



Full wwPDB X-ray Structure Validation Report i

Jan 30, 2024 – 08:11 AM EST

PDB ID : 1FQK
Title : CRYSTAL STRUCTURE OF THE HETERODIMERIC COMPLEX OF THE RGS DOMAIN OF RGS9, AND THE GT/I1 CHIMERA ALPHA SUBUNIT [(RGS9)-(GT/I1ALPHA)-(GDP)-(ALF4-)-(MG2+)]
Authors : Slep, K.C.; Kercher, M.A.; He, W.; Cowan, C.W.; Wensel, T.G.; Sigler, P.B.
Deposited on : 2000-09-05
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 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](#) ①) 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 : 2.36
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) : 2.36

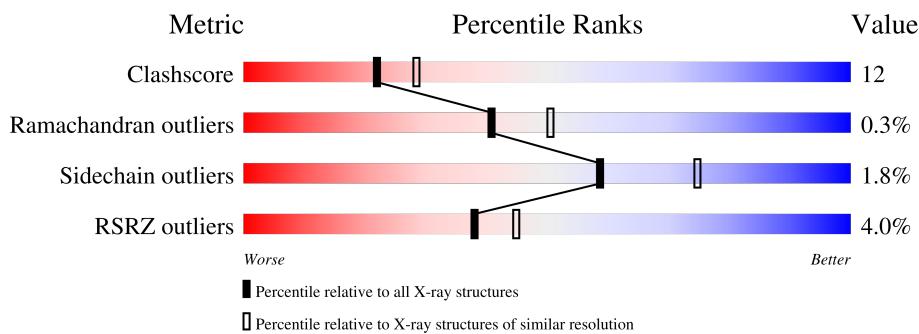
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

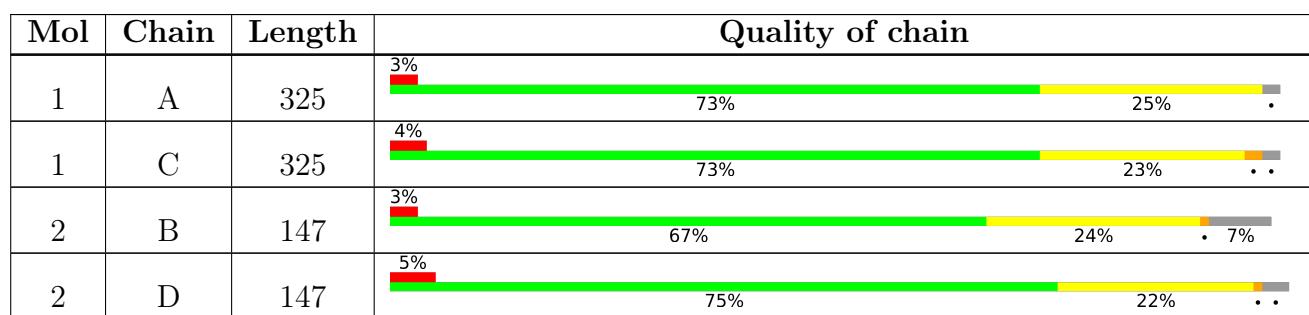
The reported resolution of this entry is 2.30 Å.

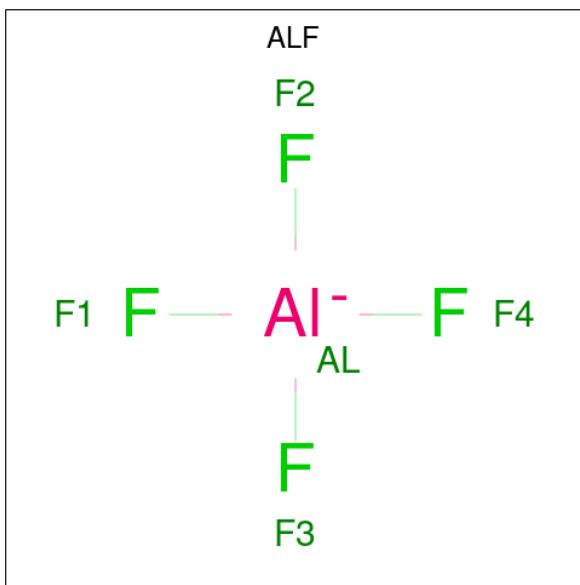
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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)

