wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:00 PM EDT

PDB ID	:	4HLQ / pdb_00004hlq
Title	:	Crystal structure of human rab1b bound to GDP and BEF3 in complex with the GAP domain of TBC1D20 from homo sapiens
Authors	:	Gazdag, E.M.; Gavriljuk, K.; Itzen, A.; Koetting, C.; Gerwert, K.; Goody, R.S.
Deposited on	:	2012-10-17
Resolution	:	3.30 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:

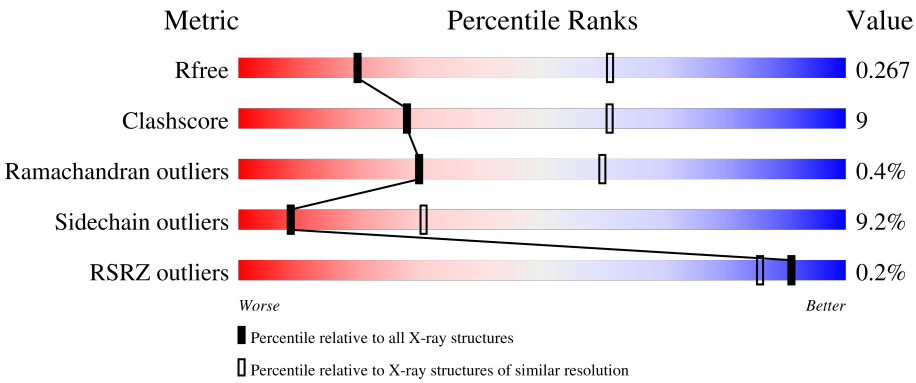
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	305	71% 19% • 8%
1	C	305	69% 21% • 8%
1	E	305	70% 20% • 8%
1	G	305	% 70% 18% • 8%

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Mol	Chain	Length	Quality of chain
1	I	305	69% 20% • 8%
2	B	175	78% 18% • •
2	D	175	70% 23% • • •
2	F	175	77% 16% 5% •
2	H	175	82% 13% • •
2	J	175	82% 15% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17765 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 TBC1 domain family member 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2242	1442	391	397	12	4	0	0
1	C	281	2240	1439	388	401	12	0	0	0
1	E	281	2246	1442	389	403	12	0	0	0
1	G	281	2118	1361	365	382	10	0	0	0
1	I	281	2237	1439	387	399	12	0	0	0

- Molecule 2 is a protein called Ras-related protein Rab-1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1332	845	218	265	4	0	0	0
2	D	170	1327	845	217	261	4	0	0	0
2	F	172	1321	839	219	260	3	0	0	0
2	H	170	1202	752	203	245	2	4	0	0
2	J	171	1259	799	205	251	4	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q9H0U4
B	1	HIS	-	expression tag	UNP Q9H0U4
B	2	MET	-	expression tag	UNP Q9H0U4
D	0	GLY	-	expression tag	UNP Q9H0U4
D	1	HIS	-	expression tag	UNP Q9H0U4

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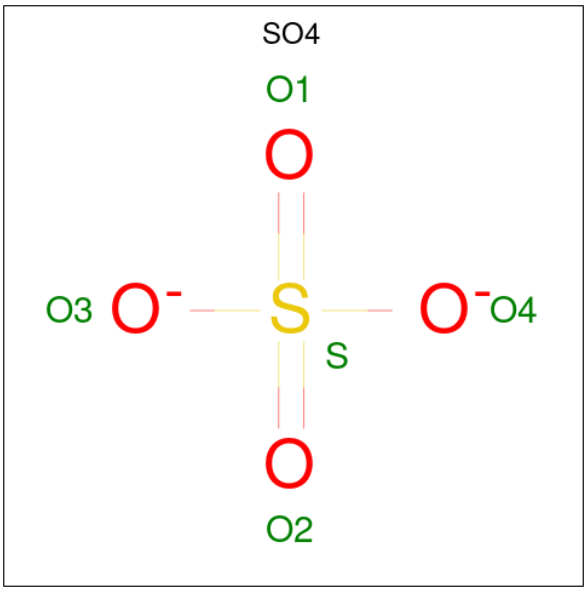
Chain	Residue	Modelled	Actual	Comment	Reference
D	2	MET	-	expression tag	UNP Q9H0U4
F	0	GLY	-	expression tag	UNP Q9H0U4
F	1	HIS	-	expression tag	UNP Q9H0U4
F	2	MET	-	expression tag	UNP Q9H0U4
H	0	GLY	-	expression tag	UNP Q9H0U4
H	1	HIS	-	expression tag	UNP Q9H0U4
H	2	MET	-	expression tag	UNP Q9H0U4
J	0	GLY	-	expression tag	UNP Q9H0U4
J	1	HIS	-	expression tag	UNP Q9H0U4
J	2	MET	-	expression tag	UNP Q9H0U4

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

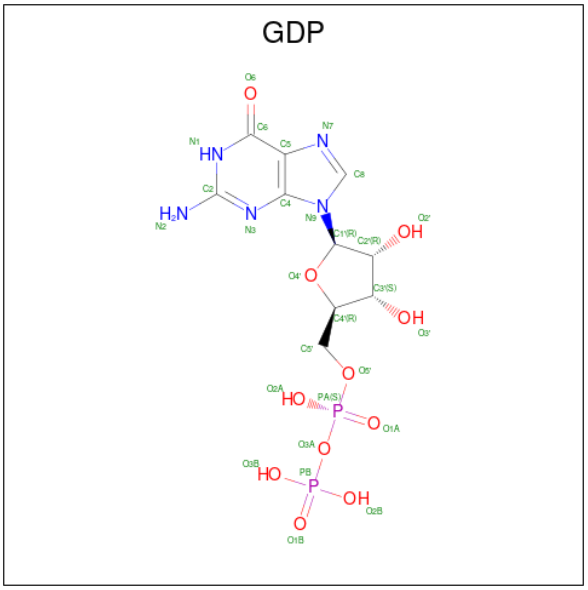


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
3	C	1	5	4	1		0	0
3	E	1	5	4	1		0	0
3	E	1	5	4	1		0	0
3	I	1	5	4	1		0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

