



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:30 am BST

PDB ID : 5J5Y
Title : Translation initiation factor 4E in complex with m2(7,2'O)GppCCl2ppG mRNA 5' cap analog
Authors : Warminski, M.; Nowak, E.; Rydzik, A.M.; Kowalska, J.; Jemielity, J.; Nowotny, M.
Deposited on : 2016-04-04
Resolution : 1.75 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

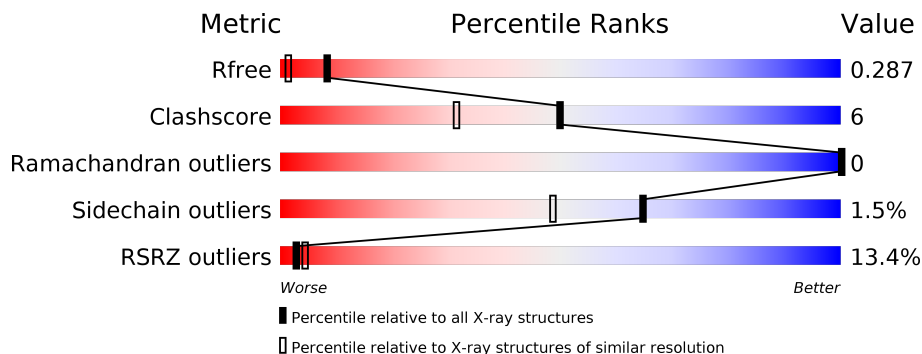
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	190	 3% 85% 11%
1	B	190	 0% 85% 10% 5%
1	C	190	 22% 67% 14% 18%
1	D	190	 23% 68% 16% 15%

2 Entry composition [i](#)

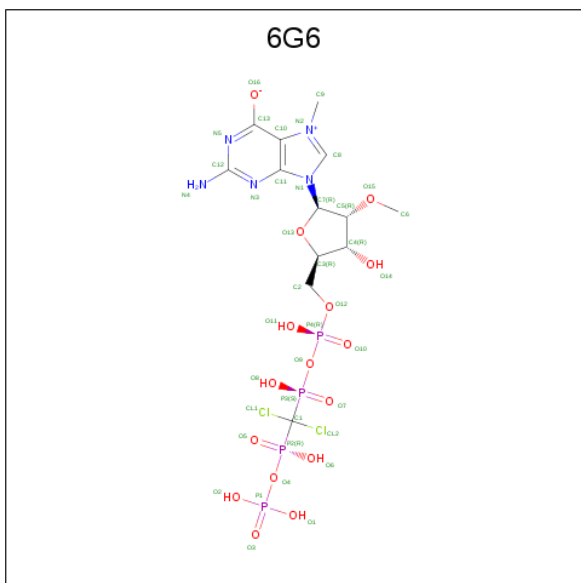
There are 4 unique types of molecules in this entry. The entry contains 5784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Eukaryotic translation initiation factor 4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	Total 1499	C 960	N 261	O 272	S 6	0	3	0
1	B	181	Total 1484	C 950	N 255	O 273	S 6	0	3	0
1	C	155	Total 1197	C 767	N 204	O 220	S 6	0	2	0
1	D	162	Total 1251	C 795	N 220	O 232	S 4	0	2	0

- Molecule 2 is 2-amino-9- $\{5\text{-O-}[(R)\text{-}\{(S)\text{-}\{dichloro[(R)\text{-hydroxy(phosphonoxy)phosphoryl}]\text{methyl}\}(\text{hydroxy)phosphoryl}]\text{oxy}\}(\text{hydroxy)phosphoryl}\text{-2-O-methyl-beta-D-ribofuranosyl}\}\text{-7-methyl-9H-purin-7-ium-6-olate}$ (three-letter code: 6G6) (formula: $\text{C}_{13}\text{H}_{21}\text{Cl}_2\text{N}_5\text{O}_{16}\text{P}_4$).