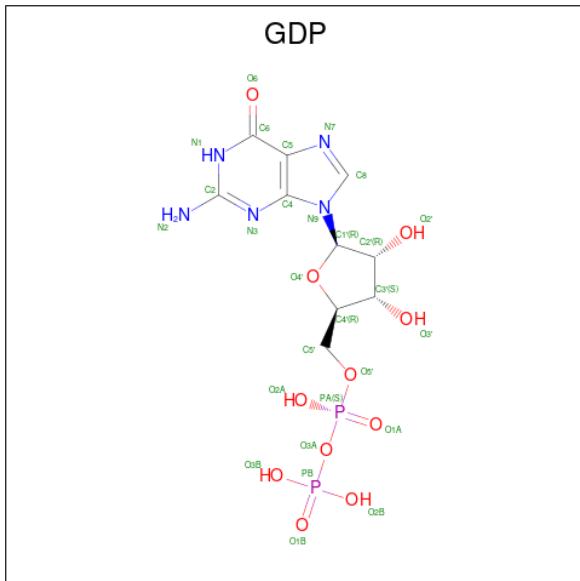
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	Al 1	F 4	0	0
4	C	1	Total 5	Al 1	F 4	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	28	10	5	11	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O P 28 10 5 11 2	0	0

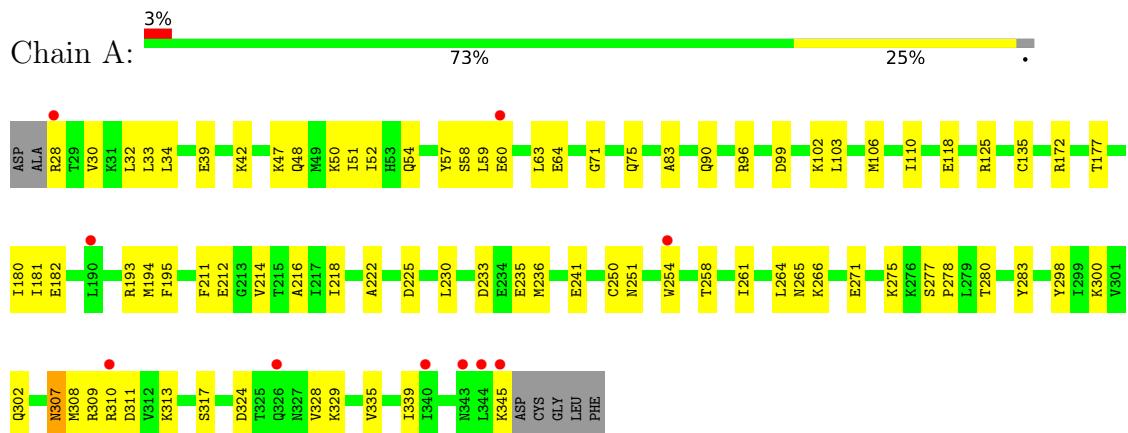
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	47	Total O 47 47	0	0
6	B	10	Total O 10 10	0	0
6	C	43	Total O 43 43	0	0
6	D	16	Total O 16 16	0	0

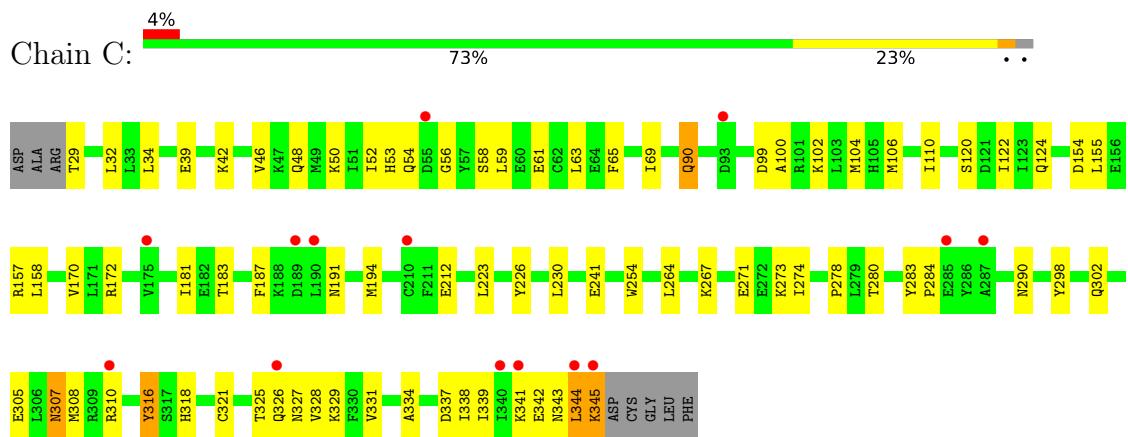
3 Residue-property plots

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.

