wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 11:38 PM EDT

PDB ID	:	1S8F
Title	:	Crystal structure of Rab9 complexed to GDP reveals a dimer with an active conformation of switch II
Authors	:	Wittmann, J.G.; Rudolph, M.G.
Deposited on	:	2004-02-02
Resolution	:	1.77 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:

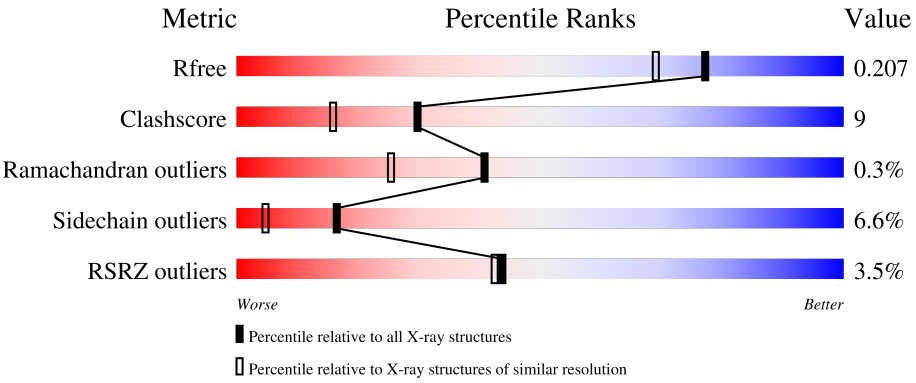
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	177	3% 76% 17% • 5%
1	B	177	3% 70% 24% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3039 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 Ras-related protein Rab-9A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	1	0
			1352	859	225	263	5			
1	B	173	Total	C	N	O	S	0	3	0
			1360	869	223	261	7			

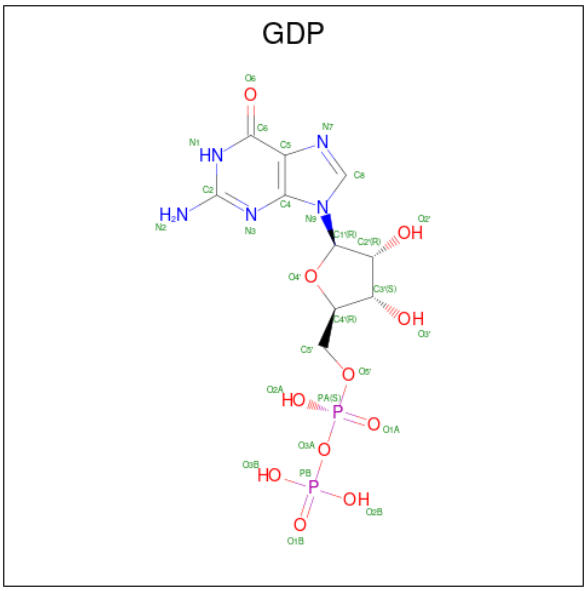
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	999	GLY	-	cloning artifact	UNP P24408
A	1000	ALA	-	cloning artifact	UNP P24408
B	3999	GLY	-	cloning artifact	UNP P24408
B	4000	ALA	-	cloning artifact	UNP P24408

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

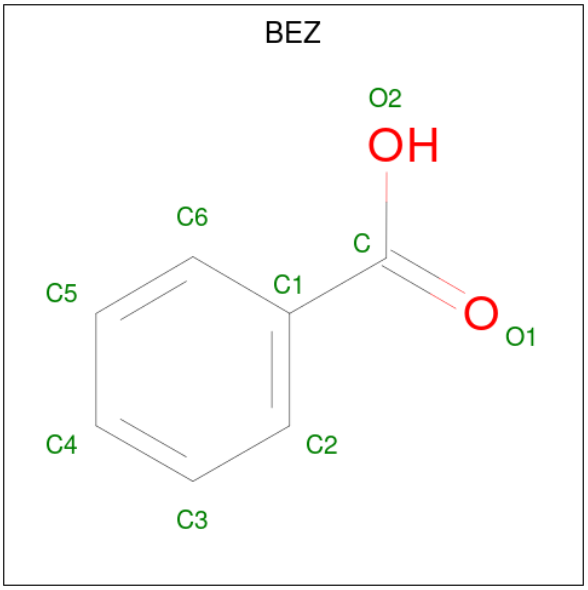
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Sr	0	0
			1	1		
2	B	1	Total	Sr	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 4 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	7	2		
4	A	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 7 2	0	0
4	B	1	Total C O 9 7 2	0	0

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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is water.

