wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 02:22 PM EDT

PDB ID	:	1GG2
Title	:	G PROTEIN HETEROTRIMER MUTANT GI_ALPHA_1(G203A) BETA_1 GAMMA_2 WITH GDP BOUND
Authors	:	Wall, M.A.; Sprang, S.R.
Deposited on	:	1996-11-13
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 following versions of software and data (see references (1)) were used in the production of this report:

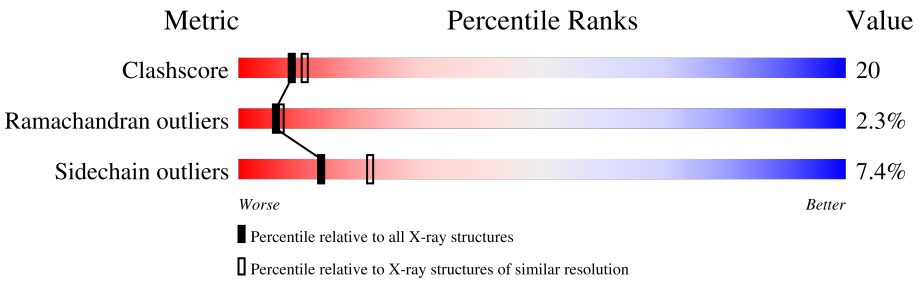
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	353	63% 31% • •
2	B	340	49% 48% • •
3	G	71	38% 31% 6% • 24%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6156 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 GI ALPHA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2760	1746	470	528	16	60	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	GLY	engineered mutation	UNP P10824

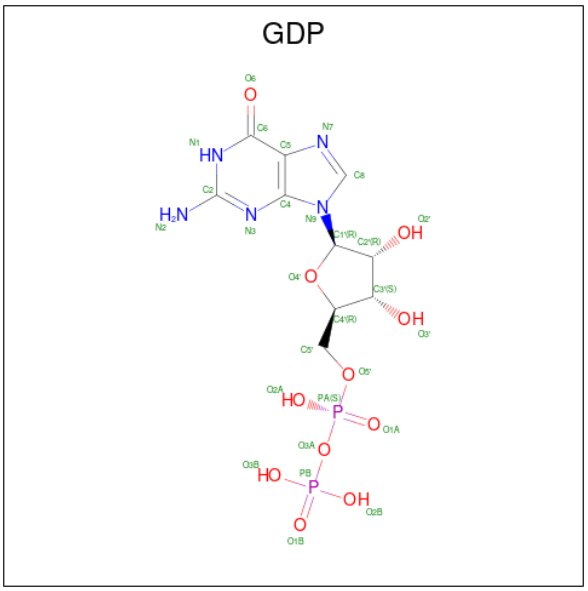
- Molecule 2 is a protein called G PROTEIN GI BETA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	339	2607	1607	468	511	21	27	0	0

- Molecule 3 is a protein called G PROTEIN GI GAMMA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	54	413	260	71	79	3	0	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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	195	195	195	0	0
			Total	O		
5	B	136	136	136	0	0
			Total	O		
5	G	17	17	17	0	0

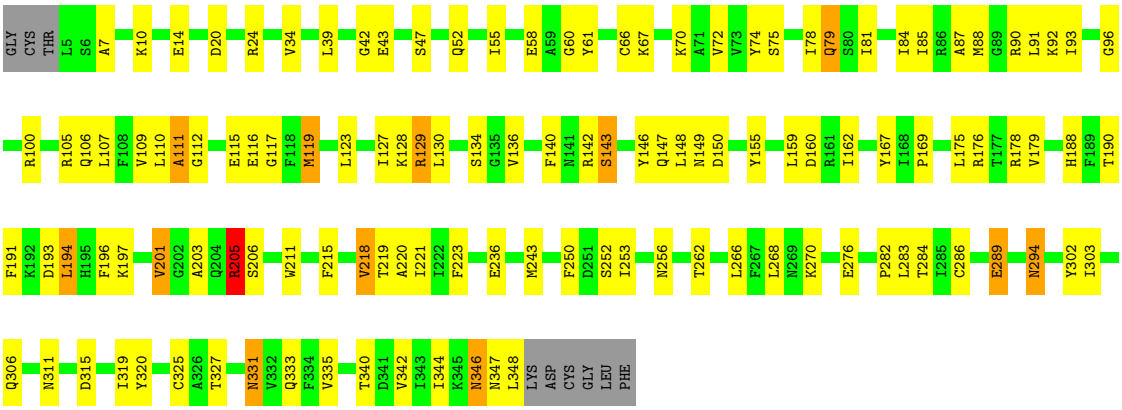
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

