wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 09:27 AM EDT

PDB ID	:	2G83 / pdb_00002g83
Title	:	Structure of activated G-alpha-i1 bound to a nucleotide-state-selective peptide: Minimal determinants for recognizing the active form of a G protein alpha subunit
Authors	:	Johnston, C.A.; Ramer, J.K.; Blaesius, R.; Kuhlman, B.; Arshavsky, V.Y.; Siderovski, D.P.
Deposited on	:	2006-03-01
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 (1)) were used in the production of this report:

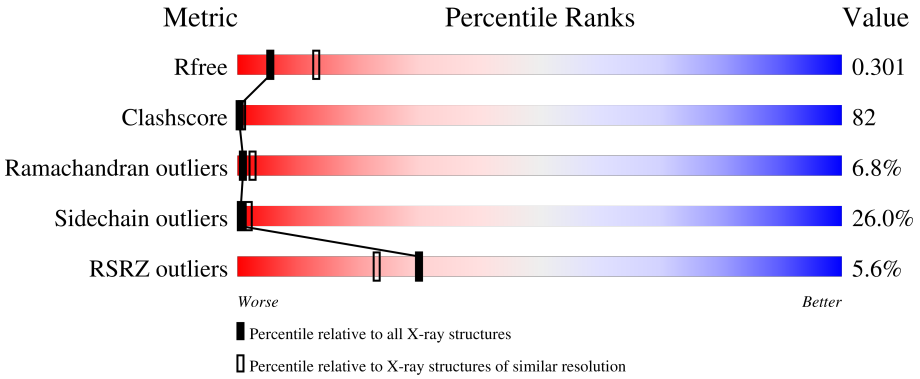
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	313	4% · 32% 45% 19% ·
1	B	313	6% · 28% 40% 26% ·
2	C	11	18% 27% 18% 45% 9%
2	D	11	18% 9% 36% 36% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GDP	A	355	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5190 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.

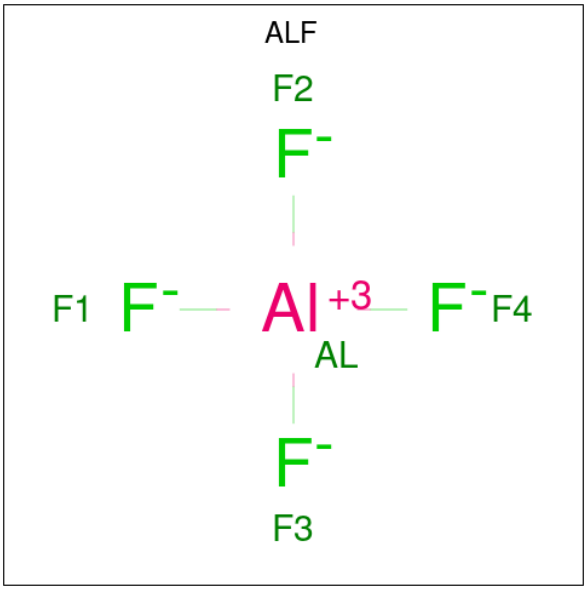
- Molecule 1 is a protein called Guanine nucleotide-binding protein G(i), alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2450	1561	411	464	14			
1	B	303	Total	C	N	O	S	0	0	0
			2450	1561	411	464	14			

- Molecule 2 is a protein called KB-1753 phage display peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			96	63	17	16			
2	D	11	Total	C	N	O	0	0	0
			96	63	17	16			

