wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 04:39 PM EDT

PDB ID	:	1TL7
Title	:	Complex Of Gs- With The Catalytic Domains Of Mammalian Adenylyl Cyclase: Complex With 2'(3')-O-(N-methylanthraniloyl)-guanosine 5'-triphosphate and Mn
Authors	:	Mou, T.C.; Gille, A.; Seifert, R.J.; Sprang, S.R.
Deposited on	:	2004-06-09
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

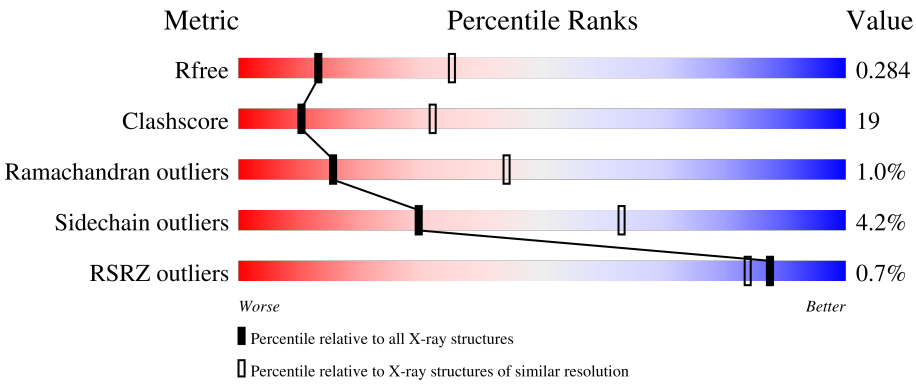
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of 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 <=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	217	% 47% 36% • 13%
2	B	212	54% 32% • 11%
3	C	402	54% 28% 18%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 5770 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 Adenylate cyclase, type V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	189	1476	929	259	271	17	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	476	MET	VAL	conflict	UNP P30803

- Molecule 2 is a protein called Adenylate cyclase, type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	189	1467	936	242	279	10	0	0	0

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s), alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	330	2702	1714	470	505	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	71	GLY	-	conflict	UNP P04896
C	?	-	GLN	deletion	UNP P04896
C	79	ASN	ALA	conflict	UNP P04896
C	81	LYS	ARG	conflict	UNP P04896
C	395	GLY	-	expression tag	UNP P04896
C	396	GLY	-	expression tag	UNP P04896
C	397	HIS	-	expression tag	UNP P04896
C	398	HIS	-	expression tag	UNP P04896
C	399	HIS	-	expression tag	UNP P04896

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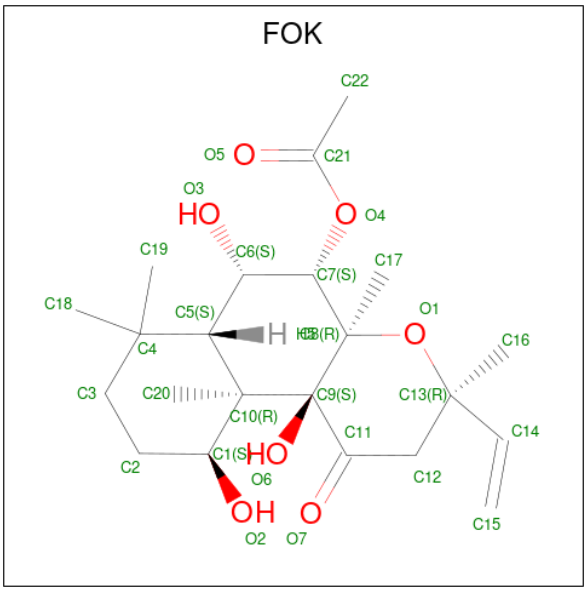
Chain	Residue	Modelled	Actual	Comment	Reference
C	400	HIS	-	expression tag	UNP P04896
C	401	HIS	-	expression tag	UNP P04896
C	402	HIS	-	expression tag	UNP P04896