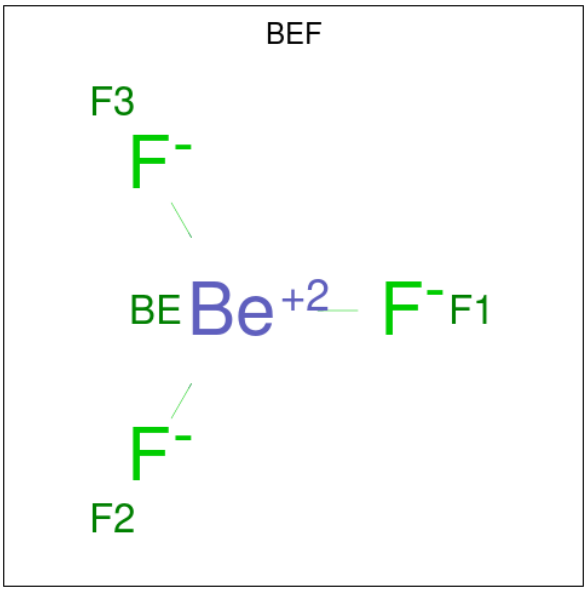
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0
4	D	1	1	1	0	0
4	F	1	1	1	0	0
4	H	1	1	1	0	0
4	J	1	1	1	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	28	10	5	11	2	0	0
5	D	1	28	10	5	11	2	0	0
5	F	1	28	10	5	11	2	0	0
5	H	1	28	10	5	11	2	0	0
5	J	1	28	10	5	11	2	0	0

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
6	B	1	4	1	3	0	0
6	D	1	4	1	3	0	0
6	F	1	4	1	3	0	0
6	H	1	4	1	3	0	0
6	J	1	4	1	3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	9	9	9	0	0
7	B	4	4	4	0	0
7	C	7	7	7	0	0
7	D	4	4	4	0	0
7	E	8	8	8	0	0
7	F	4	4	4	0	0
7	G	4	4	4	0	0

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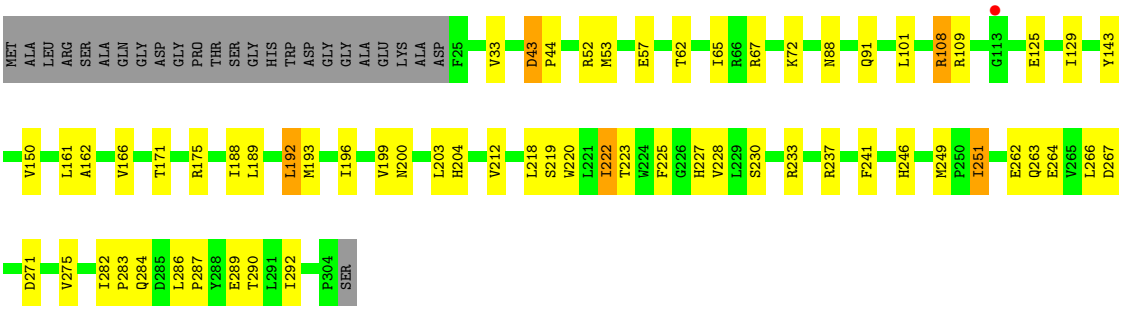
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	H	2	2	2	0	0
			Total	O		
7	I	7	7	7	0	0
			Total	O		
7	J	2	2	2	0	0

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.

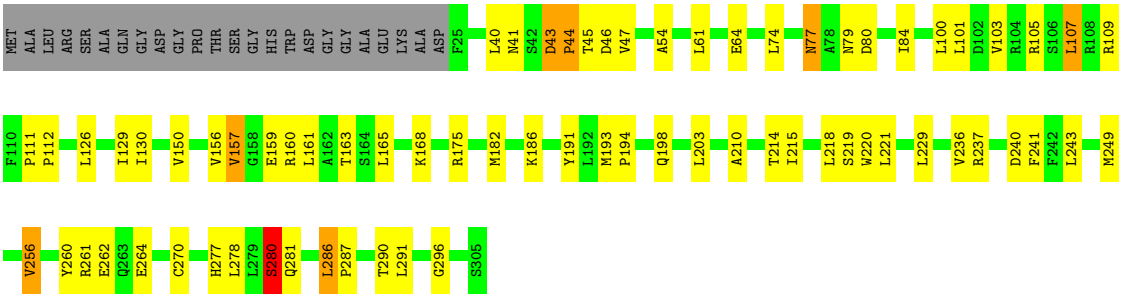
• Molecule 1: TBC1 domain family member 20

Chain A:



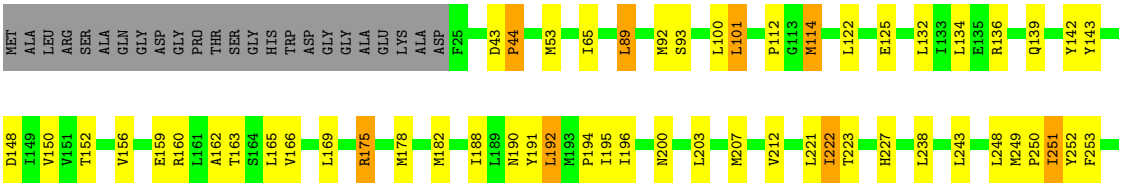
• Molecule 1: TBC1 domain family member 20

Chain C:



• Molecule 1: TBC1 domain family member 20

Chain E:



I257 V258 R261 E264 V265 L266 M272 H277 S280 Q284 S293 R294 A295 S305

• Molecule 1: TBC1 domain family member 20

Chain G:

MET ALA LEU ARG SER ALA GLN GLY ASP GLY PRO THR SER GLY HIS TRP ASP GLY GLY ALA GLU LYS ALA ASP F25 K30 I36 D43 P44 T45 D46 V47 L50 M53 S56 E57 T62 D63 E64 I65 R66 W70 L73 L74 N75 N79 I84 K87

N88 L89 Q98 R109 M114 Q118 E125 I129 L132 I133 Q139 V150 V151 V156 E159 T163 S164 L165 V166 L174 D179 P180 D183 H187 I188 L189 L192 M193 P194 I195 I196 H204 Q208 I215 S219 W220 L221 I222 T223

W224 F225 G226 V235 L238 Y239 D240 L243 L248 V256 P283 S305

• Molecule 1: TBC1 domain family member 20

Chain I:

MET ALA LEU ARG SER ALA GLN GLY ASP GLY PRO THR SER GLY HIS TRP ASP GLY GLY ALA GLU LYS ALA ASP F25 R29 K32 V33 T45 A49 M53 E57 L61 I65 R66 R67 K72 D80 P81 P82 P83 I84 S85 G86 K87 Q91 L101 D102

V103 P111 M114 L122 Q123 E124 E125 L126 I127 R136 Q139 Y143 V150 V151 T152 V166 L169 S170 T171 H172 F177 M178 D179 M182 D183 N184 I188 L189 M193 P194 L203 M207 T214 W220 L221 I222 T223 W224 H227 V228 D231

F232 V235 L238 F241 F242 L243 H246 P247 L248 M249 P250 I251 L266 D269 Q281 A295 L298 F302 S305

• Molecule 2: Ras-related protein Rab-1B

Chain B:

GLY HIS MET P3 L8 D16 S17 G18 K21 T34 T40 I41 G42 V43 I47 R48 T49 I50 E51 K58 L59 Q60 F70 I73 I84 I106 S111 N115 K116 L117 L118 V119 K122 D132 N133 T134 T135 I145 P146 F147 L148 T156 N157

V158 E159 M163 T164 M165 R172 M173 G174

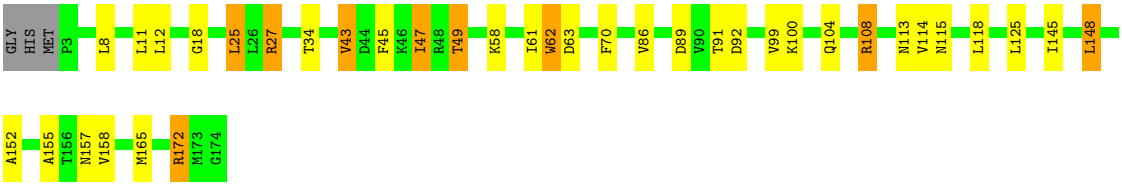
• Molecule 2: Ras-related protein Rab-1B

Chain D:

GLY HIS MET PRO E4 Y5 L8 F9 K10 L11 L12 L13 D16 S17 G18 V19 G20 K21 L24 L25 L26 R27 F28 T34 E35 S36 S39 T40 V43 K46 I47 R48 W62 F70 I73 T74 A81 I84 I85 D89 V90 T91 D92 S95 V99

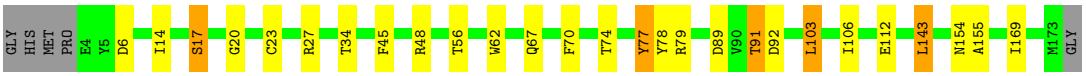
• Molecule 2: Ras-related protein Rab-1B

Chain F:



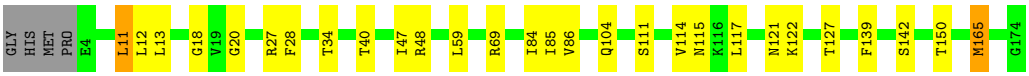
• Molecule 2: Ras-related protein Rab-1B

Chain H:



• Molecule 2: Ras-related protein Rab-1B

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.17Å 118.64Å 290.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 3.30 49.22 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-3.30) 99.9 (49.22-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.206 , 0.274 0.202 , 0.267	Depositor DCC
R_{free} test set	2334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	79.9	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 80.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17765	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, SO4, MG, 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	0.46	0/2298	0.91	2/3130 (0.1%)
1	C	0.49	0/2296	0.91	2/3129 (0.1%)
1	E	0.45	0/2302	0.85	2/3137 (0.1%)
1	G	0.49	0/2172	0.92	1/2975 (0.0%)
1	I	0.45	0/2293	0.91	4/3125 (0.1%)
2	B	0.45	0/1353	0.81	0/1832
2	D	0.46	0/1348	0.82	1/1825 (0.1%)
2	F	0.45	0/1342	0.79	0/1818
2	H	0.83	1/1221 (0.1%)	0.90	2/1667 (0.1%)
2	J	0.48	0/1280	0.80	0/1744
All	All	0.50	1/17905 (0.0%)	0.87	14/24382 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	79	ARG	CD-NE	-23.58	1.13	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	79	ARG	CG-CD-NE	10.60	135.32	112.00
1	C	280	SER	N-CA-C	9.46	124.83	112.72
1	G	87	LYS	N-CA-C	6.11	117.94	109.15
2	H	79	ARG	CD-NE-CZ	-5.88	116.16	124.40
2	D	156	THR	N-CA-C	5.77	118.96	110.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ARG	Sidechain
1	A	43	ASP	Peptide
1	C	280	SER	Peptide
1	C	43	ASP	Peptide