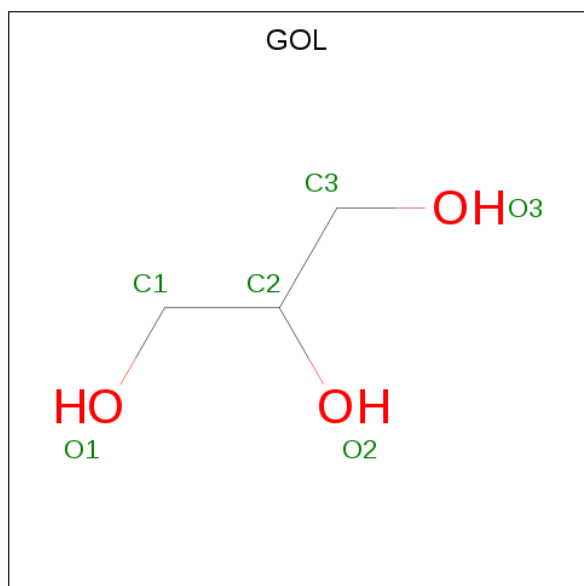
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			P
2	A	1	Total 36	C 13	Cl 2	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			P
2	B	1	40	13	2	5	16	4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	6	3	3	0	0

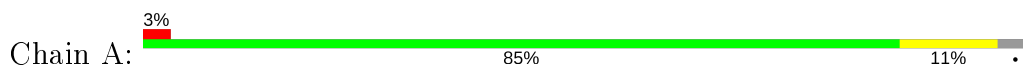
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	101	102	102	0	1
4	B	111	112	112	0	1
4	C	28	28	28	0	0
4	D	29	29	29	0	0

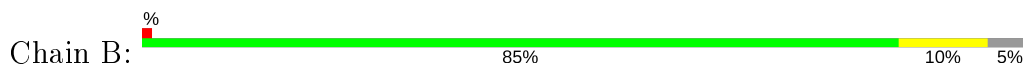
3 Residue-property plots [i](#)

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.

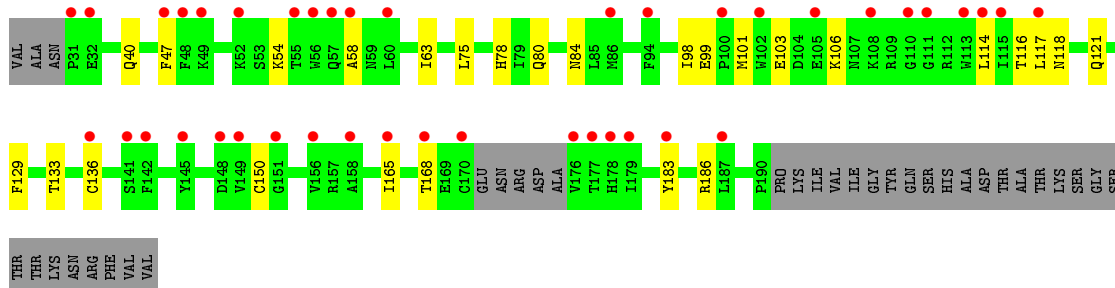
- Molecule 1: Eukaryotic translation initiation factor 4E



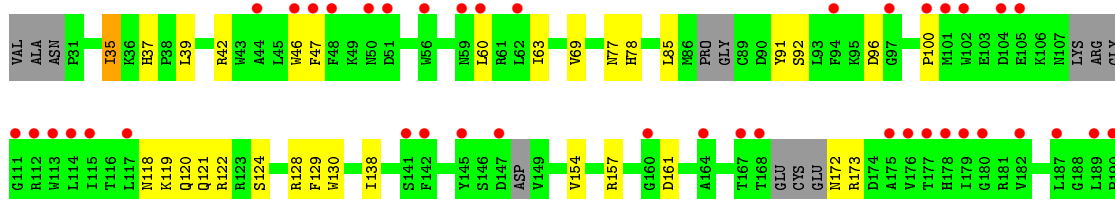
- Molecule 1: Eukaryotic translation initiation factor 4E



- Molecule 1: Eukaryotic translation initiation factor 4E



- Molecule 1: Eukaryotic translation initiation factor 4E



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.04Å 38.06Å 146.74Å 88.36° 95.63° 103.54°	Depositor
Resolution (Å)	37.00 – 1.75 37.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	90.6 (37.00-1.75) 80.4 (37.00-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.236 , 0.286 0.239 , 0.287	Depositor DCC
R_{free} test set	3650 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.086 for -h,-k,h+1	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5784	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 6G6

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	0.49	1/1543 (0.1%)	0.65	0/2090
1	B	0.43	0/1532	0.61	0/2077
1	C	0.36	1/1233 (0.1%)	0.50	0/1679
1	D	0.32	0/1281	0.53	0/1737
All	All	0.41	2/5589 (0.0%)	0.58	0/7583

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	99	GLU	C-N	7.02	1.47	1.34
1	C	99	GLU	C-N	5.61	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	90	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	1499	0	1445	11	0
1	B	1484	0	1415	11	0
1	C	1197	0	1082	16	0
1	D	1251	0	1113	23	0
2	A	36	0	0	1	0
2	B	40	0	0	0	0
3	B	6	0	8	1	0
4	A	102	0	0	0	0
4	B	112	0	0	2	0
4	C	28	0	0	1	0
4	D	29	0	0	1	0
All	All	5784	0	5063	61	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 6.

