



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:30 pm BST

PDB ID : 3K3B
Title : Co-crystal structure of the human kinesin Eg5 with a novel tetrahydro-beta-carboline
Authors : Bussiere, D.E.; Bellamacina, C.; Le, V.
Deposited on : 2009-10-02
Resolution : 2.40 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

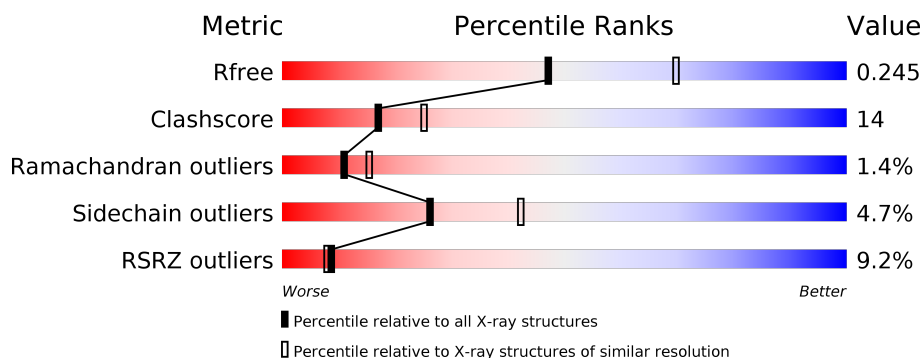
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	368	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	368	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5582 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-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2586	1622	445	509	10			
1	B	331	Total	C	N	O	S	0	0	0
			2567	1607	442	508	10			

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

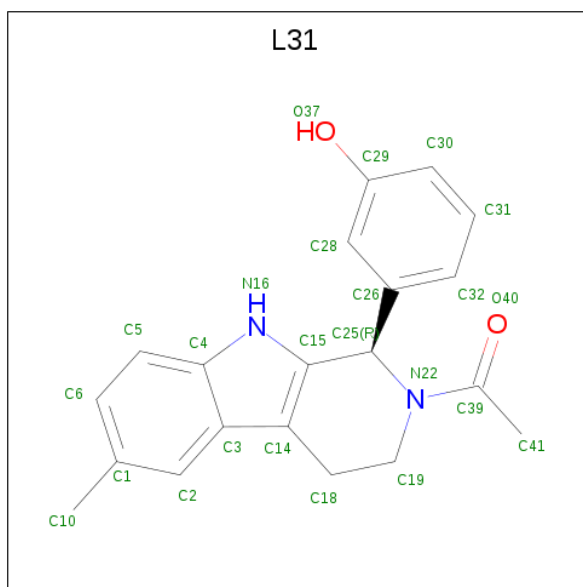
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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



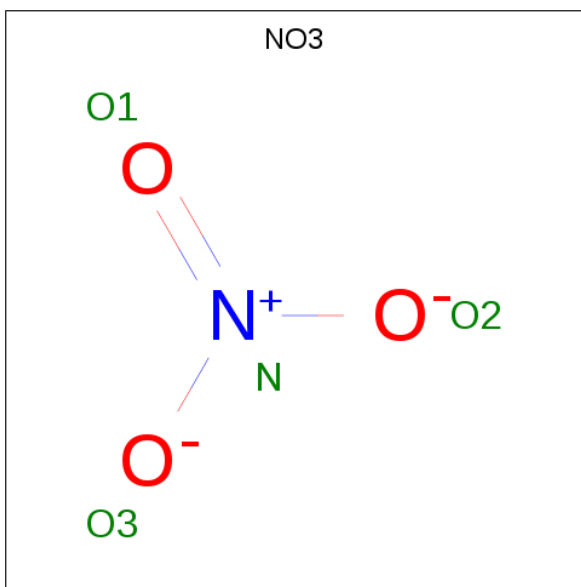
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 3-[(1R)-2-acetyl-6-methyl-2,3,4,9-tetrahydro-1H-beta-carbolin-1-yl]phenol (three-letter code: L31) (formula: C₂₀H₂₀N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			24	20	2	2			
4	B	1	Total	C	N	O		0	0
			24	20	2	2			

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO₃).

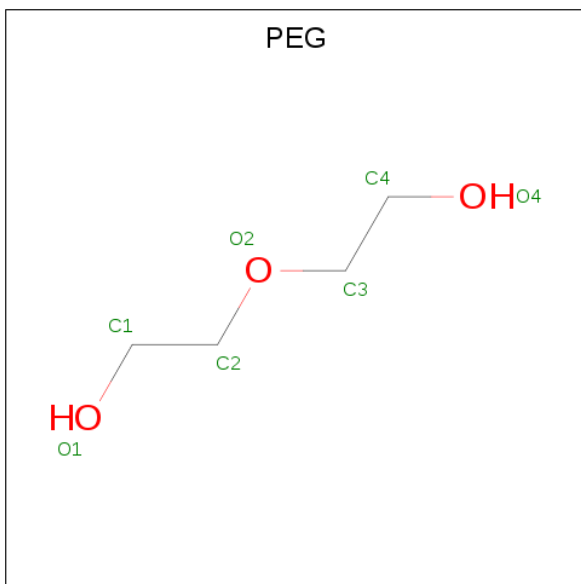


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		

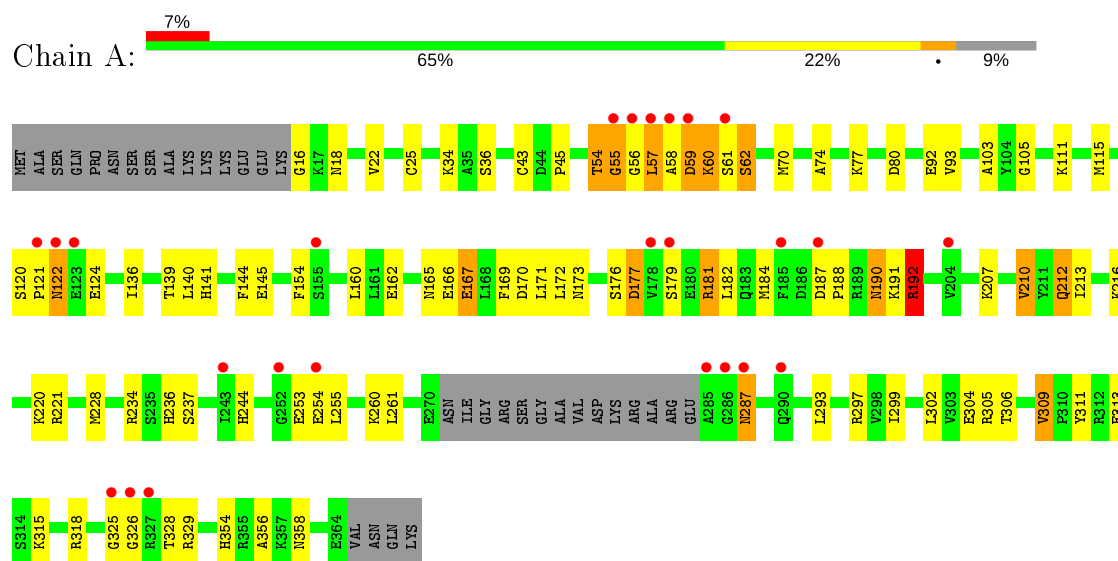
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	162	Total	O	0	0
			162	162		
8	B	147	Total	O	0	0
			147	147		

