



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:15 am BST

PDB ID : 2X7D
Title : Crystal structure of human kinesin Eg5 in complex with (S)-dimethylenastron
Authors : Kaan, H.Y.K.; Ulaganathan, V.; Rath, O.; Laggner, C.; Prokopcova, H.;
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Deposited on : 2010-02-26
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

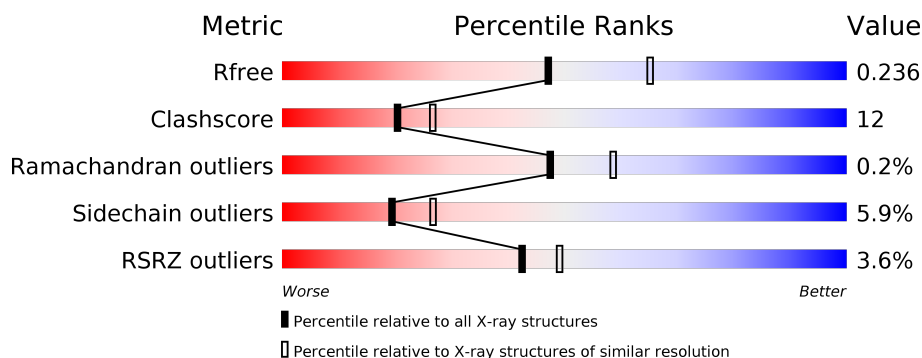
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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>3%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>• 9%</div> </div> </div>
1	B	368	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>• 9%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5990 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.

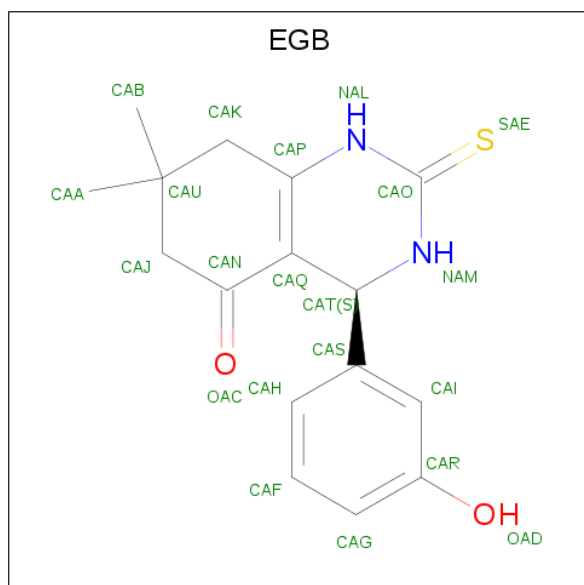
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	10	0
			2670	1674	461	524	11			
1	B	334	Total	C	N	O	S	0	11	0
			2689	1689	465	524	11			

- 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
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is (4S)-4-(3-HYDROXYPHENYL)-7,7-DIMETHYL-2-THIOXO-2,3,4,6,7,8-HEXAHYDROQUINAZOLIN-5(1H)-ONE (three-letter code: EGB) (formula: C₁₆H₁₈N₂O₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 21 16 2 2 1	0	0
4	B	1	Total C N O S 21 16 2 2 1	0	0

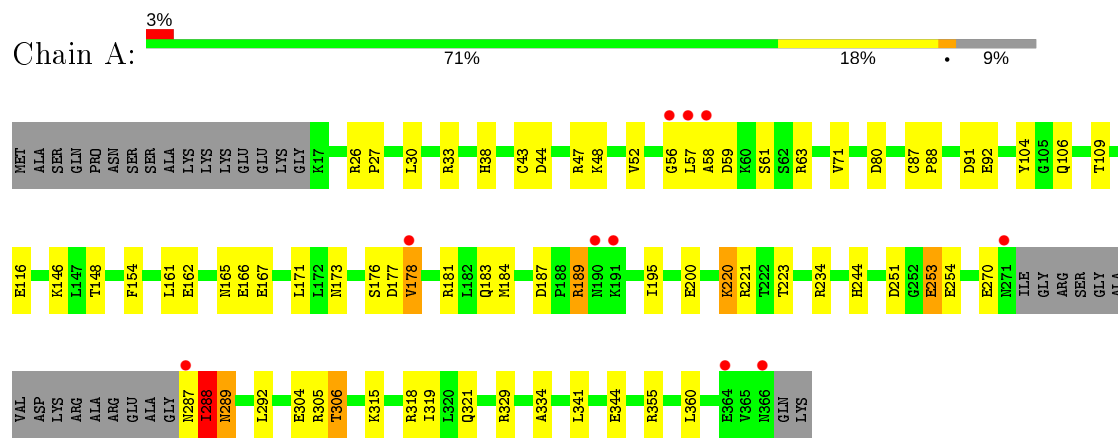
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	286	Total O 286 286	0	0
5	B	245	Total O 245 245	0	0

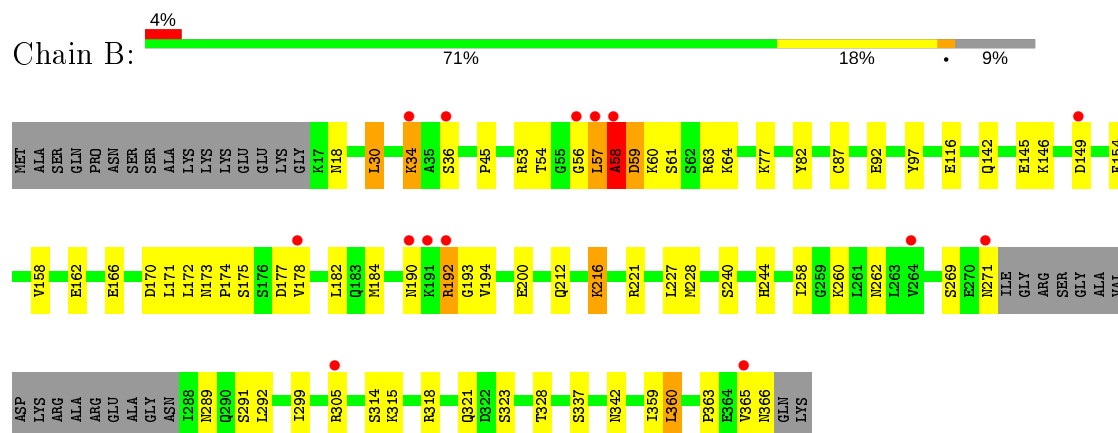
3 Residue-property plots [i](#)

