



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 12:43 PM BST

PDB ID : 6EG8
Title : Structure of the GDP-bound Gs heterotrimer
Authors : Hilger, D.; Liu, X.; Aschauer, P.; Kobilka, B.K.
Deposited on : 2018-08-19
Resolution : 2.80 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 : 2.13.1
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) : 2.13.1

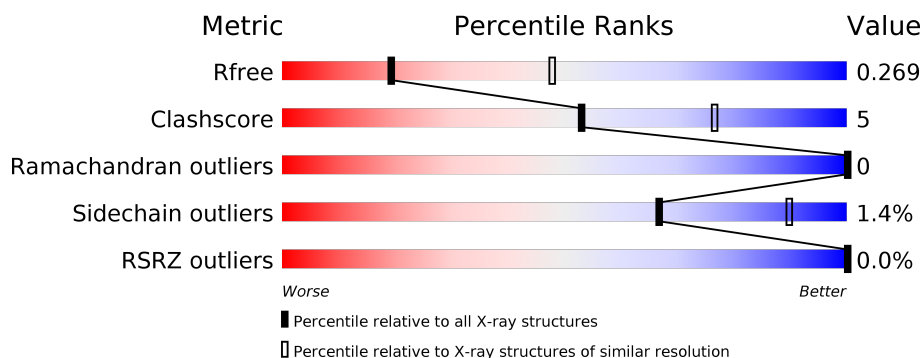
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	345	<div> <div style="width: 79%;"></div> <div style="width: 19%;"></div> <div style="width: 2%;"></div> </div> <div>79% 19% .</div>
1	B	345	<div> <div style="width: 82%;"></div> <div style="width: 17%;"></div> <div style="width: 1%;"></div> </div> <div>82% 17% .</div>
1	D	345	<div> <div style="width: 76%;"></div> <div style="width: 22%;"></div> <div style="width: 2%;"></div> </div> <div>76% 22% ..</div>
1	F	345	<div> <div style="width: 81%;"></div> <div style="width: 17%;"></div> <div style="width: 2%;"></div> </div> <div>81% 17% .</div>
2	C	71	<div> <div style="width: 73%;"></div> <div style="width: 7%;"></div> <div style="width: 20%;"></div> </div> <div>73% 7% 20%</div>
2	E	71	<div> <div style="width: 82%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> </div> <div>82% .. 15%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	71	 79% 20%
2	H	71	 76% 20%
3	I	381	 83% 14%
3	J	381	 87% 9%
3	K	381	 85% 13%
3	L	381	 84% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24622 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(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	3	0
			2598	1602	463	511	22			
1	B	341	Total	C	N	O	S	0	4	0
			2629	1619	473	516	21			
1	D	341	Total	C	N	O	S	0	2	0
			2618	1613	468	515	22			
1	F	340	Total	C	N	O	S	0	1	0
			2605	1605	468	511	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P62873
A	-3	PRO	-	expression tag	UNP P62873
A	-2	GLY	-	expression tag	UNP P62873
A	-1	SER	-	expression tag	UNP P62873
A	0	SER	-	expression tag	UNP P62873
A	1	GLY	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
D	-4	GLY	-	expression tag	UNP P62873
D	-3	PRO	-	expression tag	UNP P62873
D	-2	GLY	-	expression tag	UNP P62873
D	-1	SER	-	expression tag	UNP P62873
D	0	SER	-	expression tag	UNP P62873
D	1	GLY	-	expression tag	UNP P62873
F	-4	GLY	-	expression tag	UNP P62873
F	-3	PRO	-	expression tag	UNP P62873

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P62873
F	-1	SER	-	expression tag	UNP P62873
F	0	SER	-	expression tag	UNP P62873
F	1	GLY	-	expression tag	UNP P62873

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	57	Total	C	N	O	S	0	1	0
			446	279	80	84	3			
2	E	60	Total	C	N	O	S	0	0	0
			449	280	79	87	3			
2	G	57	Total	C	N	O	S	0	0	0
			434	271	76	84	3			
2	H	57	Total	C	N	O	S	0	0	0
			430	268	75	84	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	SER	CYS	engineered mutation	UNP P59768
E	68	SER	CYS	engineered mutation	UNP P59768
G	68	SER	CYS	engineered mutation	UNP P59768
H	68	SER	CYS	engineered mutation	UNP P59768

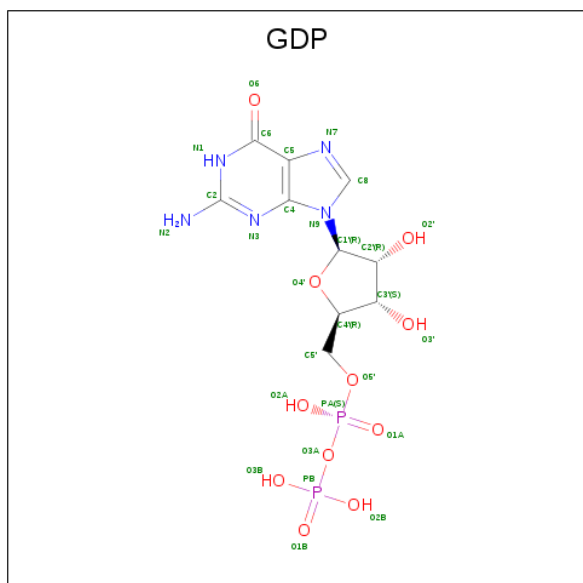
- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	372	Total	C	N	O	S	0	1	0
			3071	1936	542	580	13			
3	J	371	Total	C	N	O	S	0	0	0
			3044	1922	538	571	13			
3	K	371	Total	C	N	O	S	0	0	0
			3048	1924	539	572	13			
3	L	370	Total	C	N	O	S	0	0	0
			3047	1923	538	573	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	expression tag	UNP P63092
I	1	PRO	-	expression tag	UNP P63092
I	2	GLY	-	expression tag	UNP P63092
I	3	SER	-	expression tag	UNP P63092
J	0	GLY	-	expression tag	UNP P63092
J	1	PRO	-	expression tag	UNP P63092
J	2	GLY	-	expression tag	UNP P63092
J	3	SER	-	expression tag	UNP P63092
K	0	GLY	-	expression tag	UNP P63092
K	1	PRO	-	expression tag	UNP P63092
K	2	GLY	-	expression tag	UNP P63092
K	3	SER	-	expression tag	UNP P63092
L	0	GLY	-	expression tag	UNP P63092
L	1	PRO	-	expression tag	UNP P63092
L	2	GLY	-	expression tag	UNP P63092
L	3	SER	-	expression tag	UNP P63092