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

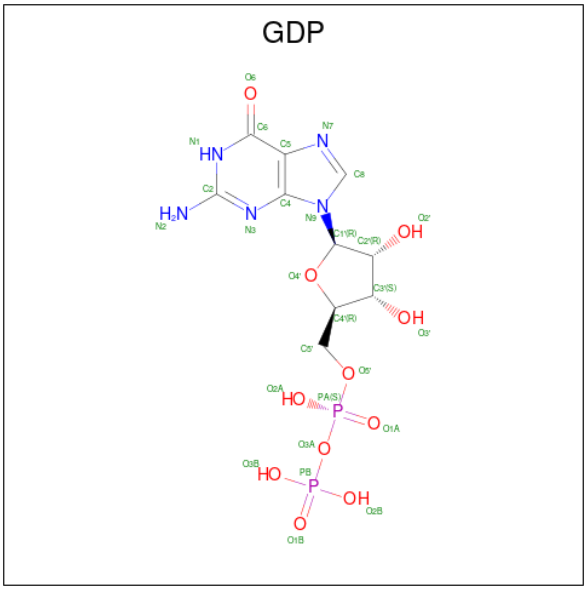


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Al F 5 1 4	0	0
3	B	1	Total Al F 5 1 4	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 28 10 5 11 2	0	0
5	B	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	17	Total O 17 17	0	0

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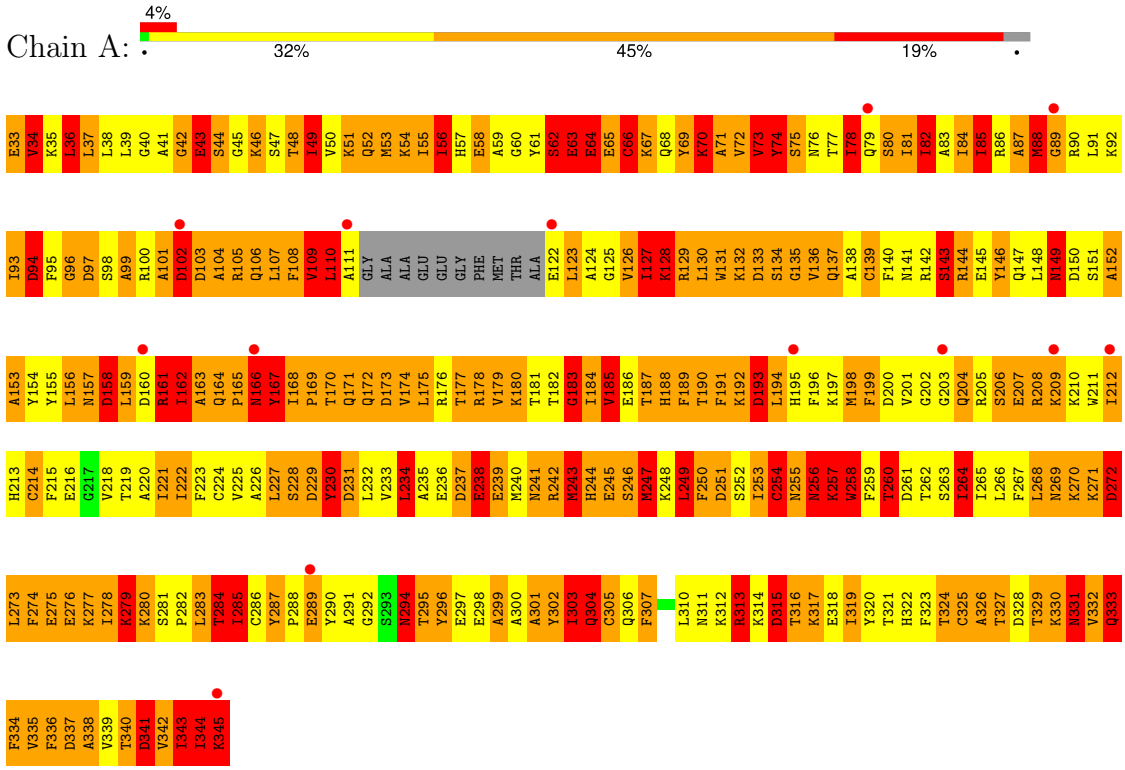
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	12	Total O 12 12	0	0
6	C	1	Total O 1 1	0	0

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.

