



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 02:25 am BST

PDB ID : 5IZK
Title : The crystal structure of human eEFSec in complex with GDP
Authors : Dobosz-Bartoszek, M.; Simonovic, M.
Deposited on : 2016-03-25
Resolution : 3.25 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

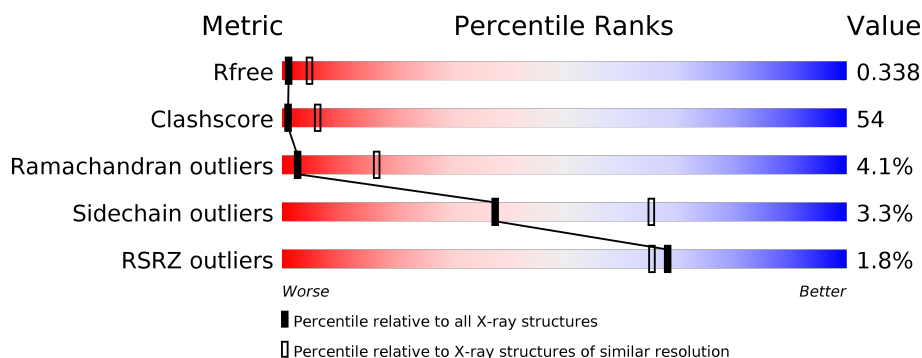
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	616	
1	B	616	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6060 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 Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3216	2046	566	585	19			
1	B	451	Total	C	N	O	S	0	1	0
			2767	1746	499	514	8			

There are 40 discrepancies between the modelled and reference sequences:

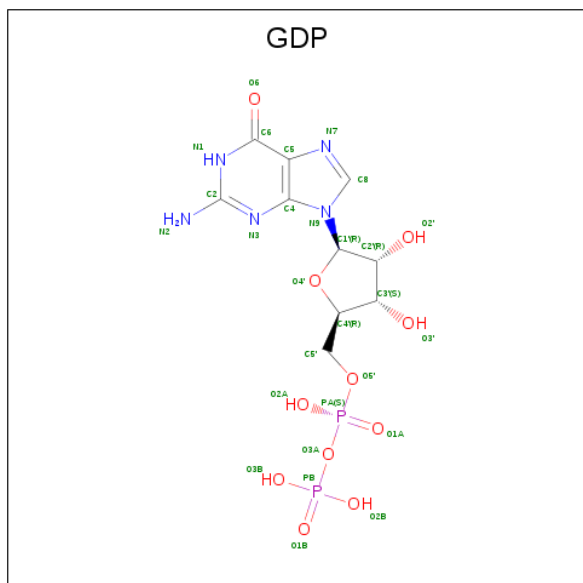
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P57772
A	-18	GLY	-	expression tag	UNP P57772
A	-17	SER	-	expression tag	UNP P57772
A	-16	SER	-	expression tag	UNP P57772
A	-15	HIS	-	expression tag	UNP P57772
A	-14	HIS	-	expression tag	UNP P57772
A	-13	HIS	-	expression tag	UNP P57772
A	-12	HIS	-	expression tag	UNP P57772
A	-11	HIS	-	expression tag	UNP P57772
A	-10	HIS	-	expression tag	UNP P57772
A	-9	SER	-	expression tag	UNP P57772
A	-8	SER	-	expression tag	UNP P57772
A	-7	GLY	-	expression tag	UNP P57772
A	-6	LEU	-	expression tag	UNP P57772
A	-5	VAL	-	expression tag	UNP P57772
A	-4	PRO	-	expression tag	UNP P57772
A	-3	ARG	-	expression tag	UNP P57772
A	-2	GLY	-	expression tag	UNP P57772
A	-1	SER	-	expression tag	UNP P57772
A	0	HIS	-	expression tag	UNP P57772
B	-19	MET	-	initiating methionine	UNP P57772
B	-18	GLY	-	expression tag	UNP P57772
B	-17	SER	-	expression tag	UNP P57772
B	-16	SER	-	expression tag	UNP P57772
B	-15	HIS	-	expression tag	UNP P57772