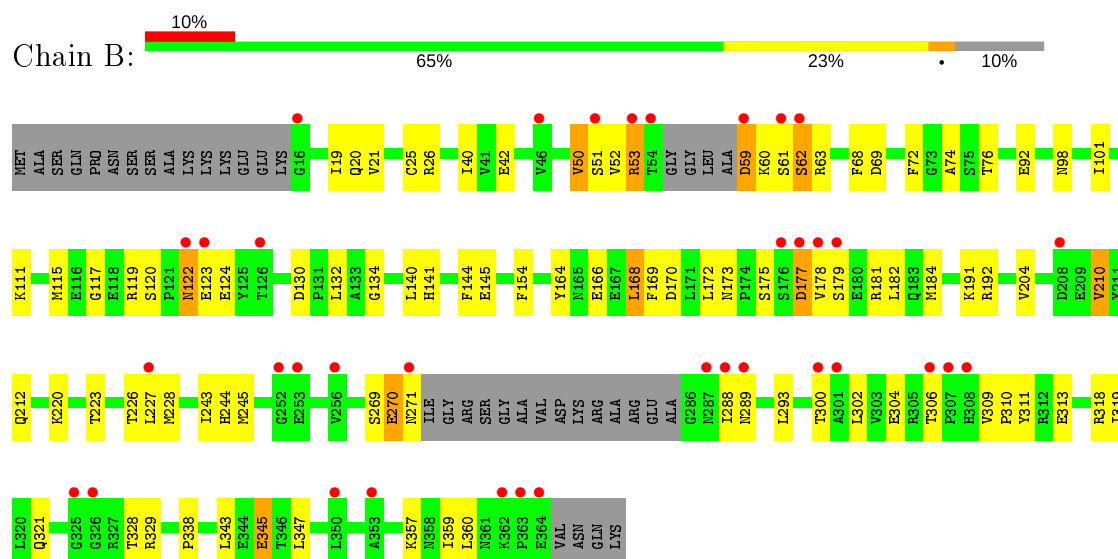
3 Residue-property plots [i](#)

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-like protein KIF11



- Molecule 1: Kinesin-like protein KIF11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.97Å 92.67Å 102.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.96 – 2.40 39.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.96-2.40) 94.4 (39.96-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.205 , 0.243 0.204 , 0.245	Depositor DCC
R_{free} test set	1510 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	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	0.94	EDS
Total number of atoms	5582	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5497e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, CL, L31, PEG, NO3

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	0.36	0/2627	0.51	0/3558
1	B	0.36	0/2605	0.51	0/3530
All	All	0.36	0/5232	0.51	0/7088

There are no bond length outliers.

There are no bond angle outliers.

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	2586	0	2569	84	0
1	B	2567	0	2542	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
4	A	24	0	20	3	0
4	B	24	0	20	0	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	7	0	10	0	0
8	A	162	0	0	10	0
8	B	147	0	0	4	0
All	All	5582	0	5185	146	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 14.