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	2242	0	2195	45	0
1	C	2240	0	2190	46	0
1	E	2246	0	2195	45	0
1	G	2118	0	1943	36	0
1	I	2237	0	2189	50	0
2	B	1332	0	1278	21	0
2	D	1327	0	1300	26	0
2	F	1321	0	1268	20	0
2	H	1202	0	1014	19	0
2	J	1259	0	1123	14	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	I	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	12	2	0
5	D	28	0	12	0	0
5	F	28	0	12	1	0
5	H	28	0	12	7	0
5	J	28	0	12	3	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
6	F	4	0	0	0	0
6	H	4	0	0	1	0
6	J	4	0	0	1	0
7	A	9	0	0	1	0
7	B	4	0	0	0	0
7	C	7	0	0	0	0
7	D	4	0	0	0	0
7	E	8	0	0	0	0
7	F	4	0	0	0	0
7	G	4	0	0	1	0
7	H	2	0	0	0	0
7	I	7	0	0	0	0
7	J	2	0	0	0	0
All	All	17765	0	16755	311	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 311 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:E:114:MET:HE1	1:E:122:LEU:HD12	1.38	1.03
1:G:79:ASN:H	1:G:79:ASN:HD22	1.06	0.96
1:E:175:ARG:O	1:E:175:ARG:HD3	1.77	0.83
1:G:98:GLN:HG2	2:H:67:GLN:HE21	1.41	0.83
1:I:177:PHE:HZ	1:I:221:LEU:HD22	1.47	0.80

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	278/305 (91%)	264 (95%)	14 (5%)	0	100	100
1	C	279/305 (92%)	266 (95%)	11 (4%)	2 (1%)	18	49
1	E	279/305 (92%)	267 (96%)	11 (4%)	1 (0%)	30	60
1	G	279/305 (92%)	266 (95%)	9 (3%)	4 (1%)	9	33
1	I	279/305 (92%)	276 (99%)	3 (1%)	0	100	100
2	B	170/175 (97%)	161 (95%)	9 (5%)	0	100	100
2	D	168/175 (96%)	163 (97%)	5 (3%)	0	100	100
2	F	170/175 (97%)	159 (94%)	10 (6%)	1 (1%)	21	52
2	H	168/175 (96%)	156 (93%)	11 (6%)	1 (1%)	21	52
2	J	169/175 (97%)	161 (95%)	7 (4%)	1 (1%)	21	52
All	All	2239/2400 (93%)	2139 (96%)	90 (4%)	10 (0%)	30	60

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	56	SER
2	H	155	ALA
2	F	114	VAL
1	E	44	PRO
1	G	46	ASP

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	239/271 (88%)	225 (94%)	14 (6%)	18	46
1	C	241/271 (89%)	217 (90%)	24 (10%)	7	27
1	E	242/271 (89%)	224 (93%)	18 (7%)	13	38
1	G	206/271 (76%)	182 (88%)	24 (12%)	5	20
1	I	240/271 (89%)	220 (92%)	20 (8%)	10	34
2	B	138/151 (91%)	126 (91%)	12 (9%)	9	32
2	D	141/151 (93%)	124 (88%)	17 (12%)	5	20
2	F	135/151 (89%)	119 (88%)	16 (12%)	5	20
2	H	103/151 (68%)	93 (90%)	10 (10%)	8	28
2	J	117/151 (78%)	107 (92%)	10 (8%)	10	33
All	All	1802/2110 (85%)	1637 (91%)	165 (9%)	8	30

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	156	VAL
1	I	203	LEU
1	G	183	ASP
2	H	91	THR
1	I	251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	144	GLN
1	I	200	ASN
1	G	26	ASN
1	I	198	GLN
2	J	121	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
3	SO4	A	401	-	4,4,4	0.22	0	6,6,6	0.21	0
3	SO4	C	401	-	4,4,4	0.26	0	6,6,6	0.09	0
5	GDP	F	202	4,6	29,30,30	1.29	4 (13%)	45,47,47	1.65	8 (17%)
3	SO4	E	402	-	4,4,4	0.25	0	6,6,6	0.12	0
5	GDP	D	202	6	29,30,30	1.35	3 (10%)	45,47,47	1.63	8 (17%)
6	BEF	F	203	5	0,3,3	-	-	-		
5	GDP	H	202	4,6	29,30,30	1.27	3 (10%)	45,47,47	1.72	9 (20%)
5	GDP	J	202	4,6	29,30,30	1.29	3 (10%)	45,47,47	1.77	10 (22%)
6	BEF	B	203	5	0,3,3	-	-	-		
6	BEF	D	203	5	0,3,3	-	-	-		
6	BEF	J	203	5	0,3,3	-	-	-		
5	GDP	B	202	4,6	29,30,30	1.34	4 (13%)	45,47,47	1.63	9 (20%)
3	SO4	E	401	-	4,4,4	0.26	0	6,6,6	0.09	0
6	BEF	H	203	5	0,3,3	-	-	-		
3	SO4	I	401	-	4,4,4	0.24	0	6,6,6	0.16	0

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
5	GDP	F	202	4,6	-	2/16/32/32	0/3/3/3
5	GDP	D	202	6	-	1/16/32/32	0/3/3/3
5	GDP	J	202	4,6	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	H	202	4,6	-	6/16/32/32	0/3/3/3
5	GDP	B	202	4,6	-	4/16/32/32	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	202	GDP	C5-N7	-3.02	1.33	1.39
5	D	202	GDP	C5-C6	-3.00	1.33	1.44
5	D	202	GDP	C5-N7	-2.94	1.33	1.39
5	B	202	GDP	C5-C6	-2.89	1.33	1.44
5	H	202	GDP	C5-C6	-2.74	1.34	1.44

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	202	GDP	C2-N3-C4	5.28	121.39	112.30
5	F	202	GDP	C2-N3-C4	5.05	121.00	112.30
5	H	202	GDP	C2-N3-C4	4.93	120.79	112.30
5	J	202	GDP	C5-C4-N3	-4.87	120.63	128.39
5	D	202	GDP	C2-N3-C4	4.70	120.39	112.30