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-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	69.52Å 79.72Å 159.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.30 29.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.58-2.30) 99.9 (29.58-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.241 0.176 , 0.236	Depositor DCC
R_{free} test set	2003 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 38.97 % 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 3.4053e-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: EGB, 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	0.67	2/2740 (0.1%)	0.82	4/3709 (0.1%)
1	B	0.65	0/2761	0.98	3/3733 (0.1%)
All	All	0.66	2/5501 (0.0%)	0.90	7/7442 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CD-OE2	-6.85	1.18	1.25
1	A	270	GLU	CD-OE1	-5.48	1.19	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ALA	CB-CA-C	29.94	155.01	110.10
1	B	59	ASP	N-CA-CB	-14.85	83.88	110.60
1	B	58	ALA	N-CA-C	-10.25	83.31	111.00
1	A	288	ILE	N-CA-CB	-7.44	93.69	110.80
1	A	59	ASP	N-CA-C	5.91	126.96	111.00
1	A	234	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	59	ASP	N-CA-CB	-5.25	101.14	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	ASP	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	2670	0	2686	59	0
1	B	2689	0	2730	76	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	21	0	18	1	0
4	B	21	0	18	1	0
5	A	286	0	0	13	0
5	B	245	0	0	12	0
All	All	5990	0	5476	135	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 12.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:SER:OG	1:B:63[A]:ARG:NH1	1.73	1.19
1:B:82[A]:TYR:CE1	1:B:87[A]:CYS:SG	2.48	1.06
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.41	0.98
1:B:82[A]:TYR:OH	1:B:142:GLN:HG3	1.65	0.97
1:A:116:GLU:OE2	1:A:221:ARG:NH2	1.99	0.95
1:A:92[A]:GLU:OE1	1:A:329[A]:ARG:HD2	1.68	0.94
1:A:355:ARG:NH2	5:A:2276:HOH:O	2.06	0.89
1:A:44:ASP:OD2	1:A:47[A]:ARG:NE	2.07	0.88
1:A:344[A]:GLU:OE2	5:A:2265:HOH:O	1.95	0.85
1:B:60:LYS:O	1:B:61:SER:HB3	1.74	0.84
1:B:271[A]:ASN:ND2	5:B:2190:HOH:O	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82[A]:TYR:CZ	1:B:87[A]:CYS:SG	2.71	0.83
1:A:80:ASP:OD1	5:A:2062:HOH:O	2.00	0.79
1:A:344[A]:GLU:CD	5:A:2263:HOH:O	2.22	0.78
1:B:30:LEU:CD1	1:B:34:LYS:NZ	2.47	0.77
1:B:162:GLU:HG3	1:B:171:LEU:HD23	1.65	0.77
1:A:80:ASP:OD2	5:A:2063:HOH:O	2.03	0.77
1:B:61:SER:HB2	5:B:2031:HOH:O	1.84	0.76
1:B:260:LYS:HD3	5:B:2179:HOH:O	1.85	0.76
1:B:227[A]:LEU:HD22	1:B:228:MET:HG3	1.69	0.74
1:A:162:GLU:HG3	1:A:171:LEU:CD2	2.15	0.74
1:A:58:ALA:O	5:A:2040:HOH:O	2.05	0.74
1:B:30:LEU:HD12	1:B:34:LYS:NZ	2.03	0.74
1:A:187:ASP:OD1	1:A:189:ARG:HG3	1.90	0.72
1:A:344[A]:GLU:HG3	5:A:2263:HOH:O	1.89	0.71
1:B:175:SER:O	5:B:2119:HOH:O	2.09	0.71
1:A:251:ASP:OD1	5:A:2213:HOH:O	2.09	0.71
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.54	0.71
1:B:61:SER:HG	1:B:63[A]:ARG:HH12	1.32	0.70
1:B:92:GLU:HG3	1:B:97:TYR:CD2	2.28	0.68
1:A:43:CYS:HB3	1:A:71:VAL:HG12	1.76	0.68
1:B:30:LEU:HD12	1:B:34:LYS:HZ3	1.57	0.67
1:A:344[A]:GLU:OE1	5:A:2263:HOH:O	2.13	0.67
1:A:344[A]:GLU:CG	5:A:2263:HOH:O	2.43	0.67
1:A:91:ASP:OD1	1:A:146:LYS:HE2	1.94	0.67
1:B:166:GLU:O	1:B:315:LYS:HE2	1.94	0.67
1:B:57:LEU:O	1:B:58:ALA:CB	2.43	0.66
1:B:184:MET:HE3	1:B:318:ARG:NH1	2.10	0.66
1:B:193:GLY:HA2	5:B:2128:HOH:O	1.96	0.66
1:A:162:GLU:OE2	1:A:221:ARG:NH1	2.30	0.65
1:A:33:ARG:NH1	5:A:2009:HOH:O	2.29	0.65
1:B:184:MET:HE3	1:B:318:ARG:HD3	1.78	0.65
1:B:58:ALA:O	5:B:2032:HOH:O	2.14	0.65
1:A:184:MET:HE3	1:A:318:ARG:HD3	1.79	0.64
1:B:30:LEU:CD1	1:B:34:LYS:HZ3	2.11	0.64
1:B:56:GLY:O	1:B:60:LYS:O	2.14	0.64
1:B:227[A]:LEU:CD2	1:B:228:MET:HG3	2.29	0.63
1:A:184:MET:CE	1:A:318:ARG:NH1	2.62	0.62
1:B:212[B]:GLN:OE1	1:B:216:LYS:HE2	2.01	0.60
1:A:43:CYS:HB3	1:A:71:VAL:CG1	2.32	0.60
