



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:16 pm BST

PDB ID : 3COB  
Title : Structural Dynamics of the Microtubule binding and regulatory elements in the Kinesin-like Calmodulin binding protein  
Authors : Vinogradova, M.V.; Malanina, G.G.; Reddy, V.; Reddy, A.S.N.; Fletterick, R.J.  
Deposited on : 2008-03-27  
Resolution : 2.20 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](mailto: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

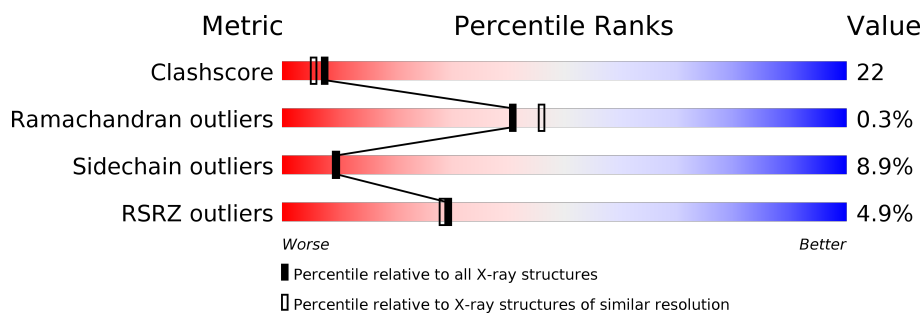
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	369	
1	C	369	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5738 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-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2792	1743	489	548	12			
1	C	340	Total	C	N	O	S	0	0	0
			2675	1669	467	527	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

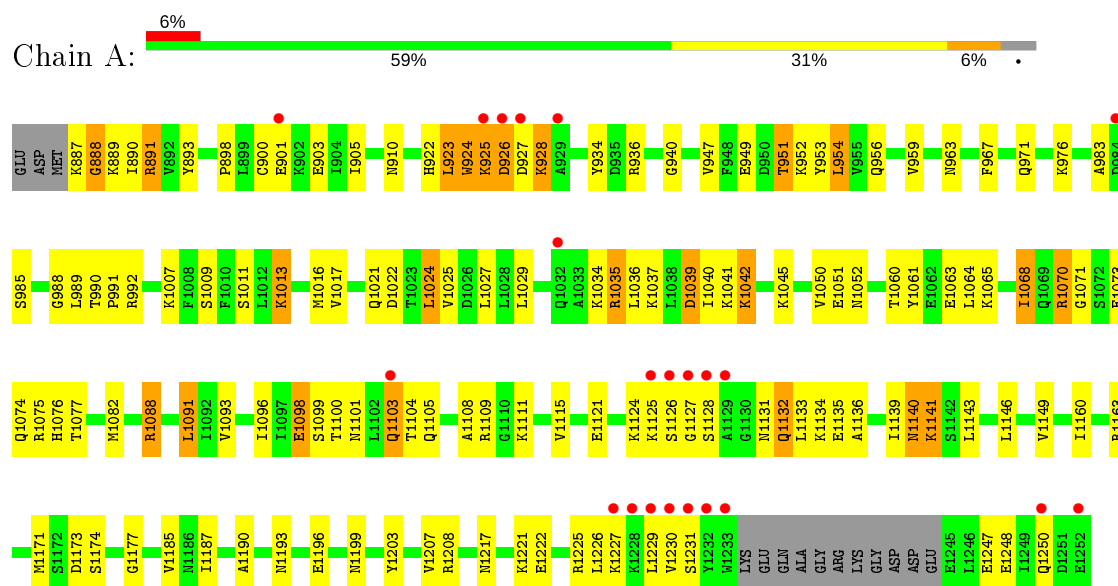
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	C	123	Total	O	0	0
			123	123		

