wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 12:38 AM EDT

PDB ID	:	3AB3
Title	:	Crystal structure of p115RhoGEF RGS domain in complex with G alpha 13
Authors	:	Kukimoto-Niino, M.; Mishima, C.; Shirouzu, M.; Kozasa, T.; Yokoyama, S.
Deposited on	:	2009-11-30
Resolution	:	2.40 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:

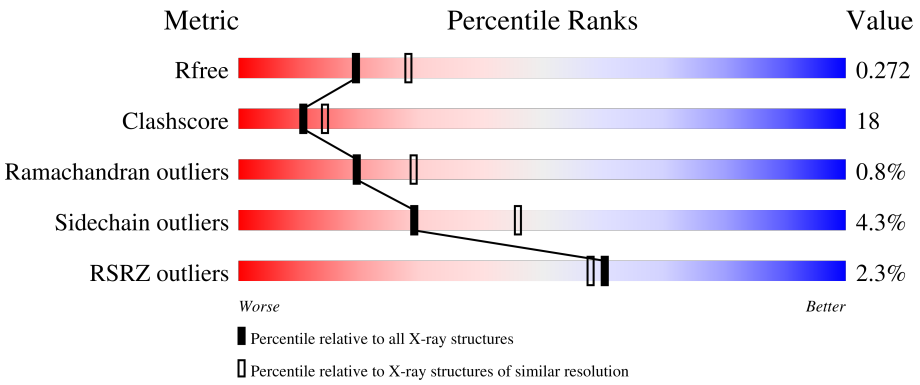
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	362	59% 29% • 11%
1	C	362	57% 28% • 12%
2	B	246	4% 46% 26% • 26%
2	D	246	4% 39% 26% • 33%

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	ALF	C	602	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8246 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(k) subunit alpha, Guanine nucleotide-binding protein subunit alpha-13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2660	1694	472	484	10	0	0	0
1	C	318	2627	1674	466	477	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ARG	-	linker	UNP Q9DC51
A	45	SER	-	linker	UNP Q9DC51
A	46	ALA	-	linker	UNP Q9DC51
C	44	ARG	-	linker	UNP Q9DC51
C	45	SER	-	linker	UNP Q9DC51
C	46	ALA	-	linker	UNP Q9DC51

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	182	1475	931	267	268	9	0	0	0
2	D	165	1329	841	237	242	9	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP Q92888
B	-11	ALA	-	expression tag	UNP Q92888
B	-10	MET	-	expression tag	UNP Q92888
B	-9	GLY	-	expression tag	UNP Q92888
B	-8	ILE	-	expression tag	UNP Q92888

Continued on next page...

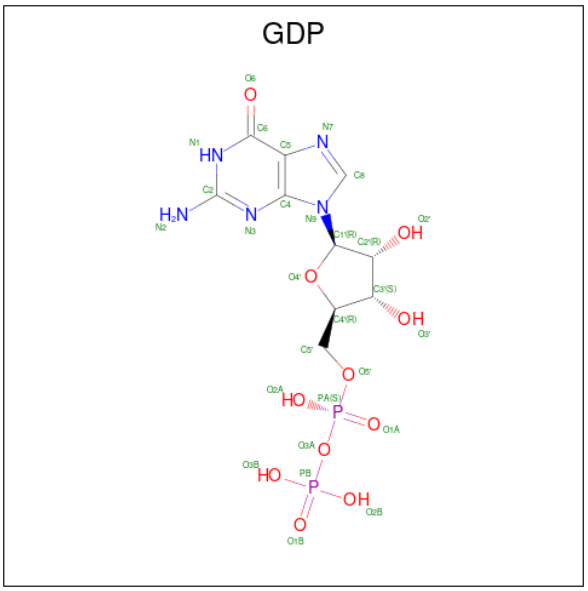
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP Q92888
B	-6	CYS	-	expression tag	UNP Q92888
B	-5	GLY	-	expression tag	UNP Q92888
B	-4	GLY	-	expression tag	UNP Q92888
B	-3	ILE	-	expression tag	UNP Q92888
B	-2	LEU	-	expression tag	UNP Q92888
B	-1	VAL	-	expression tag	UNP Q92888
B	0	PRO	-	expression tag	UNP Q92888
D	-12	GLY	-	expression tag	UNP Q92888
D	-11	ALA	-	expression tag	UNP Q92888
D	-10	MET	-	expression tag	UNP Q92888
D	-9	GLY	-	expression tag	UNP Q92888
D	-8	ILE	-	expression tag	UNP Q92888
D	-7	GLN	-	expression tag	UNP Q92888
D	-6	CYS	-	expression tag	UNP Q92888
D	-5	GLY	-	expression tag	UNP Q92888
D	-4	GLY	-	expression tag	UNP Q92888
D	-3	ILE	-	expression tag	UNP Q92888
D	-2	LEU	-	expression tag	UNP Q92888
D	-1	VAL	-	expression tag	UNP Q92888
D	0	PRO	-	expression tag	UNP Q92888