All (61) 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:118:ASN:H	1:A:121:GLN:HE21	1.37	0.72
1:B:60:LEU:HD21	1:B:100:PRO:HG2	1.75	0.68
1:A:103:GLU:OE1	2:A:300:6G6:N4	2.26	0.68
1:D:128:ARG:HH11	1:D:129:PHE:HE1	1.43	0.66
1:C:133:THR:HG23	1:C:165:ILE:HD11	1.77	0.65
1:C:47:PHE:HB2	1:C:63:ILE:HD11	1.81	0.63
1:D:119:LYS:HB2	1:D:120:GLN:HE21	1.61	0.63
1:D:119:LYS:HB2	1:D:120:GLN:NE2	2.13	0.63
1:A:118:ASN:H	1:A:121:GLN:NE2	1.97	0.62
1:D:39:LEU:HD13	1:D:138:ILE:HB	1.82	0.60
1:C:103:GLU:OE1	1:C:103:GLU:N	2.35	0.60
1:A:122:ARG:NH2	1:A:161:ASP:OD1	2.36	0.58
1:B:56:TRP:HZ3	1:B:101:MET:HE2	1.69	0.57
1:D:157:ARG:N	1:D:161:ASP:OD2	2.28	0.57
1:C:98:ILE:HG12	1:C:106:LYS:HD3	1.87	0.56
1:A:47:PHE:HB2	1:A:63:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD22	1:A:149:VAL:HG11	1.89	0.54
1:D:47:PHE:HB2	1:D:63:ILE:HD11	1.89	0.54
1:D:118:ASN:N	1:D:121:GLN:OE1	2.41	0.54
1:D:85:LEU:HD11	1:D:91:TYR:CE2	2.43	0.54
1:D:122:ARG:NH2	1:D:157:ARG:O	2.41	0.53
1:D:37[A]:HIS:HB2	1:D:69:VAL:HG12	1.91	0.53
1:A:122:ARG:NH2	1:A:157:ARG:O	2.43	0.53
1:B:36:LYS:HE3	1:B:68:THR:HG21	1.92	0.52
1:B:119:LYS:HG3	4:B:494:HOH:O	2.11	0.50
1:A:46:TRP:HB2	1:A:92:SER:HB2	1.94	0.50
1:C:114:LEU:HD22	1:C:116:THR:HG23	1.94	0.49
1:D:172:ASN:OD1	1:D:173:ARG:N	2.46	0.49
1:D:42:ARG:HG2	1:D:96:ASP:HB2	1.95	0.49
1:C:118:ASN:OD1	1:C:121:GLN:N	2.46	0.48
1:C:136:CYS:SG	1:C:186:ARG:HD3	2.53	0.48
1:B:95:LYS:HZ2	3:B:302:GOL:H32	1.79	0.48
1:C:54:LYS:HB3	1:C:58:ALA:HB3	1.95	0.47
1:A:190:PRO:HG2	1:A:193:ILE:HG12	1.96	0.47
1:C:150:CYS:SG	1:C:168:THR:HB	2.55	0.47
1:B:46:TRP:HB2	1:B:92:SER:HB2	1.98	0.46
1:B:144:ASP:N	1:B:144:ASP:OD1	2.45	0.46
1:A:35:ILE:HG22	1:A:36:LYS:O	2.16	0.46
1:B:35:ILE:O	1:B:35:ILE:HG13	2.15	0.45
1:C:165:ILE:HD13	1:C:183:TYR:CZ	2.52	0.45
1:D:130:TRP:CE3	1:D:154:VAL:HB	2.51	0.45
1:D:91:TYR:HB2	1:D:154:VAL:CG1	2.47	0.45
1:D:121:GLN:HA	1:D:124:SER:OG	2.16	0.44
1:D:35:ILE:HG13	1:D:35:ILE:O	2.17	0.44
1:C:80:GLN:NE2	1:C:84[B]:ASN:HD22	2.17	0.43
1:C:101:MET:HG3	1:C:103:GLU:HG2	2.00	0.43
1:D:60:LEU:HD21	1:D:100:PRO:HG2	1.99	0.43