1:A:187:ASP:OD1	1:A:187:ASP:C	2.39	0.59
1:A:184:MET:HE2	1:A:318:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:HE3	1:B:318:ARG:CZ	2.34	0.57
1:A:166:GLU:O	1:A:315:LYS:HE2	2.03	0.57
1:B:184:MET:CE	1:B:318:ARG:NH1	2.69	0.56
1:B:82[B]:TYR:OH	1:B:142:GLN:CG	2.55	0.55
1:B:54:THR:HG21	1:B:64:LYS:HG3	1.89	0.54
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.90	0.54
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.90	0.53
1:B:18:ASN:OD1	1:B:360:LEU:CD2	2.57	0.53
1:B:363:PRO:O	5:B:2236:HOH:O	2.18	0.53
1:A:288:ILE:O	1:A:288:ILE:CG2	2.57	0.52
1:A:92[A]:GLU:OE1	1:A:329[A]:ARG:CD	2.51	0.52
1:B:146:LYS:HE2	5:B:2058:HOH:O	2.09	0.52
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.91	0.52
1:B:45:PRO:HD2	5:B:2021:HOH:O	2.11	0.51
1:A:289:ASN:HD22	1:A:292:LEU:H	1.58	0.51
1:B:171:LEU:HG	1:B:221:ARG:HG3	1.93	0.51
1:A:184:MET:HE3	1:A:318:ARG:CZ	2.40	0.51
1:B:173:ASN:HB2	1:B:200:GLU:HG3	1.92	0.51
1:B:30:LEU:CD1	1:B:34:LYS:HZ2	2.22	0.51
1:A:184:MET:HE3	1:A:318:ARG:CD	2.40	0.50
1:A:106:GLN:HG2	1:A:109:THR:CG2	2.42	0.50
1:B:57:LEU:O	1:B:58:ALA:HB2	2.12	0.50
1:B:184:MET:CE	1:B:318:ARG:HD3	2.41	0.50
1:A:288:ILE:O	1:A:288:ILE:HG23	2.12	0.49
1:A:87[A]:CYS:HB2	1:A:88:PRO:HD3	1.94	0.49
1:B:154:PHE:HA	1:B:244:HIS:O	2.12	0.49
1:A:289:ASN:ND2	1:A:292:LEU:H	2.10	0.49
1:B:192:ARG:HG2	1:B:192:ARG:NH1	2.25	0.49
1:B:82[B]:TYR:OH	1:B:142:GLN:HG3	2.13	0.49
1:B:291:SER:HA	1:B:314:SER:HB2	1.95	0.49
1:B:158:VAL:HA	1:B:240:SER:O	2.14	0.47
1:A:187:ASP:HB2	1:A:195:ILE:HG13	1.96	0.47
1:B:92:GLU:HG3	1:B:97:TYR:HD2	1.80	0.47
1:B:323:SER:HA	1:B:328:THR:HB	1.97	0.46
1:A:173:ASN:CB	1:A:200:GLU:HG3	2.46	0.46
1:B:30:LEU:HD11	1:B:34:LYS:NZ	2.29	0.46
1:B:53:ARG:HG3	5:B:2031:HOH:O	2.16	0.45
1:B:162:GLU:OE1	1:B:221:ARG:NE	2.43	0.45
1:A:178:VAL:HG22	1:A:220:LYS:HE2	1.98	0.45
1:A:104:TYR:O	1:A:334:ALA:HA	2.17	0.44
1:B:173:ASN:HA	1:B:174:PRO:HD3	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLN:HG2	1:A:109:THR:HG21	1.99	0.44
1:B:173:ASN:CB	1:B:200:GLU:HG3	2.47	0.44
1:B:184:MET:HE3	1:B:318:ARG:CD	2.46	0.44
1:B:321:GLN:NE2	5:B:2209:HOH:O	2.50	0.44
1:A:178:VAL:HG21	1:A:223:THR:HB	2.00	0.44
1:A:253[A]:GLU:HG3	1:A:254:GLU:N	2.32	0.43
1:A:306:THR:O	5:A:2240:HOH:O	2.22	0.43
1:B:116:GLU:HB3	4:B:1369:EGB:NAM	2.34	0.43
1:B:258:ILE:O	1:B:366:ASN:ND2	2.49	0.43
1:A:116:GLU:HB3	4:A:1369:EGB:HAM	1.84	0.43
1:B:82[A]:TYR:OH	1:B:87[A]:CYS:SG	2.76	0.43
1:A:161:LEU:HD21	1:A:319:ILE:HD13	2.01	0.42
1:B:82[A]:TYR:HE1	1:B:87[A]:CYS:SG	2.30	0.42
1:A:26:ARG:HB2	1:A:27:PRO:HD2	2.01	0.42
1:B:337:SER:CB	1:B:342:ASN:HD22	2.31	0.42
1:B:61:SER:HG	1:B:63[A]:ARG:NH1	1.99	0.42
1:A:184:MET:CE	1:A:318:ARG:CZ	2.97	0.42
1:A:56:GLY:HA3	1:A:61[A]:SER:HA	2.01	0.42
1:A:154:PHE:HA	1:A:244:HIS:O	2.19	0.42
1:B:18:ASN:OD1	1:B:360:LEU:HD23	2.19	0.42
1:B:53:ARG:HH21	1:B:63[A]:ARG:NH2	2.17	0.42
1:A:253[B]:GLU:OE1	1:A:253[B]:GLU:HA	2.19	0.42
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.92	0.42
1:B:212[B]:GLN:HB3	1:B:212[B]:GLN:HE21	1.72	0.42
1:B:57:LEU:O	1:B:58:ALA:HB3	2.20	0.42
1:A:173:ASN:HA	1:A:200:GLU:HG3	2.01	0.42
1:A:184:MET:HE3	1:A:318:ARG:NE	2.35	0.41
1:B:57:LEU:HD12	1:B:57:LEU:H	1.84	0.41
1:B:240:SER:OG	1:B:262:ASN:ND2	2.52	0.41
1:B:162:GLU:CG	1:B:171:LEU:HD23	2.44	0.41
1:A:173:ASN:HB2	1:A:200:GLU:HG3	2.03	0.41
1:B:269:SER:HA	1:B:292:LEU:HD21	2.03	0.41
1:A:304:GLU:O	1:A:305:ARG:HB2	2.21	0.40
1:B:291:SER:HA	1:B:314:SER:CB	2.52	0.40
1:A:47[A]:ARG:CZ	5:A:2031:HOH:O	2.70	0.40
1:A:52:VAL:O	1:A:63:ARG:HA	2.22	0.40
1:B:194:VAL:N	5:B:2128:HOH:O	2.49	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	341/368 (93%)	333 (98%)	8 (2%)	0	100	100
1	B	340/368 (92%)	329 (97%)	10 (3%)	1 (0%)	41	50
All	All	681/736 (92%)	662 (97%)	18 (3%)	1 (0%)	47	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	ALA