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	202	GDP	C5'-O5'-PA-O3A
5	F	202	GDP	O4'-C4'-C5'-O5'
5	H	202	GDP	C5'-O5'-PA-O3A
5	H	202	GDP	C5'-O5'-PA-O1A
5	H	202	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SO4	1	0
5	F	202	GDP	1	0
5	H	202	GDP	7	0
5	J	202	GDP	3	0
6	J	203	BEF	1	0

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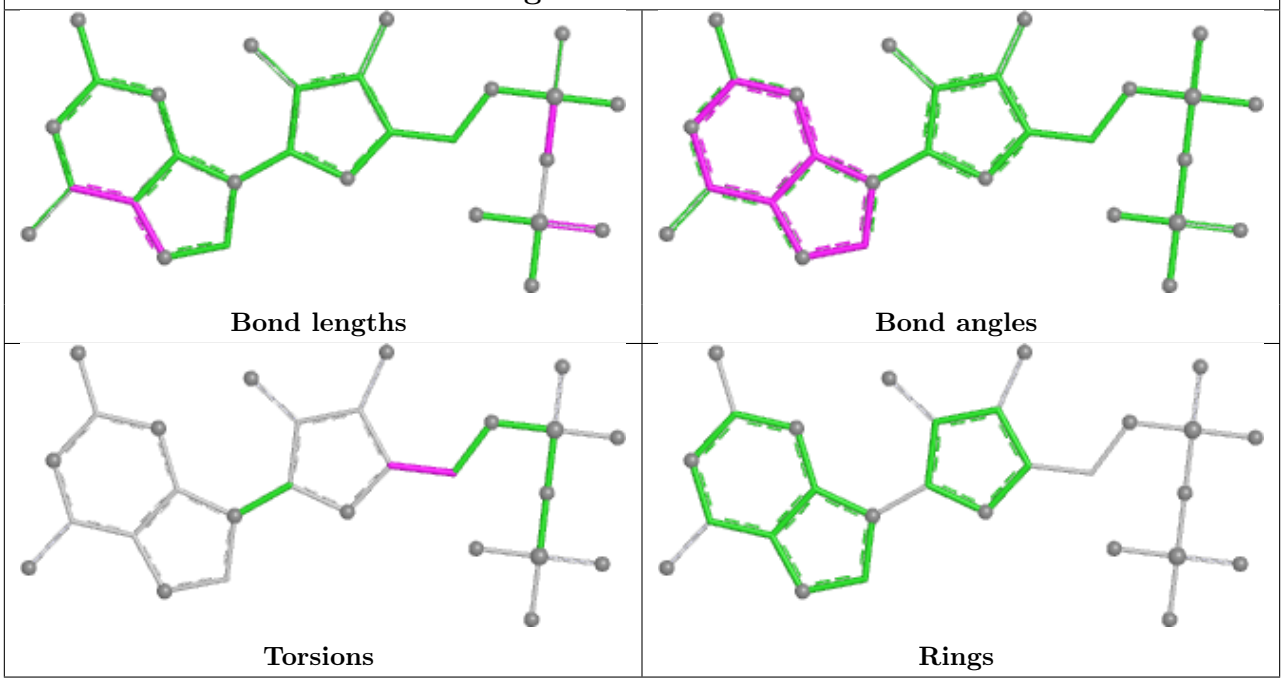
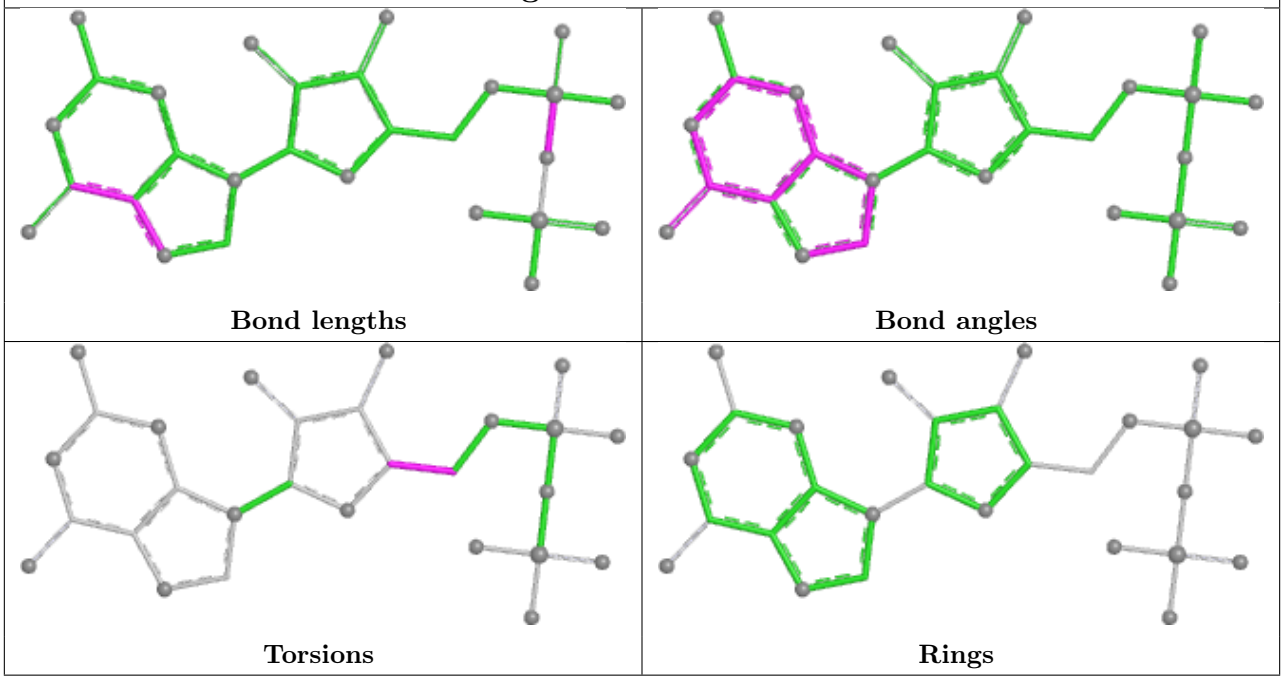
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	202	GDP	2	0
6	H	203	BEF	1	0

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.