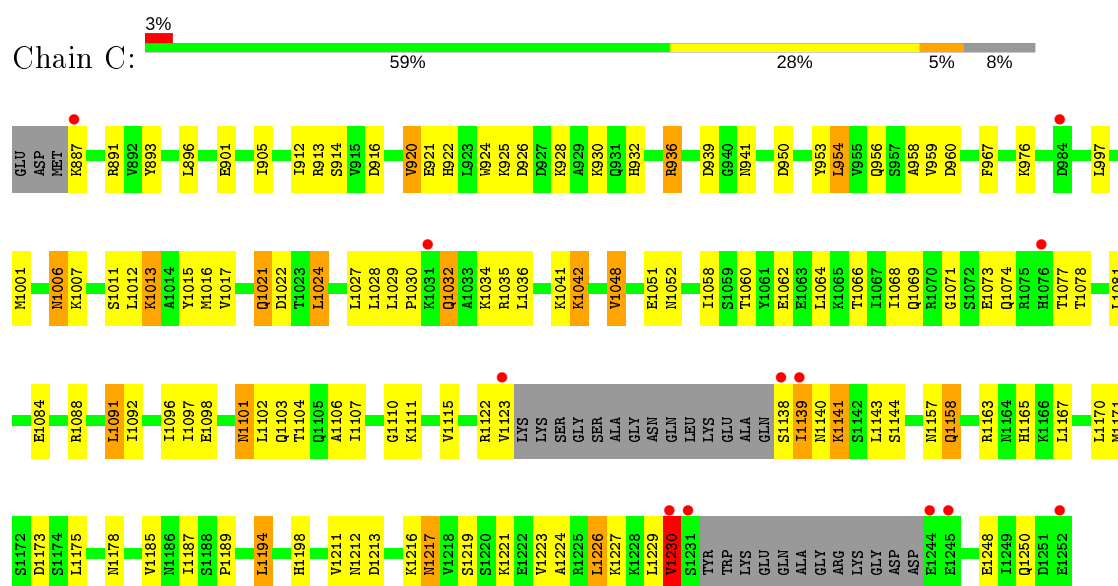
### 3 Residue-property plots

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-like protein



#### • Molecule 1: Kinesin heavy chain-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.15Å 84.91Å 89.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.54 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.9 (25.00-2.20) 95.5 (24.54-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.267 0.221 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.39	0/2830	0.62	0/3805
1	C	0.41	0/2709	0.62	1/3642 (0.0%)
All	All	0.40	0/5539	0.62	1/7447 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	936	ARG	CB-CA-C	5.09	120.58	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2792	0	2821	128	0
1	C	2675	0	2703	118	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	0	0
3	C	27	0	12	0	0
4	A	92	0	0	12	0
4	C	123	0	0	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5738	0	5548	245	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 22.

