wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 07:10 PM EDT

PDB ID	:	2BCJ
Title	:	Crystal Structure of G Protein-Coupled Receptor Kinase 2 in Complex with Galpha-q and Gbetagamma Subunits
Authors	:	Tesmer, J.J.G.
Deposited on	:	2005-10-19
Resolution	:	3.06 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:

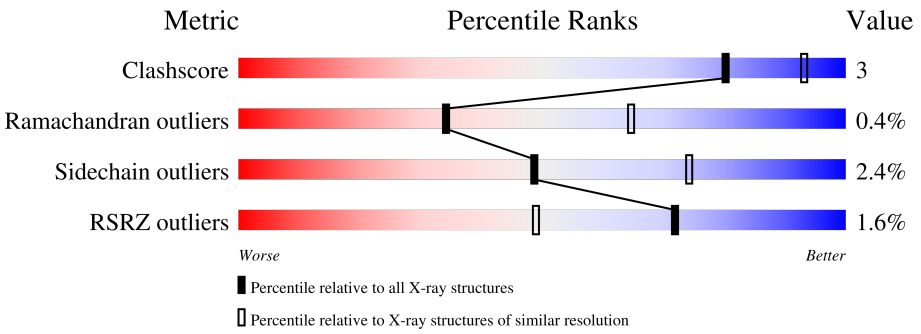
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.06 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	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	689	2%, 84%, 6%, 9%
2	B	340	84%, 15%, •
3	G	71	%, 80%, 10%, 10%
4	Q	353	2%, 84%, 6%, 10%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10878 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 G-protein-coupled receptor kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	624	5113	3263	889	925	36	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	ALA	SER	engineered mutation	UNP P21146

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	340	2610	1609	468	512	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ACE	-	acetylation	UNP P62871

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	64	501	316	88	94	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	68	SER	CYS	engineered mutation	UNP P63212

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(q) subunit alpha chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	Q	317	2615	1671	440	492	12	0	0	0

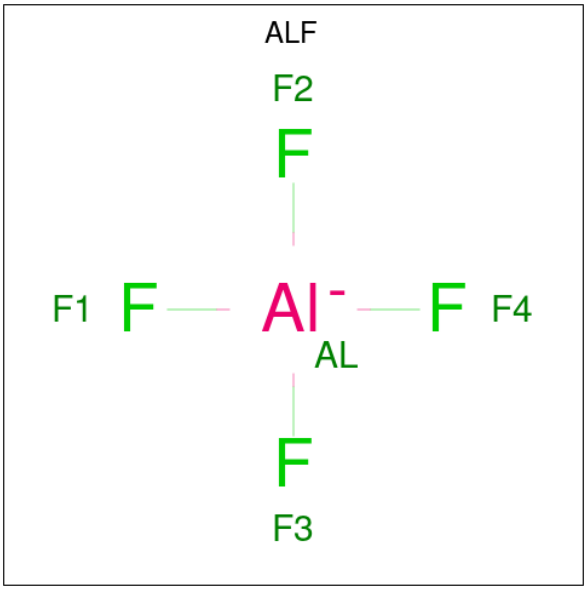
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	35	ARG	-	linker	UNP P10824
Q	36	SER	-	linker	UNP P10824

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

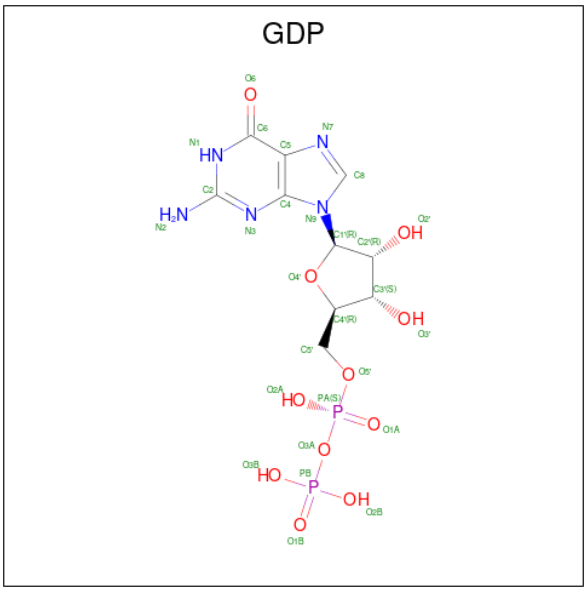
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	Q	1	1	1	0	0