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

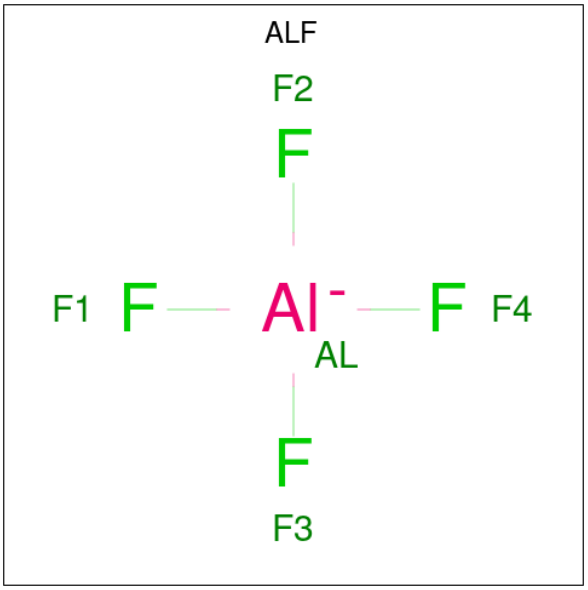
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	C	1	1	1	0	0

- Molecule 4 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		
4	A	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
4	C	1	28	10	5	11	2	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

- Molecule 6 is water.

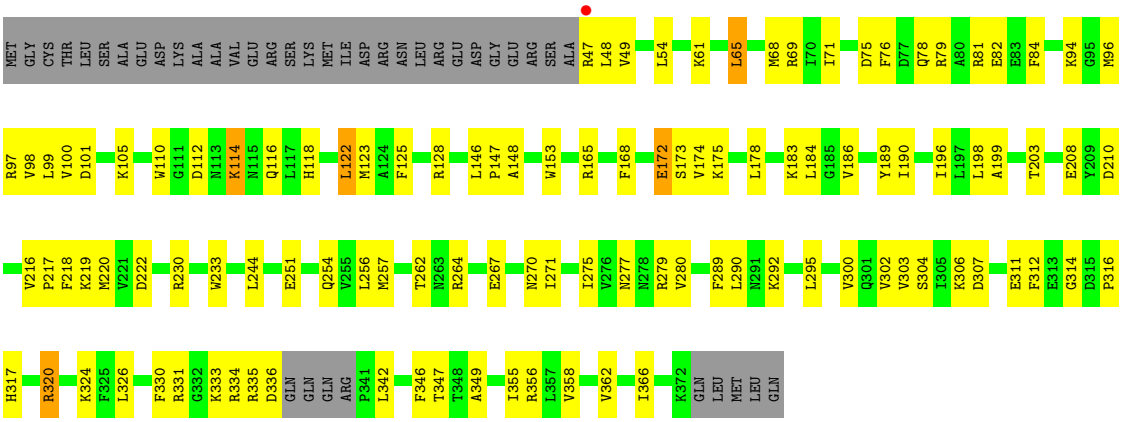
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	41	41	41	0	0
			Total	O		
6	B	12	12	12	0	0
			Total	O		
6	C	30	30	30	0	0
			Total	O		
6	D	4	4	4	0	0

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.