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

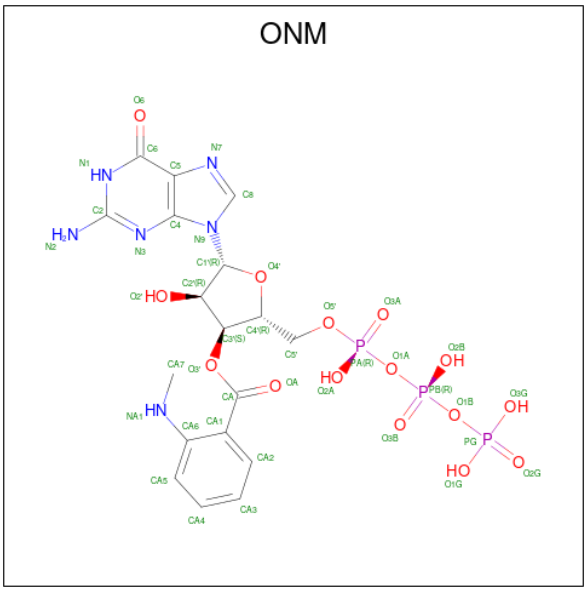
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0

- Molecule 5 is FORSKOLIN (three-letter code: FOK) (formula: $C_{22}H_{34}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 29 22 7	0	0

- Molecule 6 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: ONM) (formula: $C_{18}H_{23}N_6O_{15}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	42	18	6	15	3	0	0

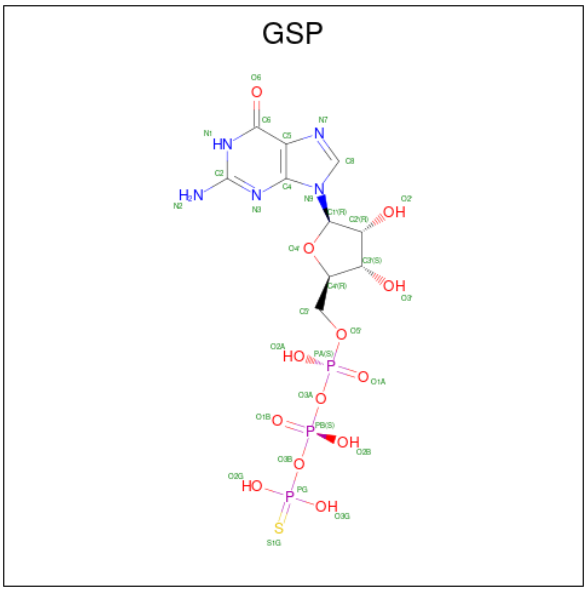
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	C	1	1	1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	C	1	1	1	0	0

- Molecule 9 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
9	C	1	32	10	5	13	3	1	0	0

- Molecule 10 is water.

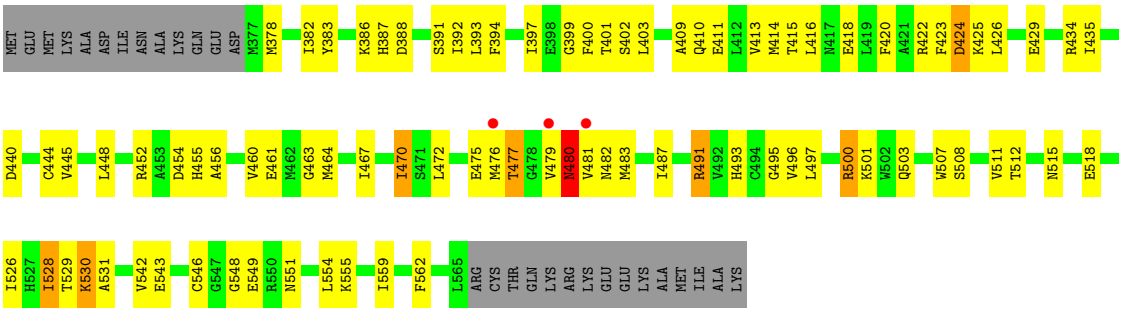
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	1	1	1	0	0
10	B	9	9	9	0	0
10	C	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