- 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	I	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	J	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	K	1	Total 28	C 10	N 5	O 11	P 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		

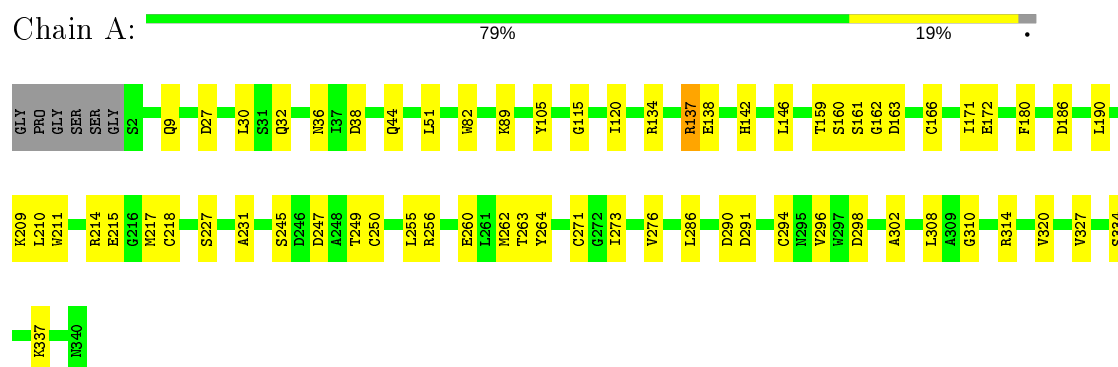
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	11	Total	O	0	0
			11	11		
6	C	1	Total	O	0	0
			1	1		
6	D	7	Total	O	0	0
			7	7		
6	F	8	Total	O	0	0
			8	8		
6	I	15	Total	O	0	0
			15	15		
6	J	16	Total	O	0	0
			16	16		
6	K	11	Total	O	0	0
			11	11		
6	L	10	Total	O	0	0
			10	10		

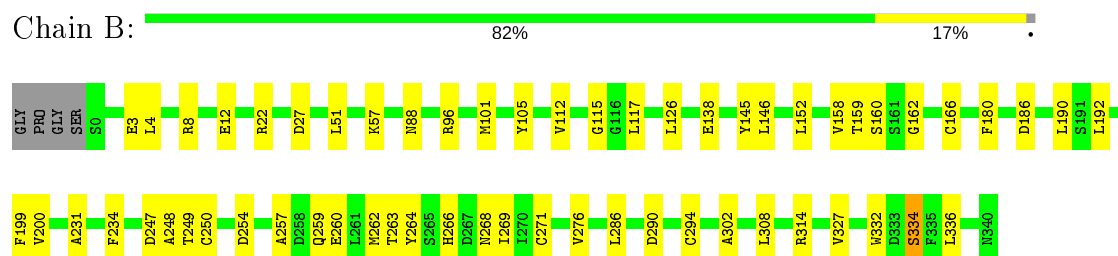
3 Residue-property plots [i](#)

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.

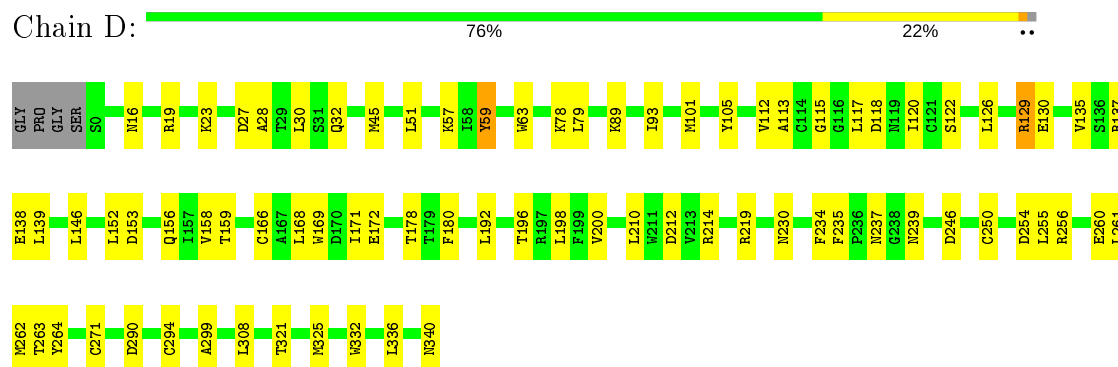
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1




- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

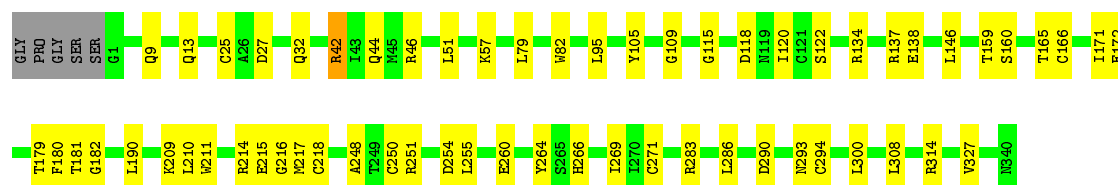


- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain F:  81% 17%




- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:  73% 7% 20%




- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain E:  82% 15%




- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:  79% 20%




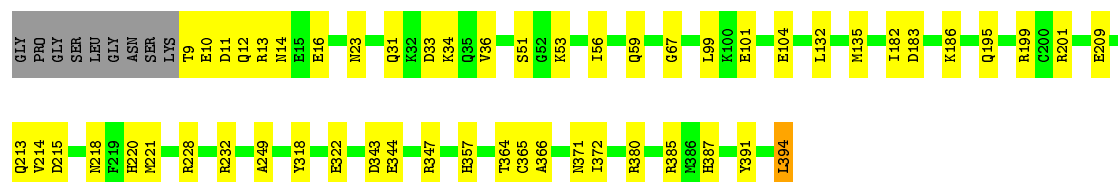
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain H:  76% 20%




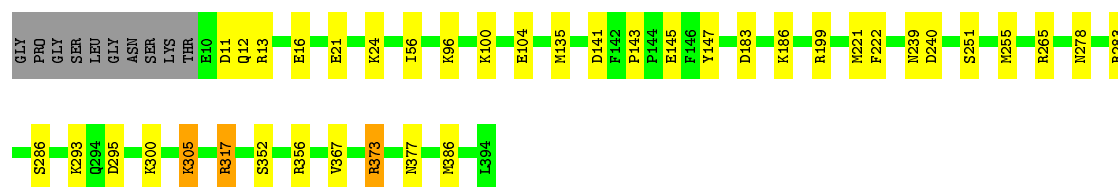
- Molecule 3: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain I:  83% 14%




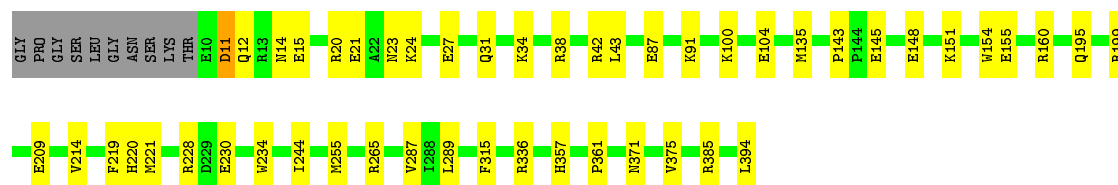
- Molecule 3: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain J:  87% 9% . .




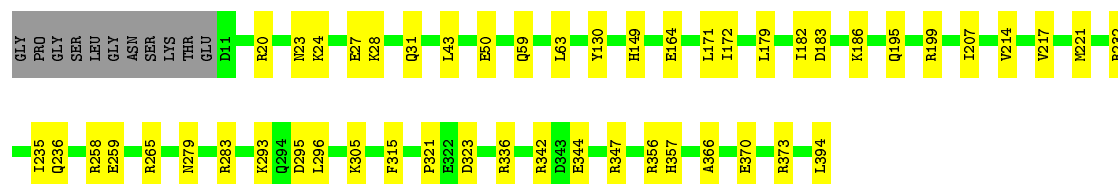
- Molecule 3: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain K:  85% 13% .



- Molecule 3: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain L:  84% 13% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.86Å 100.81Å 179.33Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	48.43 – 2.80 49.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.43-2.80) 97.5 (49.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, R_{free}	0.217 , 0.269 0.217 , 0.269	Depositor DCC
R_{free} test set	1994 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.207 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24622	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.24% 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, 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	0.24	0/2651	0.46	0/3597
1	B	0.25	0/2685	0.47	0/3640
1	D	0.31	1/2670 (0.0%)	0.52	3/3618 (0.1%)
1	F	0.24	0/2652	0.46	0/3596
2	C	0.23	0/455	0.35	0/613
2	E	0.23	0/455	0.35	0/616
2	G	0.23	0/440	0.35	0/595
2	H	0.23	0/436	0.36	0/591
3	I	0.24	0/3132	0.41	1/4230 (0.0%)
3	J	0.26	0/3105	0.40	1/4193 (0.0%)
3	K	0.23	0/3109	0.38	0/4198
3	L	0.23	0/3108	0.39	0/4196
All	All	0.25	1/24898 (0.0%)	0.43	5/33683 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	ARG	CG-CD	-6.45	1.35	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ARG	NE-CZ-NH2	8.65	124.62	120.30
3	I	394	LEU	CB-CG-CD1	-7.18	98.79	111.00
1	D	129	ARG	CA-CB-CG	-6.58	98.91	113.40
3	J	317	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	D	129	ARG	NE-CZ-NH1	-5.07	117.76	120.30

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	2598	0	2483	36	2
1	B	2629	0	2527	33	1
1	D	2618	0	2526	49	3
1	F	2605	0	2499	43	0
2	C	446	0	457	4	0
2	E	449	0	442	2	0
2	G	434	0	433	1	0
2	H	430	0	425	3	0
3	I	3071	0	3015	29	1
3	J	3044	0	2987	25	3
3	K	3048	0	2993	29	2
3	L	3047	0	2995	29	0
4	I	28	0	12	3	0
4	J	28	0	12	1	0
4	K	28	0	12	0	0
4	L	28	0	12	3	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	8	0	0	1	0
6	B	11	0	0	0	0
6	C	1	0	0	0	0
6	D	7	0	0	0	0
6	F	8	0	0	0	0
6	I	15	0	0	0	0
6	J	16	0	0	3	0
6	K	11	0	0	0	0
6	L	10	0	0	2	0
All	All	24622	0	23830	260	6

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 5.