All (146) 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:121:PRO:HA	1:A:122:ASN:CB	1.78	1.14
1:A:121:PRO:HA	1:A:122:ASN:HB2	1.43	1.00
1:A:191:LYS:O	1:A:192:ARG:HB2	1.61	0.98
1:B:269:SER:C	1:B:271:ASN:H	1.73	0.88
1:A:121:PRO:HA	1:A:122:ASN:HB3	1.54	0.86
1:B:124:GLU:HG2	8:B:482:HOH:O	1.76	0.86
1:A:120:SER:O	1:A:122:ASN:HB2	1.76	0.84
1:B:179:SER:HA	1:B:228:MET:SD	2.18	0.84
1:A:325:GLY:HA3	8:A:390:HOH:O	1.78	0.83
1:B:59:ASP:C	1:B:61:SER:H	1.84	0.79
1:A:325:GLY:CA	8:A:390:HOH:O	2.29	0.79
1:B:40:ILE:HD12	1:B:343:LEU:HD13	1.63	0.79
1:A:167:GLU:HG2	1:A:181:ARG:HG2	1.64	0.78
1:A:121:PRO:CA	1:A:122:ASN:CB	2.63	0.75
1:A:167:GLU:CG	1:A:181:ARG:HG2	2.16	0.74
1:B:269:SER:C	1:B:271:ASN:N	2.40	0.72
1:A:121:PRO:CA	1:A:122:ASN:HB2	2.18	0.71
1:A:166:GLU:O	1:A:315:LYS:NZ	2.24	0.70
1:B:42:GLU:OE2	1:B:63:ARG:NH2	2.25	0.69
1:A:179:SER:HA	1:A:228:MET:SD	2.32	0.69
1:B:40:ILE:CD1	1:B:343:LEU:HD13	2.23	0.68
1:B:191:LYS:O	1:B:192:ARG:HB2	1.93	0.68
1:B:289:ASN:O	1:B:293:LEU:HG	1.94	0.67
1:A:58:ALA:HB1	1:A:61:SER:HB2	1.77	0.66
1:A:122:ASN:HA	1:A:124:GLU:H	1.61	0.66
1:A:326:GLY:HA2	1:A:328:THR:HG22	1.78	0.66
1:B:122:ASN:HB2	8:B:482:HOH:O	1.97	0.64
1:B:26:ARG:O	1:B:338:PRO:HG3	1.98	0.63
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.80	0.63
1:B:271:ASN:HD22	1:B:289:ASN:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:HIS:HD2	8:A:515:HOH:O	1.80	0.63
1:B:59:ASP:C	1:B:61:SER:N	2.51	0.63
1:A:326:GLY:HA2	1:A:328:THR:N	2.15	0.61
1:B:168:LEU:HD21	1:B:319:ILE:HD11	1.83	0.60
1:A:234:ARG:HH22	1:B:343:LEU:HD23	1.67	0.60
1:A:166:GLU:HG3	1:A:287:ASN:HB3	1.84	0.59
1:A:122:ASN:CA	1:A:124:GLU:H	2.15	0.59
1:A:160:LEU:HB3	1:A:172:LEU:HD13	1.86	0.58
1:A:173:ASN:HB3	1:A:176:SER:CB	2.34	0.58
1:B:212:GLN:HG3	8:B:512:HOH:O	2.03	0.57
1:A:105:GLY:O	1:A:111:LYS:HE2	2.04	0.57
1:B:68:PHE:HA	1:B:359:ILE:HD12	1.85	0.57
1:B:51:SER:HB2	1:B:63:ARG:HD2	1.87	0.57
1:B:120:SER:HA	1:B:132:LEU:HD12	1.87	0.56
1:B:177:ASP:C	1:B:179:SER:H	2.07	0.56
1:A:207:LYS:O	1:A:210:VAL:HG13	2.07	0.55
1:B:178:VAL:HG21	1:B:223:THR:HG22	1.90	0.54
1:A:293:LEU:O	1:A:297:ARG:HG3	2.07	0.54
1:A:253:GLU:OE1	1:A:253:GLU:HA	2.08	0.54
1:B:270:GLU:OE1	1:B:270:GLU:N	2.38	0.53
1:A:154:PHE:HA	1:A:244:HIS:O	2.07	0.53
1:B:269:SER:O	1:B:271:ASN:N	2.42	0.53
1:A:36:SER:HB3	8:A:450:HOH:O	2.09	0.53
1:B:140:LEU:O	1:B:144:PHE:HD2	1.92	0.53
1:A:184:MET:HE2	1:A:315:LYS:HD3	1.92	0.52
1:A:325:GLY:N	8:A:390:HOH:O	2.41	0.52
1:B:53:ARG:HD3	1:B:63:ARG:CZ	2.40	0.51
1:A:103:ALA:HB2	1:A:115:MET:HE2	1.92	0.51
1:A:139:THR:HG21	1:A:261:LEU:HD23	1.93	0.51
1:B:345:GLU:HA	1:B:345:GLU:OE1	2.10	0.50
1:A:25:CYS:O	1:A:74:ALA:HA	2.12	0.50
1:A:54:THR:HB	1:A:62:SER:HB3	1.93	0.50
1:A:59:ASP:C	1:A:61:SER:H	2.16	0.49
1:A:304:GLU:HB2	1:A:306:THR:HG23	1.94	0.49
1:B:50:VAL:CG1	1:B:68:PHE:HE1	2.25	0.49
1:A:184:MET:CE	1:A:315:LYS:HD3	2.43	0.49
1:A:260:LYS:HD2	8:A:502:HOH:O	2.13	0.49
1:B:175:SER:HA	1:B:220:LYS:NZ	2.28	0.49
1:A:34:LYS:HE2	3:B:371:ADP:O3'	2.13	0.48
1:A:141:HIS:O	1:A:145:GLU:HG2	2.13	0.48
1:B:304:GLU:HB2	1:B:306:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TYR:CD2	1:B:321:GLN:HG3	2.48	0.48
1:A:184:MET:HE3	1:A:318:ARG:NH2	2.29	0.48
1:A:162:GLU:HG3	1:A:171:LEU:HD11	1.96	0.47
1:A:56:GLY:O	1:A:57:LEU:HB2	2.14	0.47
1:A:234:ARG:NH2	8:A:431:HOH:O	2.46	0.47
1:B:154:PHE:HA	1:B:244:HIS:O	2.13	0.47
1:B:61:SER:O	1:B:62:SER:C	2.52	0.47
1:A:212:GLN:HG2	1:A:213:ILE:N	2.30	0.47
1:A:55:GLY:HA2	1:A:58:ALA:O	2.14	0.47
1:A:59:ASP:HA	1:A:60:LYS:C	2.35	0.47
1:A:57:LEU:HG	1:B:164:TYR:HE1	1.80	0.47
1:A:176:SER:O	1:A:177:ASP:CB	2.63	0.47
1:A:136:ILE:HD13	4:A:371:L31:H6	1.98	0.46
1:B:72:PHE:HB3	1:B:76:THR:OG1	2.15	0.46
1:A:54:THR:HB	1:A:62:SER:CB	2.46	0.46
1:B:101:ILE:HG22	1:B:115:MET:HE1	1.97	0.46
1:B:177:ASP:C	1:B:179:SER:N	2.69	0.46
1:A:212:GLN:O	1:A:216:LYS:HG3	2.15	0.45
1:B:21:VAL:O	1:B:68:PHE:HB3	2.16	0.45
1:B:302:LEU:HD21	1:B:311:TYR:OH	2.16	0.45
1:A:234:ARG:NH2	1:B:343:LEU:HD23	2.30	0.45
1:A:165:ASN:O	1:A:166:GLU:HB2	2.17	0.45
1:A:190:ASN:ND2	1:A:191:LYS:O	2.50	0.45
1:A:56:GLY:O	1:A:57:LEU:CB	2.64	0.45
1:A:221:ARG:HH12	1:A:237:SER:HB2	1.81	0.45
1:A:326:GLY:CA	1:A:328:THR:HG22	2.45	0.45
1:A:111:LYS:NZ	8:A:386:HOH:O	2.49	0.45
1:A:111:LYS:HE3	3:A:370:ADP:O2B	2.17	0.45
1:B:310:PRO:HB3	1:B:313:GLU:OE2	2.17	0.45
1:B:169:PHE:CE2	1:B:181:ARG:HG3	2.52	0.44
1:B:288:ILE:O	1:B:289:ASN:C	2.55	0.44
1:B:300:THR:O	1:B:304:GLU:HG2	2.18	0.44
1:A:299:ILE:HG21	1:A:356:ALA:HB1	1.99	0.44
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.99	0.44
1:B:111:LYS:HE2	8:B:382:HOH:O	2.18	0.44
1:B:141:HIS:O	1:B:145:GLU:HG2	2.18	0.44
1:B:92:GLU:HG3	1:B:329:ARG:HG3	2.00	0.44
1:B:117:GLY:HA3	1:B:134:GLY:N	2.33	0.43
1:A:36:SER:C	8:A:450:HOH:O	2.56	0.43
1:A:253:GLU:HG3	1:A:255:LEU:CD2	2.48	0.43
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HH21	4:A:371:L31:H10B	1.83	0.43
1:A:162:GLU:HA	1:A:236:HIS:O	2.18	0.43
1:A:16:GLY:HA2	1:A:18:ASN:N	2.33	0.43
1:B:40:ILE:HA	1:B:53:ARG:HG3	2.01	0.43
1:B:52:VAL:HG11	1:B:347:LEU:HD21	2.00	0.43
1:B:204:VAL:HG11	1:B:210:VAL:HG12	2.01	0.42
1:B:357:LYS:HD3	1:B:359:ILE:HD11	2.01	0.42
1:A:297:ARG:NH2	1:A:313:GLU:OE2	2.52	0.42
1:A:160:LEU:HD22	4:A:371:L31:C10	2.50	0.42
1:A:92:GLU:HG3	1:A:329:ARG:HG3	2.01	0.42
1:A:77:LYS:HE3	1:A:80:ASP:OD2	2.19	0.42
1:A:43:CYS:O	1:A:45:PRO:HD3	2.19	0.42
1:A:184:MET:HE2	1:A:315:LYS:CD	2.49	0.42
1:A:309:VAL:HG22	1:A:311:TYR:CE1	2.54	0.42
1:B:20:GLN:HA	1:B:69:ASP:OD2	2.19	0.41
1:B:119:ARG:NH1	1:B:130:ASP:OD1	2.54	0.41
1:B:98:ASN:O	1:B:328:THR:HB	2.20	0.41
1:B:311:TYR:CG	1:B:321:GLN:HG3	2.55	0.41
1:B:25:CYS:O	1:B:74:ALA:HA	2.19	0.41
1:A:93:VAL:HG21	1:A:261:LEU:HB2	2.03	0.41
1:B:166:GLU:HA	5:B:369:NO3:O2	2.19	0.41
1:B:184:MET:HE3	1:B:318:ARG:HD3	2.02	0.41
1:B:191:LYS:O	1:B:192:ARG:CB	2.67	0.41
1:A:253:GLU:HG3	1:A:255:LEU:HD21	2.03	0.41
1:B:42:GLU:O	1:B:50:VAL:HA	2.21	0.41
1:A:167:GLU:HB3	1:A:169:PHE:CE1	2.55	0.41
1:A:302:LEU:HD22	1:A:325:GLY:HA2	2.01	0.41
1:B:243:ILE:HG22	1:B:245:MET:HG3	2.01	0.41
1:A:122:ASN:HA	1:A:124:GLU:N	2.33	0.40
1:A:305:ARG:NH1	8:A:462:HOH:O	2.54	0.40
1:B:170:ASP:OD2	1:B:173:ASN:HB2	2.22	0.40
1:A:140:LEU:O	1:A:144:PHE:HD2	2.05	0.40
1:A:187:ASP:OD2	1:A:188:PRO:O	2.40	0.40
1:B:226:THR:HG22	1:B:227:LEU:HD23	2.04	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	331/368 (90%)	311 (94%)	14 (4%)	6 (2%)	8	10
1	B	325/368 (88%)	303 (93%)	19 (6%)	3 (1%)	17	25
All	All	656/736 (89%)	614 (94%)	33 (5%)	9 (1%)	11	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	B	270	GLU
1	A	57	LEU
1	A	177	ASP
1	A	190	ASN
1	B	60	LYS
1	B	122	ASN
1	A	55	GLY
1	A	192	ARG