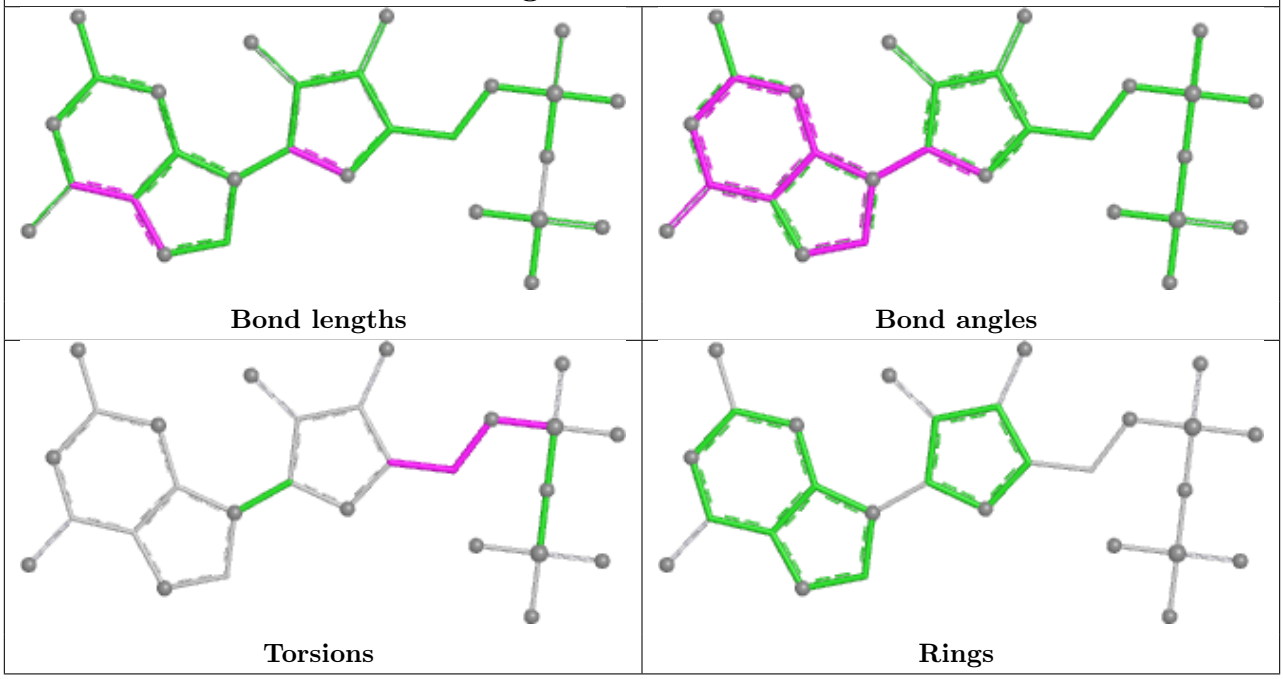
Ligand GDP F 202



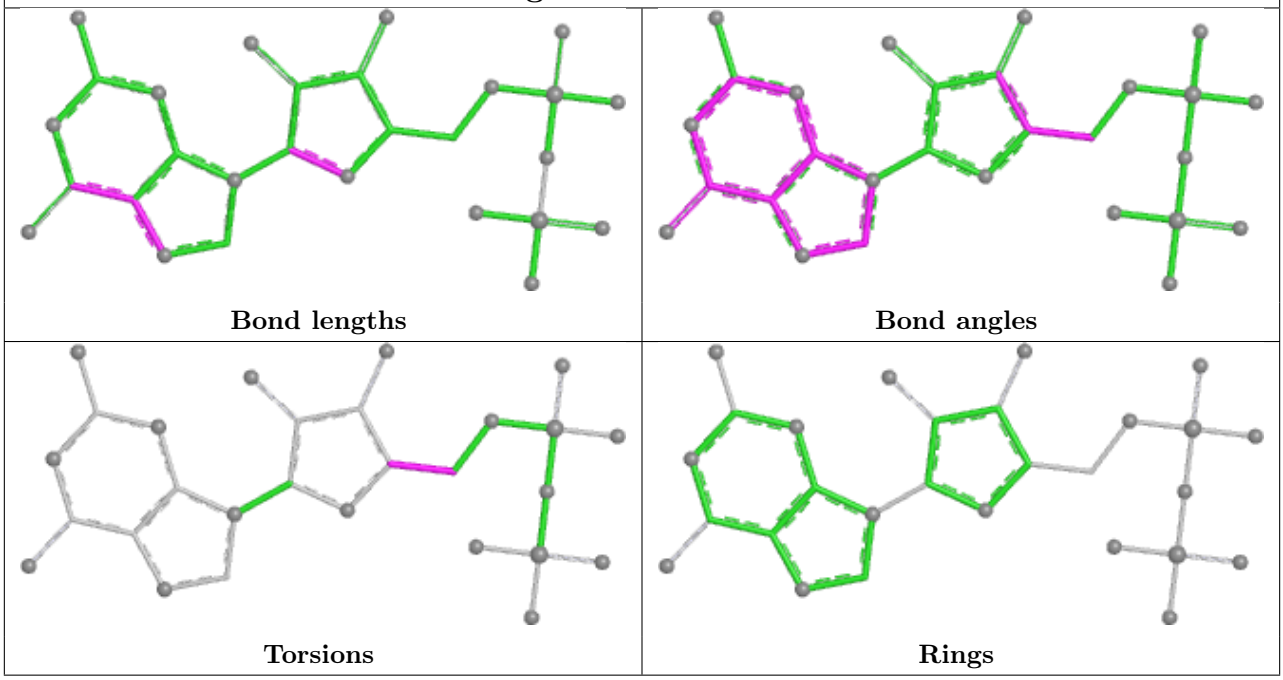
Ligand GDP D 202



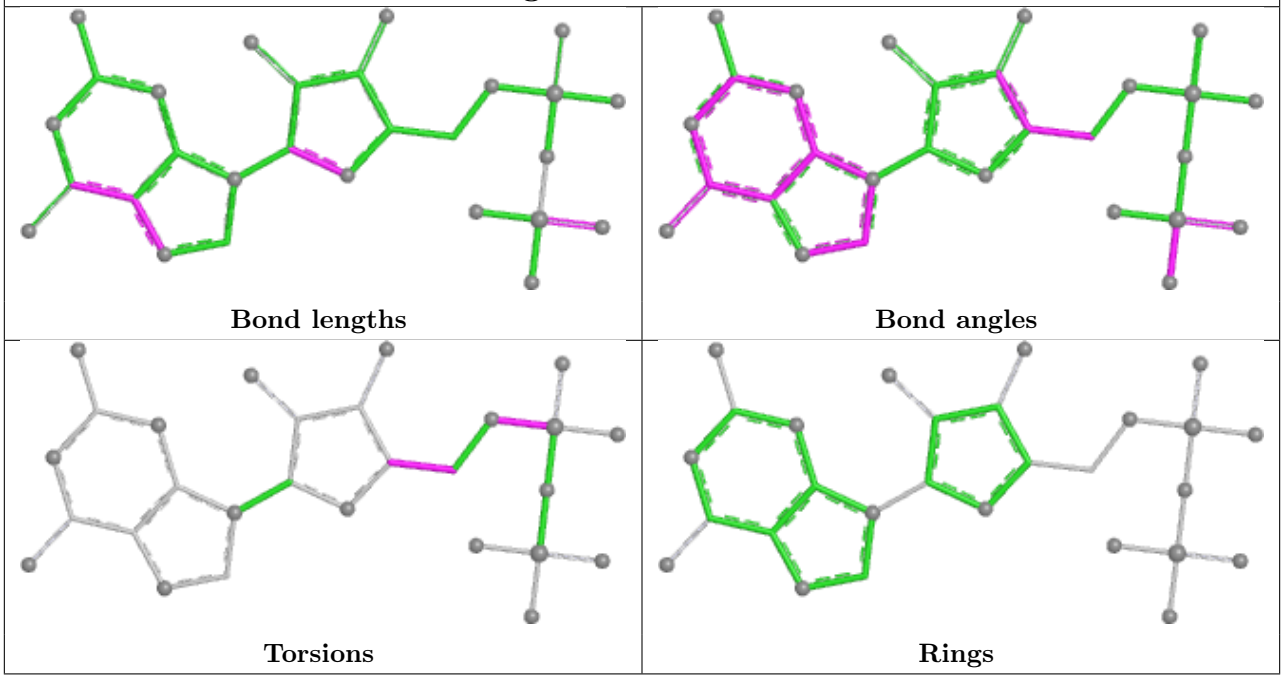
Ligand GDP H 202



Ligand GDP J 202



Ligand GDP B 202



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	280/305 (91%)	-0.45	1 (0%)	88	79	43, 62, 90, 109	1 (0%)
1	C	281/305 (92%)	-0.45	0	100	100	51, 66, 86, 110	0
1	E	281/305 (92%)	-0.38	0	100	100	51, 71, 100, 118	0
1	G	281/305 (92%)	0.04	2 (0%)	84	70	74, 96, 128, 157	0
1	I	281/305 (92%)	-0.32	1 (0%)	88	79	57, 74, 104, 117	0
2	B	172/175 (98%)	-0.31	0	100	100	51, 68, 97, 118	0