1:D:118:ASN:OD1	1:D:121:GLN:N	2.51	0.43
1:D:37[B]:HIS:HB3	1:D:69:VAL:HG12	1.99	0.43
1:B:113:TRP:O	1:B:164:ALA:HA	2.19	0.42
1:C:117:LEU:HD11	1:C:129:PHE:HD2	1.84	0.42
1:D:118:ASN:H	1:D:121:GLN:HB2	1.85	0.42
1:B:126:LEU:HD12	1:B:163:ILE:HD11	2.01	0.42
1:C:75:LEU:HD12	1:C:78:HIS:CE1	2.55	0.42
1:C:80:GLN:HE22	1:C:84[B]:ASN:HD22	1.65	0.42
1:D:46:TRP:N	1:D:92:SER:O	2.44	0.42
1:D:77:ASN:ND2	4:D:301:HOH:O	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84[A]:ASN:ND2	4:C:301:HOH:O	2.38	0.40
1:D:60:LEU:HA	1:D:60:LEU:HD12	1.84	0.40
1:B:147[A]:ASP:OD2	4:B:401:HOH:O	2.21	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	181/190 (95%)	172 (95%)	9 (5%)	0	100	100
1	B	180/190 (95%)	176 (98%)	4 (2%)	0	100	100
1	C	153/190 (80%)	144 (94%)	9 (6%)	0	100	100
1	D	150/190 (79%)	136 (91%)	14 (9%)	0	100	100
All	All	664/760 (87%)	628 (95%)	36 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	158/169 (94%)	155 (98%)	3 (2%)	57	37
1	B	156/169 (92%)	155 (99%)	1 (1%)	86	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	116/169 (69%)	115 (99%)	1 (1%)	78	67
1	D	119/169 (70%)	116 (98%)	3 (2%)	47	25
All	All	549/676 (81%)	541 (98%)	8 (2%)	65	49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	148	ASP
1	A	199	SER
1	B	148	ASP
1	C	40	GLN
1	D	35	ILE
1	D	78	HIS
1	D	202	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	155	ASN
1	B	120	GLN
1	C	80	GLN
1	D	120	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6G6	A	300	-	32,38,42	1.30	4 (12%)	29,62,69	1.34	2 (6%)
2	6G6	B	301	-	35,42,42	1.14	4 (11%)	34,69,69	1.41	6 (17%)
3	GOL	B	302	-	5,5,5	0.35	0	5,5,5	0.44	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
2	6G6	A	300	-	-	5/28/52/58	0/3/3/3
2	6G6	B	301	-	-	4/34/58/58	0/3/3/3
3	GOL	B	302	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	6G6	P3-O9	3.51	1.62	1.58
2	A	300	6G6	P2-O4	3.51	1.61	1.54
2	A	300	6G6	P3-O8	-2.79	1.50	1.56
2	B	301	6G6	P2-O4	2.73	1.61	1.58
2	B	301	6G6	P2-O6	-2.50	1.51	1.56
2	B	301	6G6	P3-O8	-2.43	1.51	1.56
2	A	300	6G6	O13-C7	2.16	1.44	1.41
2	B	301	6G6	P3-O9	2.12	1.60	1.58