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	303/322 (94%)	282 (93%)	21 (7%)	15	20
1	B	307/322 (95%)	292 (95%)	15 (5%)	25	35
All	All	610/644 (95%)	574 (94%)	36 (6%)	19	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	57	LEU
1	A	148	THR
1	A	165	ASN
1	A	167	GLU

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Mol	Chain	Res	Type
1	A	176	SER
1	A	177	ASP
1	A	178	VAL
1	A	181	ARG
1	A	183	GLN
1	A	189	ARG
1	A	220	LYS
1	A	253[A]	GLU
1	A	253[B]	GLU
1	A	287	ASN
1	A	288	ILE
1	A	289	ASN
1	A	306	THR
1	A	321	GLN
1	A	341	LEU
1	A	360	LEU
1	B	30	LEU
1	B	34	LYS
1	B	36	SER
1	B	57	LEU
1	B	77	LYS
1	B	145	GLU
1	B	177	ASP
1	B	178	VAL
1	B	190	ASN
1	B	192	ARG
1	B	216	LYS
1	B	289	ASN
1	B	305	ARG
1	B	360	LEU
1	B	365	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	262	ASN
1	A	289	ASN
1	B	262	ASN
1	B	289	ASN
1	B	290	GLN
1	B	308	HIS

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Mol	Chain	Res	Type
1	B	321	GLN
1	B	342	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	601	3	24,29,29	1.07	3 (12%)	29,45,45	1.33	4 (13%)
4	EGB	B	1369	-	23,23,23	3.63	7 (30%)	34,35,35	3.85	10 (29%)
4	EGB	A	1369	-	23,23,23	3.85	7 (30%)	34,35,35	3.78	11 (32%)
2	ADP	B	602	3	24,29,29	0.97	1 (4%)	29,45,45	1.45	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
2	ADP	A	601	3	-	0/12/32/32	0/3/3/3
4	EGB	B	1369	-	-	0/4/34/34	0/3/3/3
4	EGB	A	1369	-	-	0/4/34/34	0/3/3/3
2	ADP	B	602	3	-	1/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1369	EGB	CAO-NAM	13.11	1.46	1.33
4	A	1369	EGB	CAO-NAM	12.68	1.45	1.33
4	A	1369	EGB	CAO-NAL	8.05	1.45	1.36
4	B	1369	EGB	CAO-NAL	8.04	1.45	1.36
4	A	1369	EGB	CAK-CAP	6.37	1.57	1.50
4	A	1369	EGB	CAO-SAE	5.23	1.80	1.68
4	B	1369	EGB	CAO-SAE	4.94	1.79	1.68
4	B	1369	EGB	CAN-CAQ	-3.59	1.38	1.45
4	A	1369	EGB	CAN-CAQ	-3.21	1.39	1.45
4	A	1369	EGB	CAT-CAQ	2.89	1.54	1.51
2	A	601	ADP	O4'-C1'	2.74	1.44	1.41
4	B	1369	EGB	CAT-NAM	2.52	1.49	1.47
4	B	1369	EGB	CAK-CAP	2.47	1.53	1.50
2	B	602	ADP	C5-C4	2.41	1.47	1.40
4	B	1369	EGB	CAP-CAQ	2.37	1.39	1.36
4	A	1369	EGB	CAJ-CAN	2.33	1.54	1.51
2	A	601	ADP	C2-N3	2.15	1.35	1.32
2	A	601	ADP	C5-C4	2.02	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1369	EGB	CAO-NAL-CAP	-13.79	115.49	123.84
4	A	1369	EGB	CAO-NAL-CAP	-10.40	117.54	123.84
4	B	1369	EGB	SAE-CAO-NAL	-10.40	108.40	122.08
4	A	1369	EGB	SAE-CAO-NAM	-9.96	110.49	122.68
4	A	1369	EGB	SAE-CAO-NAL	-9.65	109.38	122.08
4	A	1369	EGB	CAT-NAM-CAO	-9.19	111.61	125.27
4	B	1369	EGB	SAE-CAO-NAM	-9.09	111.56	122.68
4	B	1369	EGB	CAT-NAM-CAO	-7.77	113.72	125.27
4	A	1369	EGB	OAC-CAN-CAQ	-4.58	116.68	121.30
4	A	1369	EGB	CAJ-CAN-CAQ	4.25	124.50	118.27
2	A	601	ADP	N3-C2-N1	-3.95	122.51	128.68
2	B	602	ADP	N3-C2-N1	-3.43	123.31	128.68
2	B	602	ADP	C2-N1-C6	3.03	123.94	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1369	EGB	CAU-CAJ-CAN	-2.97	110.08	114.48
4	B	1369	EGB	CAQ-CAT-NAM	2.92	111.42	109.09
4	A	1369	EGB	CAS-CAT-NAM	2.88	114.13	110.87
4	B	1369	EGB	CAJ-CAN-CAQ	2.86	122.46	118.27
4	B	1369	EGB	CAU-CAJ-CAN	-2.78	110.36	114.48
4	A	1369	EGB	NAL-CAO-NAM	-2.76	114.21	116.22
2	B	602	ADP	C4-C5-N7	-2.51	106.78	109.40
2	A	601	ADP	N6-C6-N1	2.40	123.55	118.57
2	A	601	ADP	O3B-PB-O2B	2.33	116.53	107.64
4	B	1369	EGB	OAC-CAN-CAQ	-2.26	119.01	121.30
2	B	602	ADP	O3'-C3'-C4'	-2.20	104.67	111.05
4	B	1369	EGB	CAS-CAT-CAQ	-2.17	109.88	112.84
2	B	602	ADP	O3'-C3'-C2'	-2.16	104.84	111.82
4	A	1369	EGB	CAR-CAI-CAS	2.16	121.96	120.11
2	A	601	ADP	C2-N1-C6	2.15	122.44	118.75
4	B	1369	EGB	CAR-CAI-CAS	2.02	121.85	120.11
4	A	1369	EGB	CAK-CAP-NAL	2.01	117.65	115.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	ADP	PA-O3A-PB-O2B