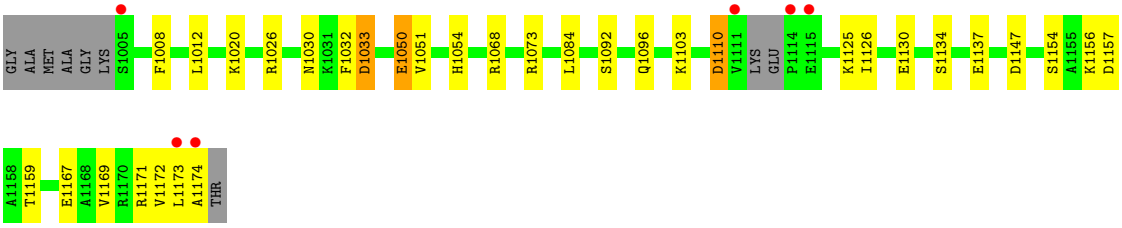
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	136	Total O 136 136	0	0
7	B	95	Total O 95 95	0	0

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.

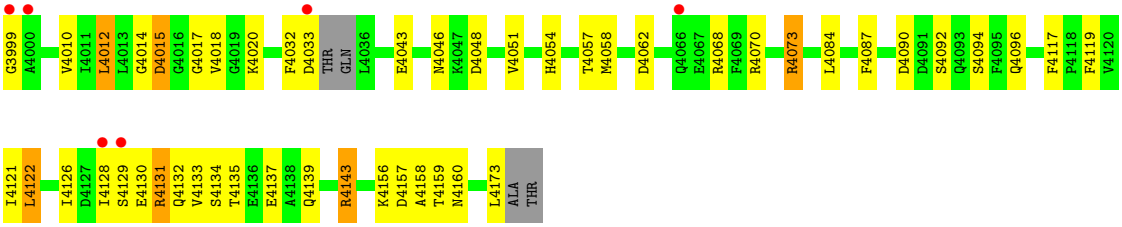
• Molecule 1: Ras-related protein Rab-9A

Chain A:



• Molecule 1: Ras-related protein Rab-9A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	98.25Å 98.25Å 79.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.77 34.73 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.77) 96.9 (34.73-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.75Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.165 , 0.221 0.159 , 0.207	Depositor DCC
R_{free} test set	1878 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.205 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3039	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, CL, SR, MG, BEZ

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	0.40	0/1387	1.10	2/1874 (0.1%)
1	B	0.38	0/1403	1.07	5/1898 (0.3%)
All	All	0.39	0/2790	1.08	7/3772 (0.2%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1073	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	4015	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	4012	LEU	CA-CB-CG	6.80	130.93	115.30
1	B	4073	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	4073	ARG	CD-NE-CZ	6.66	132.93	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1352	0	1281	23	0
1	B	1360	0	1281	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	12	1	0
3	B	28	0	12	2	0
4	A	27	0	15	0	0
4	B	9	0	5	2	0
5	B	1	0	0	0	0
6	B	1	0	0	1	0
7	A	136	0	0	5	0
7	B	95	0	0	5	0
All	All	3039	0	2606	51	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 9.

The worst 5 of 51 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)
6:B:3001:CL:CL	7:B:9069:HOH:O	2.40	0.75
1:B:4014:GLY:O	1:B:4020:LYS:HE2	1.87	0.74
1:B:4046:ASN:HB3	7:B:9137:HOH:O	1.91	0.71
1:B:4048:ASP:OD1	1:B:4057:THR:HG23	1.91	0.69
1:A:1154:SER:HB3	1:A:1157[A]:ASP:OD2	1.95	0.67

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	165/177 (93%)	162 (98%)	3 (2%)	0	100 100
1	B	172/177 (97%)	164 (95%)	7 (4%)	1 (1%)	25 11
All	All	337/354 (95%)	326 (97%)	10 (3%)	1 (0%)	41 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4130	GLU