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P57772
B	-13	HIS	-	expression tag	UNP P57772
B	-12	HIS	-	expression tag	UNP P57772
B	-11	HIS	-	expression tag	UNP P57772
B	-10	HIS	-	expression tag	UNP P57772
B	-9	SER	-	expression tag	UNP P57772
B	-8	SER	-	expression tag	UNP P57772
B	-7	GLY	-	expression tag	UNP P57772
B	-6	LEU	-	expression tag	UNP P57772
B	-5	VAL	-	expression tag	UNP P57772
B	-4	PRO	-	expression tag	UNP P57772
B	-3	ARG	-	expression tag	UNP P57772
B	-2	GLY	-	expression tag	UNP P57772
B	-1	SER	-	expression tag	UNP P57772
B	0	HIS	-	expression tag	UNP P57772

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

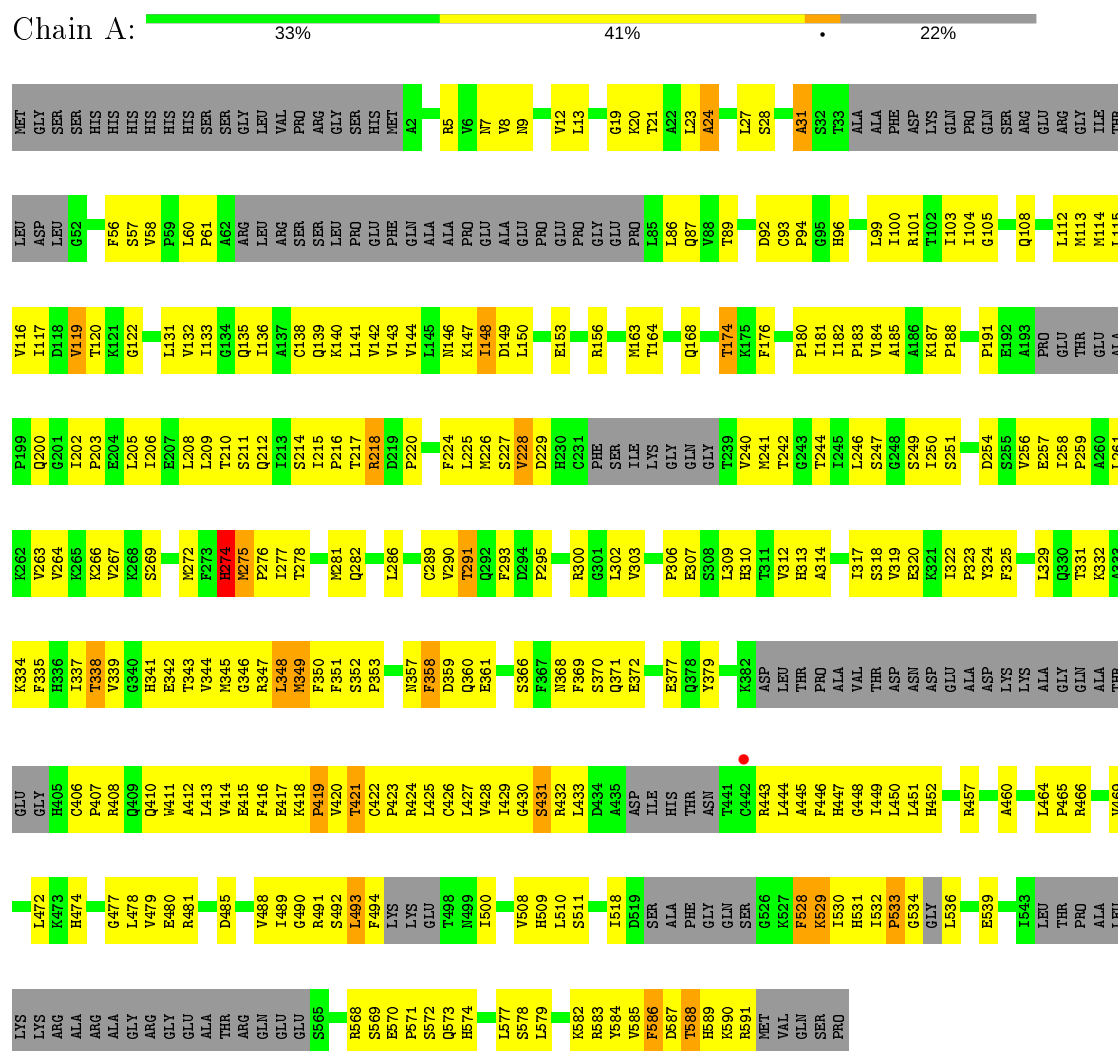


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total 15	O 15	0	0
3	B	6	Total 6	O 6	0	0

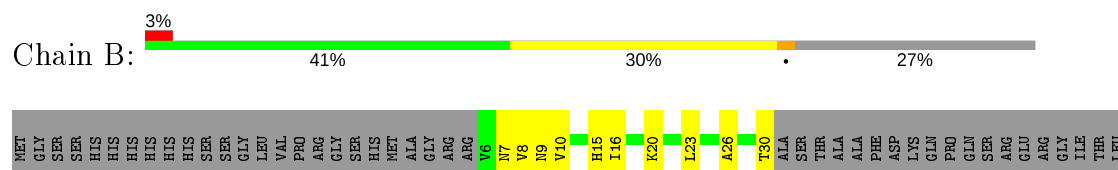
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Selenocysteine-specific elongation factor



- Molecule 1: Selenocysteine-specific elongation factor



GLN	ASP	G134	V228	L316	L454	K529
SER	LEU	Q135	ASP	L317	P485	I530
PRO	GLY	I136	CYS	S318	D456	HE31
	PHE	A137	PHE	V319	S462	LE32
	SER	C138	SER	E320	G534	P533
	C55	Q139	ILE	I321	K468	G535
	F56	K140	LYS	I322	V469	L536
	S57		LYS	F323	V470	
		I148	GLY	F324	K471	
	L60	D149	GLN	F325	L472	
	PRO	M163	THR	L329	K473	
	ALA	K166	VAL	Q330	H474	
	ARG	M167	H241	F335	K475	
	LEU	G243	T242	H336	H476	
	ARG	A179	G245	H337	G477	
	SER	P183	I245	T338	V479	
	LEU	V184	S249	H341	L478	
	PRO	A185	I250	E342	F480	
	PHE	K187	S251	T343	R481	
	GLN	P188	V263	G346	D484	
	ALA	G189	V267	R347	Y486	
	PRO	GLY	K268	I348	S487	
	GLU	ALA	S269	R349	V488	
	ALA	PRO	H270	F350	T489	
	GLU	PRO	Q271	A354	G490	
	PRO	GLU	H274	N357	S492	