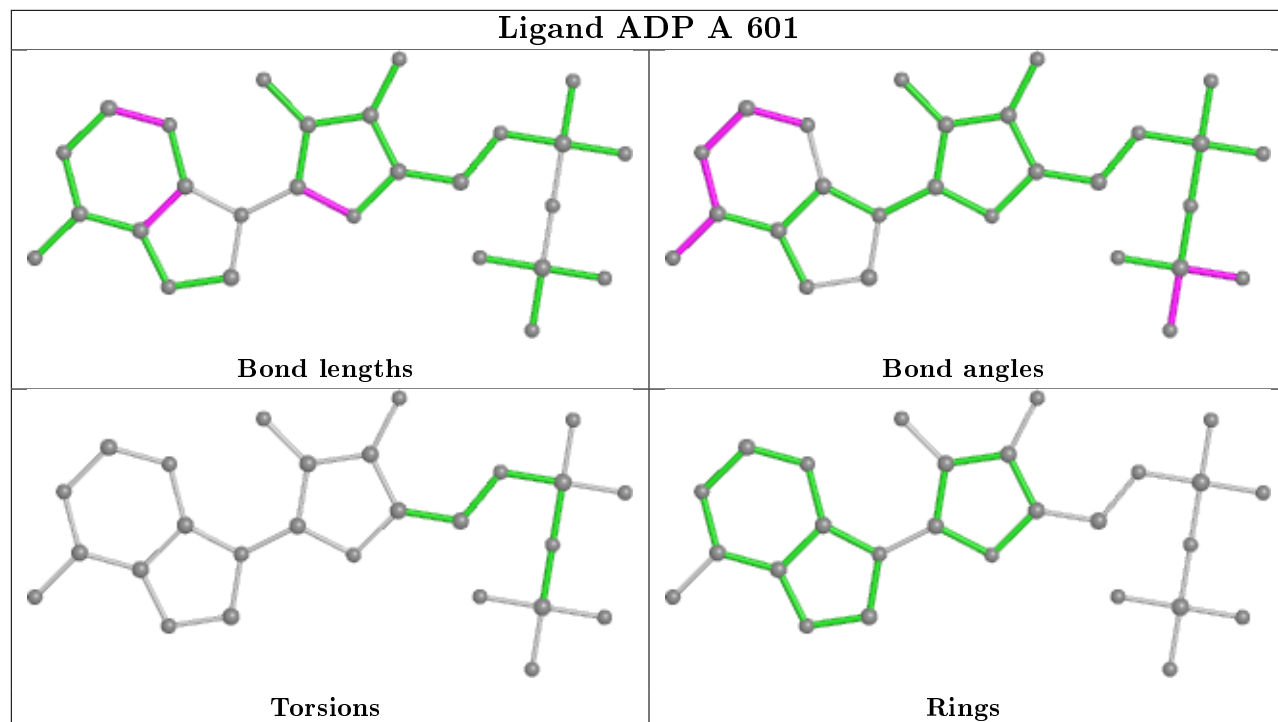
There are no ring outliers.

2 monomers are involved in 2 short contacts:

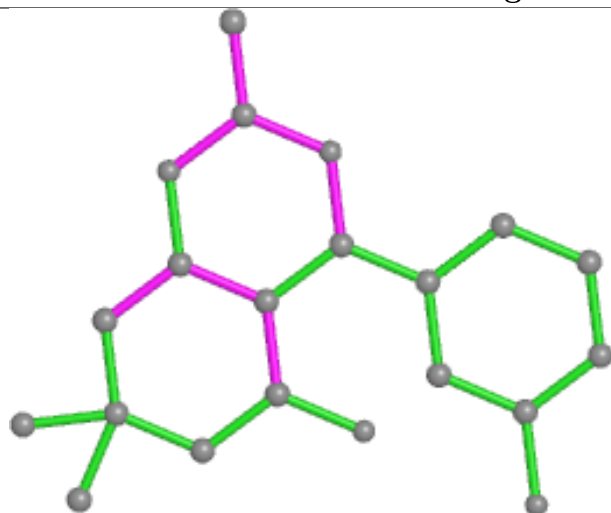
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1369	EGB	1	0
4	A	1369	EGB	1	0

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

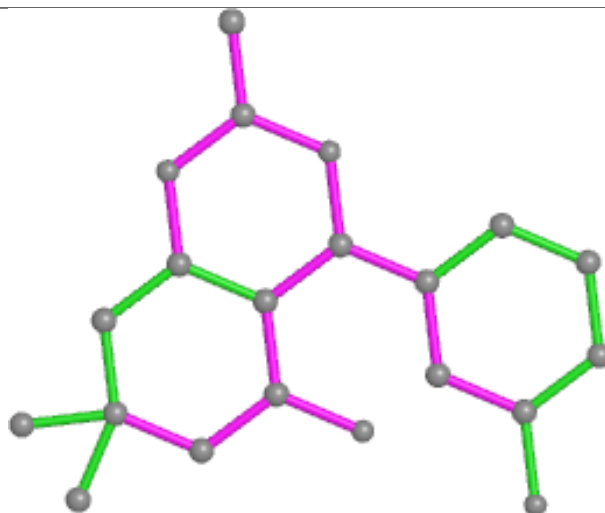
equivalents in the CSD to analyse the geometry.