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	147/152 (97%)	139 (95%)	8 (5%)	22 8
1	B	145/152 (95%)	134 (92%)	11 (8%)	13 3
All	All	292/304 (96%)	273 (94%)	19 (6%)	16 5

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4122	LEU
1	B	4132	GLN
1	B	4143	ARG
1	B	4129	SER
1	B	4012	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	GLN
1	B	4054	HIS
1	B	4093	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	BEZ	B	1503	-	9,9,9	1.93	1 (11%)	11,11,11	1.81	4 (36%)
4	BEZ	A	1501	-	9,9,9	1.88	1 (11%)	11,11,11	2.05	4 (36%)
3	GDP	A	3400	2	24,30,30	1.14	1 (4%)	30,47,47	1.68	6 (20%)
4	BEZ	A	1500	-	9,9,9	1.77	1 (11%)	11,11,11	1.85	4 (36%)
3	GDP	B	6400	5	24,30,30	1.23	3 (12%)	30,47,47	1.59	5 (16%)
4	BEZ	A	1502	2	9,9,9	1.96	1 (11%)	11,11,11	1.87	4 (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	BEZ	B	1503	-	-	0/4/4/4	0/1/1/1
4	BEZ	A	1501	-	-	0/4/4/4	0/1/1/1
3	GDP	A	3400	2	-	0/12/32/32	0/3/3/3
4	BEZ	A	1500	-	-	0/4/4/4	0/1/1/1
3	GDP	B	6400	5	-	1/12/32/32	0/3/3/3
4	BEZ	A	1502	2	-	4/4/4/4	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1502	BEZ	O1-C	5.62	1.39	1.22
4	B	1503	BEZ	O1-C	5.39	1.38	1.22
4	A	1501	BEZ	O1-C	5.20	1.38	1.22
4	A	1500	BEZ	O1-C	5.12	1.37	1.22
3	A	3400	GDP	C5-C6	-3.05	1.41	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	6400	GDP	O2'-C2'-C3'	4.32	125.80	111.82
3	A	3400	GDP	O6-C6-N1	-4.10	115.81	120.65
4	A	1502	BEZ	C3-C2-C1	-3.48	116.22	120.34
4	A	1501	BEZ	O2-C-O1	-3.46	115.66	123.35
3	B	6400	GDP	C8-N7-C5	3.42	109.50	102.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1502	BEZ	O2-C-C1-C6
4	A	1502	BEZ	O1-C-C1-C6
4	A	1502	BEZ	O2-C-C1-C2
4	A	1502	BEZ	O1-C-C1-C2
3	B	6400	GDP	PA-O3A-PB-O1B

There are no ring outliers.

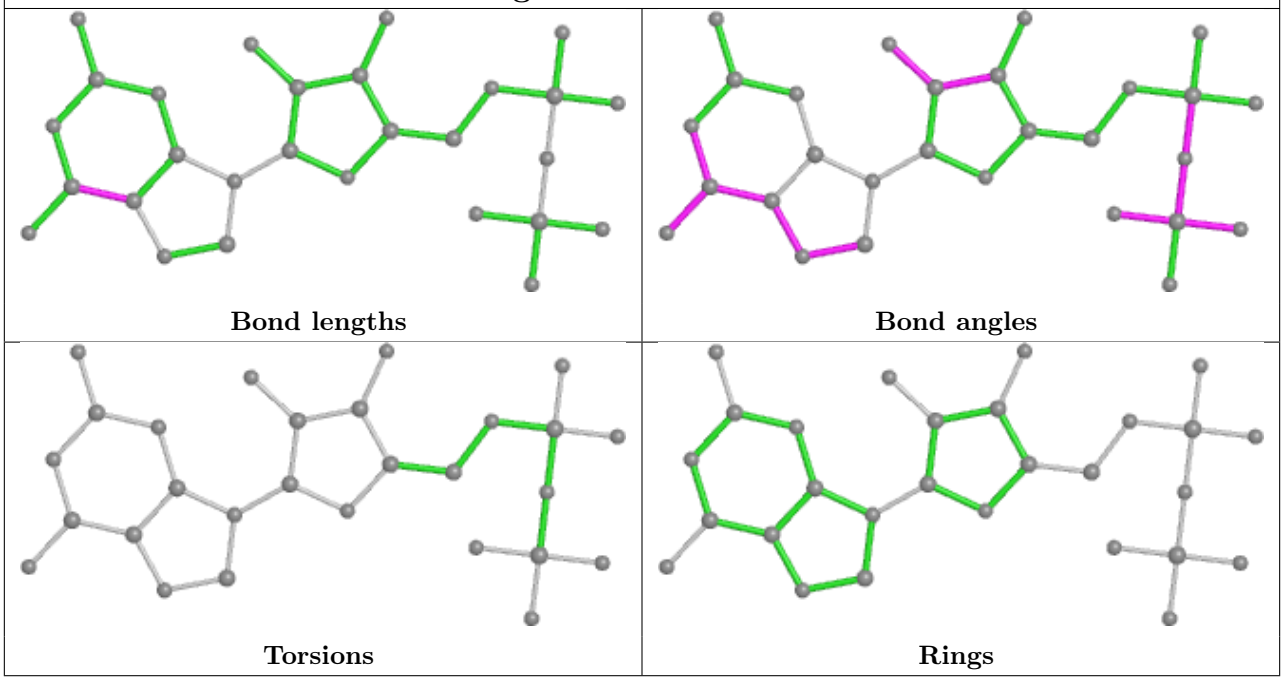
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1503	BEZ	2	0
3	A	3400	GDP	1	0
3	B	6400	GDP	2	0