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	285/322 (88%)	271 (95%)	14 (5%)	25	40
1	B	286/322 (89%)	273 (96%)	13 (4%)	27	44
All	All	571/644 (89%)	544 (95%)	27 (5%)	26	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	59	ASP
1	A	60	LYS
1	A	62	SER
1	A	167	GLU
1	A	181	ARG
1	A	192	ARG
1	A	210	VAL
1	A	212	GLN
1	A	220	LYS
1	A	254	GLU
1	A	287	ASN
1	A	309	VAL
1	A	358	ASN
1	B	19	ILE
1	B	50	VAL
1	B	53	ARG
1	B	59	ASP
1	B	62	SER
1	B	123	GLU
1	B	168	LEU
1	B	172	LEU
1	B	177	ASP
1	B	210	VAL
1	B	309	VAL
1	B	345	GLU
1	B	360	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	190	ASN
1	A	229	ASN
1	B	18	ASN
1	B	98	ASN
1	B	244	HIS
1	B	271	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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	L31	B	372	-	24,27,27	3.94	13 (54%)	30,40,40	1.60	5 (16%)
5	NO3	B	369	-	1,3,3	3.54	1 (100%)	0,3,3	0.00	-
5	NO3	A	372	-	1,3,3	3.54	1 (100%)	0,3,3	0.00	-
4	L31	A	371	-	24,27,27	3.91	13 (54%)	30,40,40	1.56	6 (20%)
3	ADP	B	371	2	24,29,29	1.01	1 (4%)	29,45,45	1.40	4 (13%)
3	ADP	A	370	2	24,29,29	1.01	1 (4%)	29,45,45	1.44	4 (13%)
7	PEG	A	374	-	6,6,6	0.46	0	5,5,5	0.26	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
4	L31	B	372	-	-	0/8/21/21	0/4/4/4
4	L31	A	371	-	-	0/8/21/21	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	371	2	-	3/12/32/32	0/3/3/3
3	ADP	A	370	2	-	3/12/32/32	0/3/3/3
7	PEG	A	374	-	-	3/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	372	L31	C39-N22	9.39	1.48	1.35
4	A	371	L31	C39-N22	9.25	1.48	1.35
4	B	372	L31	C14-C15	8.57	1.52	1.39
4	A	371	L31	C14-C15	8.51	1.52	1.39
4	B	372	L31	C32-C26	7.93	1.51	1.39
4	A	371	L31	C32-C26	7.89	1.51	1.39
4	B	372	L31	C5-C4	5.06	1.50	1.41
4	A	371	L31	C5-C4	4.88	1.50	1.41
4	A	371	L31	C30-C29	4.65	1.47	1.38
4	B	372	L31	C30-C29	4.58	1.47	1.38
4	A	371	L31	C25-N22	-4.57	1.45	1.48
4	B	372	L31	C25-N22	-4.54	1.45	1.48
4	B	372	L31	C4-N16	3.58	1.50	1.38
4	B	372	L31	C2-C1	3.56	1.44	1.37
4	A	371	L31	C4-N16	3.56	1.50	1.38
5	B	369	NO3	O1-N	3.54	1.40	1.24
5	A	372	NO3	O1-N	3.54	1.40	1.24
4	A	371	L31	C2-C1	3.50	1.44	1.37
4	B	372	L31	C6-C1	3.26	1.47	1.38
4	A	371	L31	C28-C29	3.25	1.44	1.39
4	A	371	L31	C6-C1	3.23	1.47	1.38
4	B	372	L31	C28-C29	3.22	1.43	1.39
4	B	372	L31	C19-C18	3.06	1.57	1.51
4	A	371	L31	C19-C18	3.01	1.57	1.51
3	A	370	ADP	C5-C4	2.66	1.48	1.40
3	B	371	ADP	C5-C4	2.58	1.47	1.40
4	A	371	L31	C2-C3	2.42	1.47	1.42
4	A	371	L31	C31-C30	2.41	1.44	1.38
4	B	372	L31	C2-C3	2.39	1.46	1.42
4	B	372	L31	C31-C30	2.37	1.43	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	372	L31	C41-C39-N22	4.52	122.60	117.87
4	A	371	L31	C41-C39-N22	3.89	121.94	117.87
4	A	371	L31	C18-C19-N22	3.72	114.81	109.48
3	B	371	ADP	N3-C2-N1	-3.69	122.91	128.68
3	A	370	ADP	PA-O3A-PB	-3.67	120.22	132.83
4	B	372	L31	C15-C25-N22	3.64	116.71	110.39
3	A	370	ADP	N3-C2-N1	-3.55	123.14	128.68
3	B	371	ADP	PA-O3A-PB	-3.35	121.34	132.83
4	B	372	L31	C19-C18-C14	3.24	116.98	111.64
4	A	371	L31	C15-C25-N22	3.23	116.00	110.39
4	A	371	L31	C19-C18-C14	3.13	116.80	111.64
4	B	372	L31	C18-C19-N22	2.86	113.58	109.48
3	A	370	ADP	C4-C5-N7	-2.62	106.66	109.40
3	B	371	ADP	C4-C5-N7	-2.53	106.77	109.40
4	B	372	L31	C26-C25-C15	-2.52	108.45	112.78
4	A	371	L31	C1-C2-C3	-2.15	119.20	121.64
4	A	371	L31	C26-C25-C15	-2.10	109.17	112.78
3	B	371	ADP	C2-N1-C6	2.08	122.31	118.75
3	A	370	ADP	O3B-PB-O2B	2.03	115.41	107.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