The worst 5 of 260 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)
3:I:385:ARG:HD2	3:I:394:LEU:HD11	1.33	1.06
3:K:100:LYS:NZ	3:K:104:GLU:OE2	2.04	0.91
1:D:230:ASN:ND2	1:D:246:ASP:OD1	2.13	0.81
1:D:260:GLU:OE2	1:D:263:THR:OG1	1.98	0.81
1:A:89:LYS:H	3:I:23:ASN:HD22	1.29	0.81

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:GLU:OE2	3:J:317:ARG:NH2[2_555]	1.97	0.23
1:A:36:ASN:CB	3:K:151:LYS:NZ[2_545]	1.97	0.23
1:D:138:GLU:OE2	3:J:317:ARG:CZ[2_555]	2.04	0.16
1:D:138:GLU:OE2	3:J:317:ARG:NH1[2_555]	2.06	0.14
1:A:38:ASP:OD1	3:K:148:GLU:OE2[2_545]	2.09	0.11

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	340/345 (99%)	331 (97%)	9 (3%)	0	100	100
1	B	343/345 (99%)	337 (98%)	6 (2%)	0	100	100
1	D	341/345 (99%)	329 (96%)	12 (4%)	0	100	100
1	F	339/345 (98%)	330 (97%)	9 (3%)	0	100	100
2	C	56/71 (79%)	56 (100%)	0	0	100	100
2	E	58/71 (82%)	58 (100%)	0	0	100	100
2	G	55/71 (78%)	55 (100%)	0	0	100	100
2	H	55/71 (78%)	55 (100%)	0	0	100	100
3	I	371/381 (97%)	366 (99%)	5 (1%)	0	100	100
3	J	369/381 (97%)	364 (99%)	5 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	369/381 (97%)	360 (98%)	9 (2%)	0	100	100
3	L	368/381 (97%)	363 (99%)	5 (1%)	0	100	100
All	All	3064/3188 (96%)	3004 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	280/285 (98%)	273 (98%)	7 (2%)	47	80
1	B	284/285 (100%)	281 (99%)	3 (1%)	73	92
1	D	284/285 (100%)	280 (99%)	4 (1%)	67	90
1	F	280/285 (98%)	276 (99%)	4 (1%)	67	90
2	C	47/58 (81%)	47 (100%)	0	100	100
2	E	45/58 (78%)	44 (98%)	1 (2%)	52	83
2	G	45/58 (78%)	45 (100%)	0	100	100
2	H	44/58 (76%)	43 (98%)	1 (2%)	50	82
3	I	336/341 (98%)	331 (98%)	5 (2%)	65	89
3	J	331/341 (97%)	326 (98%)	5 (2%)	65	89
3	K	332/341 (97%)	329 (99%)	3 (1%)	78	94
3	L	333/341 (98%)	328 (98%)	5 (2%)	65	89
All	All	2641/2736 (96%)	2603 (99%)	38 (1%)	67	90

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

Mol	Chain	Res	Type
1	F	266	HIS
3	I	228	ARG
3	L	342	ARG
2	H	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	232	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	23	ASN
3	J	14	ASN
3	L	261	ASN
3	I	213	GLN
3	J	93	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 8 ligands modelled in this entry, 4 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
4	GDP	I	401	5	24,30,30	1.20	2 (8%)	31,47,47	2.00	8 (25%)
4	GDP	J	401	5	24,30,30	1.18	2 (8%)	31,47,47	1.99	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	K	401	5	24,30,30	1.18	2 (8%)	31,47,47	1.95	8 (25%)
4	GDP	L	401	5	24,30,30	1.18	2 (8%)	31,47,47	1.96	8 (25%)

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	I	401	5	-	4/12/32/32	0/3/3/3
4	GDP	J	401	5	-	6/12/32/32	0/3/3/3
4	GDP	K	401	5	-	0/12/32/32	0/3/3/3
4	GDP	L	401	5	-	8/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	401	GDP	C6-C5	4.25	1.48	1.41
4	L	401	GDP	C6-C5	4.24	1.48	1.41
4	J	401	GDP	C6-C5	4.23	1.48	1.41
4	K	401	GDP	C6-C5	4.16	1.48	1.41
4	K	401	GDP	C5-C4	2.46	1.47	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	401	GDP	C2-N3-C4	4.88	120.94	115.36
4	I	401	GDP	C2-N3-C4	4.88	120.93	115.36
4	J	401	GDP	C2-N3-C4	4.86	120.91	115.36
4	L	401	GDP	C2-N3-C4	4.76	120.79	115.36
4	L	401	GDP	C5-C6-N1	-4.09	117.83	123.43

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	401	GDP	PA-O3A-PB-O3B
4	I	401	GDP	C5'-O5'-PA-O1A
4	I	401	GDP	C5'-O5'-PA-O2A
4	L	401	GDP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