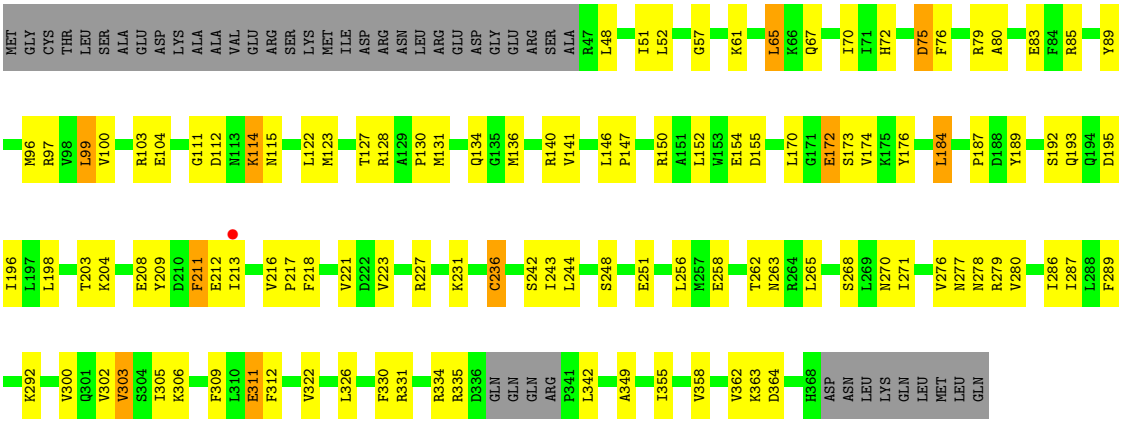
• Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha, Guanine nucleotide-binding protein subunit alpha-13

Chain A:



• Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha, Guanine nucleotide-binding protein subunit alpha-13

Chain C:



• Molecule 2: Rho guanine nucleotide exchange factor 1

Chain B: 4% 46% 26% • 26%

GLY ALA MET GLY ILE GLN CYS GLY GLY ILE LEU VAL PRO MET GLU ASP PHE ALA ARG GLY ALA ALA SER PRO GLY PRO SER ARG PRO GLY LEU VAL PRO VAL S22 I23 E29 D30 F31 E32 N33 E34 LEU GLU THR ASN SER GLU GLU GLN ASN SER GLN F46 E50 Q51 V52 K53

R54 R55 L59 L63 L68 Q69 F70 E71 P74 L75 L76 H80 A81 D82 M83 L84 G85 SER LEU GLY PRO LYS GLU ALA K93 K106 N117 V118 A119 F120 E121 LEU ASP ARG THR ARG ALA ASP LEU ILE SER GLU ASP V134 F138 V142 V143 Q144 V148

R152 Q153 L154 E155 D156 F157 R158 S159 K160 M163 G164 M165 T166 P167 Q170 W178 V179 G180 R181 D182 S185 R189 V193 R196 L197 L198 M199 H200 L201 E202 E203 M204 Q205 H206 T207 I208 S209 T210 D211 K214 S215 V219 I222 G223 L224 Y225 M226 R227 T233

• Molecule 2: Rho guanine nucleotide exchange factor 1

Chain D: 4% 39% 26% • 33%

GLY ALA MET GLY ILE GLN CYS GLY GLY ILE LEU VAL PRO MET GLU ASP PHE ALA ARG GLY ALA ALA SER PRO GLY PRO SER ARG PRO GLY LEU VAL PRO VAL S22 F31 E32 ASN GLU LEU GLU THR ASN SER GLU GLU GLN ASN SER GLN F46 Q47 S48 L49 E50 K53 R54 R55