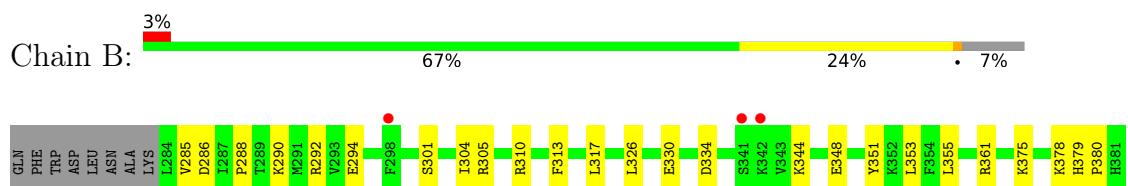
- Molecule 1: Guanine nucleotide-binding protein G(t) subunit alpha-1, Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(t) subunit alpha-1



- Molecule 1: Guanine nucleotide-binding protein G(t) subunit alpha-1, Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(t) subunit alpha-1

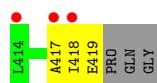
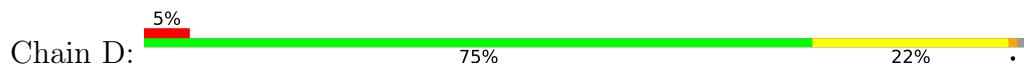


- Molecule 2: Regulator of G-protein signaling 9





- Molecule 2: Regulator of G-protein signaling 9



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.78 Å 115.07 Å 136.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 43.99 – 2.29	Depositor EDS
% Data completeness (in resolution range)	87.4 (50.00-2.30) 86.9 (43.99-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.91 (at 2.29 Å)	Xtriage
Refinement program	CNS	Depositor
R , R_{free}	0.231 , 0.268 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7634	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:355:LEU:HD21	2:D:363:ILE:HD11	2.00	0.42
1:C:339:ILE:O	1:C:343:ASN:HB2	2.18	0.42
1:A:32:LEU:HD23	1:A:194:MET:HE3	2.02	0.42
2:D:405:LEU:HD22	2:D:405:LEU:H	1.84	0.42
1:A:222:ALA:HB3	1:A:225:ASP:CG	2.40	0.42
1:C:345:LYS:HA	1:C:345:LYS:CE	2.50	0.42
1:A:28:ARG:NE	1:A:28:ARG:HA	2.33	0.42
2:B:313:PHE:O	2:B:317:LEU:HG	2.20	0.42
1:A:47:LYS:O	1:A:51:ILE:HG13	2.20	0.42
1:C:48:GLN:HG3	1:C:328:VAL:HG21	2.01	0.42
1:A:309:ARG:C	1:A:311:ASP:H	2.22	0.41
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.84	0.41
1:A:251:ASN:CG	1:A:308:MET:HG3	2.41	0.41
1:A:34:LEU:HD23	1:A:218:ILE:HB	2.01	0.41
1:C:187:PHE:HB2	6:C:382:HOH:O	2.19	0.41
1:A:106:MET:HB3	1:A:106:MET:HE2	1.96	0.41
1:A:265:ASN:O	1:A:266:LYS:HB2	2.21	0.41
2:B:379:HIS:N	2:B:380:PRO:HD3	2.36	0.41
1:C:325:THR:O	1:C:327:ASN:N	2.54	0.41
1:A:233:ASP:OD1	1:A:235:GLU:HB2	2.21	0.41
1:C:267:LYS:HE3	6:C:392:HOH:O	2.21	0.41
1:C:327:ASN:O	1:C:331:VAL:HG23	2.21	0.40
1:C:102:LYS:HD2	1:C:102:LYS:HA	1.95	0.40
1:A:32:LEU:CD1	1:A:216:ALA:HB3	2.51	0.40
1:A:39:GLU:HA	5:A:360:GDP:O3B	2.22	0.40
2:D:382:ARG:HA	6:D:77:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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.