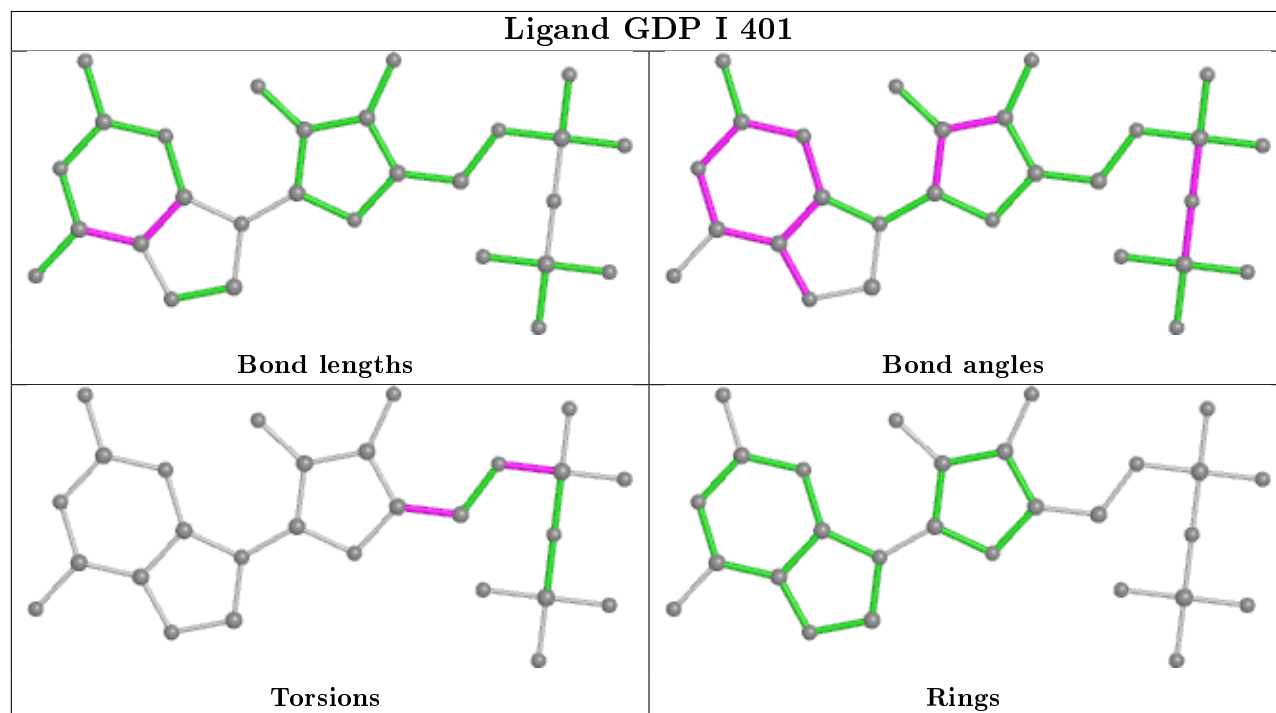
Mol	Chain	Res	Type	Atoms
4	L	401	GDP	C5'-O5'-PA-O1A

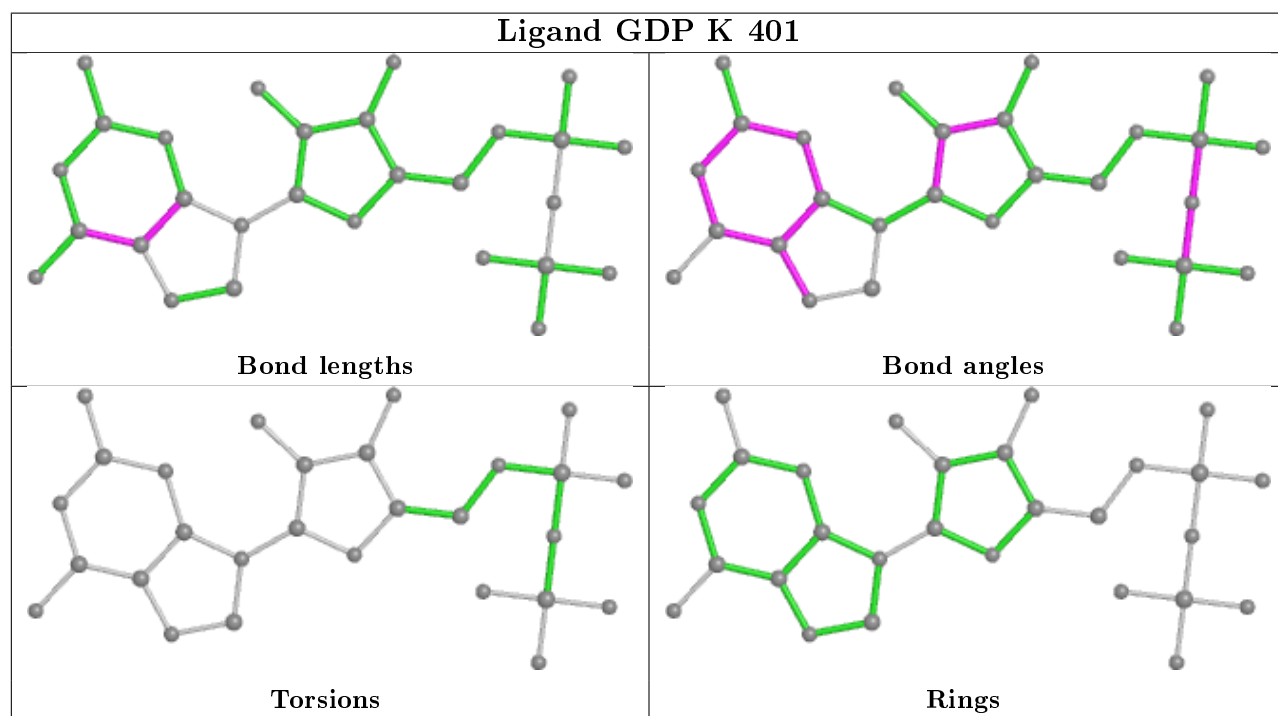
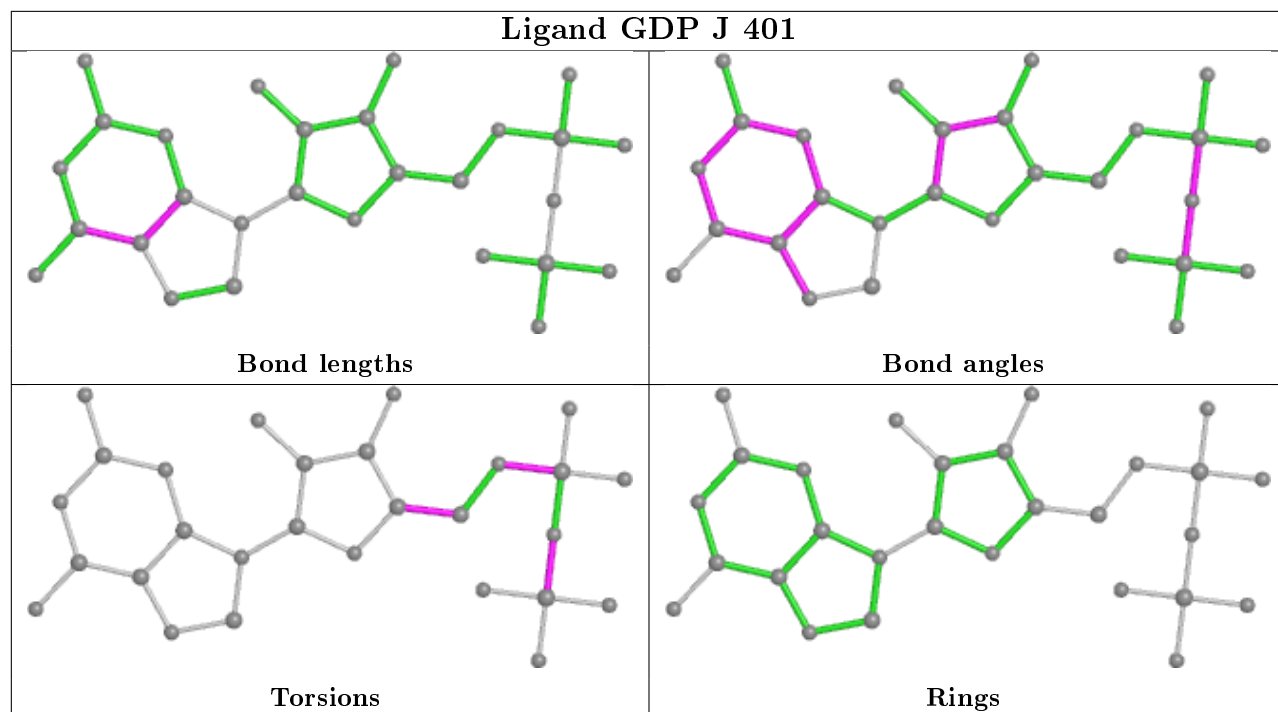
There are no ring outliers.