All (245) 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:1125:LYS:HG3	1:A:1136:ALA:HB2	1.24	1.12
1:A:924:TRP:HB3	1:A:925:LYS:HZ1	1.26	1.00
1:A:924:TRP:HB3	1:A:925:LYS:NZ	1.83	0.93
1:C:913:ARG:HE	1:C:914:SER:H	0.94	0.91
1:C:925:LYS:HB2	4:C:180:HOH:O	1.69	0.90
1:C:1111:LYS:HE2	4:C:16:HOH:O	1.71	0.89
1:C:1021:GLN:HB3	4:C:190:HOH:O	1.72	0.88
1:C:913:ARG:NE	1:C:914:SER:H	1.71	0.88
1:A:926:ASP:HB3	1:A:928:LYS:HE3	1.55	0.87
1:A:889:LYS:HD3	1:A:1208:ARG:O	1.76	0.85
1:C:1101:ASN:ND2	1:C:1103:GLN:H	1.73	0.84
1:C:1157:ASN:HB3	4:C:33:HOH:O	1.75	0.84
1:C:1139:ILE:HD11	4:C:28:HOH:O	1.77	0.84
1:C:887:LYS:HE3	1:C:1213:ASP:HB2	1.61	0.82
1:A:1077:THR:HG22	4:A:128:HOH:O	1.80	0.81
1:C:913:ARG:HE	1:C:914:SER:N	1.78	0.80
1:A:1125:LYS:HG3	1:A:1136:ALA:CB	2.11	0.79
1:A:1143:LEU:HD12	4:A:169:HOH:O	1.82	0.79
1:A:1230:VAL:O	1:A:1230:VAL:HG23	1.83	0.78
1:A:1060:THR:HG23	1:A:1063:GLU:H	1.49	0.78
1:A:926:ASP:HB3	1:A:928:LYS:CE	2.14	0.77
1:C:1250:GLN:HA	1:C:1250:GLN:HE21	1.51	0.76
1:A:924:TRP:HA	1:A:924:TRP:CE3	2.19	0.76
1:C:1011:SER:HB3	1:C:1098:GLU:HB3	1.66	0.76
1:C:1101:ASN:HD22	1:C:1103:GLN:H	1.33	0.76
1:A:1101:ASN:HD22	1:A:1104:THR:H	1.36	0.74
1:C:1250:GLN:HA	1:C:1250:GLN:NE2	2.02	0.74
1:A:1126:SER:HB2	1:A:1127:GLY:CA	2.17	0.73
1:A:924:TRP:CB	1:A:925:LYS:HZ1	2.01	0.73
1:A:1222:GLU:CD	1:A:1222:GLU:H	1.91	0.73
1:C:1048:VAL:HG22	4:C:16:HOH:O	1.89	0.73
1:C:1034:LYS:HE3	1:C:1036:LEU:HD21	1.72	0.72
1:A:891:ARG:HH11	1:A:891:ARG:HG2	1.54	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:SER:HB2	1:A:1127:GLY:HA2	1.71	0.71
1:A:1134:LYS:HD3	1:A:1135:GLU:N	2.05	0.71
1:C:1122:ARG:HH22	1:C:1144:SER:HB2	1.56	0.70
1:C:1101:ASN:HD22	1:C:1101:ASN:C	1.95	0.70
1:C:1006:ASN:HD22	1:C:1006:ASN:N	1.88	0.70
1:A:1034:LYS:HE3	1:A:1036:LEU:HD21	1.73	0.69
1:A:924:TRP:HA	1:A:924:TRP:HE3	1.53	0.69
1:A:1109:ARG:HB3	1:A:1217:ASN:ND2	2.07	0.68
1:C:920:VAL:HG12	1:C:932:HIS:HB2	1.75	0.68
1:C:1092:ILE:HD12	1:C:1170:LEU:HD13	1.76	0.68
1:C:1226:LEU:HD12	1:C:1229:LEU:HD21	1.75	0.68
1:C:1006:ASN:H	1:C:1006:ASN:HD22	1.43	0.67
1:C:891:ARG:HG2	4:C:19:HOH:O	1.95	0.67
1:C:1158:GLN:HB2	4:C:153:HOH:O	1.94	0.67
1:C:1021:GLN:HA	1:C:1139:ILE:HG12	1.79	0.65
1:C:1138:SER:O	1:C:1141:LYS:HG2	1.97	0.64
1:C:1219:SER:HB3	1:C:1223:VAL:HG13	1.78	0.64
1:A:1037:LYS:HE3	1:A:1039:ASP:OD2	1.99	0.63
1:A:1075:ARG:HD3	1:A:1091:LEU:HD12	1.80	0.63
1:A:1134:LYS:HD3	1:A:1134:LYS:C	2.19	0.63
1:C:936:ARG:NH1	1:C:950:ASP:OD2	2.32	0.62
1:C:1013:LYS:HG2	1:C:1096:ILE:HB	1.79	0.62
1:C:1006:ASN:H	1:C:1006:ASN:ND2	1.97	0.62
1:C:912:ILE:HG22	1:C:1189:PRO:HA	1.81	0.62
1:A:1196:GLU:HA	1:A:1199:ASN:HD22	1.65	0.61
1:A:1227:LYS:O	1:A:1230:VAL:HG22	2.00	0.61
1:C:926:ASP:O	1:C:928:LYS:HD2	2.00	0.61
1:A:1017:VAL:HG23	1:A:1025:VAL:O	2.01	0.61
1:C:1041:LYS:HE2	1:C:1248:GLU:OE2	2.01	0.61
1:A:947:VAL:HG12	1:A:989:LEU:HD21	1.82	0.60
1:A:1140:ASN:ND2	1:A:1140:ASN:H	1.98	0.60
1:C:1227:LYS:O	1:C:1230:VAL:CG2	2.50	0.60
1:A:1060:THR:HG22	1:A:1063:GLU:HB2	1.82	0.59
1:A:1088:ARG:NH2	1:A:1121:GLU:OE1	2.34	0.59
1:C:1029:LEU:CD2	1:C:1035:ARG:HB3	2.32	0.59
1:C:1165:HIS:HD2	1:C:1167:LEU:H	1.50	0.59
1:C:887:LYS:CE	1:C:1213:ASP:HB2	2.31	0.59
1:A:1250:GLN:HG2	4:A:96:HOH:O	2.03	0.58
1:A:1141:LYS:NZ	1:A:1141:LYS:HB3	2.18	0.58
1:C:930:LYS:HE2	1:C:1198:HIS:NE2	2.18	0.58
1:A:1101:ASN:ND2	1:A:1103:GLN:HG3	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LYS:HG2	4:A:61:HOH:O	2.03	0.58
1:A:1109:ARG:HB3	1:A:1217:ASN:HD22	1.68	0.58
1:C:939:ASP:OD2	1:C:941:ASN:HB2	2.03	0.58
1:A:891:ARG:HG2	1:A:891:ARG:NH1	2.19	0.57
1:C:956:GLN:O	1:C:959:VAL:HG22	2.05	0.57
1:A:1135:GLU:O	1:A:1139:ILE:HG13	2.03	0.57
1:C:1042:LYS:NZ	1:C:1248:GLU:O	2.37	0.57
1:C:1032:GLN:NE2	1:C:1032:GLN:H	2.03	0.57
1:C:1217:ASN:HD22	1:C:1217:ASN:C	2.06	0.57