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Mol	Chain	Res	Type
2	B	382	ARG
1	C	90	GLN
1	C	307	ASN
1	C	316	TYR
1	C	344	LEU
1	C	345	LYS
2	D	318	ARG

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

Mol	Chain	Res	Type
1	A	297	ASN
1	A	307	ASN
2	B	299	ASN
2	B	325	ASN
1	C	53	HIS
1	C	90	GLN
1	C	307	ASN
2	D	325	ASN
2	D	381	HIS

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 [\(i\)](#)

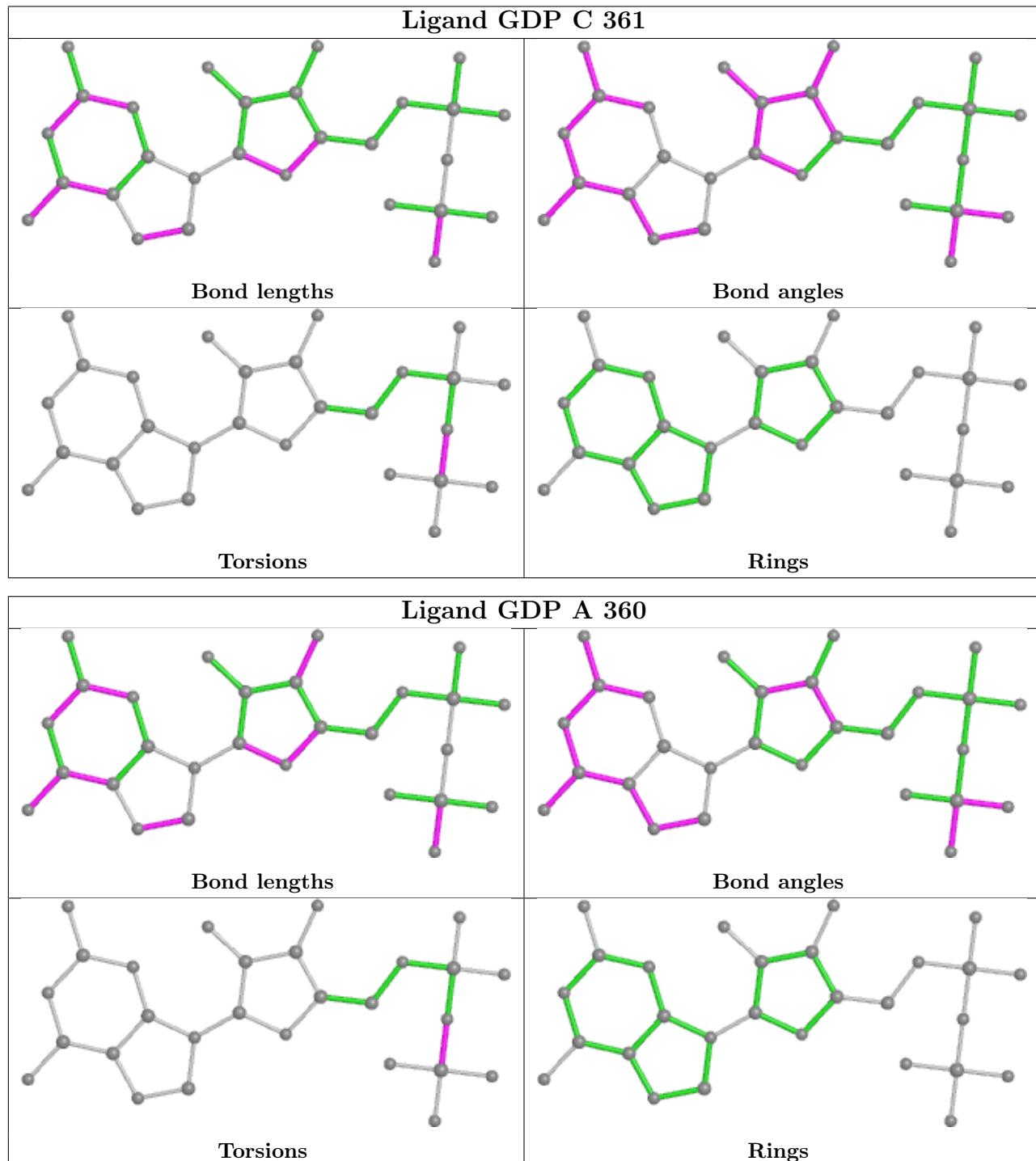
There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 6 ligands modelled in this entry, 2 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

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.