	GLY	THR	K275	F358	L493	
	GLU	GLU	P276	D359	F494	
	P84	ALA	T277	V428	K495	
	L85	PRO	T278	I429	LYS	
	L86	GLN	S279	G430	THR	
	V87	G201	K280	S431	ASN	
	V88	I202	K281	R432	ILE	
		F203	Q282	LEU	Q501	
	A97	E204	G283	ASP	L502	
		L205	L286	ALA	G505	
	I100	I206	G287	ASP	V508	
		E207	I288	ILE	H509	
	I109	L208		HIS	L510	
	I110	L209		THR	L515	
	D111	T210		ASN	G516	
	L112	S211	Q292	THR	D519	
		Q212	F293	C442	S520	
	I117	I213	D294	R443	ALA	
	D118	S214	P295	L380	F446	
	V119	ILE		S381	H447	
	T120	PRO		LYS	Q448	
	LYS	T217		ASP	T449	
	GLY			LEU	L450	
	M123	P220		THR	L451	
		F224		PRO	H452	
	Q126	L225		ALA	G453	
	V132	M226		VAL	S525	
	I133	S227		THR	G526	
				ASN	H527	
					F528	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.69Å 96.86Å 125.41Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	42.94 – 3.25 42.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.94-3.25) 91.2 (42.94-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.296 , 0.338 0.296 , 0.338	Depositor DCC
R_{free} test set	1286 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.36	0/3276	0.68	12/4477 (0.3%)
1	B	0.32	0/2816	0.66	8/3868 (0.2%)
All	All	0.34	0/6092	0.67	20/8345 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	LEU	N-CA-C	8.09	132.84	111.00
1	A	274	HIS	CB-CA-C	-7.73	94.93	110.40
1	B	565	SER	CB-CA-C	-7.32	96.19	110.10
1	B	341	HIS	N-CA-C	7.23	130.53	111.00
1	A	588	THR	N-CA-C	6.56	128.71	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	3216	0	2771	331	0
1	B	2767	0	2027	258	0
2	A	28	0	12	4	0
2	B	28	0	12	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	0	19	0
3	B	6	0	0	10	0
All	All	6060	0	4822	583	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 54.