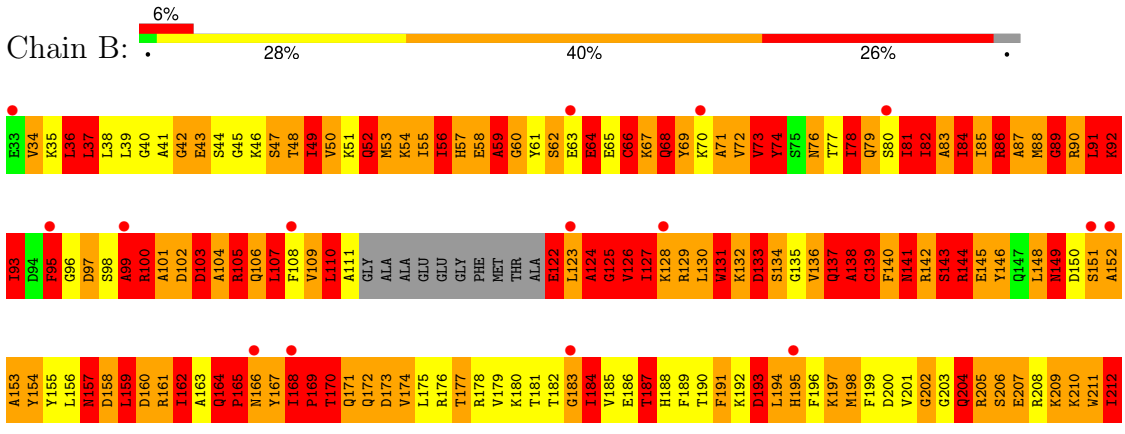
• Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

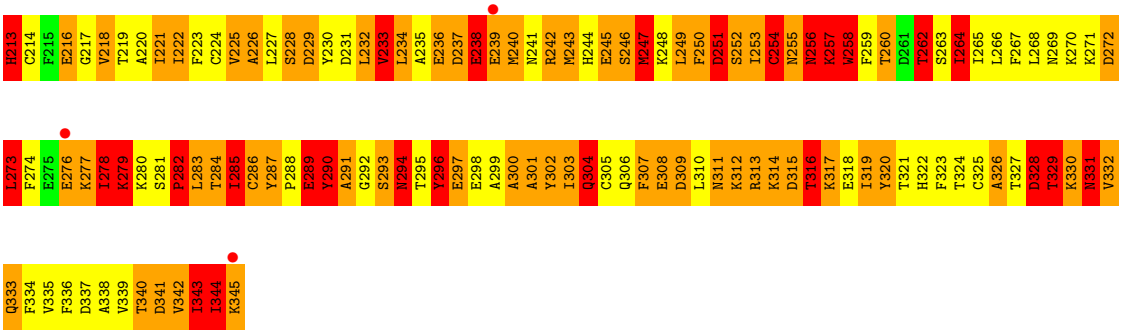
Chain A:



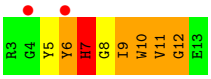
• Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

Chain B:

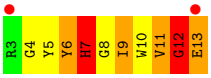




• Molecule 2: KB-1753 phage display peptide



• Molecule 2: KB-1753 phage display peptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.13Å 103.13Å 206.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.9 (50.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.300 0.271 , 0.301	Depositor DCC
R_{free} test set	3043 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: GDP, ALF, MG

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	4.77	707/2494 (28.3%)	2.91	121/3359 (3.6%)
1	B	4.23	531/2494 (21.3%)	2.45	162/3359 (4.8%)
2	C	3.78	17/100 (17.0%)	2.05	5/133 (3.8%)
2	D	4.23	22/100 (22.0%)	1.97	6/133 (4.5%)
All	All	4.49	1277/5188 (24.6%)	2.66	294/6984 (4.2%)

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	A	0	18
1	B	0	29
2	D	0	1
All	All	0	48

The worst 5 of 1277 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	VAL	C-N	-59.30	0.73	1.33
1	A	110	LEU	C-N	-33.71	0.86	1.33
1	B	104	ALA	N-CA	22.19	1.86	1.47
1	B	55	ILE	CA-CB	-19.89	1.32	1.54
1	B	226	ALA	CA-CB	-19.56	1.27	1.53

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	LEU	O-C-N	-77.33	40.38	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	109	VAL	CA-C-N	-54.51	10.61	123.99
1	A	109	VAL	C-N-CA	-54.51	10.61	123.99
1	B	95	PHE	CB-CA-C	-23.89	72.33	111.50
1	B	152	ALA	N-CA-C	20.39	136.77	111.69

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	VAL	Peptide,Mainchain
1	A	110	LEU	Mainchain
1	A	33	GLU	Peptide
1	A	88	MET	Peptide
1	A	89	GLY	Peptide

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	2450	0	2428	285	3
1	B	2450	0	2430	535	0
2	C	96	0	82	11	0
2	D	96	0	82	10	3
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	9	1	0
5	B	28	0	8	2	0
6	A	17	0	0	1	0
6	B	12	0	0	0	0
6	C	1	0	0	0	0
All	All	5190	0	5039	841	3

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 82.

