



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GOT
Title : HETEROTRIMERIC COMPLEX OF A GT-ALPHA/GI-ALPHA CHIMERA
AND THE GT-BETA-GAMMA SUBUNITS
Authors : Lambright, D.G.; Sondek, J.; Bohm, A.; Skiba, N.P.; Hamm, H.E.; Sigler, P.B.
Deposited on : 1996-08-07
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

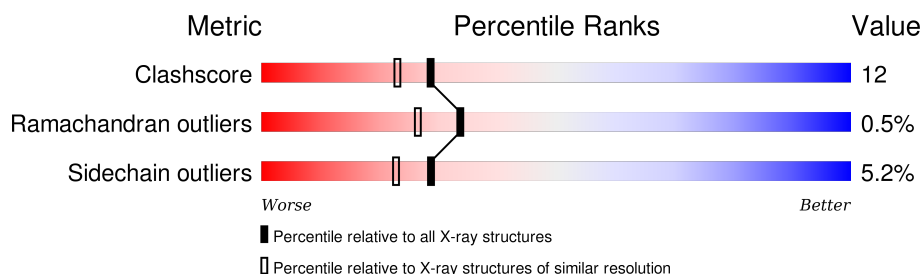
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	
2	B	340	
3	G	73	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6448 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 GT-ALPHA/GI-ALPHA CHIMERA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	Se	0	0	0
			2722	1720	453	530	7	12			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	84	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	104	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	106	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	115	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	119	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	194	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	216	ALA	CYS	CONFLICT	UNP P04695
A	220	CYS	ILE	CONFLICT	UNP P04695
A	221	VAL	ALA	CONFLICT	UNP P04695
A	225	ASP	ALA	CONFLICT	UNP P04695
A	228	LEU	MET	CONFLICT	UNP P04695
A	231	ALA	VAL	CONFLICT	UNP P04695
A	234	GLU	ASP	CONFLICT	UNP P04695
A	236	MSE	VAL	CONFLICT	UNP P04695
A	239	MSE	MET	CONFLICT	UNP P04695
A	243	MSE	LEU	CONFLICT	UNP P04695
A	244	LYS	HIS	CONFLICT	UNP P04695
A	247	ASP	ASN	CONFLICT	UNP P04695
A	252	ASN	HIS	CONFLICT	UNP P04695
A	253	LYS	ARG	CONFLICT	UNP P04695
A	254	TRP	TYR	CONFLICT	UNP P04695
A	256	THR	ALA	CONFLICT	UNP P04695
A	257	ASP	THR	CONFLICT	UNP P04695
A	261	ILE	VAL	CONFLICT	UNP P04695
A	269	LEU	VAL	CONFLICT	UNP P04695
A	271	GLU	SER	CONFLICT	UNP P04695

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Chain	Residue	Modelled	Actual	Comment	Reference
A	277	SER	ALA	CONFLICT	UNP P04695
A	278	PRO	HIS	CONFLICT	UNP P04695
A	280	THR	SER	CONFLICT	UNP P04695
A	283	TYR	PHE	CONFLICT	UNP P04695
A	285	GLU	ASP	CONFLICT	UNP P04695
A	287	ALA	ASN	CONFLICT	UNP P04695
A	289	SER	PRO	CONFLICT	UNP P04695
A	294	GLU	ASP	CONFLICT	UNP P04695
A	308	MSE	MET	MODIFIED RESIDUE	UNP P04695
A	319	MSE	MET	MODIFIED RESIDUE	UNP P04695

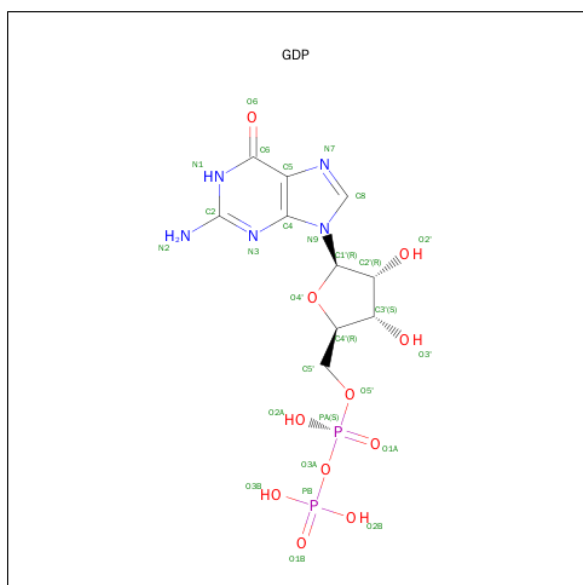
- Molecule 2 is a protein called GT-BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	0	0
			2608	1608	468	511	21			

- Molecule 3 is a protein called GT-GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	58	Total	C	N	O	S	0	0	0
			474	295	78	97	4			

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

- Molecule 5 is water.