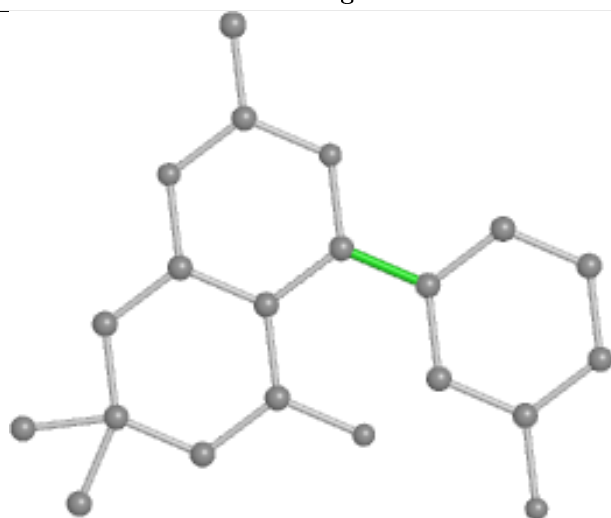
Ligand EGB B 1369



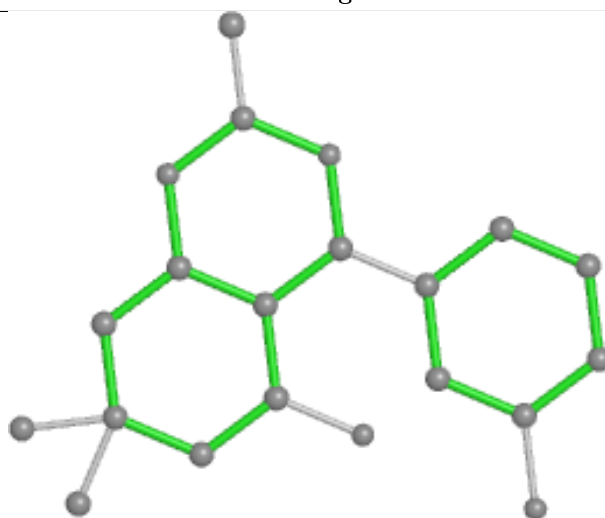
Bond lengths



Bond angles

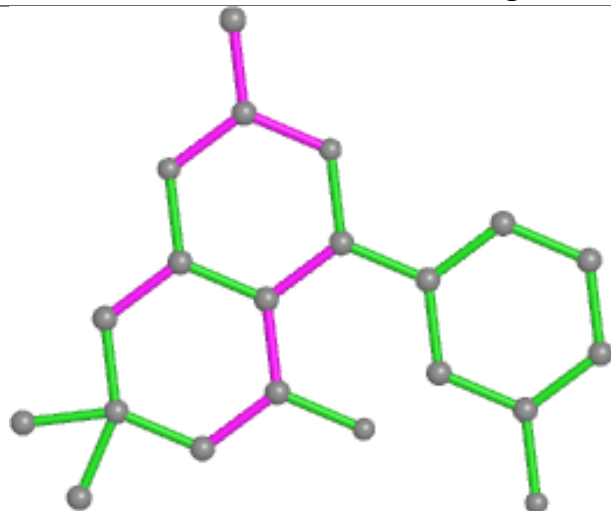


Torsions

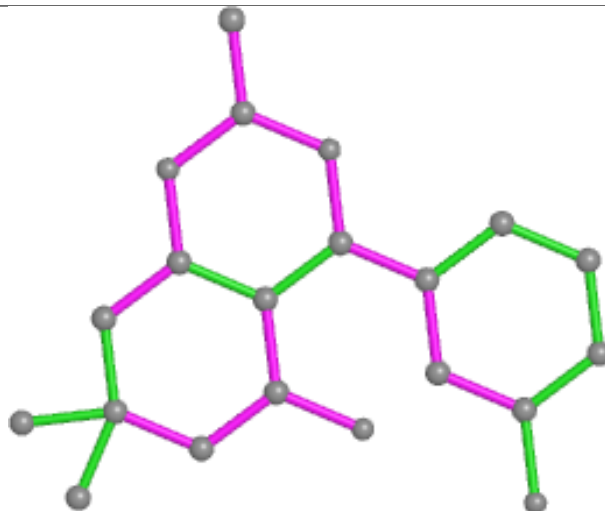


Rings

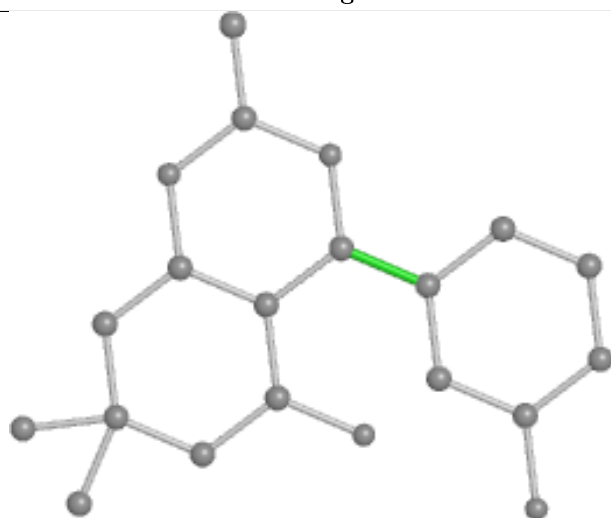
Ligand EGB A 1369



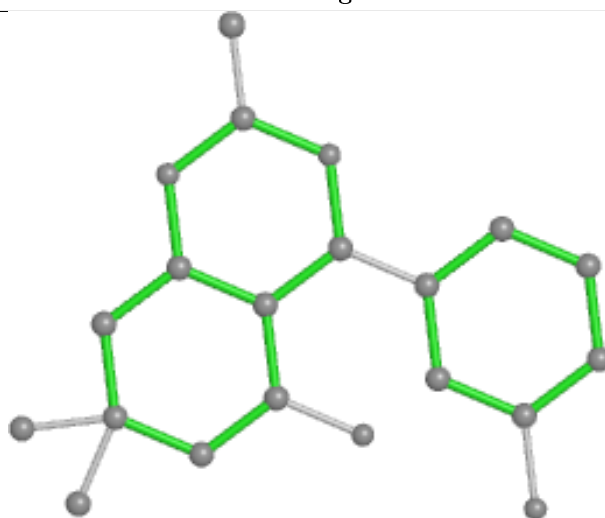
Bond lengths



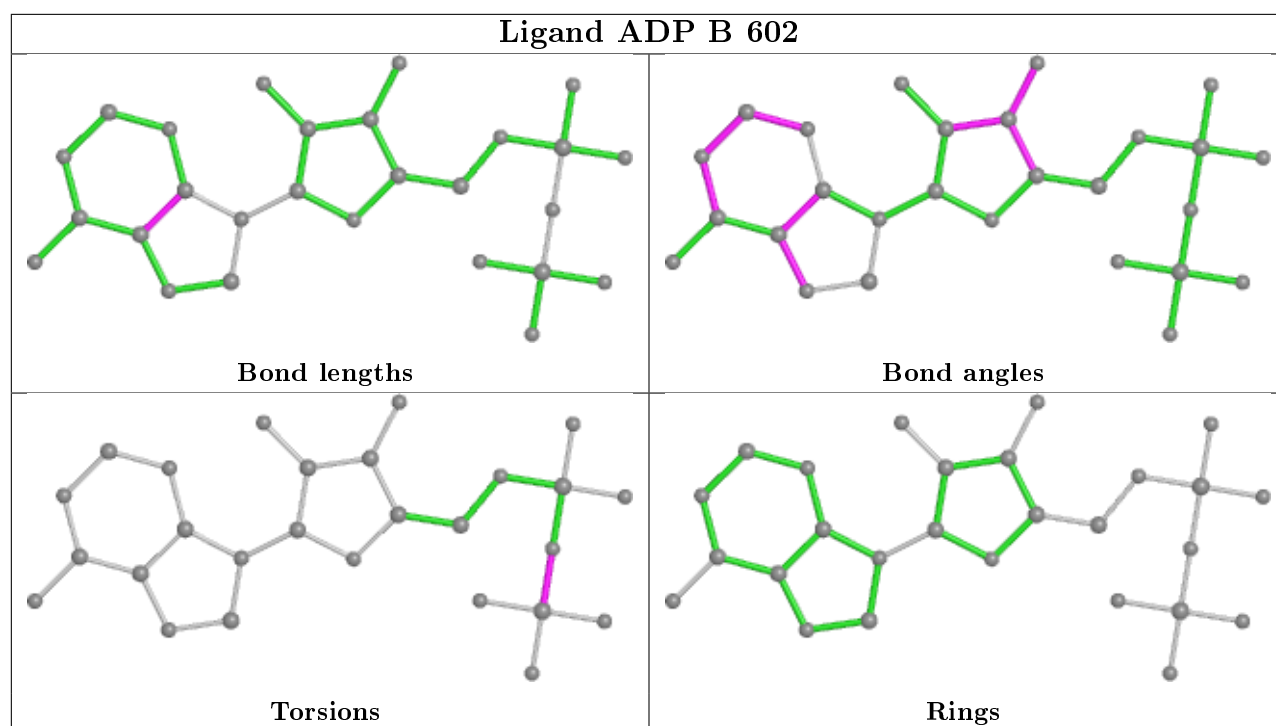
Bond angles



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%)	-0.15	10 (2%) 50 57	6, 18, 45, 60	0
1	B	334/368 (90%)	-0.07	14 (4%) 36 43	6, 17, 44, 67	0
All	All	669/736 (90%)	-0.11	24 (3%) 42 49	6, 17, 44, 67	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	ALA	11.1
1	A	57	LEU	9.4
1	B	57	LEU	7.6
1	B	149[A]	ASP	4.9
1	B	190	ASN	4.1
1	A	178	VAL	4.1
1	A	58	ALA	4.1
1	A	271	ASN	4.0
1	B	192	ARG	3.9
1	B	56	GLY	3.7
1	A	190	ASN	3.7
1	B	34	LYS	3.5
1	B	365	VAL	3.4
1	B	36	SER	3.0
1	A	287	ASN	2.8