P56 A57 H58 L59 M60 L63 Q64 H65 V66 A67 L68 Q69 P74 C77 H80 M83 L84 G85 SER LEU GLY PRO LYS GLU A92 K93 K94 L97 D98 F99 Y100 H101 S102 F103 L104 E105 K106 T107 A108 V109 L110 R111 V112 P113 V114 P115 PRO ASN VAL ALA PHE GLU LEU ASP

ARG THR ARG ALA ASP LEU ILE SER GLU ASP VAL GLN ARG ARG F138 V139 Q140 E141 V142 V143 Q144 S145 Q146 Q147 V148 G151 R158 S159 K160 R161 L162 M163 G164 M165 E176 ALA TRP VAL GLY ARG ASP R183 A188 R189 E190 R191 H192 E195 L198 L201 E202 Q205

H206 T207 I208 S209 K214 V218 V219 I222 Y225 M226 R227 H228 L229 G230 V231 R232 T233

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.48Å 70.64Å 88.08Å 77.77° 84.45° 80.11°	Depositor
Resolution (Å)	48.88 – 2.40 48.88 – 2.39	Depositor EDS
% Data completeness (in resolution range)	81.7 (48.88-2.40) 81.1 (48.88-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.280 0.200 , 0.272	Depositor DCC
R_{free} test set	3734 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8246	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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	0.48	0/2712	0.65	0/3651
1	C	0.49	0/2679	0.64	1/3607 (0.0%)
2	B	0.44	0/1502	0.62	0/2022
2	D	0.39	0/1351	0.58	0/1815
All	All	0.46	0/8244	0.63	1/11095 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184	LEU	CA-CB-CG	5.61	128.21	115.30

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	2660	0	2662	88	0
1	C	2627	0	2628	107	0
2	B	1475	0	1457	62	0
2	D	1329	0	1320	62	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	12	0	0
4	C	28	0	12	1	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	41	0	0	2	0
6	B	12	0	0	1	0
6	C	30	0	0	4	0
6	D	4	0	0	0	0
All	All	8246	0	8091	299	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 18.

The worst 5 of 299 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:320:ARG:HE	1:A:324:LYS:HE3	1.20	0.99
1:C:213:ILE:HD12	6:C:378:HOH:O	1.65	0.96
2:B:193:VAL:HA	2:B:196:ARG:NH1	1.85	0.92
2:B:211:ASP:HB3	2:B:214:LYS:HB3	1.55	0.86
2:D:226:MET:HB3	2:D:231:VAL:HB	1.55	0.86

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	318/362 (88%)	304 (96%)	14 (4%)	0	100 100
1	C	314/362 (87%)	297 (95%)	16 (5%)	1 (0%)	41 55
2	B	174/246 (71%)	160 (92%)	11 (6%)	3 (2%)	9 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	155/246 (63%)	142 (92%)	9 (6%)	4 (3%)	5	5
All	All	961/1216 (79%)	903 (94%)	50 (5%)	8 (1%)	19	29

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	148	VAL
2	D	109	VAL
2	B	203	GLU
2	B	211	ASP
2	B	33	ASN

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	294/328 (90%)	285 (97%)	9 (3%)	40	60
1	C	290/328 (88%)	277 (96%)	13 (4%)	27	44
2	B	157/207 (76%)	147 (94%)	10 (6%)	17	28
2	D	142/207 (69%)	136 (96%)	6 (4%)	30	47
All	All	883/1070 (82%)	845 (96%)	38 (4%)	29	46

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	SER
2	D	162	LEU
1	C	303	VAL
2	D	50	GLU
2	D	233	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	101	HIS
2	D	192	HIS
2	D	174	GLN
1	C	144	GLN
2	D	47	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 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 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	ALF	A	601	-	0,4,4	-	-	-		
5	ALF	C	602	-	0,4,4	-	-	-		
4	GDP	A	401	3	24,30,30	1.57	4 (16%)	30,47,47	1.87	8 (26%)
4	GDP	C	402	3	24,30,30	1.51	3 (12%)	30,47,47	1.92	11 (36%)