1:A:924:TRP:CD1	1:A:925:LYS:HE3	2.40	0.56
1:A:1021:GLN:O	1:A:1022:ASP:HB2	2.05	0.56
1:C:1068:ILE:HG22	4:C:106:HOH:O	2.05	0.56
1:A:1070:ARG:NH2	4:A:39:HOH:O	2.37	0.56
1:C:1226:LEU:O	1:C:1229:LEU:HG	2.05	0.56
1:C:887:LYS:HE3	1:C:1213:ASP:CB	2.33	0.56
1:A:1101:ASN:ND2	1:A:1104:THR:H	2.04	0.56
1:C:1178:ASN:HA	1:C:1213:ASP:O	2.05	0.56
1:A:1013:LYS:HG2	1:A:1096:ILE:HB	1.88	0.56
1:A:1071:GLY:O	1:A:1075:ARG:HG2	2.07	0.55
1:A:1126:SER:CB	1:A:1127:GLY:HA2	2.27	0.55
1:A:926:ASP:CB	1:A:928:LYS:HE3	2.30	0.55
1:C:1107:ILE:HD13	1:C:1224:ALA:HB1	1.88	0.55
1:C:913:ARG:HH21	1:C:914:SER:HB2	1.71	0.55
1:A:887:LYS:HG3	4:A:116:HOH:O	2.06	0.55
1:A:1135:GLU:HG2	1:A:1139:ILE:HD11	1.88	0.55
1:A:922:HIS:HD2	1:A:923:LEU:O	1.91	0.54
1:A:967:PHE:CB	1:A:1115:VAL:HB	2.38	0.54
1:A:1104:THR:O	1:A:1105:GLN:HB2	2.08	0.54
1:A:947:VAL:O	1:A:951:THR:HG23	2.08	0.54
1:A:1096:ILE:HD12	1:A:1096:ILE:N	2.23	0.53
1:C:1006:ASN:ND2	1:C:1006:ASN:N	2.53	0.53
1:C:912:ILE:CG2	1:C:1189:PRO:HA	2.38	0.53
1:C:925:LYS:O	1:C:926:ASP:HB2	2.07	0.53
1:C:1101:ASN:HD22	1:C:1102:LEU:N	2.06	0.53
1:C:912:ILE:HD12	1:C:921:GLU:O	2.09	0.53
1:A:1009:SER:OG	1:A:1100:THR:HB	2.09	0.53
1:A:1229:LEU:O	1:A:1231:SER:N	2.36	0.53
1:A:1017:VAL:HG22	1:A:1024:LEU:HD22	1.90	0.52
1:C:1062:GLU:O	1:C:1066:THR:HG23	2.10	0.52
1:A:901:GLU:O	1:A:905:ILE:HG12	2.10	0.52
1:C:1250:GLN:CA	1:C:1250:GLN:HE21	2.15	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:PHE:HB3	1:A:1115:VAL:HB	1.91	0.51
1:C:1017:VAL:HB	1:C:1024:LEU:HD22	1.92	0.51
1:A:1017:VAL:CG2	1:A:1024:LEU:HD22	2.40	0.51
1:C:976:LYS:HE2	4:C:87:HOH:O	2.09	0.51
1:C:1171:MET:HB3	1:C:1175:LEU:CD2	2.40	0.51
1:C:922:HIS:HE1	1:C:932:HIS:HE1	1.57	0.50
1:C:1123:VAL:H	1:C:1140:ASN:HD21	1.59	0.50
1:A:1125:LYS:HB3	1:A:1132:GLN:HG3	1.94	0.50
1:A:1141:LYS:HD3	4:A:212:HOH:O	2.11	0.50
1:C:1021:GLN:HA	1:C:1139:ILE:CD1	2.42	0.50
1:A:1105:GLN:HB3	1:A:1221:LYS:HG2	1.93	0.50
1:A:971:GLN:HE22	1:A:1193:ASN:HB3	1.77	0.50
1:A:1051:GLU:O	1:A:1052:ASN:HB2	2.12	0.49
1:A:1021:GLN:HG2	1:A:1021:GLN:O	2.11	0.49
1:A:1230:VAL:CG2	1:A:1230:VAL:O	2.55	0.49
1:C:1227:LYS:O	1:C:1230:VAL:HG22	2.13	0.49
1:C:967:PHE:CB	1:C:1115:VAL:HB	2.42	0.49
1:A:1041:LYS:HB3	1:A:1247:GLU:O	2.13	0.48
1:A:1101:ASN:HD21	1:A:1103:GLN:HG3	1.77	0.48
1:C:1103:GLN:CD	1:C:1103:GLN:O	2.51	0.48
1:C:912:ILE:HD11	1:C:920:VAL:HG13	1.96	0.48
1:C:1069:GLN:O	1:C:1073:GLU:HG3	2.14	0.48
1:A:1101:ASN:HD22	1:A:1103:GLN:H	1.60	0.48
1:C:1006:ASN:HD22	1:C:1007:LYS:H	1.59	0.48
1:A:887:LYS:O	1:A:888:GLY:C	2.52	0.48
1:A:1173:ASP:HA	1:A:1177:GLY:HA3	1.95	0.48
1:A:890:ILE:HG21	1:A:1207:VAL:HG12	1.96	0.48
1:C:1029:LEU:HD12	1:C:1030:PRO:HD2	1.96	0.47
1:A:1141:LYS:HZ3	1:A:1141:LYS:HB3	1.79	0.47
1:A:1076:HIS:O	4:A:127:HOH:O	2.20	0.47
1:C:1032:GLN:N	1:C:1032:GLN:NE2	2.62	0.47
1:C:896:LEU:HG	1:C:1187:ILE:HD11	1.96	0.47
1:A:1075:ARG:CG	1:A:1091:LEU:HD12	2.45	0.47
1:A:927:ASP:OD2	1:A:927:ASP:O	2.32	0.47
1:C:1032:GLN:HE21	1:C:1032:GLN:H	1.61	0.47
1:A:983:ALA:C	1:A:985:SER:H	2.19	0.46
1:C:1071:GLY:O	1:C:1074:GLN:HB3	2.16	0.46
1:C:1077:THR:HB	4:C:152:HOH:O	2.16	0.46
1:C:913:ARG:HH21	1:C:914:SER:CB	2.28	0.46
1:C:1217:ASN:C	1:C:1217:ASN:ND2	2.68	0.46
1:C:1101:ASN:ND2	1:C:1101:ASN:C	2.67	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1048:VAL:HG13	1:C:1173:ASP:CG	2.36	0.46
1:C:997:LEU:O	1:C:1001:MET:HG3	2.15	0.46
1:A:1099:SER:OG	1:A:1108:ALA:HB3	2.15	0.46
1:C:1029:LEU:HD22	1:C:1035:ARG:HB3	1.97	0.46
1:A:1045:LYS:HG3	1:A:1217:ASN:OD1	2.16	0.46
1:C:887:LYS:HB3	1:C:1212:ASN:O	2.16	0.46
1:C:958:ALA:O	1:C:1110:GLY:HA3	2.16	0.46
1:A:1024:LEU:HD11	1:A:1040:ILE:HD11	1.98	0.46
1:A:1185:VAL:HG13	1:A:1185:VAL:O	2.15	0.46
1:C:1171:MET:HB3	1:C:1175:LEU:HD23	1.98	0.46
1:A:953:TYR:CZ	1:A:954:LEU:HD22	2.51	0.45