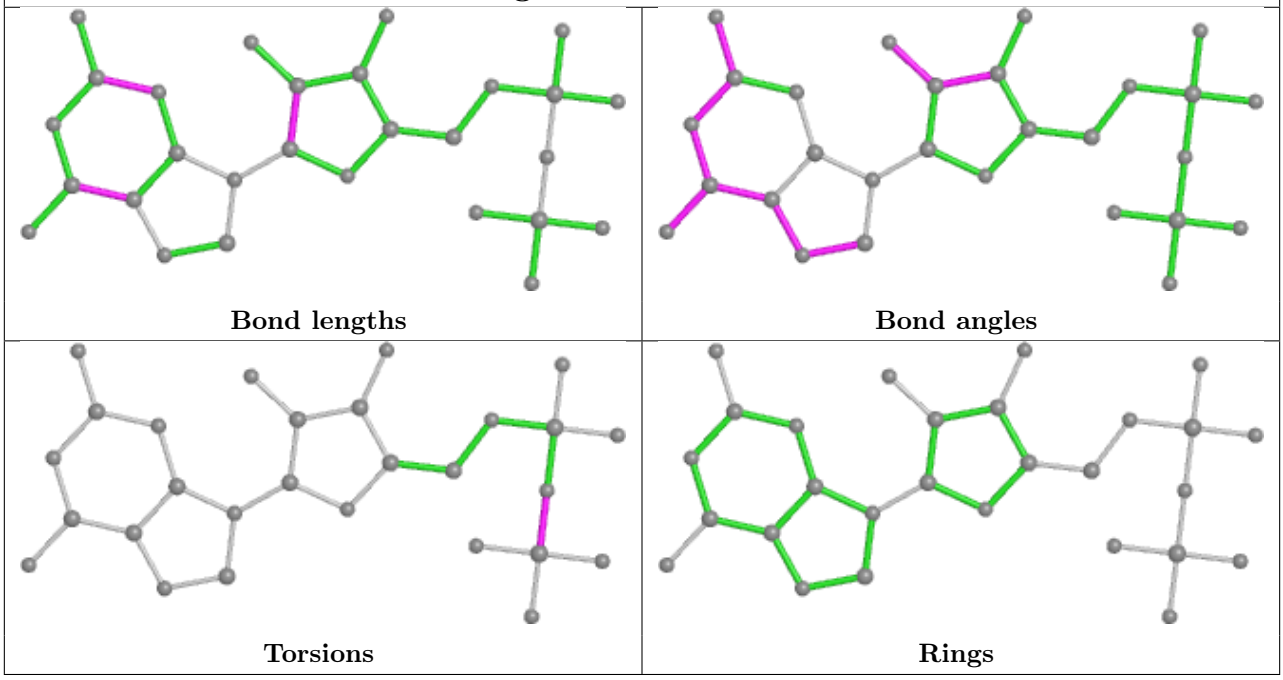
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3400



Ligand GDP B 6400



5.7 Other polymers

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

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	168/177 (94%)	-0.02	6 (3%)	42	41	13, 24, 48, 82	0
1	B	173/177 (97%)	0.15	6 (3%)	44	42	16, 29, 56, 100	0
All	All	341/354 (96%)	0.07	12 (3%)	44	42	13, 27, 54, 100	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3999	GLY	3.2
1	B	4128	ILE	3.1
1	A	1174	ALA	3.1
1	B	4066	GLN	2.9
1	A	1111	VAL	2.8

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 monosaccharides in this entry.