The worst 5 of 841 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:100:ARG:CZ	1:B:129:ARG:HD2	1.19	1.55
1:B:167:TYR:CE1	1:B:169:PRO:HG3	1.51	1.46
1:B:126:VAL:C	1:B:130:LEU:CD1	1.89	1.45
1:B:126:VAL:C	1:B:130:LEU:HD12	1.40	1.40
1:B:104:ALA:N	1:B:104:ALA:CA	1.86	1.39

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:OD2	2:D:6:TYR:O[2_455]	1.40	0.80
1:A:97:ASP:CG	2:D:6:TYR:O[2_455]	2.07	0.13
1:A:97:ASP:OD1	2:D:6:TYR:O[2_455]	2.15	0.05

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	299/313 (96%)	240 (80%)	43 (14%)	16 (5%)	1 4
1	B	299/313 (96%)	232 (78%)	41 (14%)	26 (9%)	0 1
2	C	9/11 (82%)	8 (89%)	1 (11%)	0	100 100
2	D	9/11 (82%)	5 (56%)	4 (44%)	0	100 100
All	All	616/648 (95%)	485 (79%)	89 (14%)	42 (7%)	1 2

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLY
1	B	93	ILE
1	B	105	ARG

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Mol	Chain	Res	Type
1	B	138	ALA
1	B	160	ASP

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	267/272 (98%)	211 (79%)	56 (21%)	1 4
1	B	267/272 (98%)	182 (68%)	85 (32%)	0 1
2	C	8/8 (100%)	7 (88%)	1 (12%)	4 15
2	D	8/8 (100%)	7 (88%)	1 (12%)	4 15
All	All	550/560 (98%)	407 (74%)	143 (26%)	0 2

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	240	MET
1	B	257	LYS
1	B	294	ASN
1	A	303	ILE
1	A	294	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	171	GLN
1	B	172	GLN
1	B	304	GLN
1	B	195	HIS
1	A	269	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 oligosaccharides in this entry.

5.6 Ligand geometry

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 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	GDP	B	355	4,3	29,30,30	3.53	20 (68%)	45,47,47	2.95	21 (46%)
5	GDP	A	355	-	29,30,30	4.05	22 (75%)	45,47,47	2.75	26 (57%)
3	ALF	B	359	5	4,4,4	0.63	0	-		
3	ALF	A	357	-	4,4,4	0.68	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
5	GDP	B	355	4,3	-	1/16/32/32	0/3/3/3
5	GDP	A	355	-	-	4/16/32/32	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	355	GDP	PA-O3A	-8.73	1.50	1.59
5	B	355	GDP	C6-N1	-8.66	1.22	1.38
5	A	355	GDP	C6-N1	-8.21	1.23	1.38
5	B	355	GDP	C5-N7	-6.58	1.25	1.39
5	A	355	GDP	C5-N7	-5.72	1.27	1.39

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	355	GDP	C5-C4-N3	-8.29	115.19	128.39
5	A	355	GDP	O3B-PB-O3A	6.10	125.11	104.64
5	A	355	GDP	C5-C4-N3	-6.10	118.69	128.39
5	B	355	GDP	N9-C4-N3	5.65	137.25	125.95
5	B	355	GDP	O2B-PB-O3A	-5.38	86.59	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	355	GDP	C5'-O5'-PA-O3A
5	A	355	GDP	C5'-O5'-PA-O1A
5	A	355	GDP	C5'-O5'-PA-O2A
5	A	355	GDP	PB-O3A-PA-O2A
5	B	355	GDP	PA-O3A-PB-O2B

There are no ring outliers.