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	6G6	N3-C12-N5	-4.25	121.55	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	6G6	N3-C12-N5	-4.09	121.77	127.22
2	A	300	6G6	C12-N3-C11	3.32	119.15	115.36
2	B	301	6G6	P1-O4-P2	-3.15	121.54	132.62
2	B	301	6G6	C12-N3-C11	2.72	118.46	115.36
2	B	301	6G6	O15-C5-C7	2.54	114.13	109.09
2	B	301	6G6	C7-N1-C11	-2.31	122.58	126.64
2	B	301	6G6	O16-C13-C10	2.18	123.74	119.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	6G6	CL1-C1-P2-O4
2	A	300	6G6	CL2-C1-P2-O4
2	A	300	6G6	CL1-C1-P2-O6
2	A	300	6G6	CL2-C1-P2-O6
2	B	301	6G6	C7-C5-O15-C6
3	B	302	GOL	C1-C2-C3-O3
3	B	302	GOL	O2-C2-C3-O3
2	B	301	6G6	P4-O9-P3-O7
2	B	301	6G6	P1-O4-P2-O5
2	A	300	6G6	P3-O9-P4-O10
2	B	301	6G6	P4-O9-P3-O8

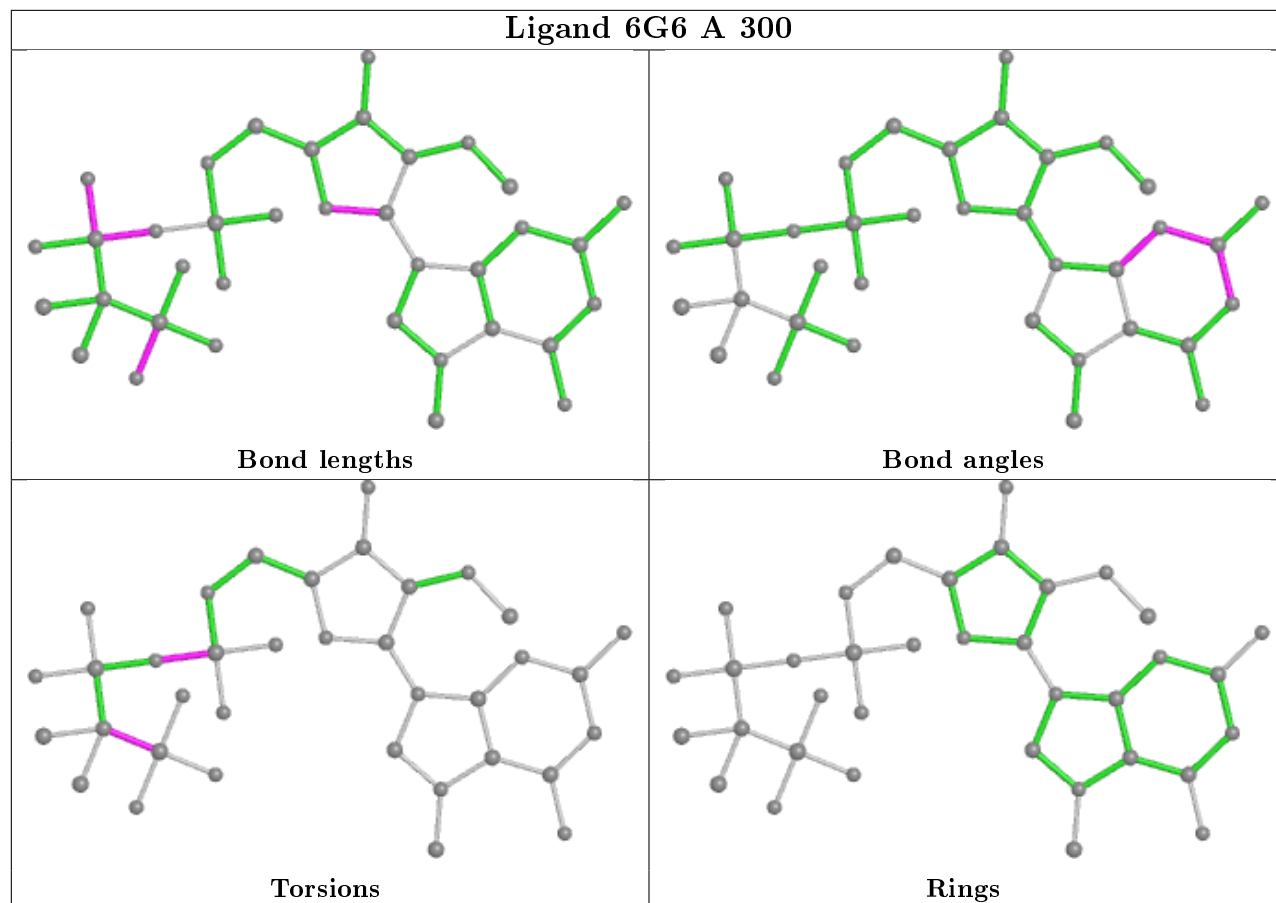
There are no ring outliers.