- Molecule 6 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
6	Q	1	5	1	4	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	Q	5	5	5	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: G-protein-coupled receptor kinase 2

Chain A: 2% 84% 6% 9%

MET ALA ASP LEU GLU ALA VAL LEU ALA ASP VAL SER TYR LEU MET ALA MET GLU LYS SER LYS ALA THR PRO ALA ALA ARG A28 P35 R40 S41 V42 E48 V53 F85 K91 H135 L136 V137 Q140 C154 L157 R158 Q176 I197 E204

D212 Q231 L235 V246 G249 I254 H262 T263 P264 D265 K266 L267 D278 N310 D335 S350 E360 V361 A367 Y368 R392 M409 A410 V411 R431 G475 GLU VAL ASN ALA ALA ASP ALA PHE ASP ILE GLY SER PHE ASP GLU GLU D492 T493

I496 K497 L498 H549 D552 M568 G569 N570 P571 F572 L573 R591 L600 E639 L640 R648 Y651 R652 K667 PRO ARG ALA PRO VAL VAL GLU LEU SER LYS VAL PRO LEU ILE GLN ARG GLY SER ALA ASN GLY LEU

• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 84% 15%

ACE1 S2 E3 L4 L7 L14 C25 L30 I33 V40 M45 L51 H54 L55 W63 L70 V71 K78 L79 I80 I81 W82 D83 T87 Y105 S108 Y124 V135 L152 D153 D154 E172 H183 S191 P194 D195 T196

S201 A208 K209 L210 A231 I232 C233 N237 G238 C250 D254 L255 Q259 E260 L261 Y264 I273 T274 S275 L284 F292 N295 L308 D322 A328 I338 W339 N340

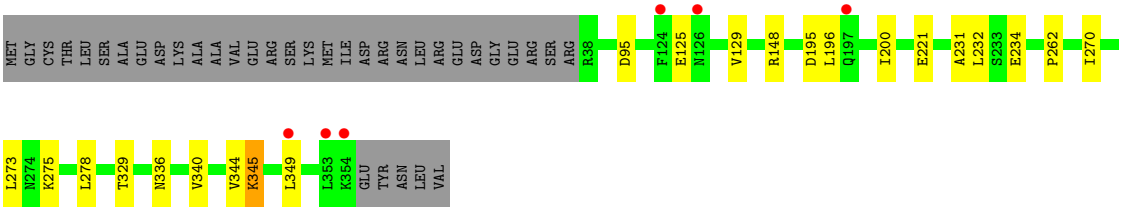
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G: % 80% 10% 10%

MET ALA SER N4 R13 A33 A34 L51 A56 F61 R62 E63 F66 F67 SER ALA ILE LEU

• Molecule 4: Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(q) subunit alpha chimera

Chain Q: 2% 84% 6% 10%


MET
GLY
CYS
THR
LEU
SER
ALA
GLU
ASP
LYS
ALA
ALA
VAL
GLU
ARG
SER
LYS
MET
ILE
ASP
ARG
ASN
LEU
ARG
GLU
ASP
GLY
GLU
ARG
SER
ARG
R38
D95
F124
E125
N126
V129
R148
D195
L196
Q197
I200
E221
A231
L232
S233
E234
P262
I270
L273
N274
K275
L278
T329
N336
V340
V344
K345
L349
L353
K354
GLU
TYR
ASN
LEU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.92Å 129.95Å 122.76Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	46.78 – 3.06 46.80 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.78-3.06) 98.8 (46.80-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.243 , 0.292 0.246 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	82.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.9	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	0.93	EDS
Total number of atoms	10878	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: ACE, GDP, MG, ALF

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	0.34	0/5228	0.49	0/7025
2	B	0.33	0/2655	0.53	0/3599
3	G	0.36	0/509	0.44	0/685
4	Q	0.33	0/2671	0.49	0/3610
All	All	0.34	0/11063	0.50	0/14919

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	5113	0	5116	17	0
2	B	2610	0	2514	30	0
3	G	501	0	510	7	0
4	Q	2615	0	2582	11	0
5	Q	1	0	0	0	0
6	Q	5	0	0	0	0
7	Q	28	0	12	0	0
8	Q	5	0	0	0	0
All	All	10878	0	10734	58	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 3.