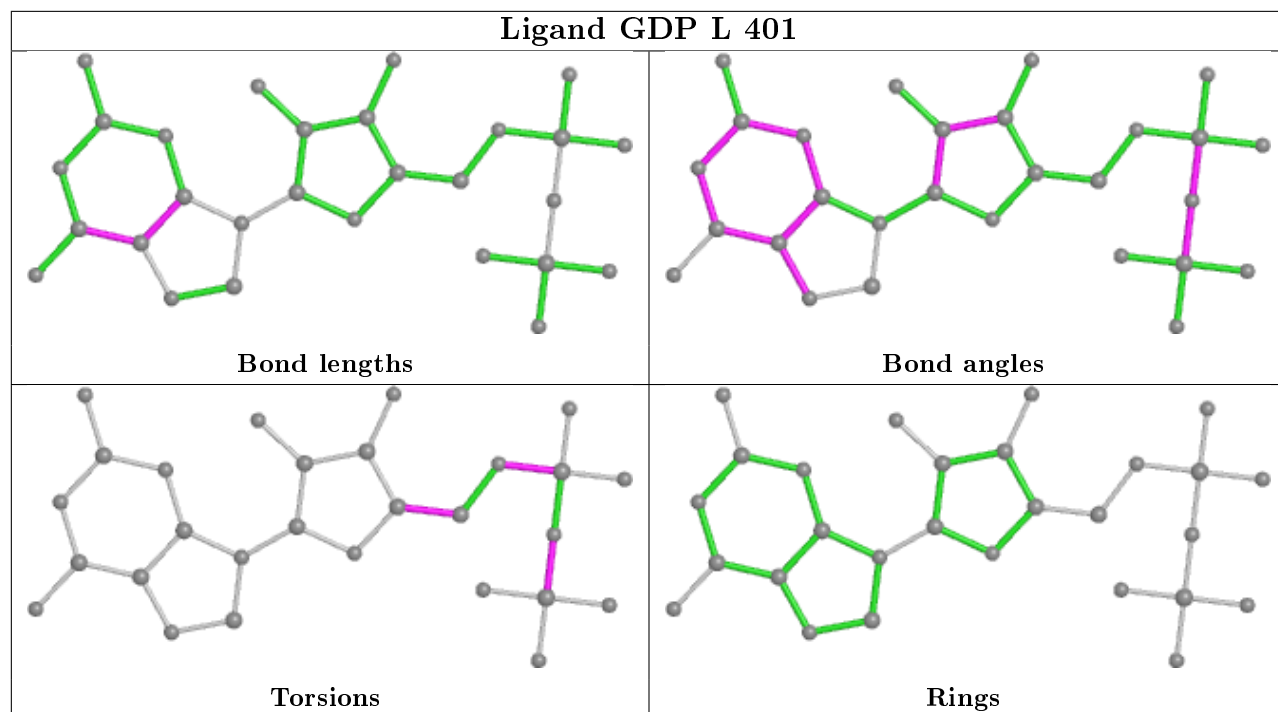
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	401	GDP	3	0
4	J	401	GDP	1	0
4	L	401	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 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 ⓘ

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, 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	339/345 (98%)	-0.47	0 100 100	19, 38, 66, 86	0
1	B	341/345 (98%)	-0.44	0 100 100	23, 39, 66, 86	0
1	D	341/345 (98%)	-0.40	0 100 100	24, 39, 69, 113	0
1	F	340/345 (98%)	-0.41	0 100 100	24, 40, 70, 95	0
2	C	57/71 (80%)	-0.34	0 100 100	34, 53, 83, 86	0
2	E	60/71 (84%)	-0.28	1 (1%) 70 63	37, 56, 98, 104	0
2	G	57/71 (80%)	-0.40	0 100 100	38, 55, 86, 105	0
2	H	57/71 (80%)	-0.35	0 100 100	34, 51, 85, 99	0
3	I	372/381 (97%)	-0.44	0 100 100	21, 38, 70, 115	0
3	J	371/381 (97%)	-0.44	0 100 100	22, 42, 71, 112	0
3	K	371/381 (97%)	-0.47	0 100 100	21, 37, 68, 97	0
3	L	370/381 (97%)	-0.45	0 100 100	21, 40, 70, 108	0
All	All	3076/3188 (96%)	-0.43	1 (0%) 100 100	19, 41, 71, 115	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	6	THR	2.9