6.4 Ligands

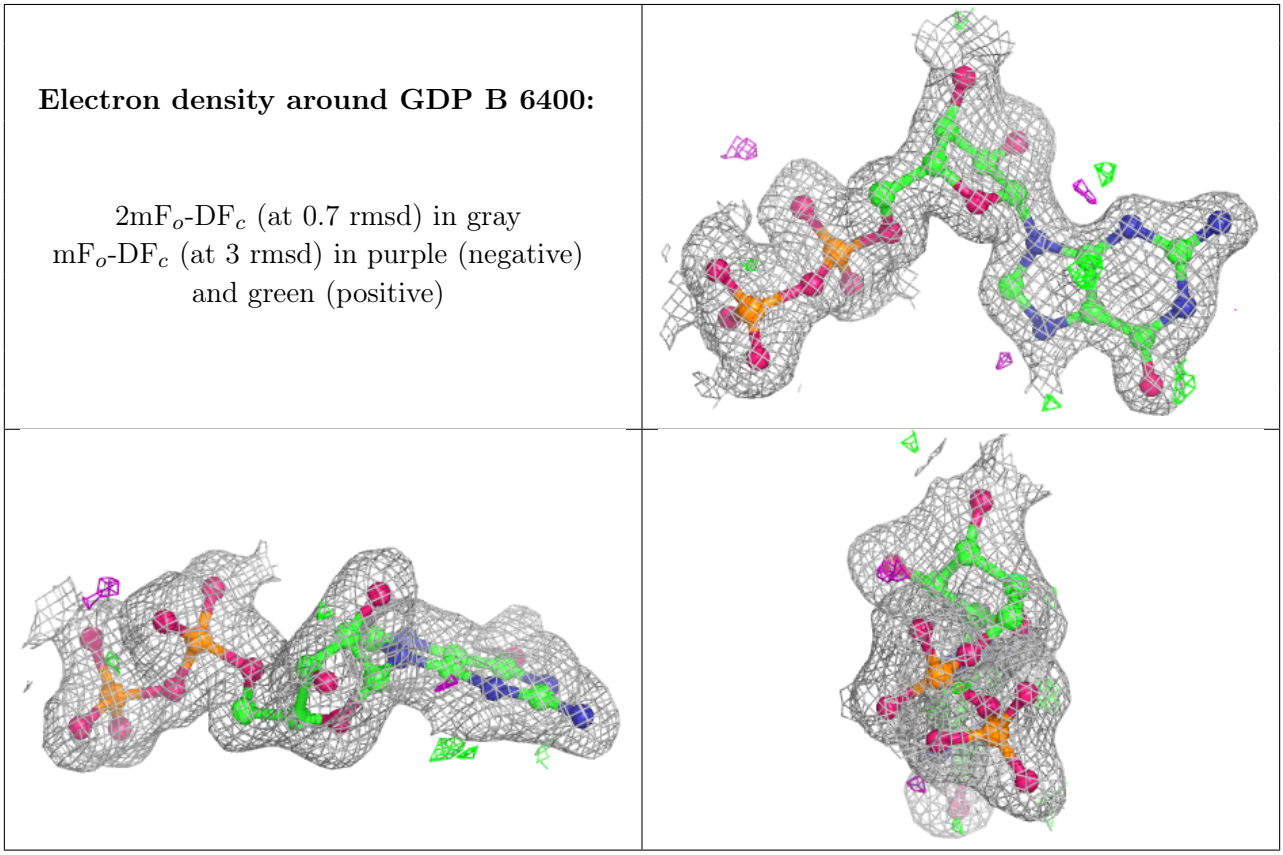
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BEZ	B	1503	9/9	0.90	0.11	21,26,31,42	0
4	BEZ	A	1502	9/9	0.94	0.10	19,25,27,30	0
3	GDP	B	6400	28/28	0.96	0.09	20,28,43,60	0
4	BEZ	A	1500	9/9	0.96	0.09	16,18,24,36	0
3	GDP	A	3400	28/28	0.97	0.08	16,21,29,36	0
4	BEZ	A	1501	9/9	0.97	0.08	11,18,20,20	0
6	CL	B	3001	1/1	0.97	0.08	37,37,37,37	0
5	MG	B	5401	1/1	0.98	0.05	20,20,20,20	0
2	SR	A	2401	1/1	1.00	0.03	20,20,20,20	0
2	SR	B	2001	1/1	1.00	0.09	37,37,37,37	1