The worst 5 of 58 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)
4:Q:270:ILE:HD13	4:Q:344:VAL:HG13	1.80	0.62
4:Q:231:ALA:HB3	4:Q:234:GLU:HG3	1.82	0.61
1:A:350:SER:HA	1:A:361:VAL:HG12	1.83	0.61
2:B:295:ASN:HD22	2:B:295:ASN:N	1.99	0.60
2:B:25:CYS:HB2	2:B:259:GLN:HE22	1.67	0.59

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	620/689 (90%)	581 (94%)	35 (6%)	4 (1%)	25	55
2	B	338/340 (99%)	315 (93%)	22 (6%)	1 (0%)	41	70
3	G	62/71 (87%)	59 (95%)	3 (5%)	0	100	100
4	Q	315/353 (89%)	300 (95%)	14 (4%)	1 (0%)	41	70
All	All	1335/1453 (92%)	1255 (94%)	74 (6%)	6 (0%)	34	64

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	SER
1	A	335	ASP
4	Q	221	GLU
1	A	231	GLN
1	A	249	GLY

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	561/611 (92%)	546 (97%)	15 (3%)	44	71
2	B	282/282 (100%)	271 (96%)	11 (4%)	32	63
3	G	53/58 (91%)	53 (100%)	0	100	100
4	Q	290/321 (90%)	287 (99%)	3 (1%)	76	89
All	All	1186/1272 (93%)	1157 (98%)	29 (2%)	49	74

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	651	TYR
4	Q	148	ARG
2	B	71	VAL
2	B	295	ASN
2	B	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	259	GLN
4	Q	266	ASN
2	B	295	ASN
4	Q	299	GLN
4	Q	109	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	GDP	Q	360	6,5	24,30,30	0.92	1 (4%)	30,47,47	1.16	4 (13%)
6	ALF	Q	362	5,8,7	0,4,4	-	-	-		

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
7	GDP	Q	360	6,5	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	360	GDP	C6-N1	-2.16	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	360	GDP	C8-N7-C5	2.43	107.62	102.99
7	Q	360	GDP	C5-C6-N1	2.36	118.12	113.95
7	Q	360	GDP	C3'-C2'-C1'	2.15	104.21	100.98
7	Q	360	GDP	O2B-PB-O3A	2.04	111.48	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

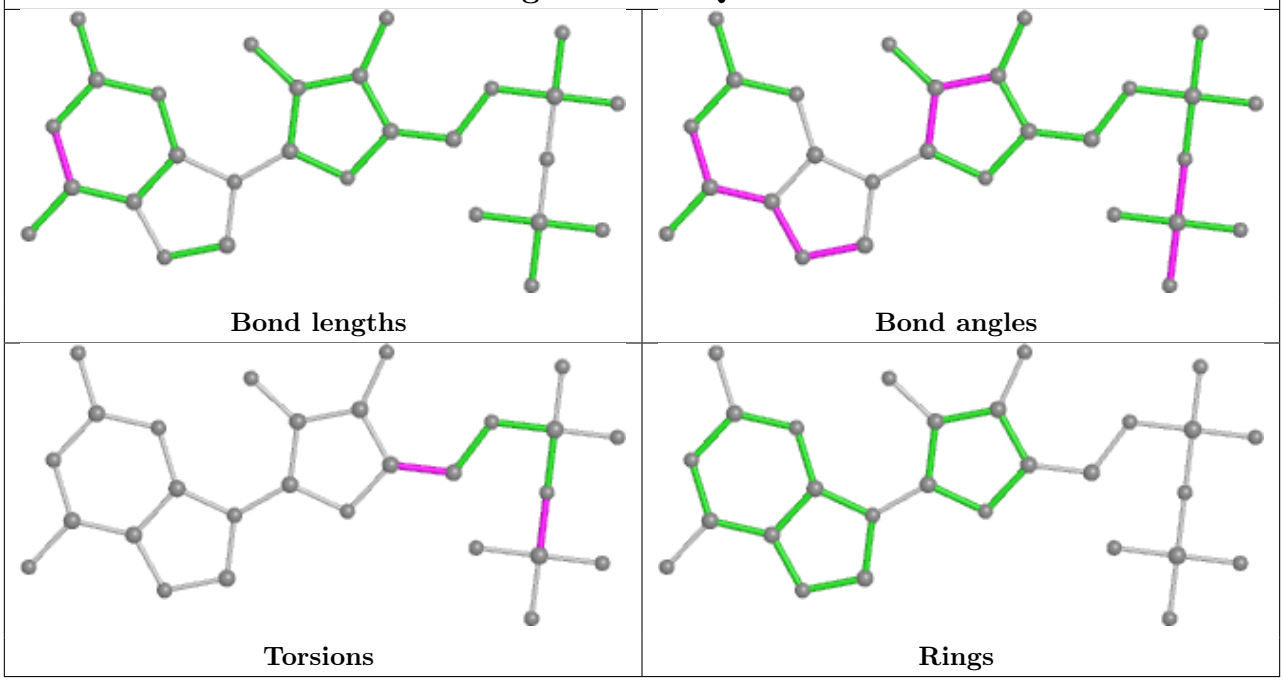
Mol	Chain	Res	Type	Atoms
7	Q	360	GDP	PA-O3A-PB-O2B
7	Q	360	GDP	PA-O3A-PB-O3B
7	Q	360	GDP	O4'-C4'-C5'-O5'
7	Q	360	GDP	C3'-C4'-C5'-O5'
7	Q	360	GDP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 GDP Q 360