The worst 5 of 583 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:477:GLY:HA2	1:B:492:SER:CB	1.25	1.59
1:B:477:GLY:CA	1:B:492:SER:CB	2.02	1.36
1:B:476:HIS:O	1:B:492:SER:CB	1.79	1.31
1:B:490:GLY:O	1:B:528:PHE:CD2	1.84	1.30
1:B:311:THR:CA	1:B:421:THR:HG22	1.65	1.24

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	459/616 (74%)	340 (74%)	99 (22%)	20 (4%)	2	15
1	B	428/616 (70%)	330 (77%)	82 (19%)	16 (4%)	3	19
All	All	887/1232 (72%)	670 (76%)	181 (20%)	36 (4%)	3	17

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	ILE
1	A	275	MET

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Mol	Chain	Res	Type
1	A	277	ILE
1	A	324	TYR
1	A	369	PHE

5.3.2 Protein sidechains ⓘ

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	261/524 (50%)	251 (96%)	10 (4%)	33	62
1	B	160/524 (30%)	156 (98%)	4 (2%)	47	71
All	All	421/1048 (40%)	407 (97%)	14 (3%)	38	65

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	THR
1	A	528	PHE
1	B	324	TYR
1	A	358	PHE
1	B	135	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	310	HIS
1	A	341	HIS
1	A	410	GLN
1	A	509	HIS

5.3.3 RNA ⓘ

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](#)

2 ligands are 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$
2	GDP	A	1001	-	24,30,30	1.69	5 (20%)	31,47,47	1.91	5 (16%)
2	GDP	B	1001	-	24,30,30	1.69	5 (20%)	31,47,47	1.93	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
2	GDP	A	1001	-	-	3/12/32/32	0/3/3/3
2	GDP	B	1001	-	-	3/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GDP	C6-C5	-4.51	1.33	1.41
2	B	1001	GDP	C6-C5	-4.51	1.33	1.41
2	A	1001	GDP	C6-N1	4.09	1.40	1.33
2	B	1001	GDP	C6-N1	4.05	1.40	1.33
2	A	1001	GDP	C5-C4	-2.66	1.33	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	GDP	N3-C2-N1	-5.95	119.28	127.22
2	A	1001	GDP	N3-C2-N1	-5.88	119.38	127.22
2	B	1001	GDP	C2-N3-C4	4.71	120.74	115.36
2	A	1001	GDP	C2-N3-C4	4.66	120.67	115.36
2	B	1001	GDP	PA-O3A-PB	-3.75	119.97	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