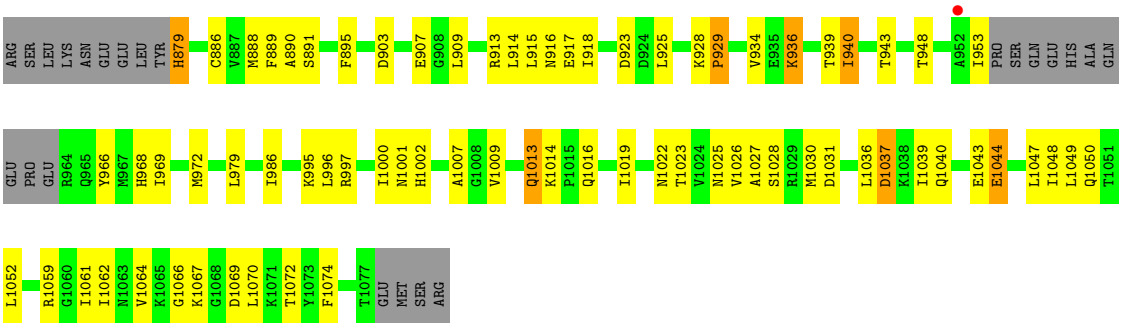
• Molecule 1: Adenylate cyclase, type V

Chain A:



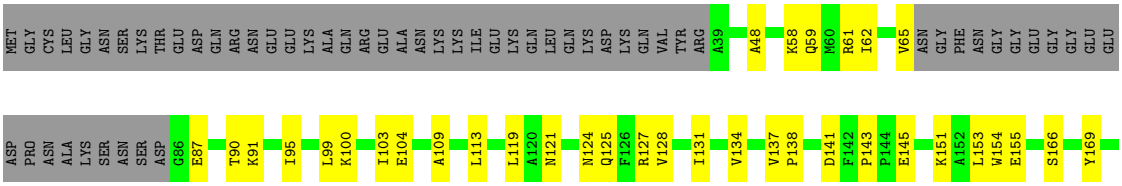
• Molecule 2: Adenylate cyclase, type II

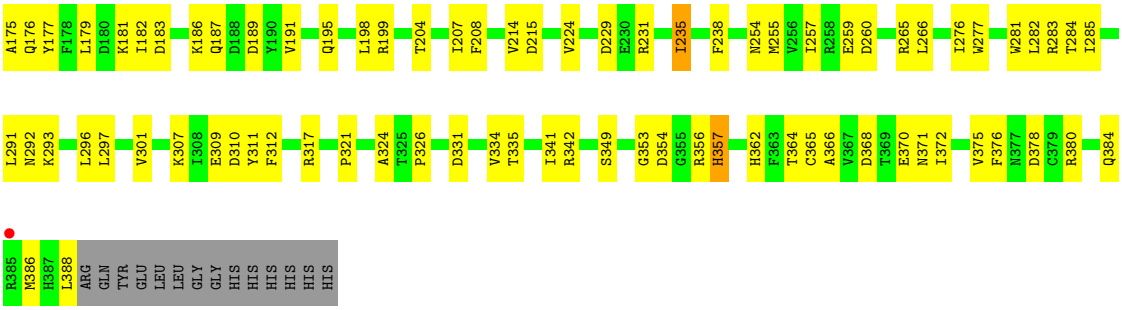
Chain B:



• Molecule 3: Guanine nucleotide-binding protein G(s), alpha subunit

Chain C:




A175 Q176 Y177 F178 L179 D180 K181 I182 D183 K186 Q187 D188 D189 Y190 V191 Q195 L198 R199 T204 I207 F208 V214 D215 V224 D229 E230 R231 I235 F238 N254 M255 V256 I257 R258 E259 D260 R265 L266 I276 W277 W281 L282 R283 T284 I285
L291 N292 K293 L296 L297 V301 K307 I308 E309 D310 Y311 F312 R317 P321 A324 T325 P326 D331 V334 T335 I341 R342 S349 G353 D354 G355 R356 H357 H362 F363 T364 C365 A366 V367 D368 T369 E370 N371 I372 V375 F376 N377 D378 G379 R380 Q384
R385 M386 H387 L388 ARG GLN TYR GLU LEU LEU GLY GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.23Å 133.60Å 70.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 2.80 48.44 – 2.69	Depositor EDS
% Data completeness (in resolution range)	81.2 (14.99-2.80) 76.5 (48.44-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.298 0.249 , 0.284	Depositor DCC
R_{free} test set	1104 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	1.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	5770	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ONM, CL, MG, GSP, FOK, MN

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	0.33	0/1504	0.61	0/2027
2	B	0.38	0/1492	0.58	0/2014
3	C	0.36	0/2759	0.58	0/3733
All	All	0.35	0/5755	0.59	0/7774