1:C:893:TYR:CD1	1:C:936:ARG:HB3	2.51	0.45
1:C:901:GLU:O	1:C:905:ILE:HG12	2.16	0.45
1:A:1075:ARG:CD	1:A:1091:LEU:HD12	2.46	0.45
1:C:1081:LEU:HB2	4:C:196:HOH:O	2.17	0.45
1:C:1229:LEU:O	1:C:1230:VAL:C	2.54	0.45
1:A:990:THR:HB	1:A:991:PRO:CD	2.46	0.45
1:A:898:PRO:HD3	1:A:940:GLY:O	2.17	0.45
1:A:1060:THR:CG2	1:A:1063:GLU:HB2	2.47	0.44
1:C:953:TYR:CE1	1:C:954:LEU:HD13	2.52	0.44
1:A:1103:GLN:HE21	1:A:1103:GLN:HB2	1.48	0.44
1:A:1141:LYS:NZ	1:A:1141:LYS:CB	2.80	0.44
1:A:1217:ASN:HB2	4:A:168:HOH:O	2.17	0.44
1:C:1021:GLN:HA	1:C:1139:ILE:CG1	2.45	0.44
1:A:1040:ILE:CD1	1:A:1050:VAL:HG22	2.47	0.44
1:A:991:PRO:HD3	1:A:1068:ILE:HD13	1.99	0.44
1:C:916:ASP:C	1:C:916:ASP:OD1	2.55	0.44
1:C:913:ARG:HH22	1:C:939:ASP:HA	1.83	0.44
1:A:925:LYS:HG3	1:A:925:LYS:H	1.34	0.44
1:A:1146:LEU:HD13	1:A:1171:MET:CE	2.48	0.44
1:A:1190:ALA:HB3	1:A:1193:ASN:HD22	1.83	0.44
1:A:1074:GLN:O	1:A:1074:GLN:HG3	2.17	0.43
1:C:887:LYS:HD3	1:C:1211:VAL:CG1	2.48	0.43
1:A:1229:LEU:C	1:A:1231:SER:N	2.71	0.43
1:C:1051:GLU:O	1:C:1052:ASN:HB2	2.18	0.43
1:C:1012:LEU:HB3	1:C:1058:ILE:HB	1.99	0.43
1:C:1185:VAL:O	1:C:1185:VAL:HG13	2.19	0.43
1:A:1011:SER:HB3	1:A:1098:GLU:HB3	2.00	0.43
1:A:1077:THR:HG23	4:A:166:HOH:O	2.17	0.43
1:C:960:ASP:HB3	1:C:1216:LYS:HE3	2.01	0.43
1:A:1061:TYR:CE2	1:A:1065:LYS:HD2	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:TYR:HD1	1:A:1208:ARG:HD2	1.84	0.43
1:C:1106:ALA:C	1:C:1107:ILE:HD12	2.39	0.43
1:A:1082:MET:HA	1:A:1082:MET:CE	2.48	0.43
1:A:925:LYS:N	1:A:925:LYS:HZ2	2.16	0.43
1:A:991:PRO:HD3	1:A:1068:ILE:CD1	2.48	0.43
1:C:1173:ASP:OD1	1:C:1173:ASP:N	2.52	0.43
1:C:926:ASP:HB3	1:C:928:LYS:HE3	2.01	0.43
1:A:956:GLN:NE2	1:A:959:VAL:CG2	2.82	0.43
1:C:1107:ILE:HD12	1:C:1107:ILE:N	2.34	0.43
1:A:1149:VAL:HG13	1:A:1160:ILE:CG2	2.48	0.43
1:A:1037:LYS:HE3	1:A:1039:ASP:CG	2.39	0.42
1:C:924:TRP:CE3	1:C:924:TRP:HA	2.53	0.42
1:A:976:LYS:HE2	4:A:4:HOH:O	2.19	0.42
1:C:1194:LEU:HA	1:C:1194:LEU:HD23	1.84	0.42
1:A:1042:LYS:HD2	1:A:1247:GLU:HB2	2.01	0.42
1:A:924:TRP:HB3	1:A:925:LYS:HZ2	1.76	0.42
1:A:949:GLU:OE2	1:A:952:LYS:HE2	2.20	0.42
1:C:1163:ARG:HH11	1:C:1248:GLU:HB3	1.85	0.42
1:A:1126:SER:CB	1:A:1127:GLY:CA	2.84	0.41
1:A:900:CYS:SG	1:A:903:GLU:HG3	2.60	0.41
1:C:1103:GLN:OE1	1:C:1103:GLN:O	2.37	0.41
1:A:1064:LEU:HA	1:A:1064:LEU:HD23	1.85	0.41
1:C:1223:VAL:HG22	1:C:1227:LYS:HD2	2.03	0.41
1:A:1187:ILE:HD13	4:A:92:HOH:O	2.20	0.41
1:C:1017:VAL:O	1:C:1091:LEU:HD23	2.20	0.41
1:C:1021:GLN:CA	1:C:1139:ILE:HG12	2.48	0.41
1:C:1143:LEU:HD13	1:C:1143:LEU:HA	1.92	0.41
1:A:1029:LEU:HD22	1:A:1035:ARG:HB3	2.01	0.41
1:C:1103:GLN:C	1:C:1103:GLN:CD	2.79	0.41
1:A:954:LEU:HA	1:A:954:LEU:HD13	1.91	0.41
1:C:1024:LEU:HA	1:C:1024:LEU:HD23	1.90	0.41
1:A:1007:LYS:HA	1:A:1007:LYS:HD3	1.87	0.41
1:A:1093:VAL:HG13	1:A:1093:VAL:O	2.20	0.41
1:A:925:LYS:C	1:A:927:ASP:H	2.23	0.41
1:A:925:LYS:NZ	1:A:926:ASP:H	2.19	0.41
1:A:1226:LEU:HD21	1:C:1227:LYS:CG	2.50	0.40
1:C:1016:MET:HG2	1:C:1027:LEU:HD12	2.03	0.40
1:C:1015:TYR:HA	1:C:1028:LEU:HD12	2.03	0.40
1:C:1042:LYS:HE3	4:C:14:HOH:O	2.21	0.40
1:A:1163:ARG:HH11	1:A:1248:GLU:HB3	1.86	0.40
1:A:925:LYS:HZ2	1:A:926:ASP:H	1.69	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:THR:O	1:C:1221:LYS:HB2	2.21	0.40
1:C:926:ASP:HB3	1:C:928:LYS:CD	2.50	0.40
1:A:1016:MET:HE3	1:A:1027:LEU:CD1	2.51	0.40
1:A:893:TYR:CD1	1:A:936:ARG:HB3	2.57	0.40
1:A:963:ASN:OD1	1:A:1111:LYS:HB3	2.20	0.40
1:A:988:GLY:O	1:A:992:ARG:HD2	2.21	0.40
1:C:1012:LEU:HD11	1:C:1097:ILE:HG23	2.03	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	351/369 (95%)	336 (96%)	14 (4%)	1 (0%)	41	46
1	C	334/369 (90%)	327 (98%)	6 (2%)	1 (0%)	41	46
All	All	685/738 (93%)	663 (97%)	20 (3%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	888	GLY
1	C	1230	VAL