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
4	GDP	A	401	3	-	3/12/32/32	0/3/3/3
4	GDP	C	402	3	-	2/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	GDP	O4'-C1'	5.17	1.48	1.41
4	A	401	GDP	O4'-C1'	4.78	1.47	1.41
4	A	401	GDP	C8-N7	-3.22	1.29	1.35
4	C	402	GDP	C8-N7	-2.97	1.30	1.35
4	A	401	GDP	C2'-C1'	-2.25	1.50	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	GDP	O3'-C3'-C4'	5.91	128.15	111.05
4	C	402	GDP	O3'-C3'-C4'	5.86	128.00	111.05
4	C	402	GDP	C8-N7-C5	3.33	109.33	102.99
4	A	401	GDP	C8-N7-C5	3.05	108.80	102.99
4	A	401	GDP	O3B-PB-O2B	2.79	118.30	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	GDP	PA-O3A-PB-O2B
4	A	401	GDP	PA-O3A-PB-O3B
4	C	402	GDP	PA-O3A-PB-O3B
4	C	402	GDP	PA-O3A-PB-O2B
4	A	401	GDP	PA-O3A-PB-O1B

There are no ring outliers.

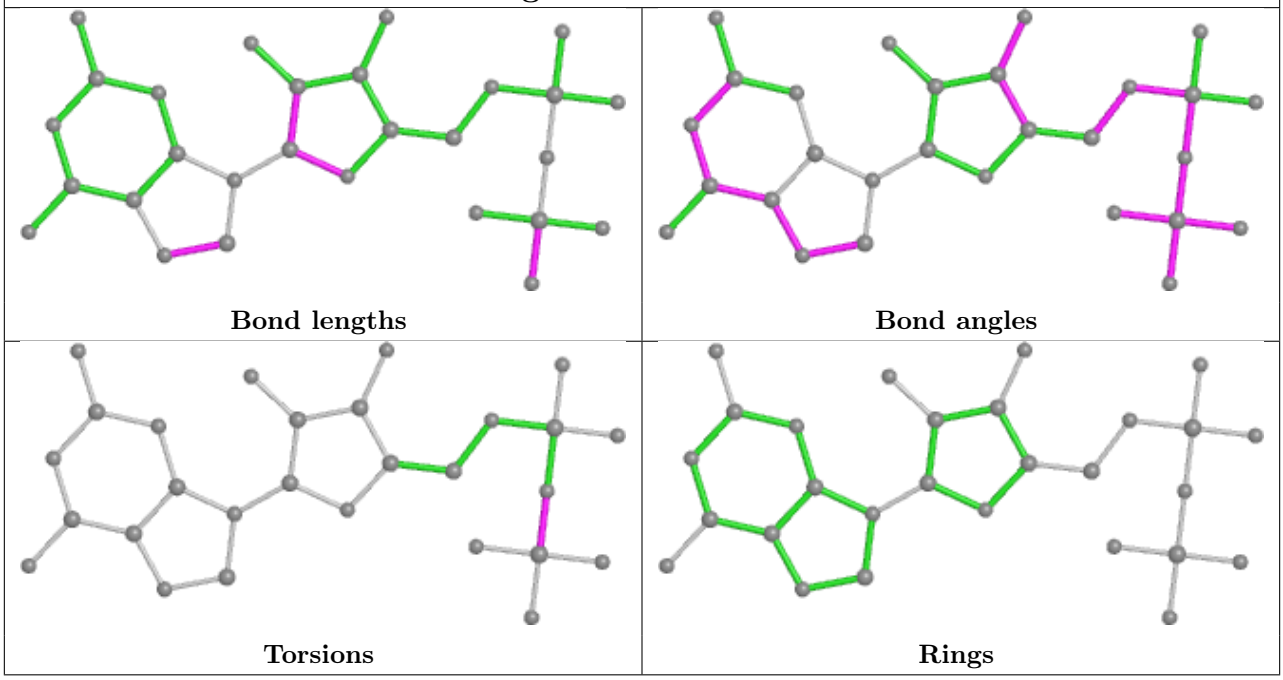
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	ALF	1	0
5	C	602	ALF	2	0
4	C	402	GDP	1	0