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 (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	1476	0	1450	82	0
2	B	1467	0	1470	64	0
3	C	2702	0	2652	78	0
4	A	2	0	0	0	0
5	A	29	0	34	2	0
6	A	42	0	19	1	0
7	C	1	0	0	0	0
8	C	1	0	0	0	0
9	C	32	0	12	1	0
10	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	9	0	0	0	0
10	C	8	0	0	2	0
All	All	5770	0	5637	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 213 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:477:THR:HB	1:A:479:VAL:HG12	1.43	0.97
1:A:554:LEU:HA	1:A:559:ILE:HD12	1.58	0.84
3:C:321:PRO:HG2	3:C:324:ALA:HB2	1.60	0.83
3:C:207:ILE:HG12	3:C:224:VAL:HG12	1.61	0.83
1:A:420:PHE:HA	1:A:423:PHE:HB2	1.63	0.81

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	187/217 (86%)	161 (86%)	24 (13%)	2 (1%)	14 41
2	B	185/212 (87%)	169 (91%)	15 (8%)	1 (0%)	29 61
3	C	326/402 (81%)	303 (93%)	19 (6%)	4 (1%)	13 39
All	All	698/831 (84%)	633 (91%)	58 (8%)	7 (1%)	15 44

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ASN

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Mol	Chain	Res	Type
3	C	48	ALA
3	C	175	ALA
2	B	929	PRO
3	C	138	PRO

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	158/182 (87%)	147 (93%)	11 (7%)	15	40
2	B	162/184 (88%)	155 (96%)	7 (4%)	29	62
3	C	297/357 (83%)	289 (97%)	8 (3%)	44	78
All	All	617/723 (85%)	591 (96%)	26 (4%)	30	63

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	940	ILE
2	B	1044	GLU
3	C	357	HIS
2	B	1037	ASP
3	C	141	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	93	GLN
3	C	362	HIS
3	C	377	ASN
3	C	371	ASN
1	A	515	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	FOK	A	101	-	28,31,31	3.42	11 (39%)	35,54,54	1.62	6 (17%)
6	ONM	A	100	4	37,45,45	3.42	14 (37%)	47,69,69	3.03	21 (44%)
9	GSP	C	405	7	26,34,34	1.49	3 (11%)	27,54,54	1.68	5 (18%)

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
5	FOK	A	101	-	-	5/7/80/80	0/3/3/3
6	ONM	A	100	4	-	6/28/48/48	0/4/4/4
9	GSP	C	405	7	-	3/17/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	101	FOK	O7-C11	13.60	1.43	1.21
6	A	100	ONM	CA4-CA5	10.06	1.60	1.38
6	A	100	ONM	OA-CA	8.83	1.46	1.22
6	A	100	ONM	CA3-CA2	8.77	1.57	1.38
6	A	100	ONM	CA5-CA6	7.61	1.52	1.39

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	100	ONM	O1G-PG-O3G	-8.55	74.97	107.64
6	A	100	ONM	PB-O1B-PG	-8.15	104.88	132.83
6	A	100	ONM	O3G-PG-O1B	5.61	123.44	104.64
6	A	100	ONM	O3'-CA-CA1	5.58	120.38	111.69
9	C	405	GSP	O6-C6-N1	5.53	127.18	120.65

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	101	FOK	O1-C13-C14-C15
5	A	101	FOK	C16-C13-C14-C15
6	A	100	ONM	O4'-C4'-C5'-O5'
5	A	101	FOK	C22-C21-O4-C7
5	A	101	FOK	O5-C21-O4-C7

There are no ring outliers.