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Mol	Chain	Res	Type	RSRZ
2	D	414	LEU	2.6
1	C	287	ALA	2.5
1	A	28	ARG	2.5
1	C	326	GLN	2.4
2	D	283	LYS	2.4
1	C	341	LYS	2.4
1	C	340	ILE	2.4
1	C	93	ASP	2.3
2	D	295	ARG	2.2
1	C	175	VAL	2.2
1	A	254	TRP	2.2
2	D	290	LYS	2.2
1	C	189	ASP	2.2
2	D	417	ALA	2.1
1	A	60	GLU	2.1
1	A	326	GLN	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 [\(i\)](#)

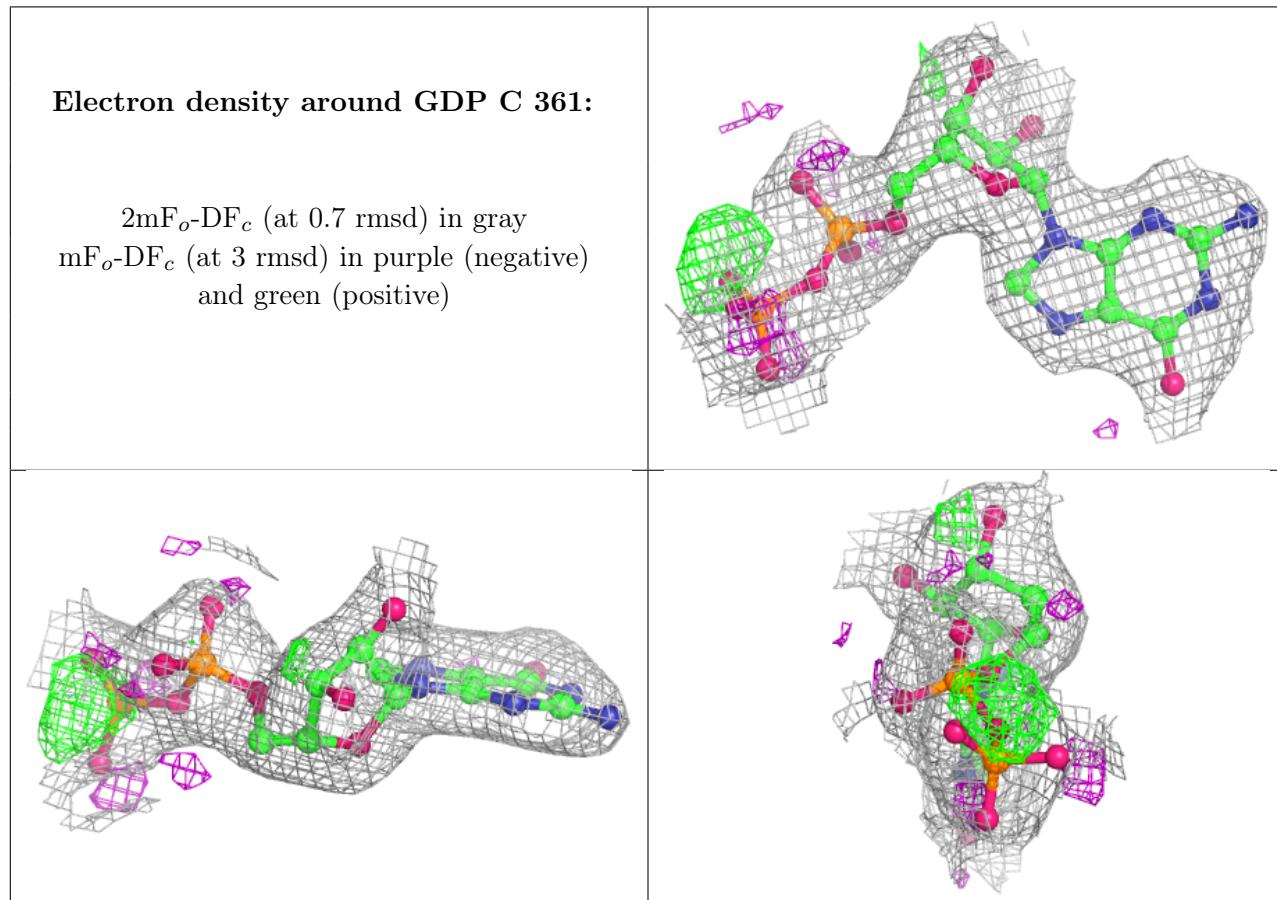
There are no monosaccharides in this entry.