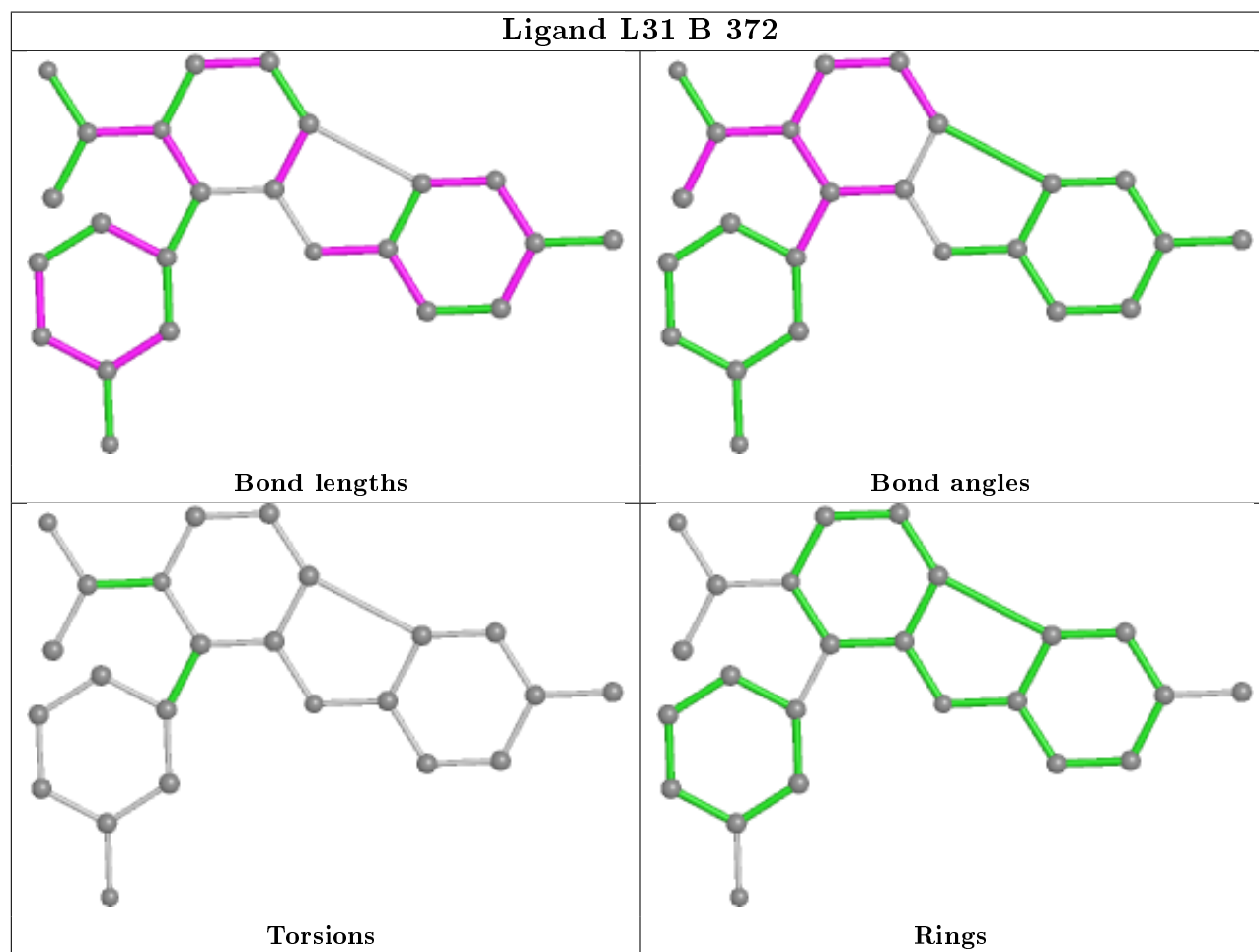
Mol	Chain	Res	Type	Atoms
3	B	371	ADP	C5'-O5'-PA-O2A
3	A	370	ADP	C5'-O5'-PA-O1A
3	A	370	ADP	C5'-O5'-PA-O2A
7	A	374	PEG	O2-C3-C4-O4
3	B	371	ADP	C5'-O5'-PA-O3A
3	A	370	ADP	C5'-O5'-PA-O3A
3	B	371	ADP	C5'-O5'-PA-O1A
7	A	374	PEG	C4-C3-O2-C2
7	A	374	PEG	C1-C2-O2-C3

There are no ring outliers.