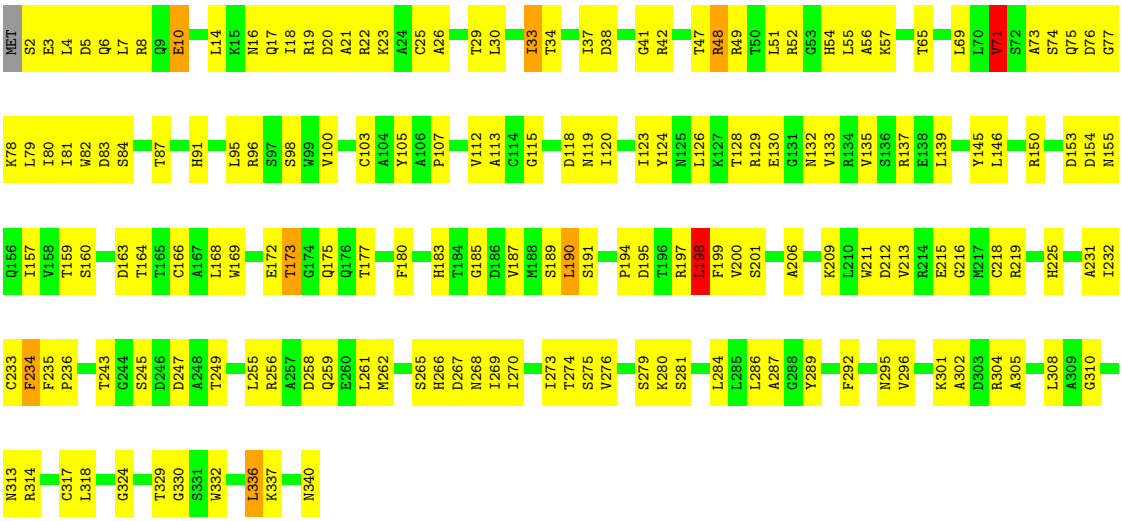
• Molecule 1: G PROTEIN GI ALPHA 1

Chain A: 63% 31%



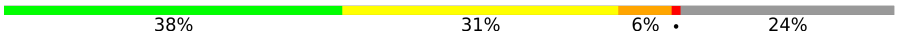
• Molecule 2: G PROTEIN GI BETA 1

Chain B: 49% 48%



• Molecule 3: G PROTEIN GI GAMMA 2

Chain G:


38%
31%
6%
24%

MET
ALA
SER
ASN
ASN
THR
ALA
S8
I9
R13
Q18
L19
K20
M21
E22
R27
I28
K29
V30
D36
L37
M38
A39
K46
E47
D48
P49
I50
L51
T52
P53
V54
P55
A56
S57
E58
N59
P60
F61
ARG
GLU
LYS
LYS
PHE
PHE
SER
ALA
ILE
LEU

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	83.78Å 83.78Å 130.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	93.0 (15.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6156	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

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

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	0.54	0/2806	0.72	1/3777 (0.0%)
2	B	0.53	1/2654 (0.0%)	0.82	4/3597 (0.1%)
3	G	0.49	0/419	0.67	0/566
All	All	0.53	1/5879 (0.0%)	0.76	5/7940 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	GLU	CD-OE2	6.61	1.32	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	41	GLY	N-CA-C	-5.27	99.93	113.10
2	B	190	LEU	CA-CB-CG	5.25	127.38	115.30
2	B	71	VAL	CB-CA-C	-5.16	101.60	111.40
1	A	325	CYS	N-CA-C	-5.04	97.38	111.00
2	B	198	LEU	CA-CB-CG	5.01	126.82	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	2760	0	2741	95	0
2	B	2607	0	2510	130	0
3	G	413	0	423	23	0
4	A	28	0	12	3	0
5	A	195	0	0	6	0
5	B	136	0	0	5	0
5	G	17	0	0	1	0
All	All	6156	0	5686	232	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 20.

The worst 5 of 232 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:72:VAL:HG11	1:A:179:VAL:HG12	1.42	0.98
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.56	0.87
1:A:340:THR:O	1:A:344:ILE:HG12	1.80	0.80
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.66	0.77
1:A:85:ILE:HA	1:A:88:MET:HE2	1.67	0.76

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	342/353 (97%)	305 (89%)	31 (9%)	6 (2%)	8 10
2	B	337/340 (99%)	298 (88%)	32 (10%)	7 (2%)	7 8
3	G	52/71 (73%)	43 (83%)	5 (10%)	4 (8%)	1 0
All	All	731/764 (96%)	646 (88%)	68 (9%)	17 (2%)	6 7