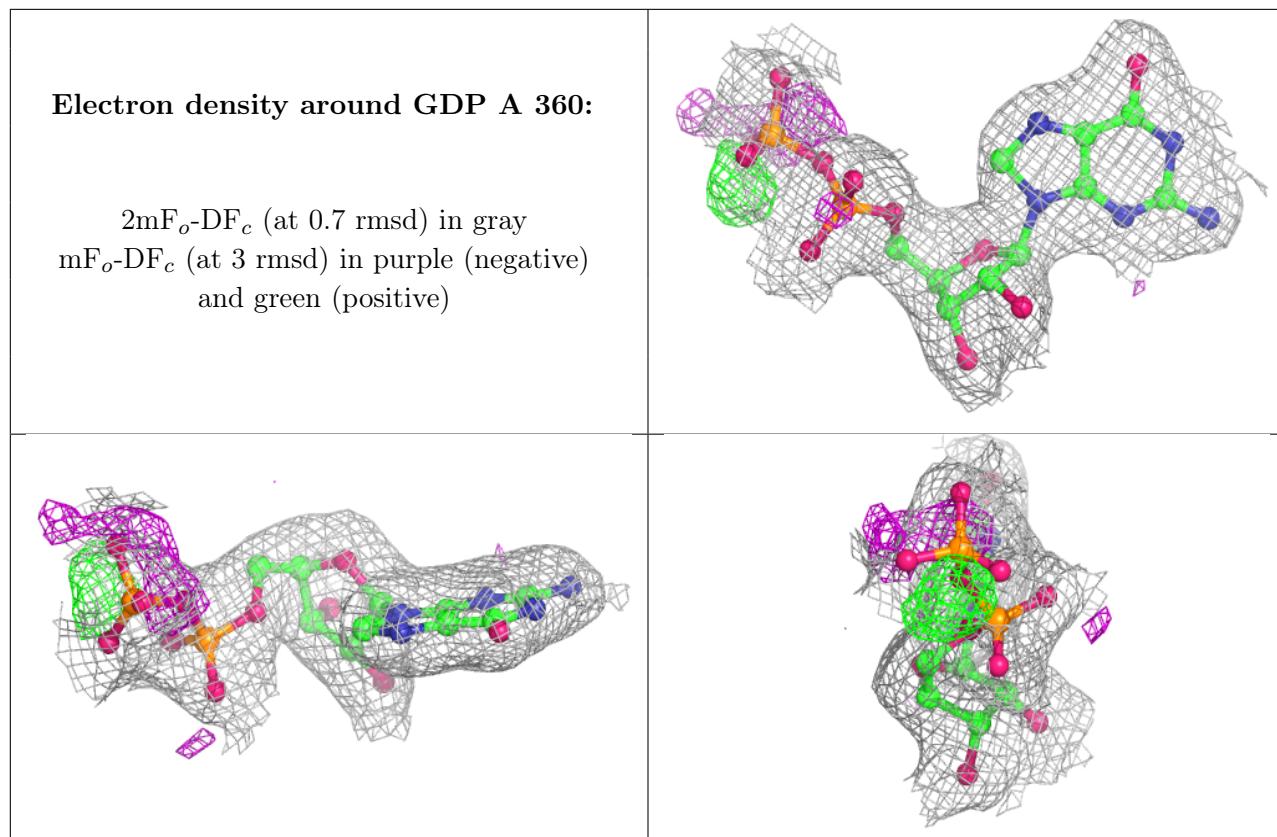
6.4 Ligands [\(i\)](#)

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
3	MG	A	352	1/1	0.92	0.29	47,47,47,47	0
5	GDP	C	361	28/28	0.95	0.20	49,52,61,67	0
5	GDP	A	360	28/28	0.96	0.20	39,45,56,60	0
4	ALF	A	362	5/5	0.97	0.23	49,50,55,55	0
3	MG	C	352	1/1	0.98	0.26	58,58,58,58	0
4	ALF	C	363	5/5	0.99	0.24	44,52,53,55	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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.