### 5.3.2 Protein sidechains [i](#)

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	315/326 (97%)	284 (90%)	31 (10%)	8	7
1	C	304/326 (93%)	280 (92%)	24 (8%)	12	12
All	All	619/652 (95%)	564 (91%)	55 (9%)	9	9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	891	ARG
1	A	910	ASN
1	A	923	LEU
1	A	924	TRP
1	A	925	LYS
1	A	926	ASP
1	A	928	LYS
1	A	951	THR
1	A	954	LEU
1	A	1013	LYS
1	A	1024	LEU
1	A	1035	ARG
1	A	1039	ASP
1	A	1042	LYS
1	A	1068	ILE
1	A	1070	ARG
1	A	1073	GLU
1	A	1088	ARG
1	A	1091	LEU
1	A	1098	GLU
1	A	1103	GLN
1	A	1124	LYS
1	A	1128	SER
1	A	1131	ASN
1	A	1132	GLN
1	A	1133	LEU
1	A	1140	ASN
1	A	1141	LYS
1	A	1174	SER
1	A	1203	TYR
1	A	1225	ARG
1	C	920	VAL
1	C	954	LEU
1	C	1006	ASN
1	C	1013	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1021	GLN
1	C	1022	ASP
1	C	1024	LEU
1	C	1032	GLN
1	C	1042	LYS
1	C	1048	VAL
1	C	1060	THR
1	C	1064	LEU
1	C	1078	THR
1	C	1084	GLU
1	C	1088	ARG
1	C	1091	LEU
1	C	1101	ASN
1	C	1139	ILE
1	C	1141	LYS
1	C	1158	GLN
1	C	1194	LEU
1	C	1217	ASN
1	C	1226	LEU
1	C	1230	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	922	HIS
1	A	931	GLN
1	A	956	GLN
1	A	971	GLN
1	A	1021	GLN
1	A	1052	ASN
1	A	1085	GLN
1	A	1101	ASN
1	A	1103	GLN
1	A	1131	ASN
1	A	1140	ASN
1	A	1157	ASN
1	A	1158	GLN
1	A	1193	ASN
1	A	1198	HIS
1	A	1199	ASN
1	C	922	HIS
1	C	931	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	932	HIS
1	C	956	GLN
1	C	1006	ASN
1	C	1032	GLN
1	C	1052	ASN
1	C	1101	ASN
1	C	1140	ASN
1	C	1157	ASN
1	C	1217	ASN
1	C	1250	GLN

### 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	$\# Z  > 2$
3	ADP	C	600	2	24,29,29	0.98	1 (4%)	29,45,45	1.59	5 (17%)
3	ADP	A	600	2	24,29,29	0.97	1 (4%)	29,45,45	1.54	5 (17%)

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
3	ADP	C	600	2	-	2/12/32/32	0/3/3/3
3	ADP	A	600	2	-	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)
3	A	600	ADP	C2-N1	3.12	1.39	1.33
3	C	600	ADP	C2-N1	3.04	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ADP	C5-C6-N6	3.82	126.15	120.35
3	C	600	ADP	N3-C2-N1	-3.63	123.00	128.68
3	C	600	ADP	C5-C6-N6	3.58	125.80	120.35
3	A	600	ADP	N3-C2-N1	-3.45	123.28	128.68
3	C	600	ADP	C3'-C2'-C1'	2.96	105.43	100.98
3	A	600	ADP	C5-C6-N1	-2.87	113.85	120.35
3	C	600	ADP	C2-N1-C6	2.83	123.60	118.75
3	C	600	ADP	C5-C6-N1	-2.79	114.03	120.35
3	A	600	ADP	C2-N1-C6	2.78	123.50	118.75
3	A	600	ADP	C3'-C2'-C1'	2.04	104.05	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