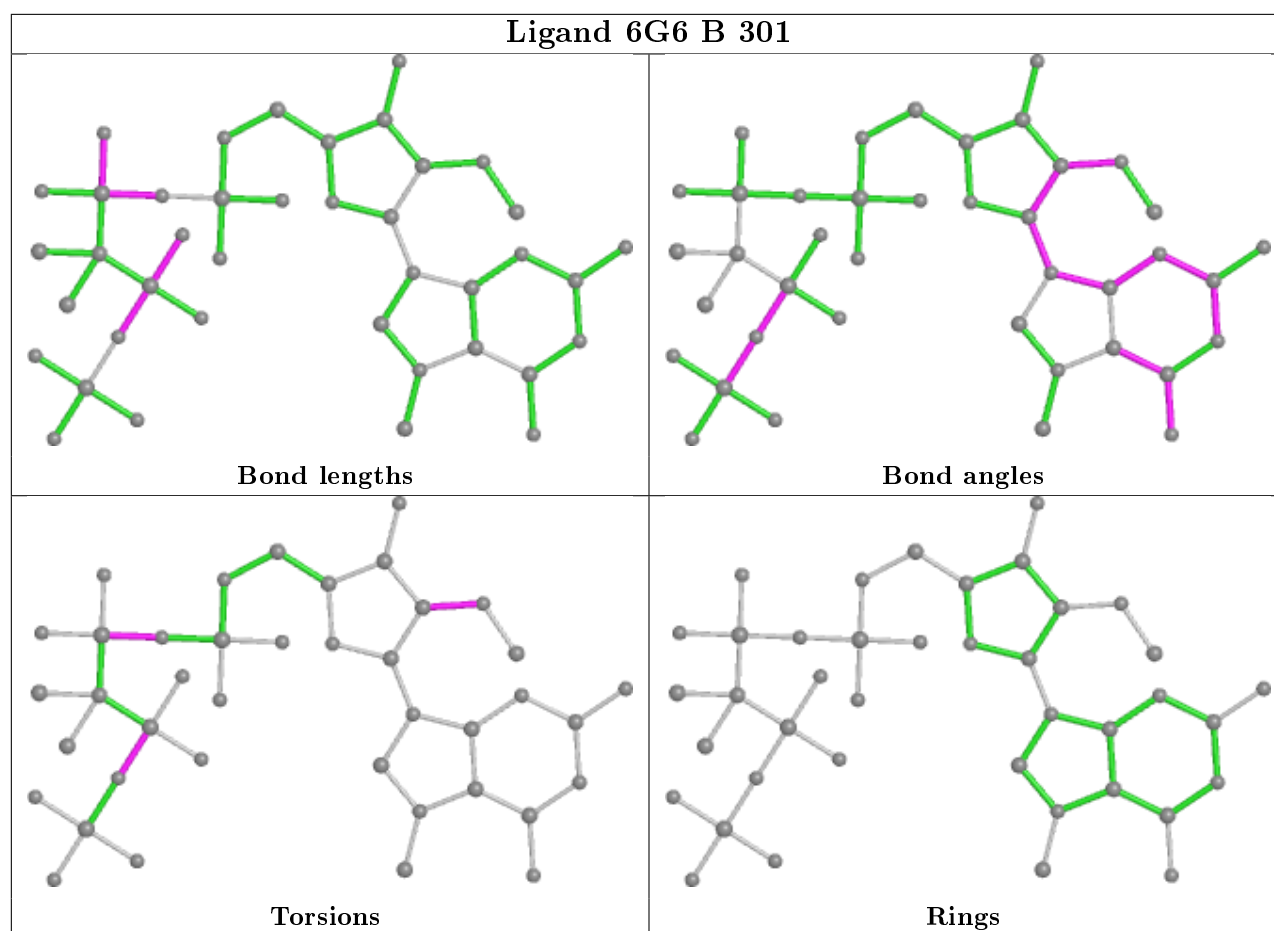
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	6G6	1	0
3	B	302	GOL	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.