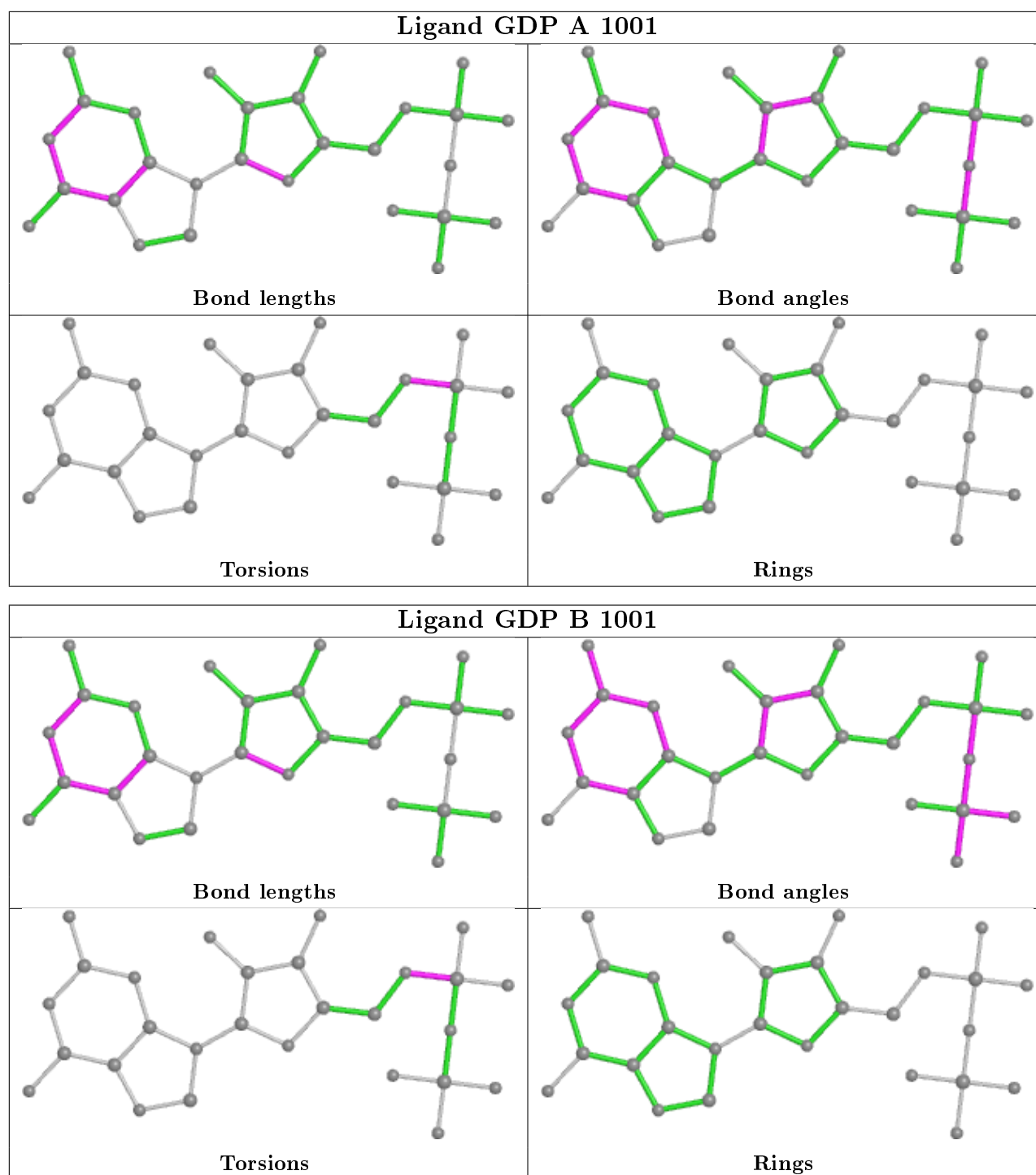
Mol	Chain	Res	Type	Atoms
2	A	1001	GDP	C5'-O5'-PA-O1A
2	B	1001	GDP	C5'-O5'-PA-O1A
2	B	1001	GDP	C5'-O5'-PA-O2A
2	A	1001	GDP	C5'-O5'-PA-O2A
2	A	1001	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GDP	4	0
2	B	1001	GDP	7	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 than 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.