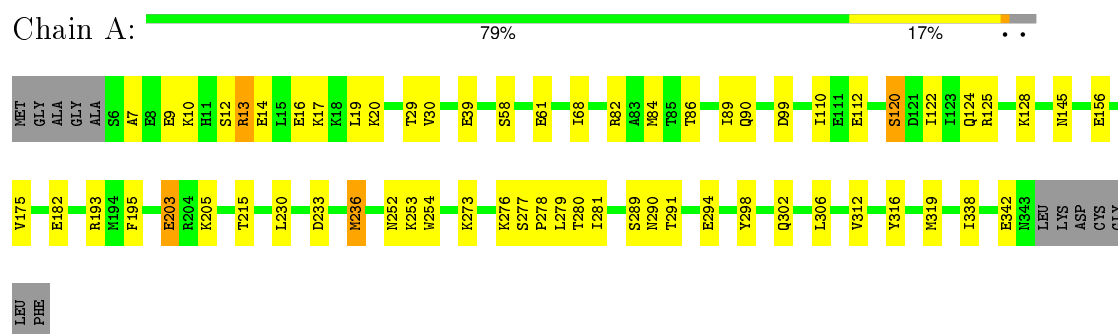
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	359	Total	O	0	0
			359	359		
5	B	221	Total	O	0	0
			221	221		
5	G	36	Total	O	0	0
			36	36		

3 Residue-property plots

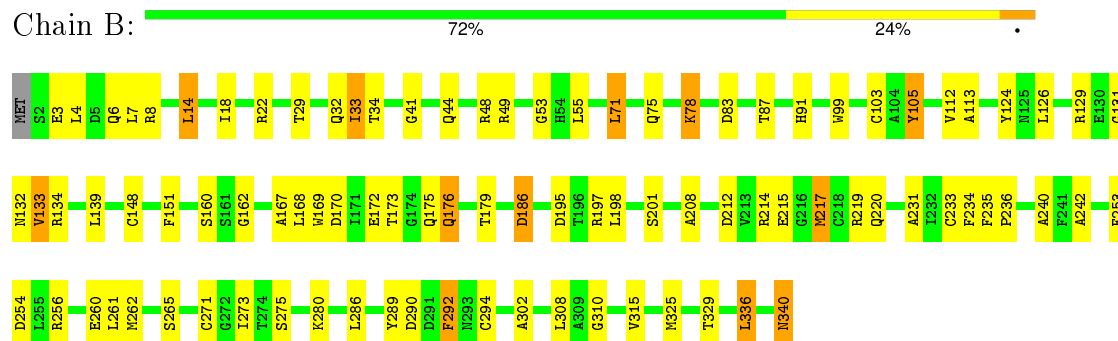
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

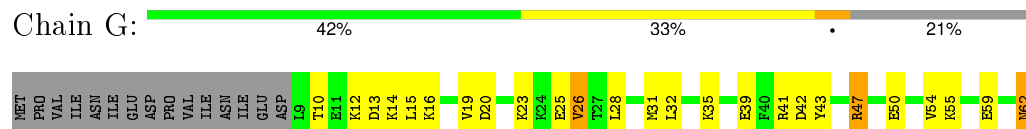
• Molecule 1: GT-ALPHA/GI-ALPHA CHIMERA



• Molecule 2: GT-BETA



• Molecule 3: GT-GAMMA



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.40 Å 91.40 Å 83.20 Å 90.00° 120.10° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (6.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXS, X-PLOR 3.1	Depositor
R, R_{free}	0.207 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6448	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	0.57	0/2754	0.65	0/3685
2	B	0.48	0/2655	0.79	2/3598 (0.1%)
3	G	0.45	0/479	0.64	0/636
All	All	0.53	0/5888	0.71	2/7919 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	ASP	N-CA-C	-5.06	97.33	111.00
2	B	315	VAL	N-CA-C	-5.05	97.36	111.00

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	2722	0	2697	45	0
2	B	2608	0	2512	71	0
3	G	474	0	469	22	0
4	G	28	0	12	0	0
5	A	359	0	0	10	0
5	B	221	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	36	0	0	1	0
All	All	6448	0	5690	133	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 12.

The worst 5 of 133 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)
2:B:129:ARG:HB3	2:B:133:VAL:HA	1.52	0.91
2:B:233:CYS:HB3	5:B:511:HOH:O	1.73	0.87
1:A:124:GLN:O	1:A:128:LYS:HG2	1.91	0.69
1:A:273:LYS:HG3	1:A:276:LYS:HE3	1.76	0.67
1:A:9:GLU:O	1:A:13:ARG:HD2	1.96	0.66

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	336/350 (96%)	325 (97%)	10 (3%)	1 (0%)	46	41
2	B	337/340 (99%)	312 (93%)	23 (7%)	2 (1%)	30	22
3	G	56/73 (77%)	55 (98%)	0	1 (2%)	11	4
All	All	729/763 (96%)	692 (95%)	33 (4%)	4 (0%)	34	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	GLU
3	G	10	THR

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Mol	Chain	Res	Type
2	B	310	GLY
2	B	53	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	300/297 (101%)	287 (96%)	13 (4%)	35	30
2	B	282/283 (100%)	267 (95%)	15 (5%)	28	22
3	G	54/71 (76%)	49 (91%)	5 (9%)	11	6
All	All	636/651 (98%)	603 (95%)	33 (5%)	29	23

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	ILE
2	B	133	VAL
3	G	26	VAL
2	B	71	LEU
2	B	78	LYS

Some 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	32	GLN
2	B	88	ASN
2	B	176	GLN
2	B	16	ASN
2	B	132	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 carbohydrates 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	G	355	-	23,30,30	1.56	4 (17%)	30,47,47	2.45	7 (23%)

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	G	355	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	355	GDP	C8-N7	-2.56	1.29	1.34
4	G	355	GDP	PB-O2B	-2.47	1.45	1.54
4	G	355	GDP	O4'-C1'	2.73	1.44	1.41
4	G	355	GDP	C6-N1	3.91	1.40	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	355	GDP	C5-C6-N1	-8.68	111.72	123.59
4	G	355	GDP	O3A-PA-O5'	-3.58	93.43	102.94
4	G	355	GDP	N3-C2-N1	-2.69	123.34	127.44
4	G	355	GDP	C1'-N9-C4	-2.25	123.54	126.94
4	G	355	GDP	PA-O3A-PB	-2.20	125.29	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.