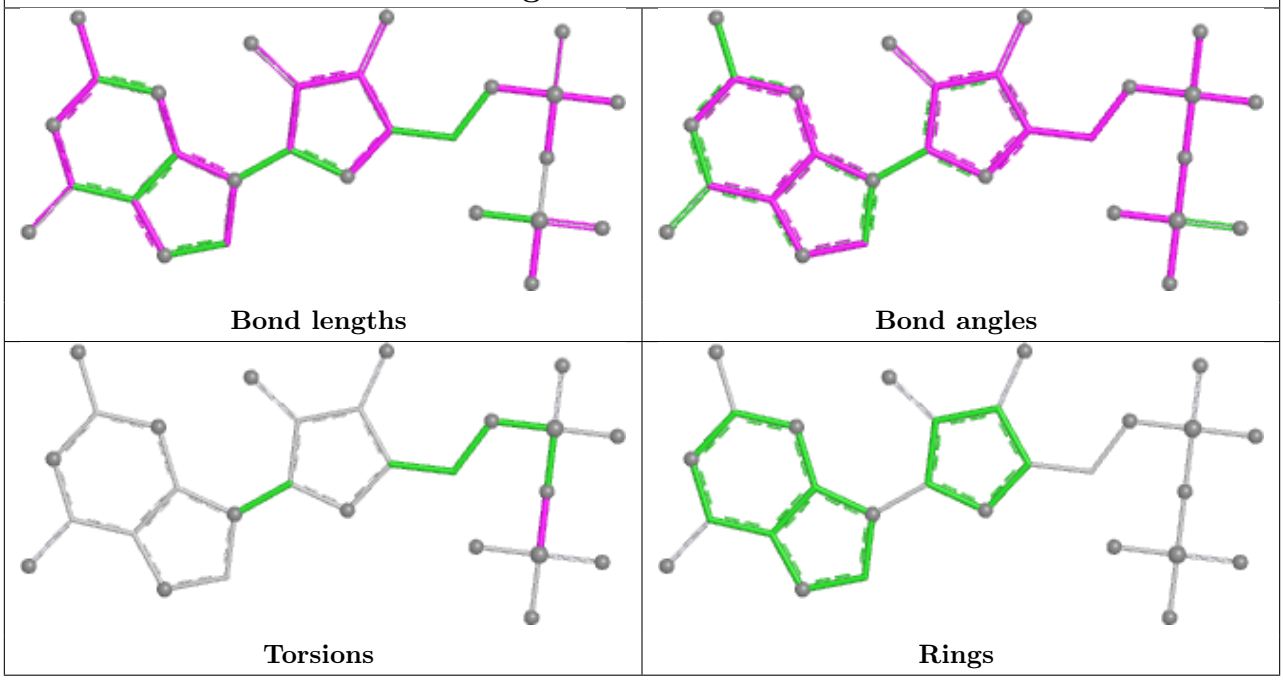
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	355	GDP	2	0
5	A	355	GDP	1	0
3	B	359	ALF	1	0