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	60	PRO
1	A	111	ALA
1	A	236	GLU
2	B	154	ASP
2	B	269	ILE

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	296/303 (98%)	275 (93%)	21 (7%)	14 23
2	B	282/283 (100%)	263 (93%)	19 (7%)	16 26
3	G	44/58 (76%)	38 (86%)	6 (14%)	3 4
All	All	622/644 (97%)	576 (93%)	46 (7%)	13 22

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	71	VAL
2	B	198	LEU
2	B	96	ARG
2	B	173	THR
2	B	234	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	36	ASN
2	B	88	ASN
2	B	266	HIS
2	B	110	ASN
1	A	331	ASN

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)

1 ligand is modelled in this entry.

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	GDP	A	355	-	24,30,30	2.17	6 (25%)	31,47,47	2.47	7 (22%)

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	355	-	-	2/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	355	GDP	O4'-C1'	6.61	1.50	1.41
4	A	355	GDP	C6-N1	4.37	1.40	1.33
4	A	355	GDP	C2'-C1'	-3.05	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	355	GDP	PB-O2B	-2.87	1.43	1.54
4	A	355	GDP	C8-N7	-2.49	1.30	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	355	GDP	C5-C6-N1	-9.08	111.02	123.43
4	A	355	GDP	C6-N1-C2	6.18	125.74	115.93
4	A	355	GDP	C3'-C2'-C1'	-3.18	96.20	100.98
4	A	355	GDP	N3-C2-N1	-2.98	123.25	127.22
4	A	355	GDP	C2-N3-C4	-2.58	112.41	115.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	355	GDP	PA-O3A-PB-O2B
4	A	355	GDP	PA-O3A-PB-O3B

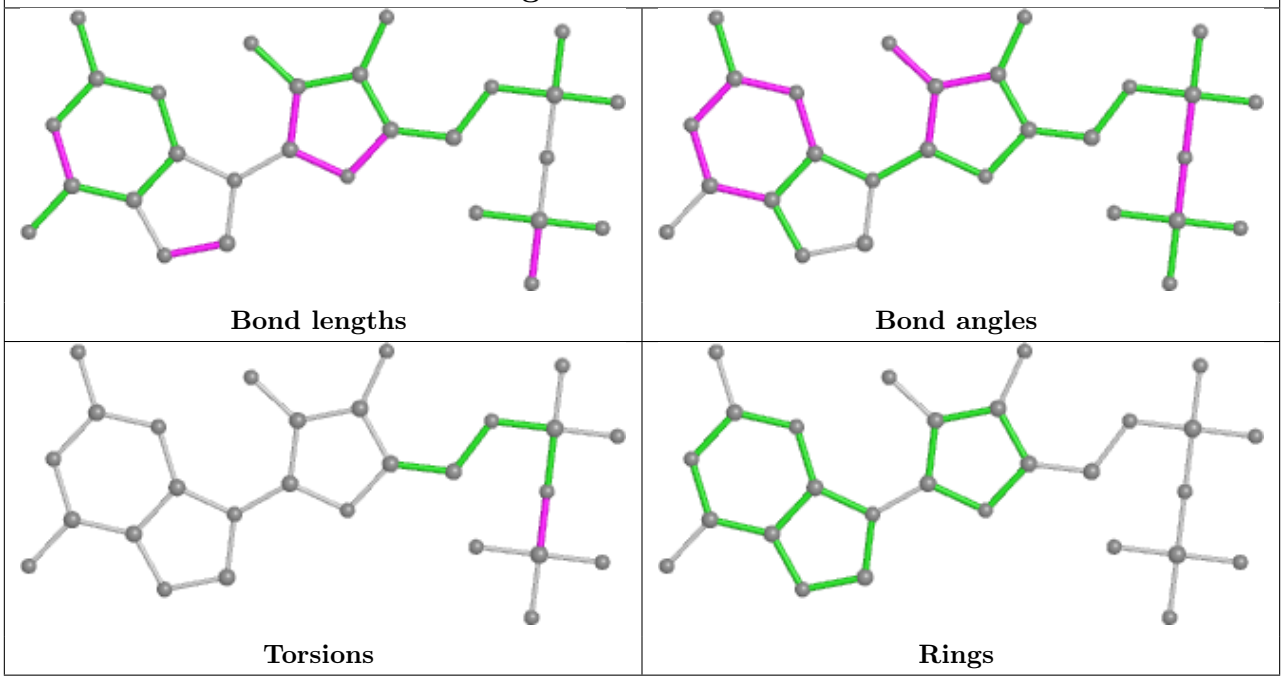
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	355	GDP	3	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 355



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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.