0
All	All	664/730 (90%)	-0.08	26 (3%) 39 38	14, 38, 70, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	VAL	4.9
1	A	281	THR	4.0
1	B	350	ARG	3.3
1	A	279	ASN	3.2
1	A	352	TYR	3.0
1	A	10	GLU	2.8
1	A	24	ASP	2.7
1	A	167	ASN	2.7
1	A	224	LEU	2.7
1	B	203	ASN	2.5
1	B	260	ASN	2.5
1	A	28	LYS	2.5
1	A	225	GLU	2.5
1	A	278	GLY	2.5
1	B	10	GLU	2.3
1	A	237	VAL	2.3
1	B	28	LYS	2.3
1	A	355	GLU	2.3
1	A	155	VAL	2.3
1	A	166	LYS	2.2
1	B	41	VAL	2.2
1	B	168	ARG	2.2
1	B	29	ALA	2.1
1	B	346	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	224	LEU	2.1
1	A	227	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

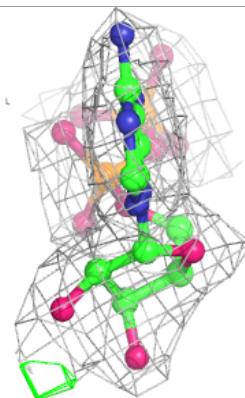
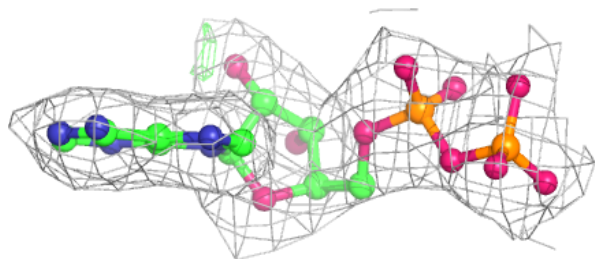
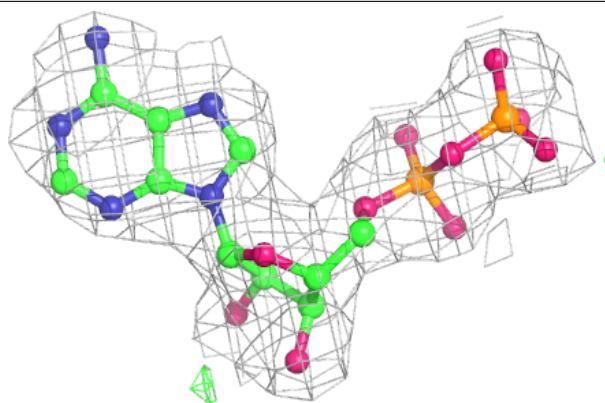
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	601	1/1	0.96	0.32	44,44,44,44	0
2	ADP	A	600	27/27	0.97	0.12	24,33,37,42	0
3	MG	B	601	1/1	0.98	0.18	20,20,20,20	0
2	ADP	B	600	27/27	0.98	0.10	19,27,30,31	0

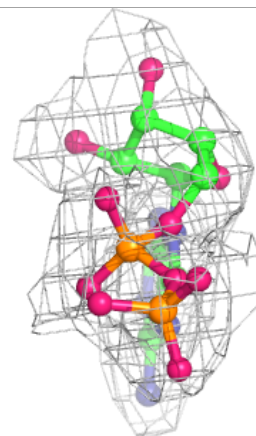
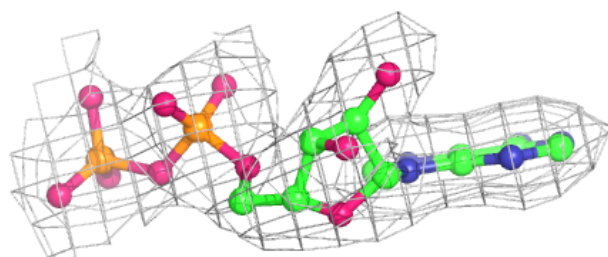
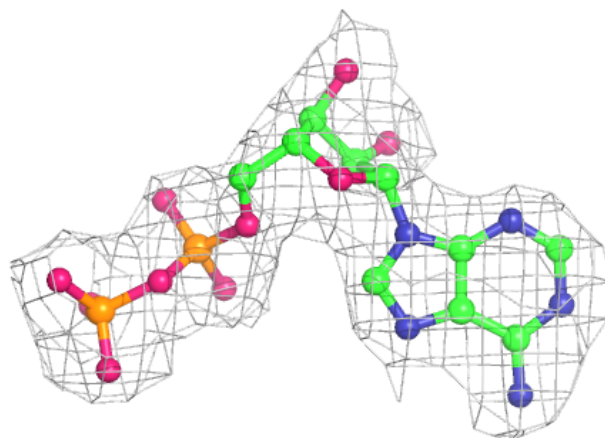
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 600:

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

**Electron density around ADP B 600:**

$2mF_o-DF_c$ (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.