2	D	170/175 (97%)	-0.31	0	100	100	59, 76, 101, 116	0
2	F	172/175 (98%)	-0.30	0	100	100	57, 72, 100, 120	0
2	H	170/175 (97%)	0.18	0	100	100	74, 101, 141, 163	1 (0%)
2	J	171/175 (97%)	-0.06	0	100	100	71, 90, 118, 131	0
All	All	2259/2400 (94%)	-0.25	4 (0%)	91	86	43, 75, 114, 163	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	305	SER	2.5
1	G	305	SER	2.4
1	A	113	GLY	2.4
1	G	223	THR	2.1

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 oligosaccharides in this entry.

6.4 Ligands (i)

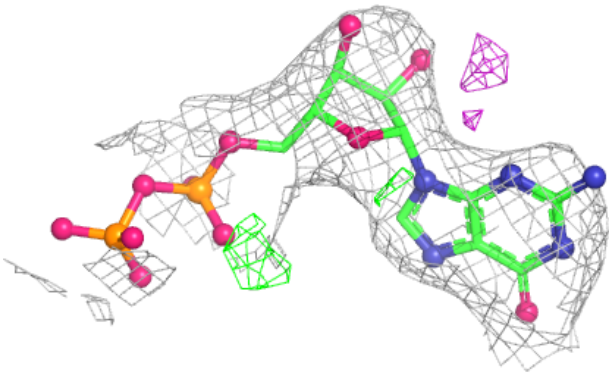
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