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.

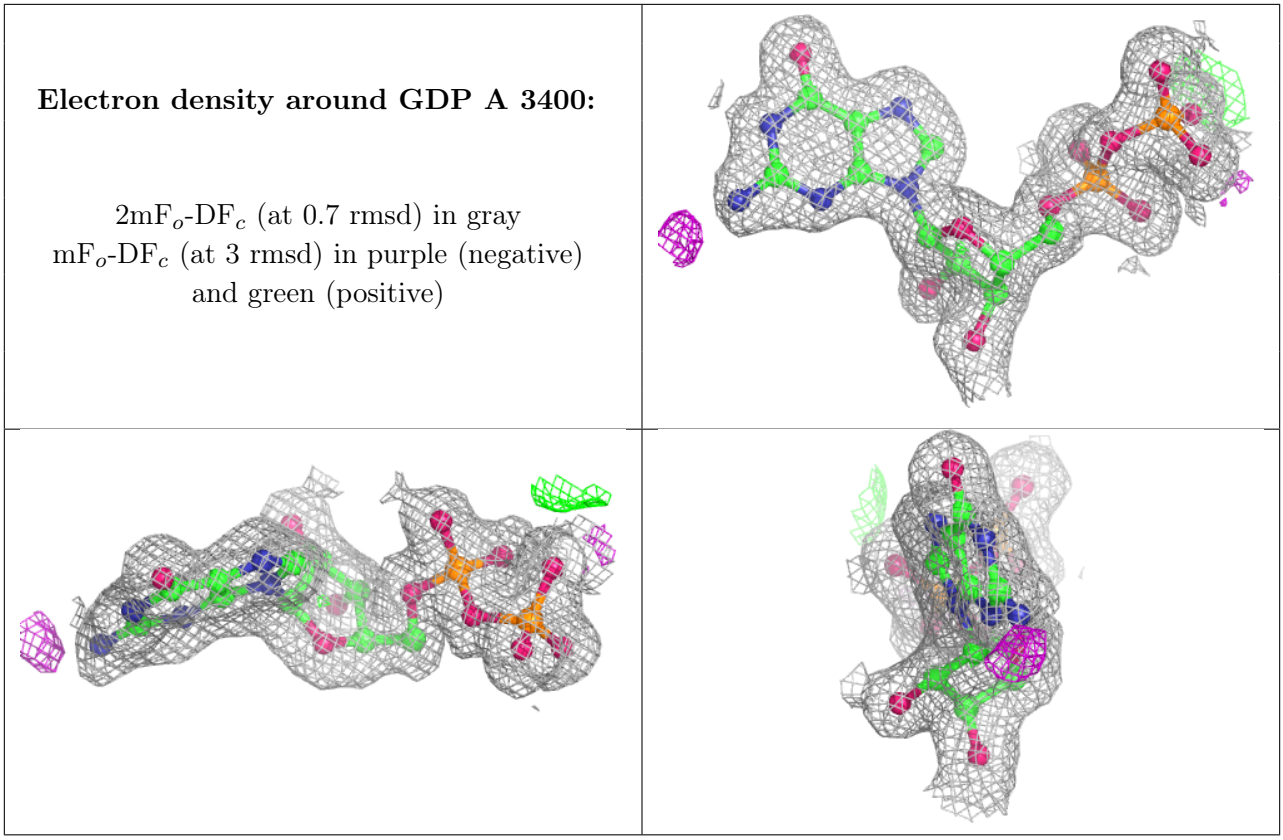
Electron density around GDP B 6400:

$2mF_o$-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 3400:

$2mF_o$-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.