1	A	56	GLY	2.7
1	B	191	LYS	2.6
1	B	264	VAL	2.5
1	A	364	GLU	2.5
1	B	305	ARG	2.4
1	A	366	ASN	2.3
1	B	178	VAL	2.2
1	A	191	LYS	2.1
1	B	271[A]	ASN	2.1

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](#)

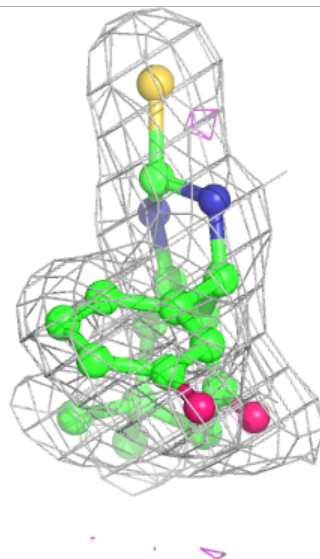
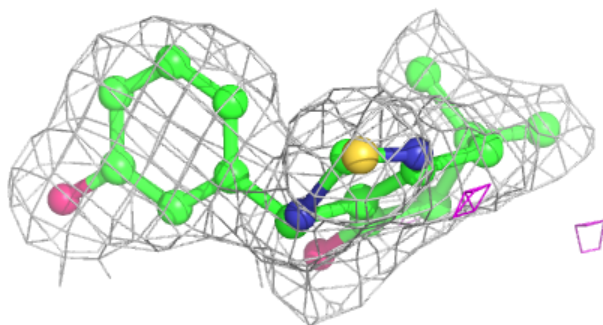
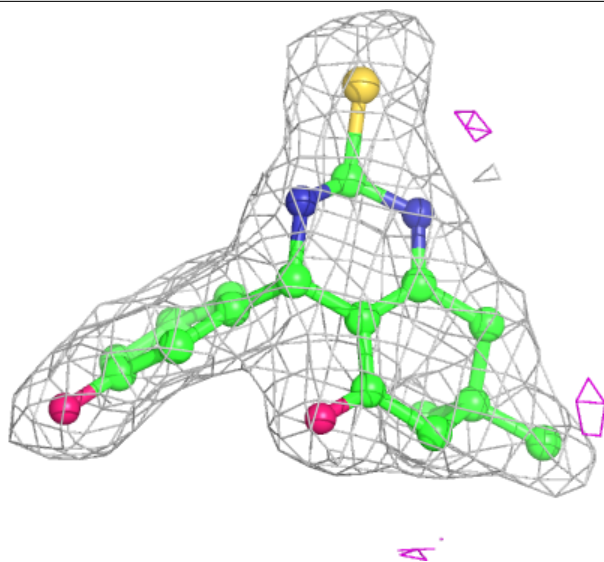
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1367	1/1	0.96	0.11	12,12,12,12	0
3	MG	A	1368	1/1	0.96	0.25	17,17,17,17	0
4	EGB	B	1369	21/21	0.98	0.12	6,8,11,14	0
4	EGB	A	1369	21/21	0.98	0.10	6,11,15,18	0
3	MG	B	1367	1/1	0.99	0.06	8,8,8,8	0
2	ADP	A	601	27/27	0.99	0.11	6,17,21,26	0
3	MG	B	1368	1/1	0.99	0.20	3,3,3,3	0
2	ADP	B	602	27/27	0.99	0.09	7,12,17,18	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.

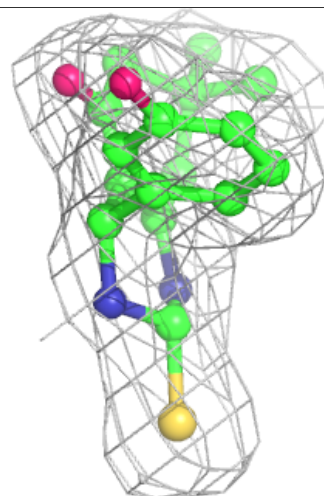
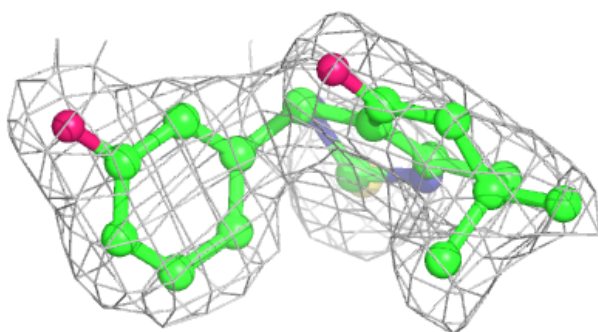
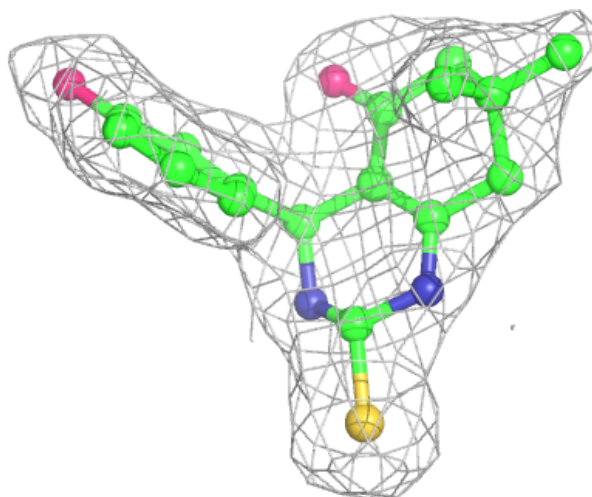
Electron density around EGB B 1369:

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



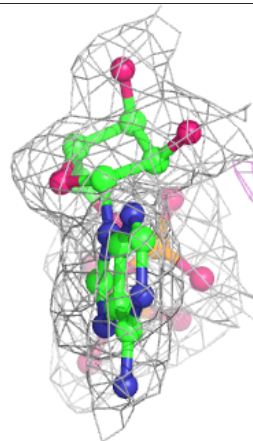
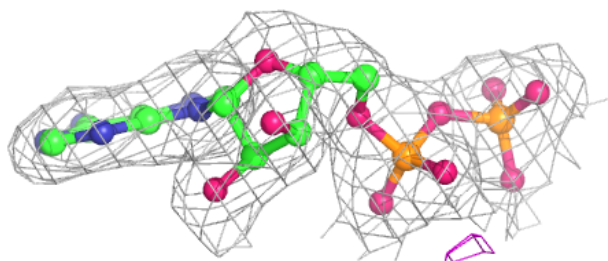
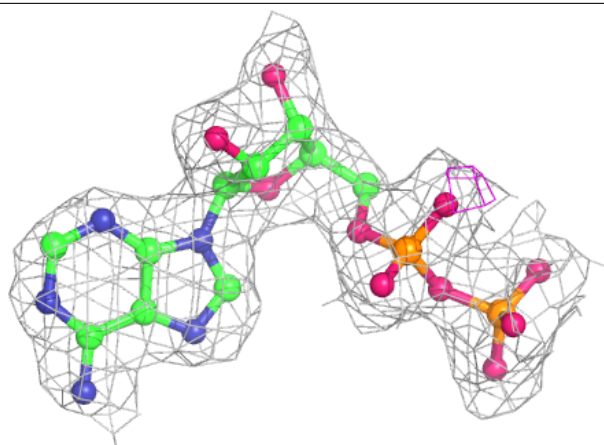
Electron density around EGB A 1369:

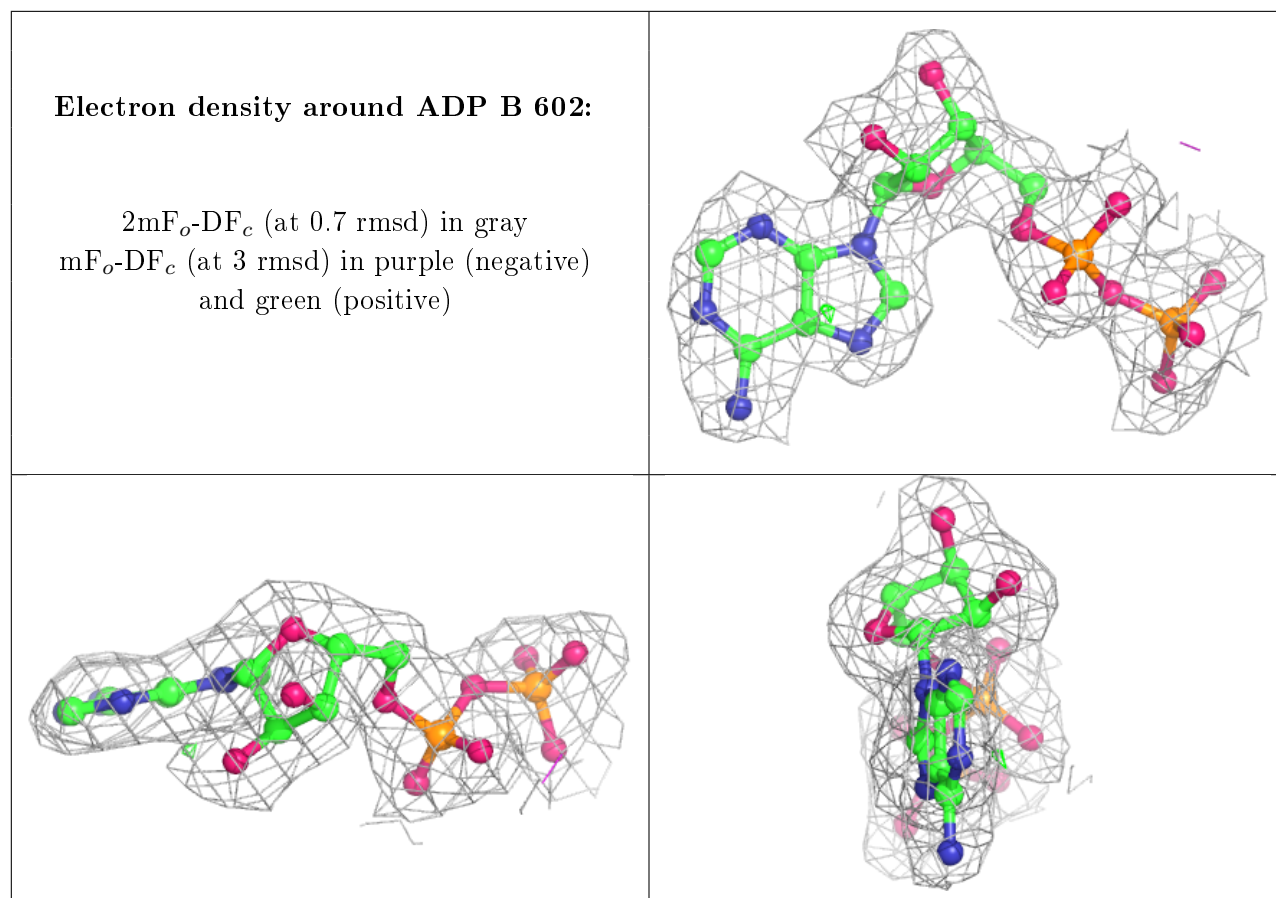
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 601:

$2mF_o - DF_c$ (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.