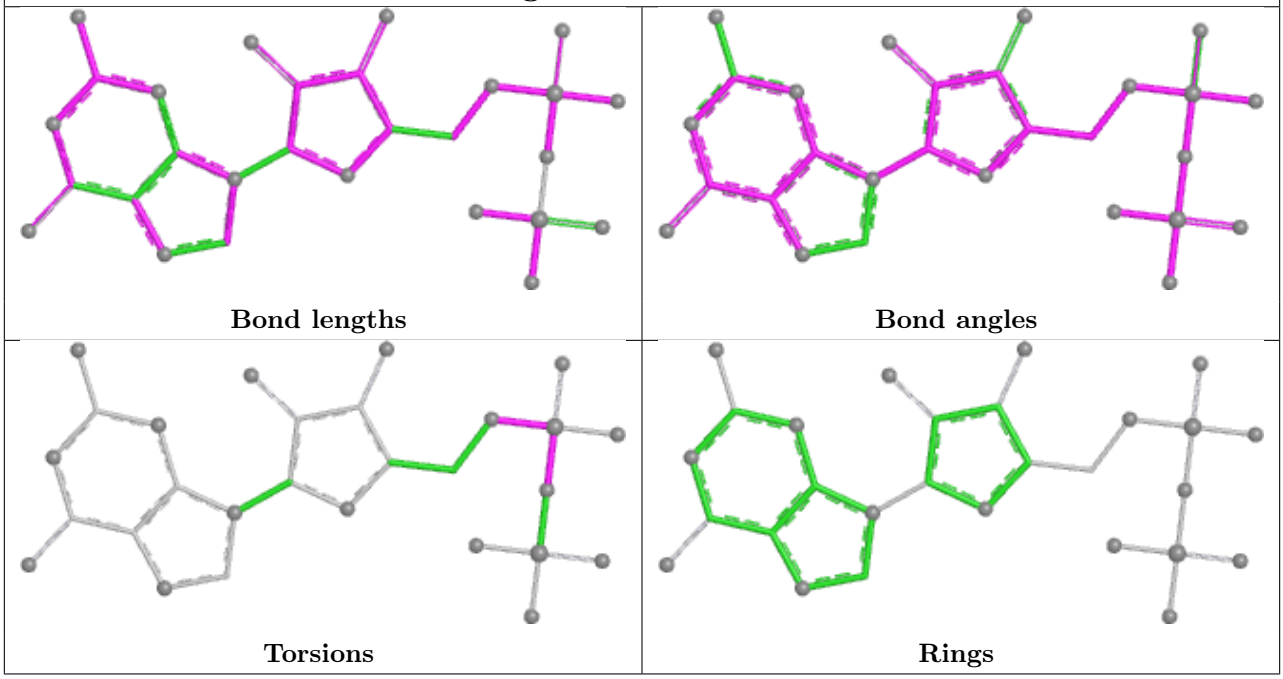
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GDP B 355



Ligand GDP A 355



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	103:ASP	C	104:ALA	N	1.18
1	A	344:ILE	C	345:LYS	N	1.15
1	A	110:LEU	C	111:ALA	N	0.86
1	A	109:VAL	C	110:LEU	N	0.73

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, 95^{th} 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	303/313 (96%)	0.20	13 (4%)	40	31	27, 50, 84, 124	0
1	B	303/313 (96%)	0.46	18 (5%)	28	21	29, 57, 110, 151	0
2	C	11/11 (100%)	1.08	2 (18%)	3	2	47, 66, 107, 109	0
2	D	11/11 (100%)	0.86	2 (18%)	3	2	45, 53, 80, 103	0
All	All	628/648 (96%)	0.36	35 (5%)	30	23	27, 53, 104, 151	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	SER	4.7
1	A	89	GLY	4.1
1	B	183	GLY	4.1
1	A	166	ASN	3.4
1	A	160	ASP	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

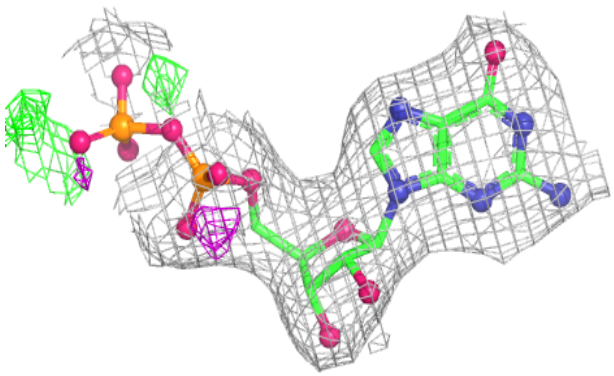
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

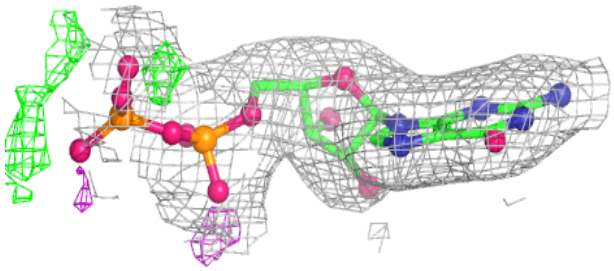
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ALF	B	359	5/5	0.88	0.13	59,61,63,65	0
4	MG	B	358	1/1	0.94	0.07	45,45,45,45	0
5	GDP	A	355	28/28	0.95	0.07	30,33,39,40	0
3	ALF	A	357	5/5	0.96	0.15	53,53,55,56	0
5	GDP	B	355	28/28	0.96	0.07	38,42,45,48	0
4	MG	A	356	1/1	0.97	0.08	29,29,29,29	0