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	480/616 (77%)	-0.54	1 (0%) 95 95	27, 69, 101, 114	0
1	B	451/616 (73%)	-0.26	16 (3%) 44 40	44, 95, 149, 168	0
All	All	931/1232 (75%)	-0.40	17 (1%) 68 65	27, 81, 129, 168	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	VAL	5.5
1	B	268	LYS	5.0
1	B	299	GLU	5.0
1	B	287	GLY	4.5
1	B	269	SER	4.1

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](#)

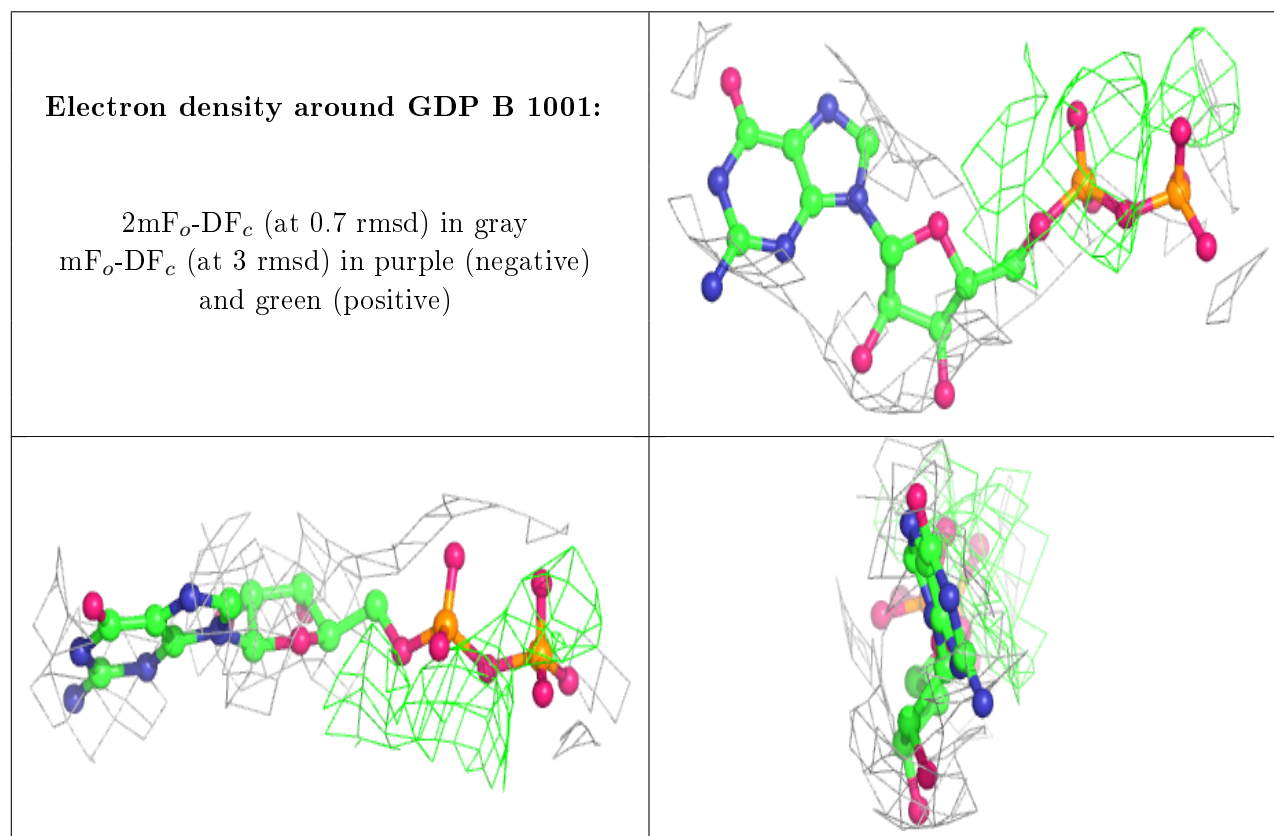
There are no carbohydrates in this entry.