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	182/190 (95%)	0.16	5 (2%) 54 60	14, 25, 47, 67	0
1	B	181/190 (95%)	0.14	1 (0%) 89 92	13, 25, 47, 69	0
1	C	155/190 (81%)	1.41	41 (26%) 0 0	28, 51, 81, 101	0
1	D	162/190 (85%)	1.38	44 (27%) 0 0	25, 56, 80, 93	0
All	All	680/760 (89%)	0.73	91 (13%) 3 4	13, 36, 74, 101	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	VAL	5.2
1	D	51	ASP	5.2
1	C	145	TYR	5.2
1	C	111	GLY	5.0
1	C	108	LYS	4.9
1	C	158	ALA	4.9
1	D	100	PRO	4.8
1	D	201	ALA	4.5
1	A	211	THR	4.4
1	C	156	VAL	4.3
1	D	56	TRP	4.3
1	C	102	TRP	4.1
1	C	113	TRP	4.0
1	C	56	TRP	4.0
1	D	111	GLY	3.8
1	D	46	TRP	3.8
1	C	60	LEU	3.7
1	D	59	ASN	3.7
1	D	113	TRP	3.7
1	D	94	PHE	3.7
1	C	86	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	178	HIS	3.6
1	C	110	GLY	3.5
1	D	177	THR	3.5
1	D	142	PHE	3.5
1	C	142	PHE	3.4
1	D	60	LEU	3.4
1	C	58	ALA	3.3
1	D	117	LEU	3.3
1	D	176	VAL	3.3
1	C	49	LYS	3.3
1	D	167	THR	3.2
1	D	190	PRO	3.2
1	A	31	PRO	3.1
1	D	50	ASN	3.1
1	C	100	PRO	3.1
1	D	102	TRP	3.1
1	C	52	LYS	3.0
1	C	115	ILE	3.0
1	D	62	LEU	3.0
1	D	48	PHE	3.0
1	C	114	LEU	3.0
1	D	187	LEU	2.9
1	C	57	GLN	2.9
1	C	170	CYS	2.8
1	C	55	THR	2.8
1	C	183	TYR	2.8
1	D	145	TYR	2.8
1	C	141	SER	2.8
1	C	151	GLY	2.7
1	C	136	CYS	2.6
1	D	215	PHE	2.6
1	C	117	LEU	2.6
1	A	204	ALA	2.6
1	C	179	ILE	2.6
1	D	179	ILE	2.6
1	D	147	ASP	2.6
1	D	178	HIS	2.5
1	D	114	LEU	2.5
1	D	180	GLY	2.5
1	C	165	ILE	2.5
1	D	214	ARG	2.4
1	D	189	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	2.4
1	D	164	ALA	2.4
1	C	32	GLU	2.4
1	C	94	PHE	2.3
1	C	187	LEU	2.3
1	C	48	PHE	2.3
1	D	44	ALA	2.3
1	D	104	ASP	2.3
1	D	168	THR	2.2
1	D	105	GLU	2.2
1	D	182	VAL	2.2
1	A	205	THR	2.2
1	C	168	THR	2.2
1	D	47	PHE	2.2
1	D	175	ALA	2.2
1	C	47	PHE	2.1
1	D	115	ILE	2.1
1	C	31	PRO	2.1
1	D	112	ARG	2.1
1	A	50	ASN	2.1
1	C	177	THR	2.1
1	D	101	MET	2.1
1	D	97	GLY	2.1
1	D	160	GLY	2.1
1	D	141	SER	2.1
1	B	109	ARG	2.0
1	C	105	GLU	2.0
1	C	149	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

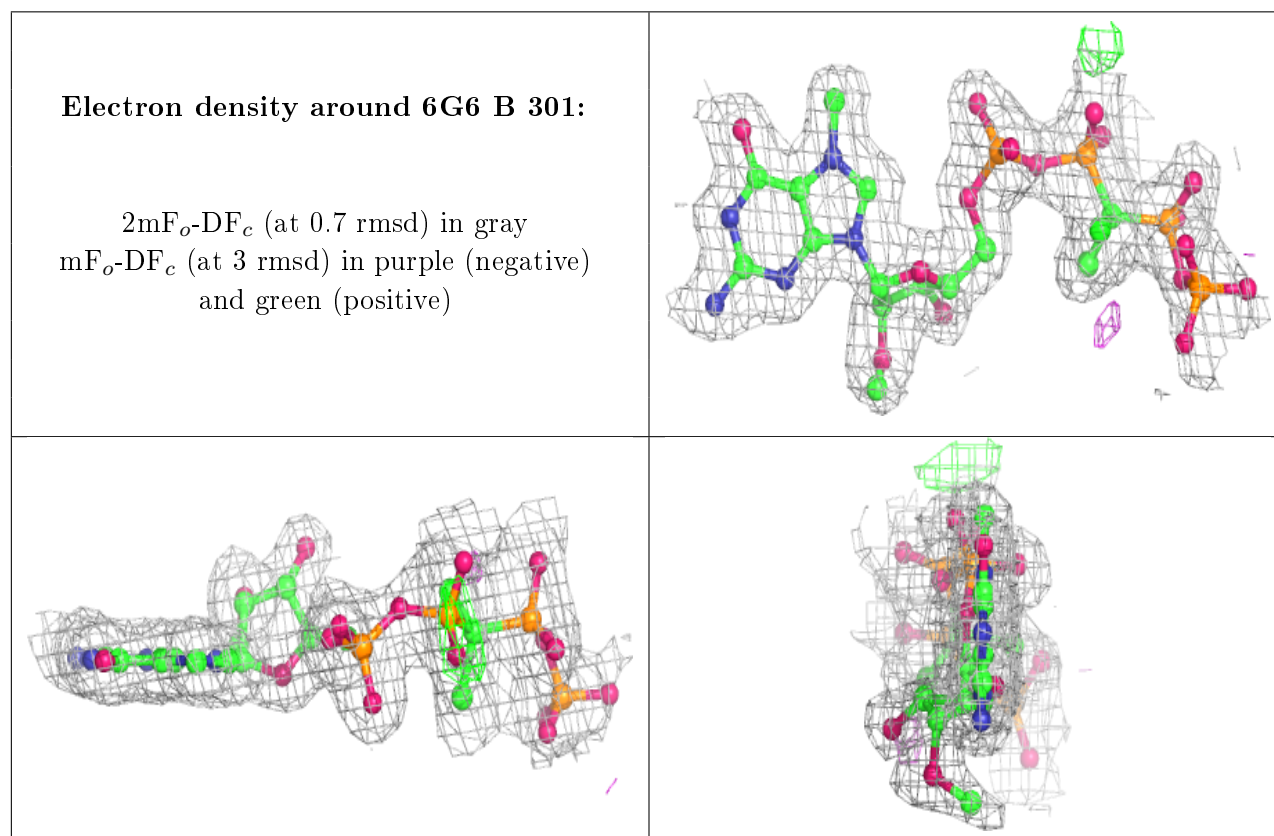
6.4 Ligands [i](#)