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	624/689 (90%)	0.22	13 (2%)	63	39	83, 106, 131, 139	0
2	B	339/340 (99%)	0.15	1 (0%)	94	85	78, 90, 118, 130	0
3	G	64/71 (90%)	0.20	1 (1%)	72	49	91, 105, 126, 128	0
4	Q	317/353 (89%)	0.24	6 (1%)	66	43	90, 106, 123, 128	0
All	All	1344/1453 (92%)	0.20	21 (1%)	72	49	78, 103, 126, 139	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	ILE	3.3
1	A	497	LYS	3.2
4	Q	124	PHE	3.2
4	Q	197	GLN	3.1
1	A	572	PHE	3.1

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 monosaccharides in this entry.

6.4 Ligands (i)

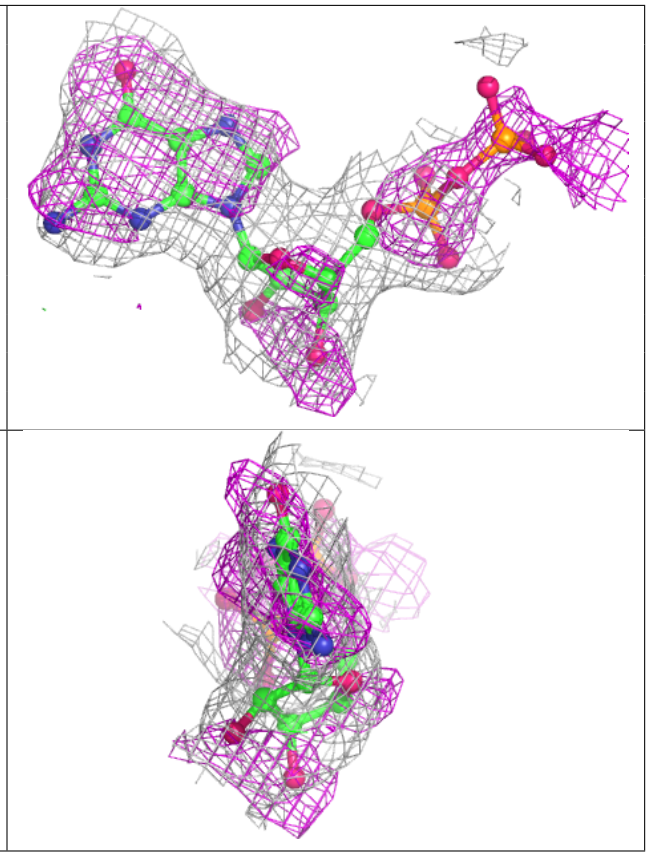
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	Q	361	1/1	0.95	0.09	87,87,87,87	0
7	GDP	Q	360	28/28	0.97	0.14	71,77,78,78	0
6	ALF	Q	362	5/5	0.98	0.10	79,81,83,83	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 GDP Q 360:

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.