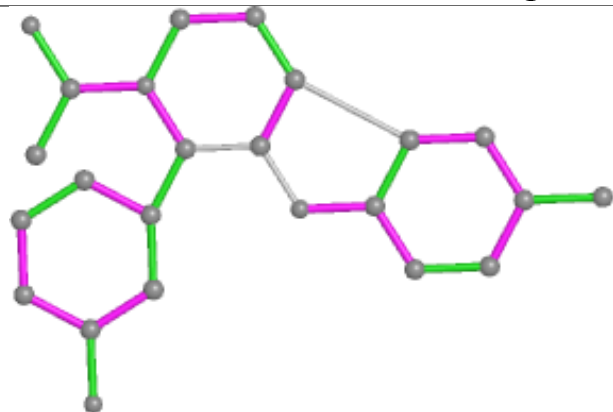
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	369	NO3	1	0
4	A	371	L31	3	0
3	B	371	ADP	1	0
3	A	370	ADP	1	0

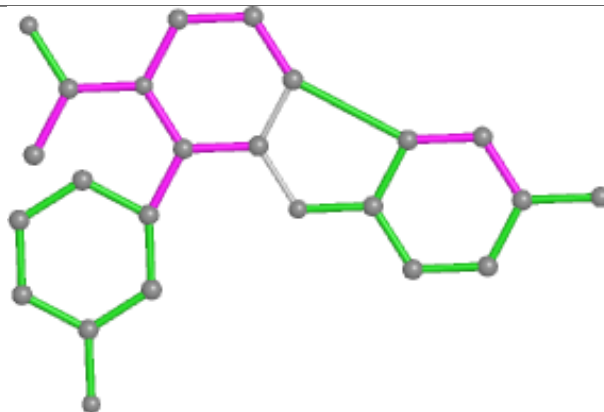
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