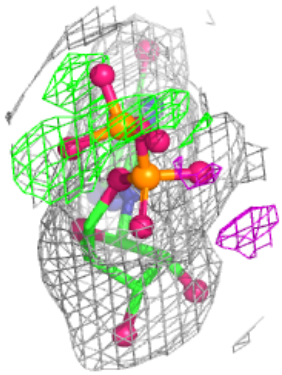
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP A 355:

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

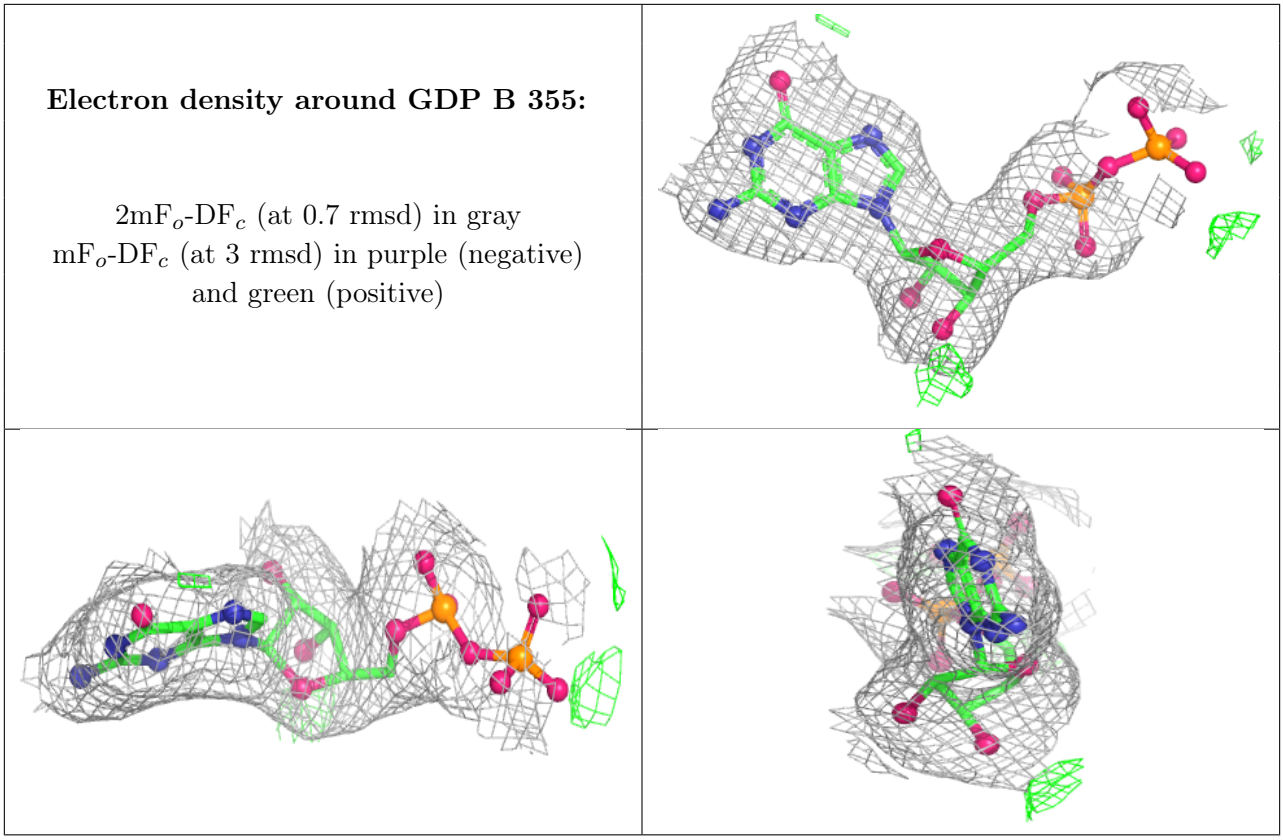






Electron density around GDP B 355:

$2mF_o$-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.