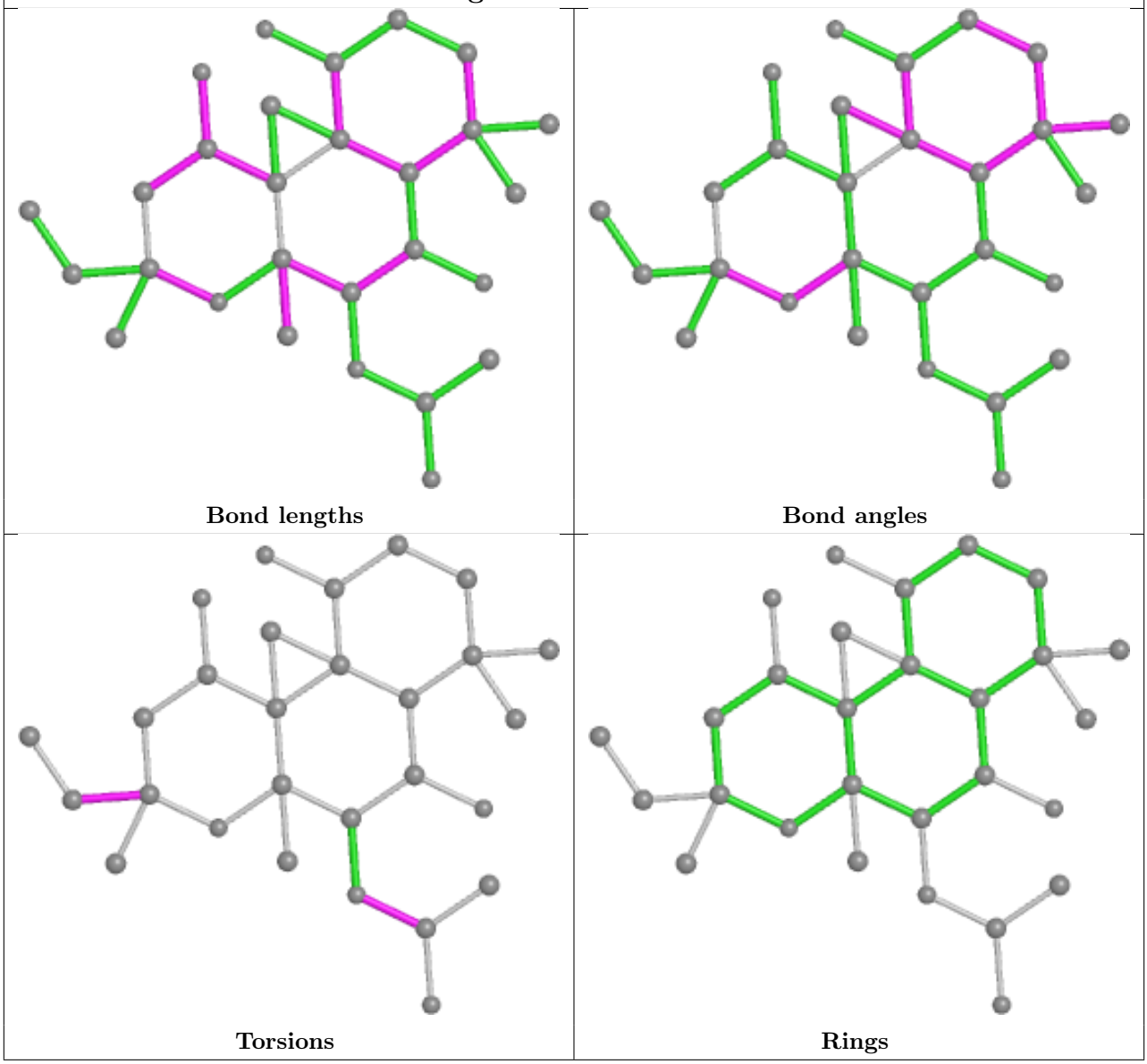
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	101	FOK	2	0
6	A	100	ONM	1	0
9	C	405	GSP	1	0

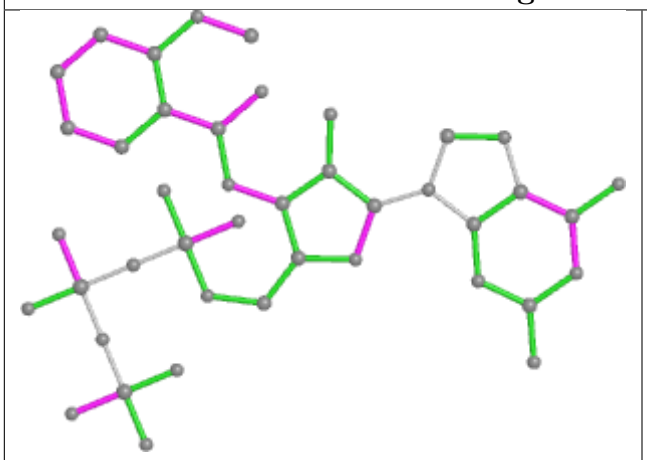
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