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 ⓘ

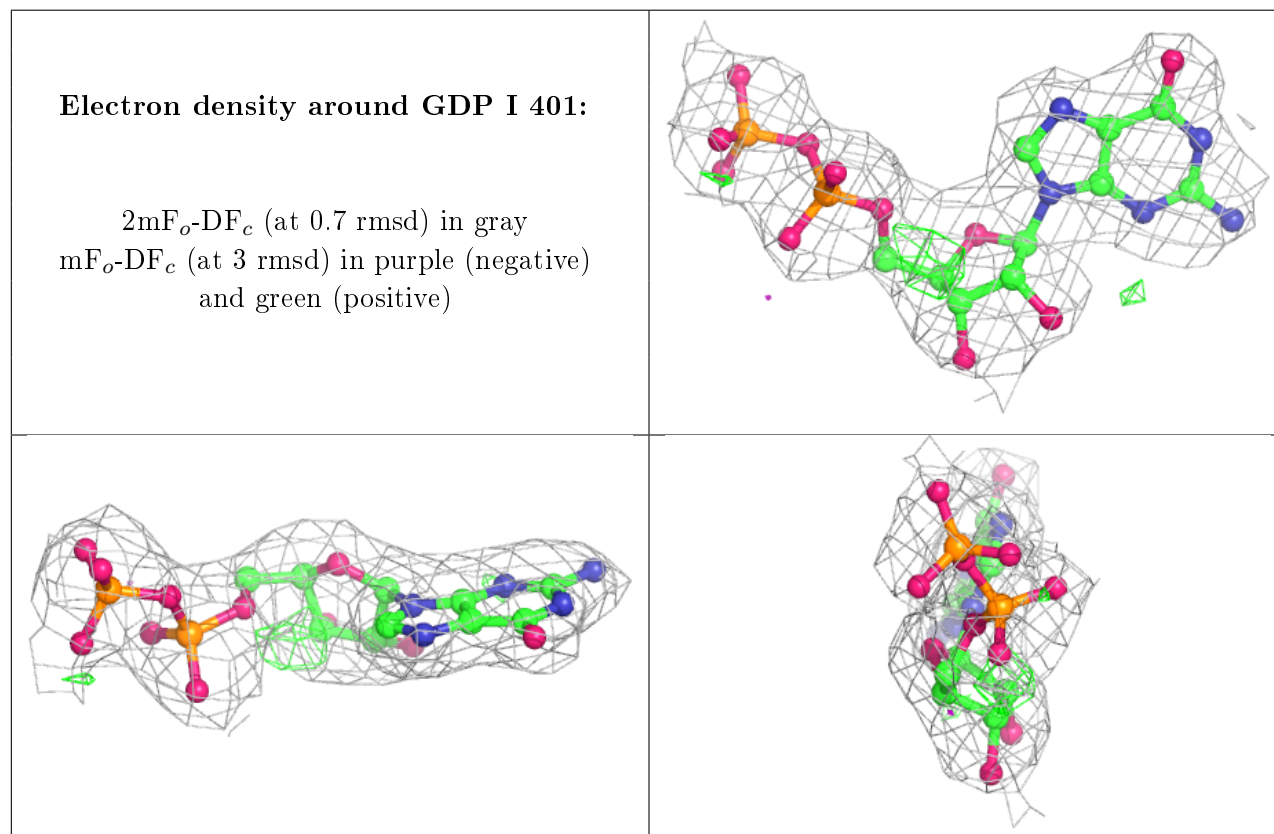
There are no monosaccharides in this entry.

6.4 Ligands [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.

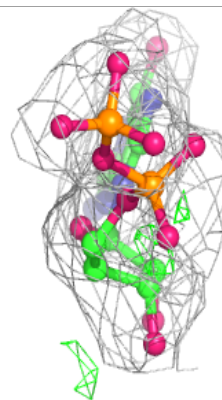
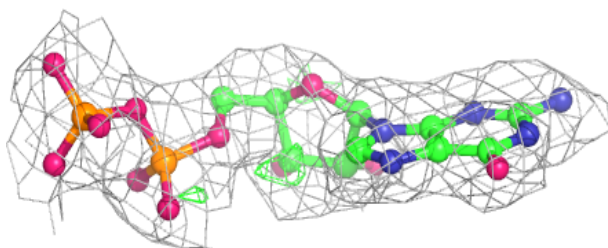
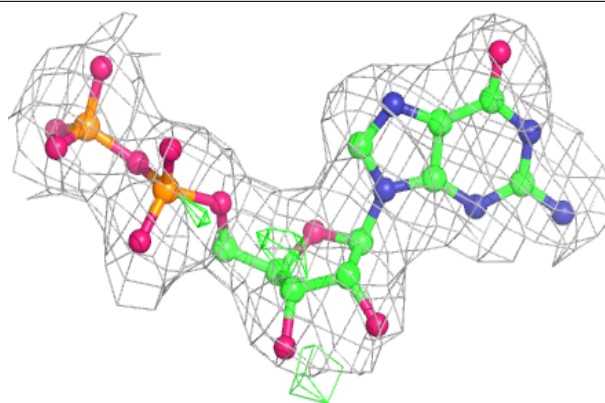
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	J	402	1/1	0.97	0.11	29,29,29,29	0
5	MG	K	402	1/1	0.97	0.07	26,26,26,26	0
4	GDP	I	401	28/28	0.98	0.15	19,29,33,35	0
5	MG	I	402	1/1	0.98	0.11	22,22,22,22	0
5	MG	L	402	1/1	0.98	0.12	19,19,19,19	0
4	GDP	K	401	28/28	0.98	0.16	22,28,32,36	0
4	GDP	J	401	28/28	0.99	0.13	19,25,32,38	0
4	GDP	L	401	28/28	0.99	0.14	19,23,31,34	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.