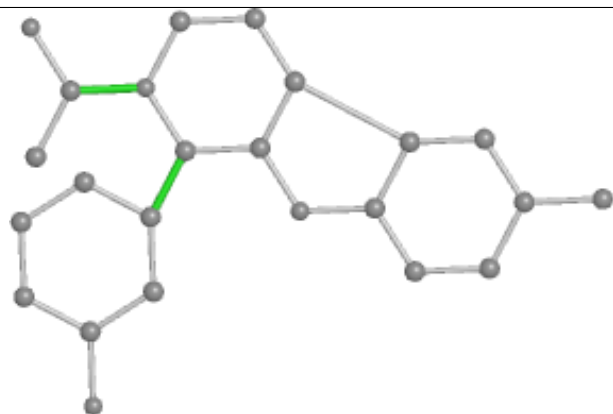
Ligand L31 A 371



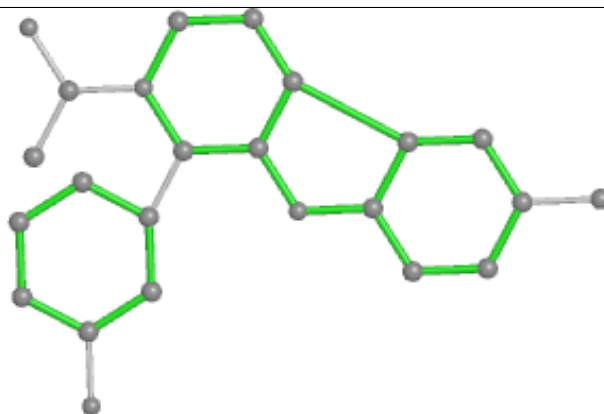
Bond lengths



Bond angles

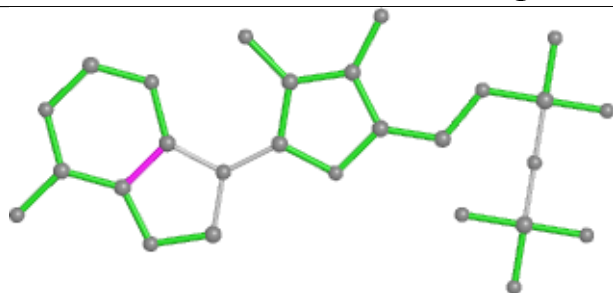


Torsions

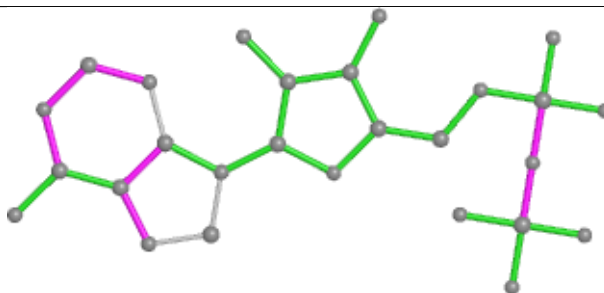


Rings

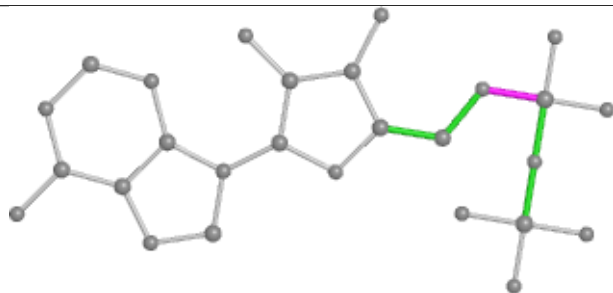
Ligand ADP B 371



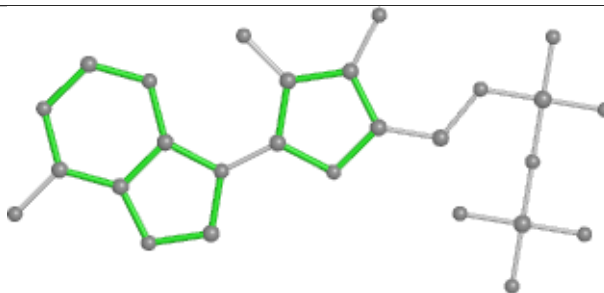
Bond lengths



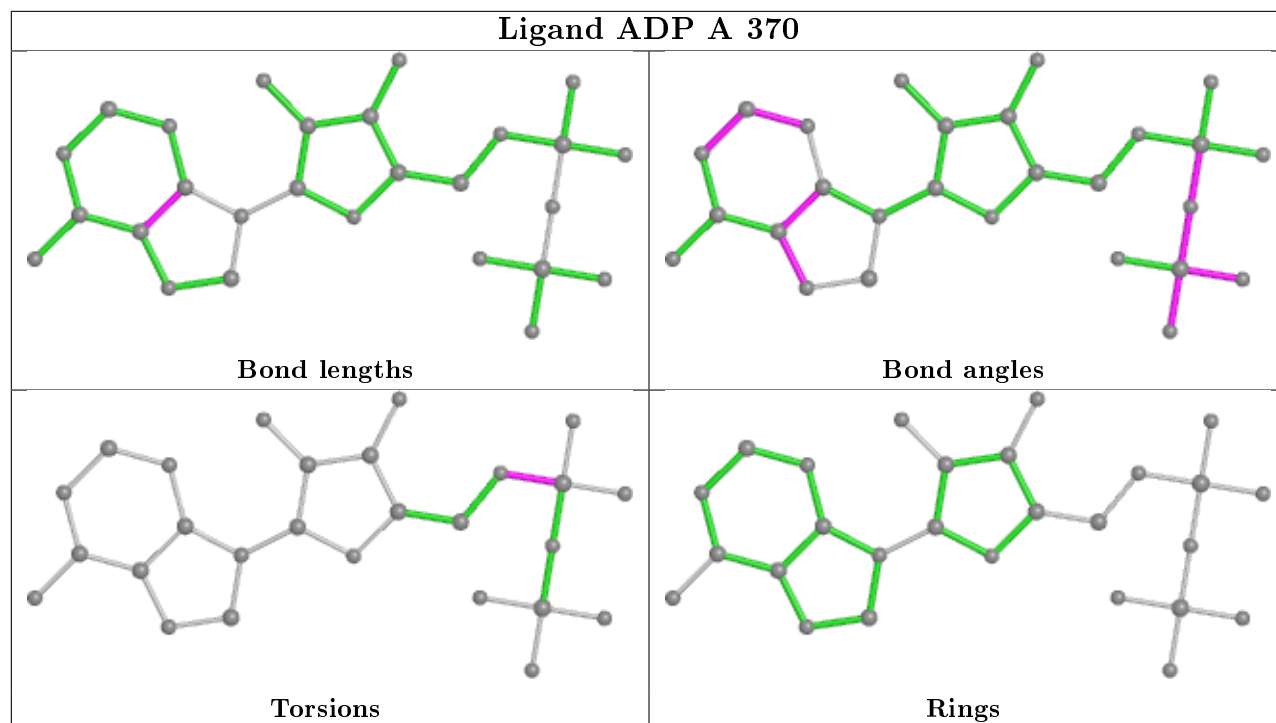
Bond angles



Torsions



Rings



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	335/368 (91%)	0.50	25 (7%) 14 13	42, 59, 100, 118	0
1	B	331/368 (89%)	0.64	36 (10%) 5 5	44, 63, 103, 118	0
All	All	666/736 (90%)	0.57	61 (9%) 9 8	42, 61, 101, 118	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	5.7
1	B	364	GLU	5.6
1	A	326	GLY	5.5
1	B	326	GLY	5.4
1	A	55	GLY	5.0
1	A	56	GLY	4.7
1	B	122	ASN	4.4
1	B	177	ASP	4.2
1	A	327	ARG	4.1
1	B	288	ILE	4.0
1	A	286	GLY	4.0
1	A	121	PRO	3.9
1	B	53	ARG	3.9
1	B	307	PRO	3.8
1	A	290	GLN	3.8
1	B	271	ASN	3.7
1	B	59	ASP	3.7
1	B	289	ASN	3.7
1	B	178	VAL	3.7
1	A	61	SER	3.6
1	B	252	GLY	3.5
1	B	363	PRO	3.5
1	A	59	ASP	3.4
1	B	287	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	285	ALA	3.3
1	B	46	VAL	3.3
1	B	253	GLU	3.2
1	B	362	LYS	3.2
1	B	16	GLY	3.2
1	A	122	ASN	3.1
1	B	61	SER	3.0
1	B	179	SER	3.0
1	A	187	ASP	2.9
1	B	62	SER	2.9
1	A	252	GLY	2.8
1	B	123	GLU	2.8
1	B	54	THR	2.8
1	B	301	ALA	2.8
1	B	300	THR	2.7
1	A	204	VAL	2.7
1	A	287	ASN	2.6
1	A	254	GLU	2.6
1	A	243	ILE	2.5
1	B	353	ALA	2.5
1	B	306	THR	2.4
1	B	176	SER	2.4
1	B	308	HIS	2.4
1	B	51	SER	2.4
1	A	185	PHE	2.3
1	B	208	ASP	2.3
1	A	178	VAL	2.3
1	A	179	SER	2.2
1	B	126	THR	2.2
1	A	58	ALA	2.1
1	A	155	SER	2.1
1	B	256	VAL	2.1
1	A	123	GLU	2.1
1	B	350	LEU	2.0
1	A	325	GLY	2.0
1	B	325	GLY	2.0
1	B	227	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

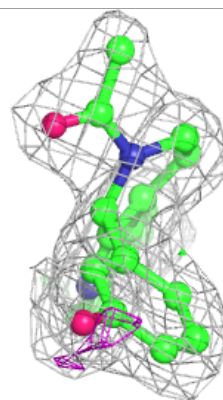
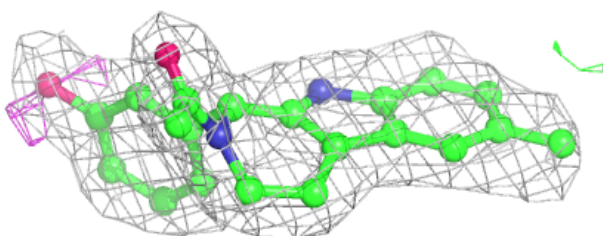
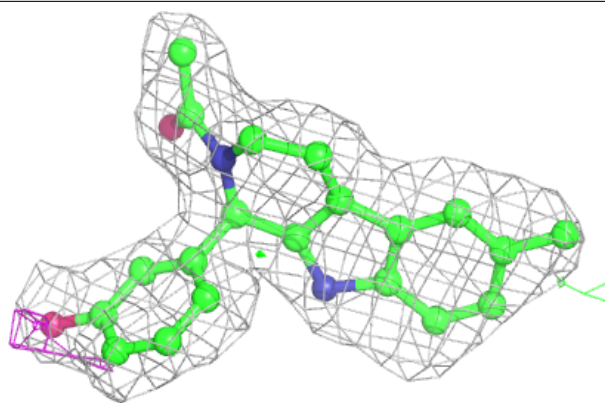
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PEG	A	374	7/7	0.79	0.27	67,79,80,82	0
2	MG	A	369	1/1	0.86	0.34	52,52,52,52	0
5	NO3	B	369	4/4	0.86	0.31	82,105,108,109	0
4	L31	A	371	24/24	0.88	0.16	35,43,46,55	0
6	CL	A	373	1/1	0.89	0.11	87,87,87,87	0
4	L31	B	372	24/24	0.91	0.17	37,48,53,89	0
5	NO3	A	372	4/4	0.91	0.13	74,78,83,88	0
2	MG	B	370	1/1	0.92	0.33	54,54,54,54	0
3	ADP	A	370	27/27	0.95	0.17	40,49,56,59	0
3	ADP	B	371	27/27	0.95	0.16	40,48,52,54	0