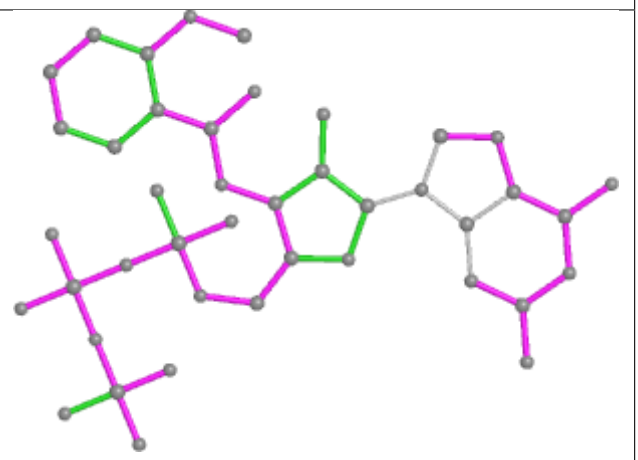
Ligand FOK A 101



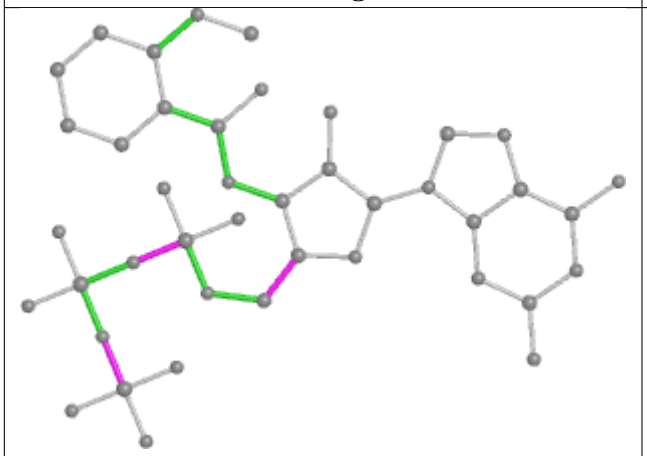
Ligand ONM A 100



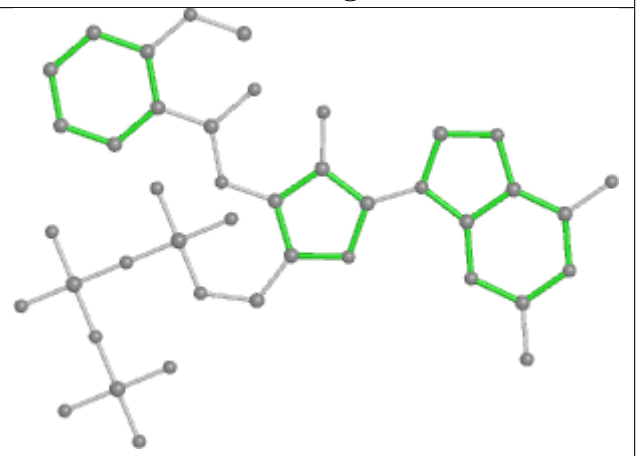
Bond lengths



Bond angles

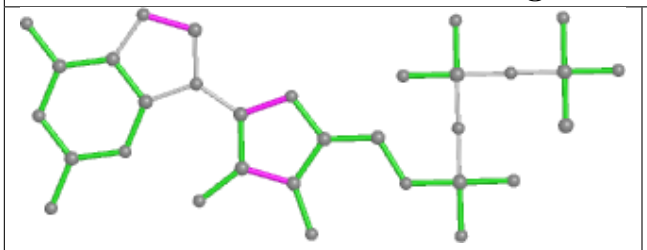


Torsions

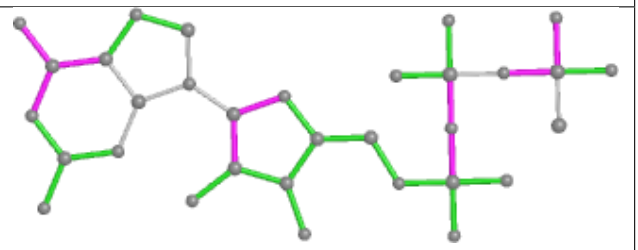


Rings

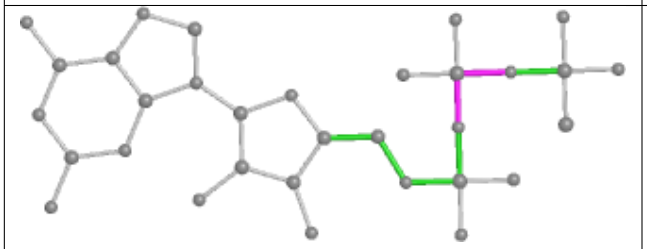
Ligand GSP C 405



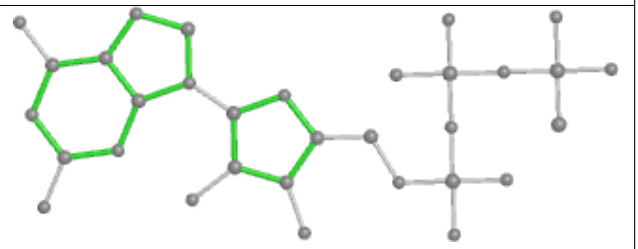
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	189/217 (87%)	-0.12	3 (1%)	72	66	22, 54, 83, 98	0
2	B	189/212 (89%)	-0.27	1 (0%)	91	88	12, 38, 73, 94	0
3	C	330/402 (82%)	-0.37	1 (0%)	94	93	18, 40, 68, 92	0