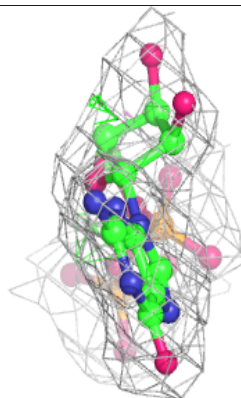
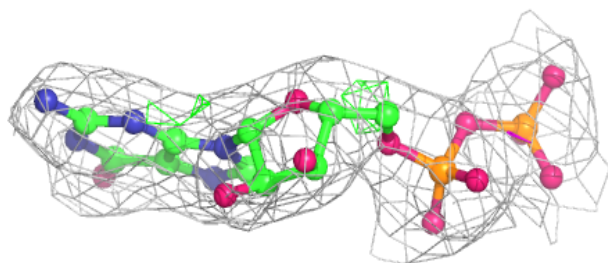
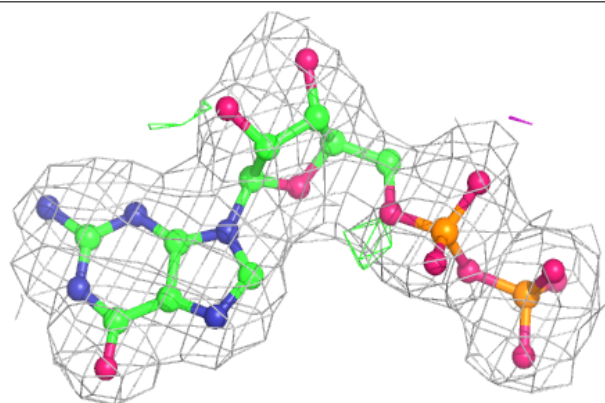


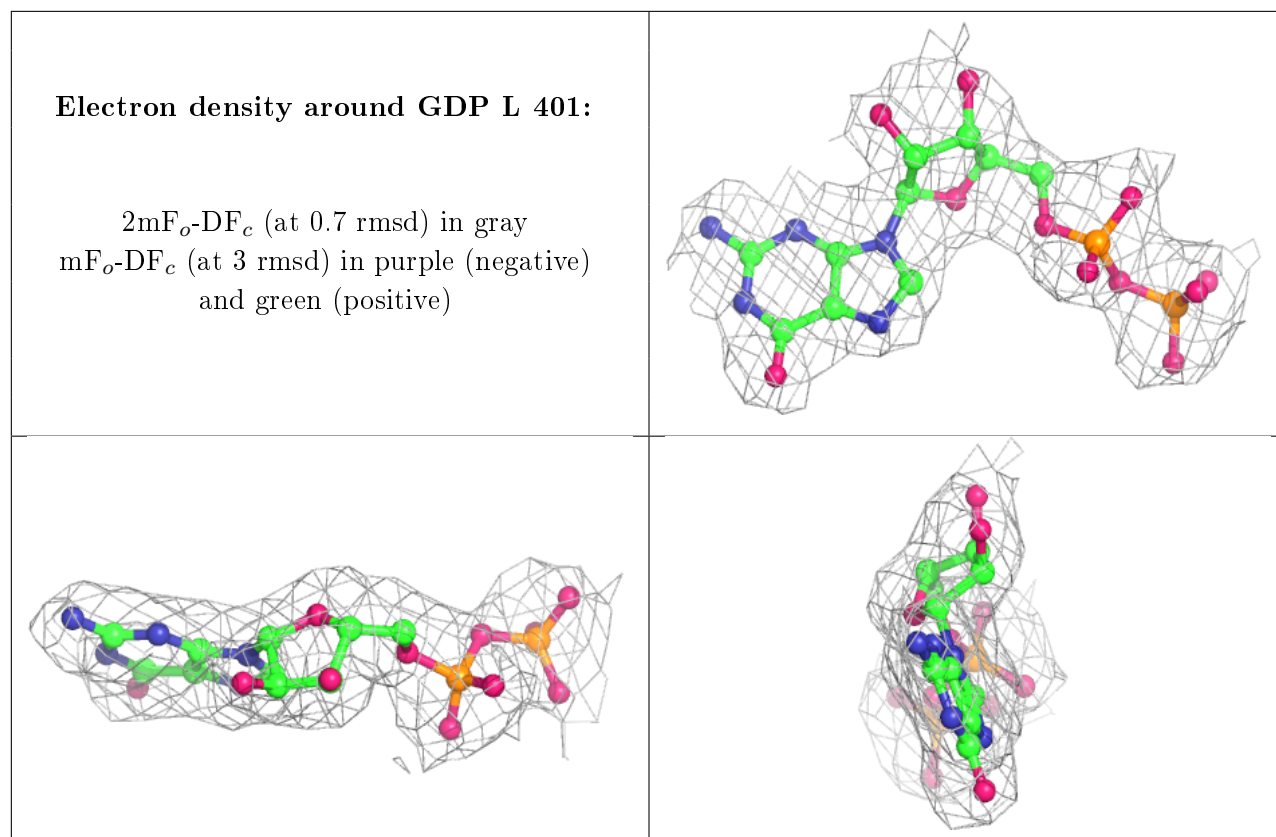
Electron density around GDP K 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP J 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.