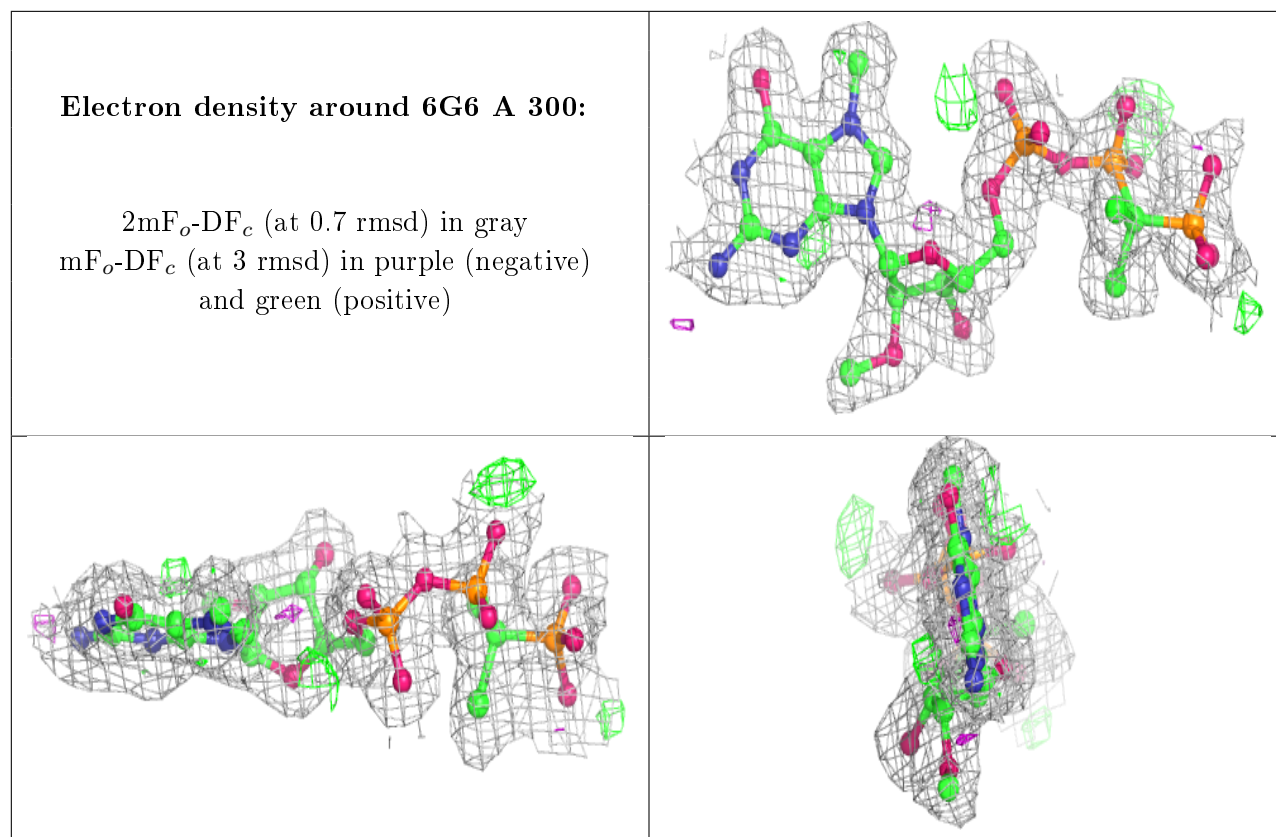
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	302	6/6	0.84	0.12	43,47,48,50	0
2	6G6	B	301	40/40	0.92	0.10	18,29,61,65	2
2	6G6	A	300	36/40	0.92	0.09	14,30,47,55	2

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.