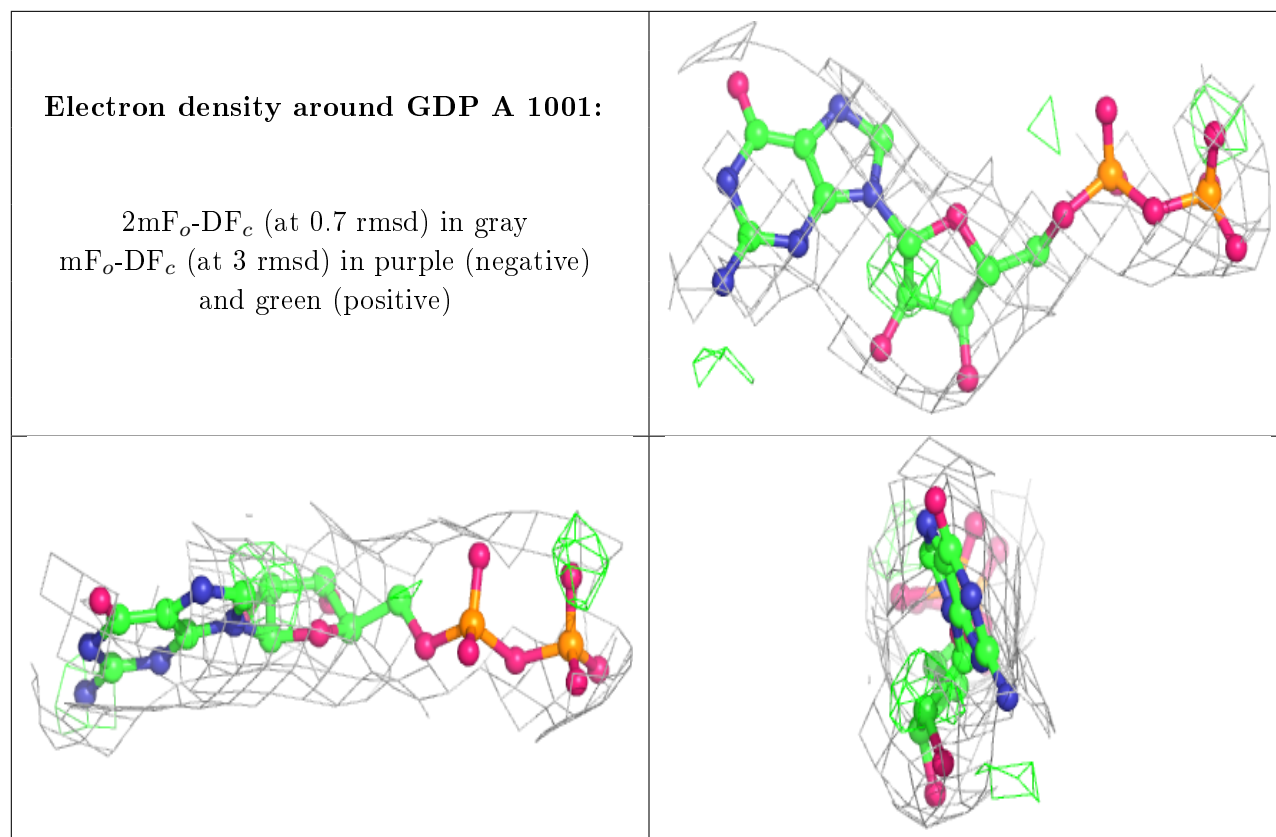
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	GDP	B	1001	28/28	0.80	0.18	122,135,153,158	0
2	GDP	A	1001	28/28	0.89	0.17	72,93,113,129	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.