All	All	708/831 (85%)	-0.28	5 (0%)	87	84	12, 43, 74, 98	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	VAL	4.3
2	B	952	ALA	3.7
1	A	476	MET	2.6
1	A	481	VAL	2.5
3	C	385	ARG	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

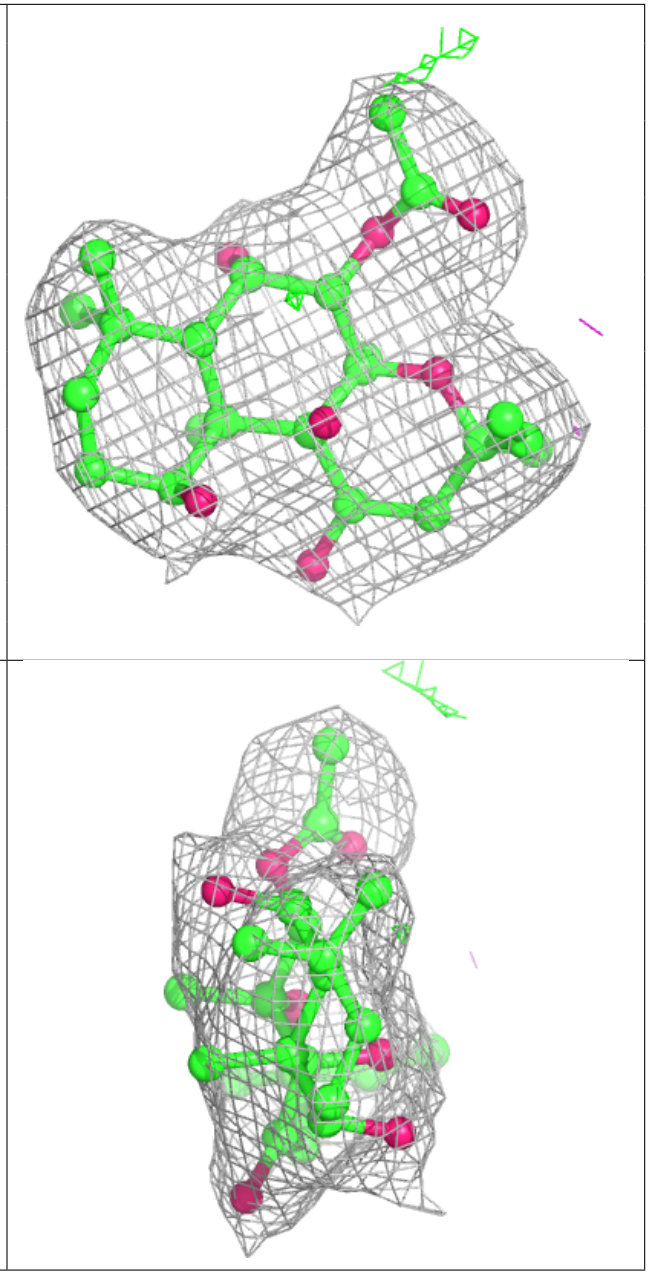
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FOK	A	101	29/29	0.91	0.24	26,30,36,40	0
6	ONM	A	100	42/42	0.91	0.22	44,54,62,64	0
7	MG	C	403	1/1	0.92	0.20	0,0,0,0	0
8	CL	C	404	1/1	0.94	0.12	49,49,49,49	0
4	MN	A	582	1/1	0.95	0.14	37,37,37,37	0
9	GSP	C	405	32/32	0.95	0.17	23,28,58,66	0
4	MN	A	581	1/1	0.96	0.15	32,32,32,32	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.