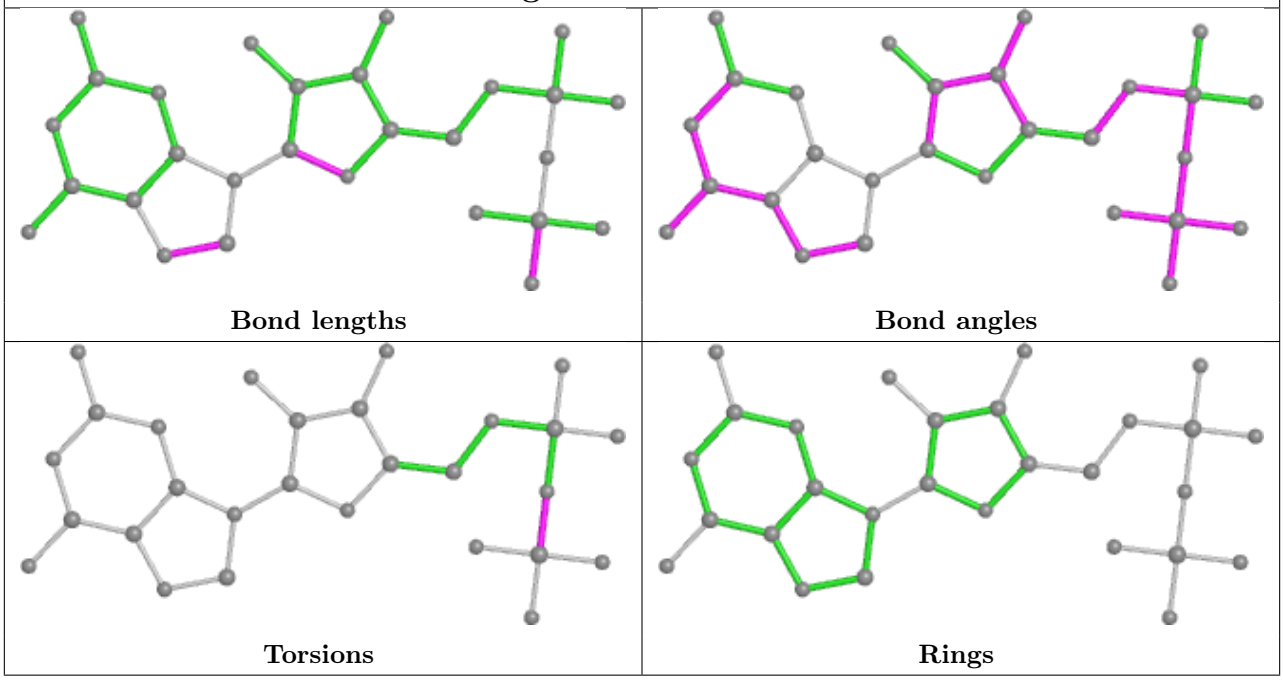
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 A 401



Ligand GDP C 402



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	322/362 (88%)	-0.25	1 (0%)	94	93	25, 42, 68, 92	0
1	C	318/362 (87%)	-0.24	1 (0%)	94	93	23, 44, 77, 104	0
2	B	182/246 (73%)	0.14	10 (5%)	25	24	27, 55, 95, 107	1 (0%)
2	D	165/246 (67%)	0.34	11 (6%)	17	16	35, 62, 97, 104	1 (0%)
All	All	987/1216 (81%)	-0.07	23 (2%)	60	58	23, 47, 86, 107	2 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	110	LEU	3.5
2	B	208	ILE	3.4
2	D	115	PRO	3.3
2	D	139	VAL	3.3
2	D	108	ALA	3.2

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)