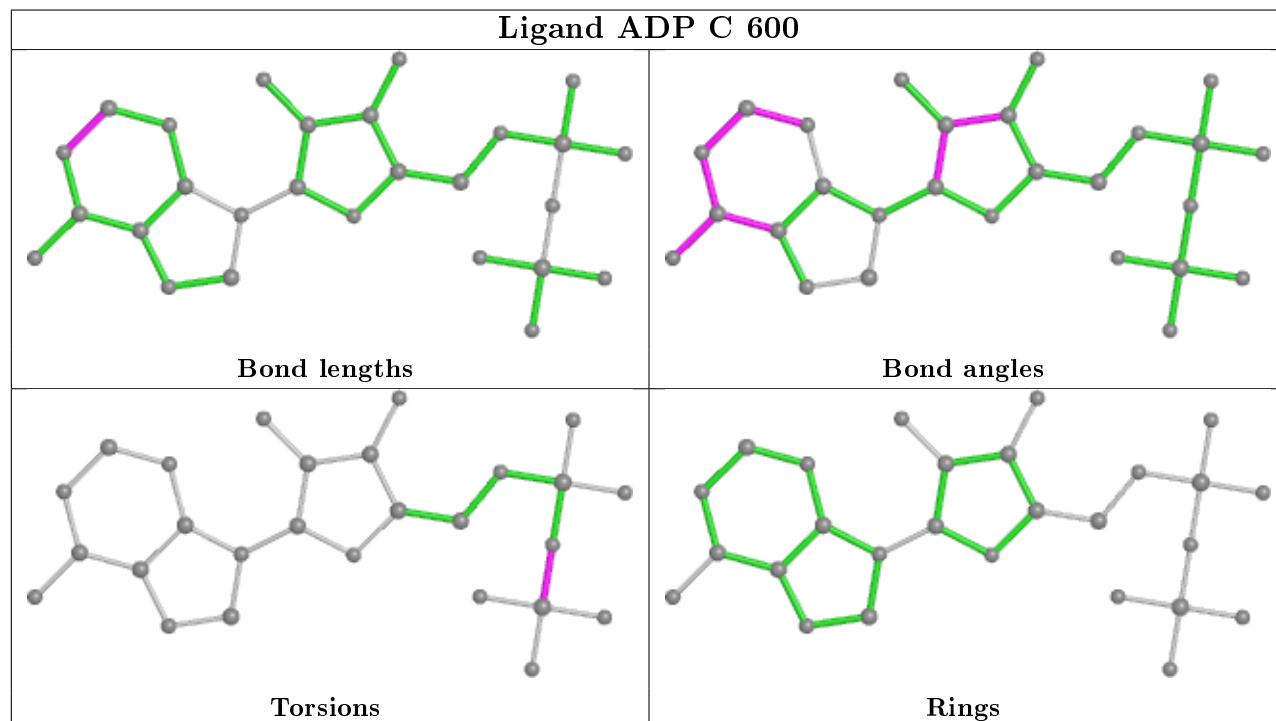
Mol	Chain	Res	Type	Atoms
3	C	600	ADP	PA-O3A-PB-O3B
3	A	600	ADP	PA-O3A-PB-O3B
3	C	600	ADP	PA-O3A-PB-O2B
3	A	600	ADP	PA-O3A-PB-O2B

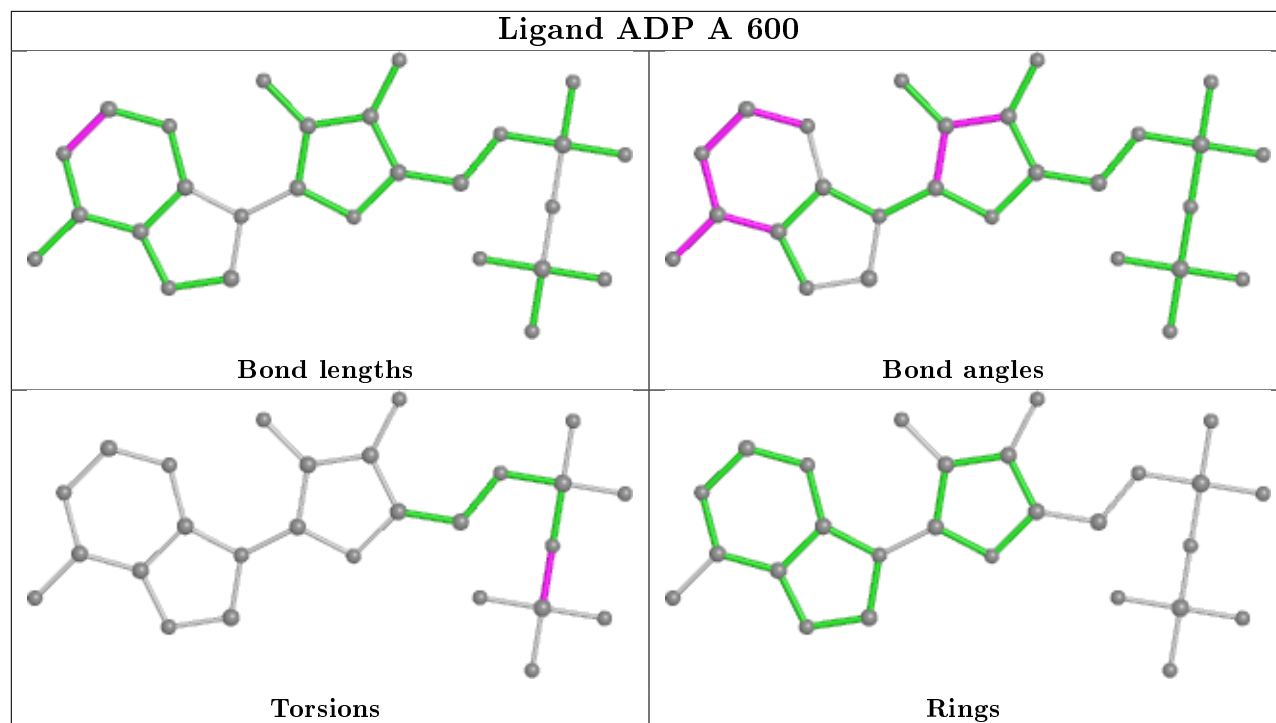
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	355/369 (96%)	0.06	22 (6%) 20 19	11, 28, 62, 84	0
1	C	340/369 (92%)	-0.18	12 (3%) 44 42	11, 24, 57, 78	0
All	All	695/738 (94%)	-0.06	34 (4%) 29 28	11, 26, 60, 84	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1127	GLY	10.1
1	A	1232	TYR	9.1
1	A	1126	SER	8.6
1	C	1138	SER	5.8
1	C	1244	GLU	5.7
1	A	927	ASP	5.3
1	C	1230	VAL	4.8
1	A	1233	TRP	4.6
1	C	887	LYS	4.6
1	C	984	ASP	4.5
1	A	1230	VAL	4.1
1	C	1123	VAL	4.0
1	A	926	ASP	3.6
1	C	1245	GLU	3.6
1	A	1129	ALA	3.5
1	A	1125	LYS	3.4
1	C	1076	HIS	3.3
1	A	1228	LYS	3.1
1	A	984	ASP	2.9
1	C	1231	SER	2.8
1	A	1231	SER	2.8
1	C	1252	GLU	2.7
1	C	1139	ILE	2.5
1	A	1229	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	925	LYS	2.4
1	A	1227	LYS	2.2
1	A	1252	GLU	2.2
1	A	901	GLU	2.2
1	A	1103	GLN	2.2
1	A	1250	GLN	2.2
1	A	1128	SER	2.1
1	C	1031	LYS	2.1
1	A	1032	GLN	2.1
1	A	929	ALA	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](#)