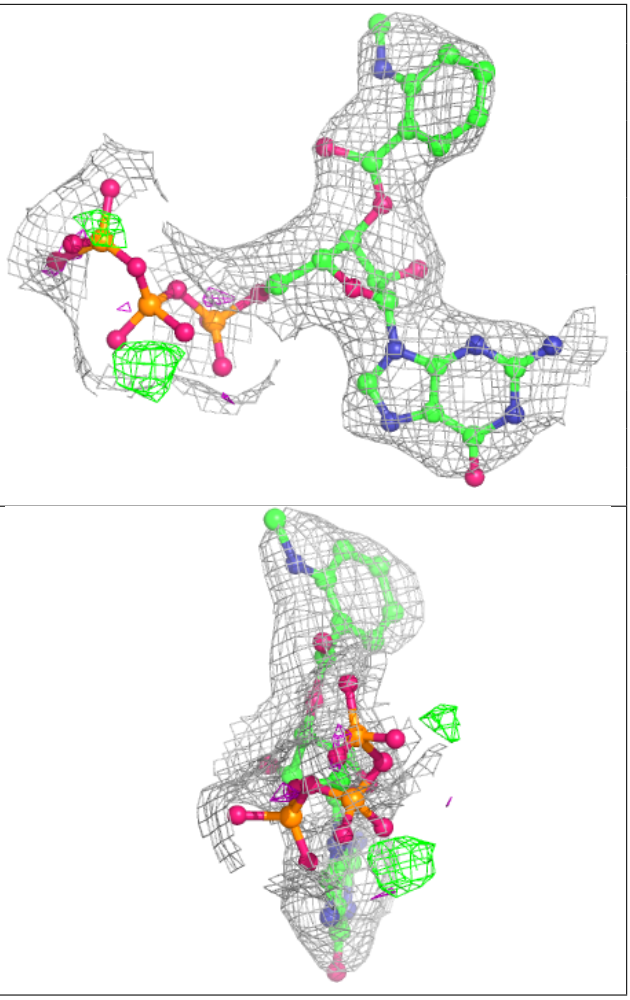
Electron density around FOK A 101:

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



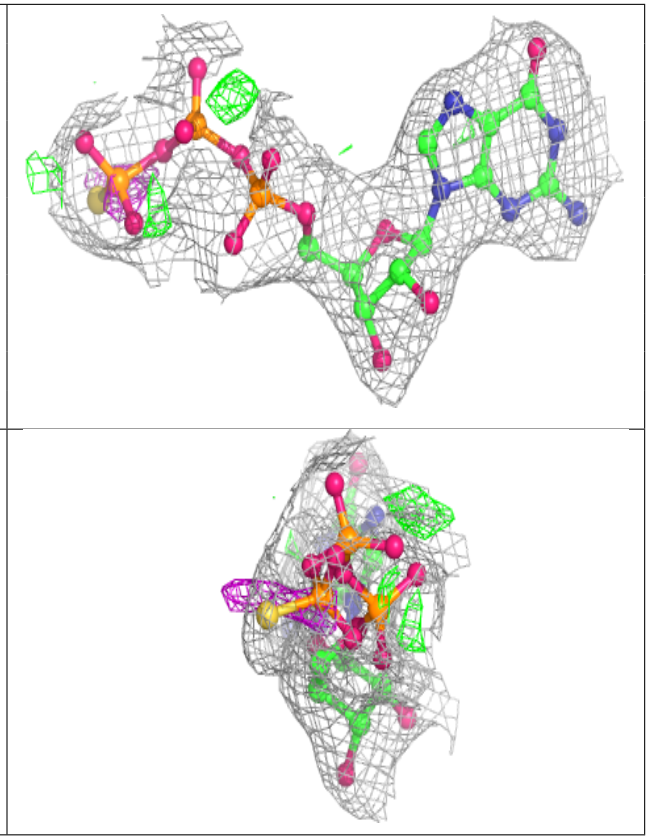
Electron density around ONM A 100:

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



Electron density around GSP C 405:

$2mF_o$-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.