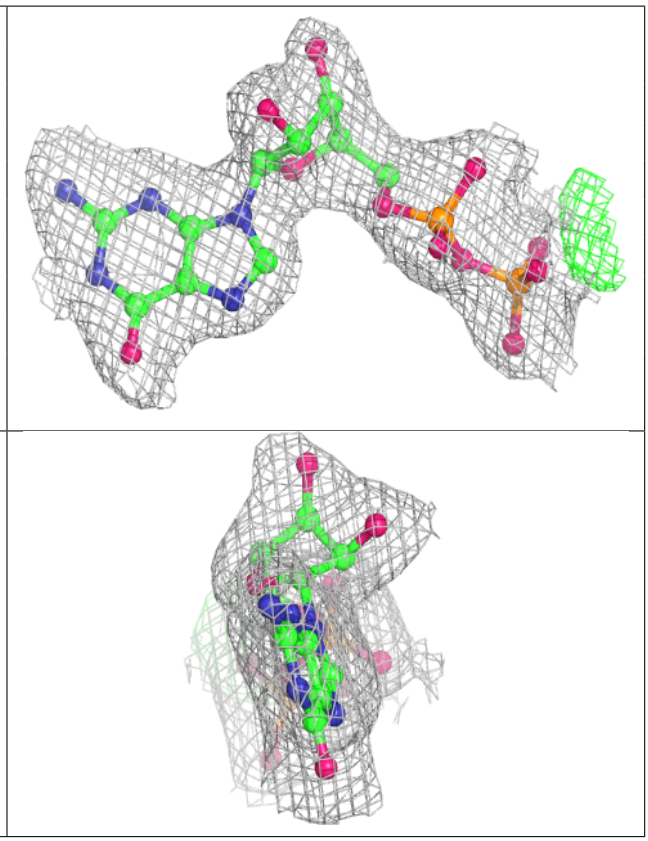
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	502	1/1	0.95	0.21	34,34,34,34	0
5	ALF	A	601	5/5	0.97	0.18	33,41,45,51	0
5	ALF	C	602	5/5	0.97	0.23	47,47,49,61	0
3	MG	A	501	1/1	0.98	0.20	30,30,30,30	0
4	GDP	C	402	28/28	0.98	0.16	22,31,39,40	0
4	GDP	A	401	28/28	0.99	0.16	19,26,34,40	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.

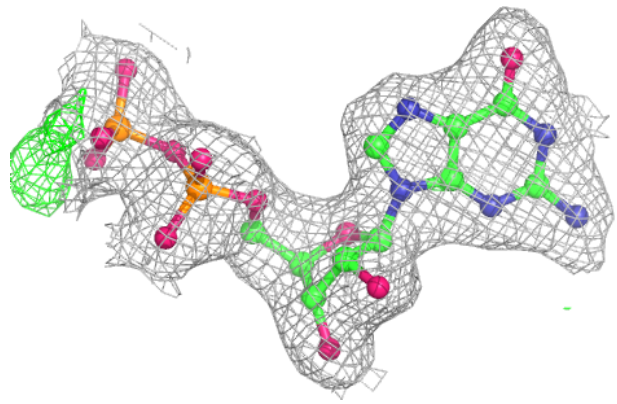
Electron density around GDP C 402:

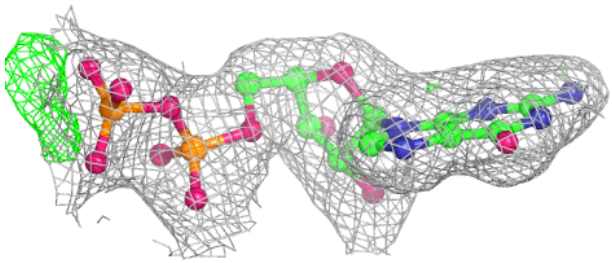
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

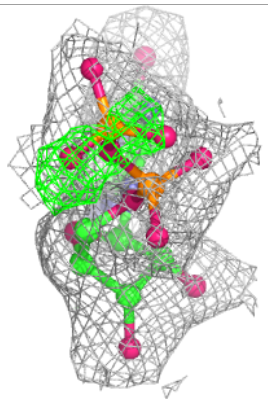


Electron density around GDP A 401:

$2mF_o$-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.