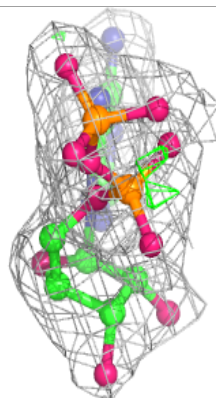
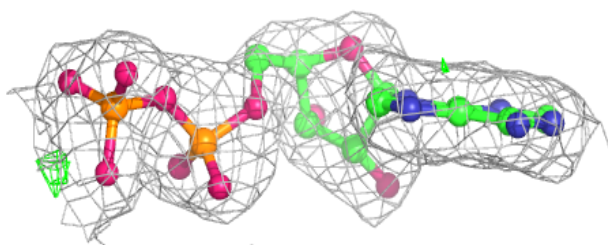
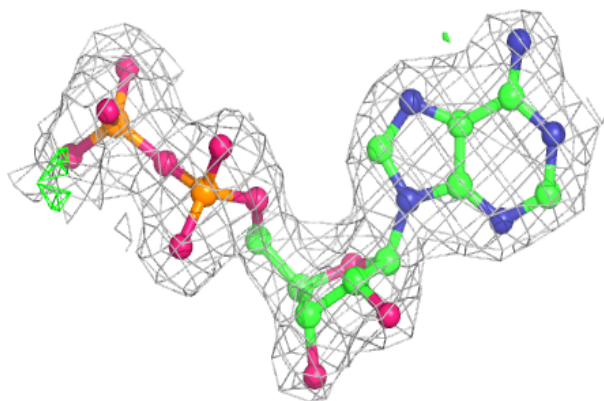
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	601	1/1	0.92	0.18	19,19,19,19	0
2	MG	C	602	1/1	0.94	0.12	18,18,18,18	0
3	ADP	C	600	27/27	0.97	0.12	14,23,30,41	0
3	ADP	A	600	27/27	0.97	0.11	14,21,30,31	0

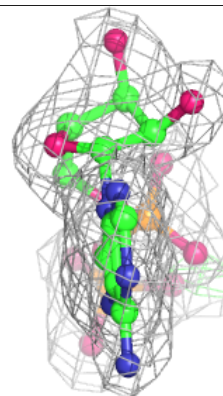
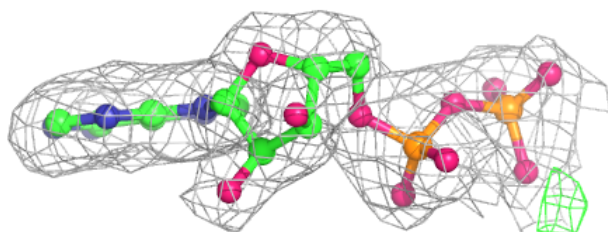
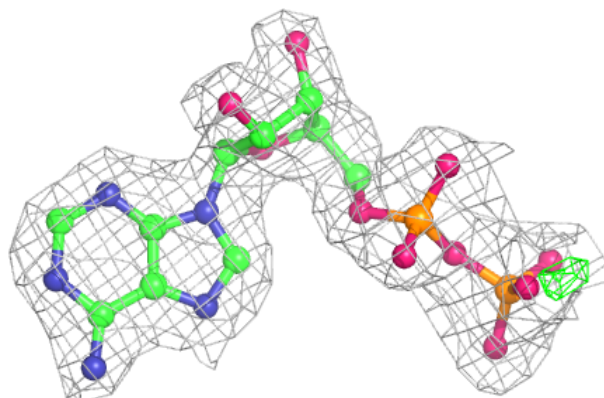
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP C 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 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.