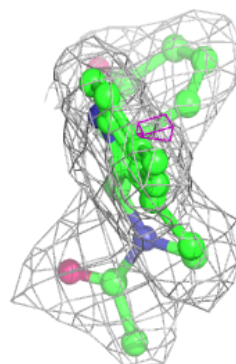
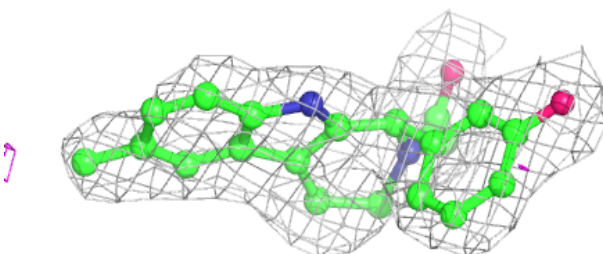
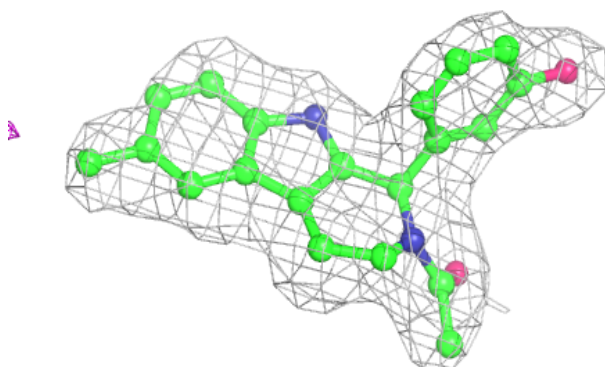
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L31 A 371:

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

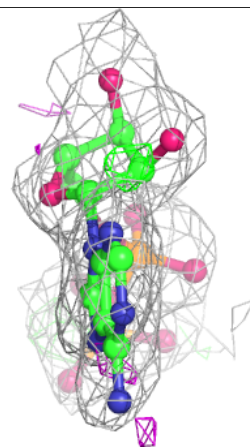
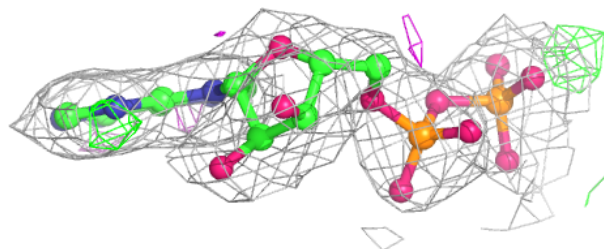
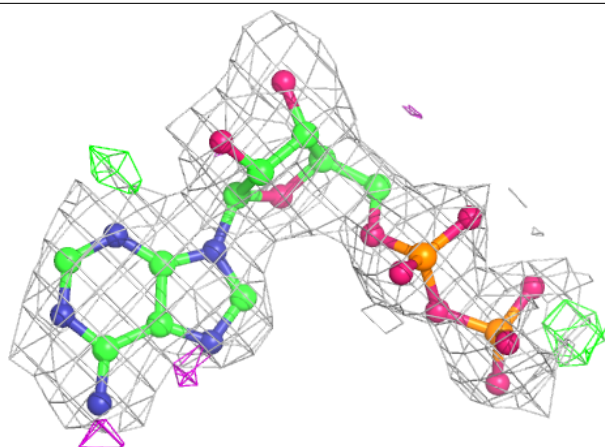
**Electron density around L31 B 372:**

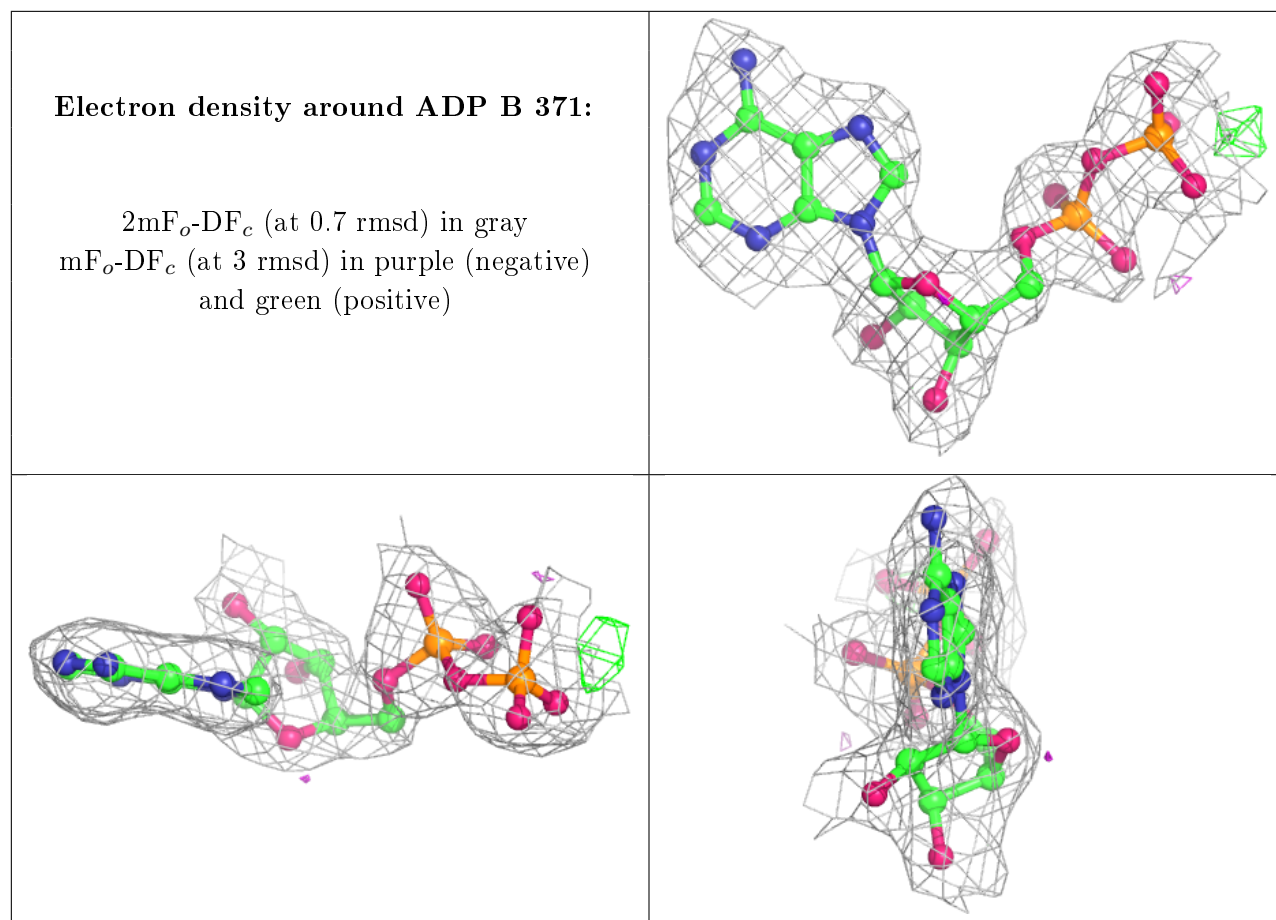
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 370:

$2mF_o - DF_c$ (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.