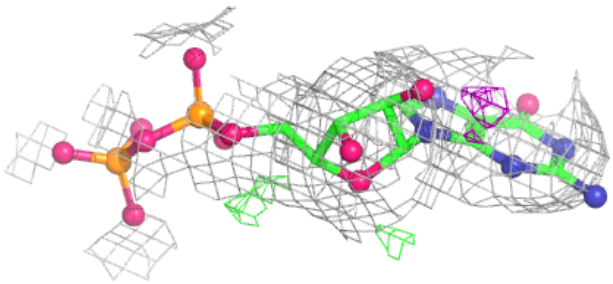
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	401	5/5	0.78	0.10	101,101,102,102	0
3	SO4	C	401	5/5	0.78	0.17	124,124,124,124	0
3	SO4	E	401	5/5	0.84	0.08	106,106,107,107	0
6	BEF	H	203	4/4	0.84	0.10	103,104,104,104	0
4	MG	F	201	1/1	0.89	0.08	61,61,61,61	0
5	GDP	J	202	28/28	0.91	0.09	84,90,92,93	0
6	BEF	D	203	4/4	0.92	0.09	75,75,76,76	0
5	GDP	H	202	28/28	0.92	0.07	64,70,80,80	0
4	MG	D	201	1/1	0.93	0.12	55,55,55,55	0
3	SO4	I	401	5/5	0.93	0.08	107,107,107,107	0
6	BEF	J	203	4/4	0.93	0.09	95,96,96,96	0
6	BEF	F	203	4/4	0.94	0.06	70,70,70,71	0
3	SO4	E	402	5/5	0.95	0.06	105,105,105,105	0
5	GDP	B	202	28/28	0.95	0.07	51,56,57,58	0
5	GDP	F	202	28/28	0.95	0.07	54,59,64,64	0
5	GDP	D	202	28/28	0.96	0.07	63,64,67,68	0
4	MG	B	201	1/1	0.96	0.07	65,65,65,65	0
4	MG	H	201	1/1	0.97	0.04	61,61,61,61	0
6	BEF	B	203	4/4	0.97	0.06	64,64,64,64	0
4	MG	J	201	1/1	0.97	0.07	61,61,61,61	0

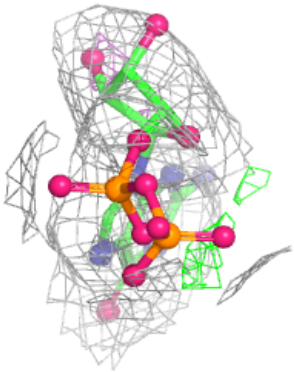
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP J 202:

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

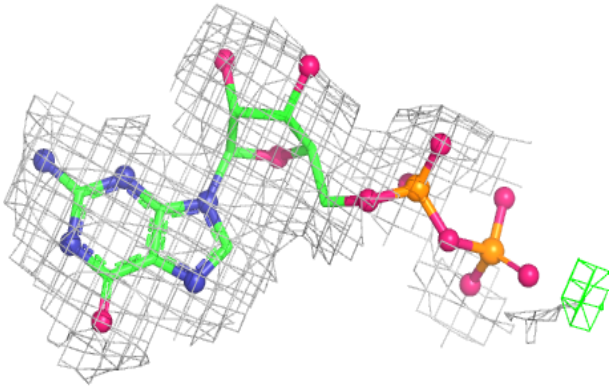


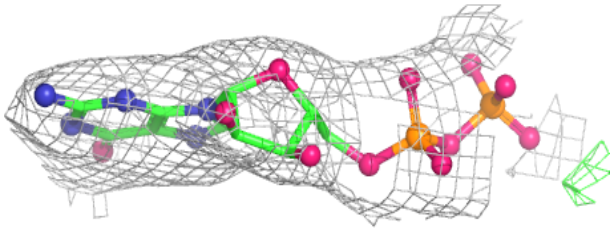


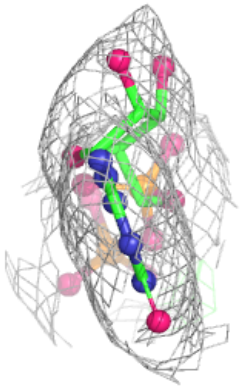


Electron density around GDP H 202:

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

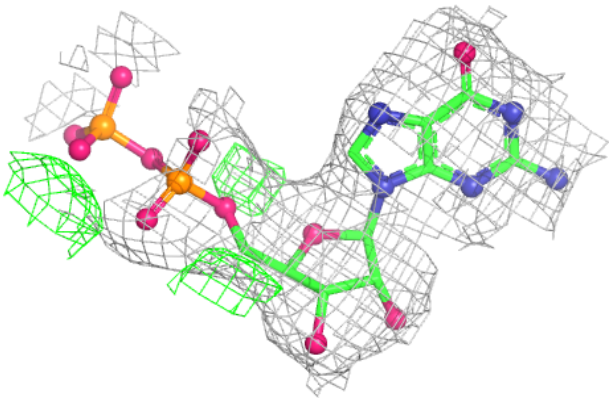


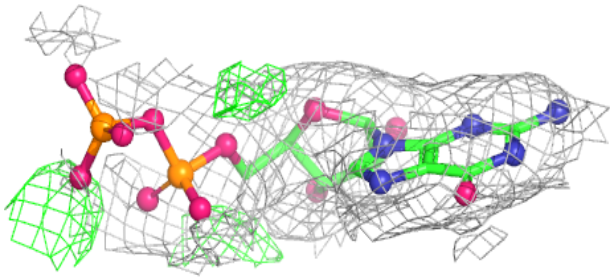


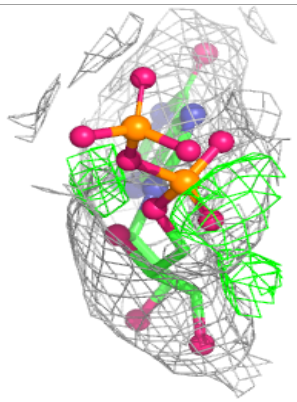


Electron density around GDP B 202:

$2mF_o$-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 F 202:

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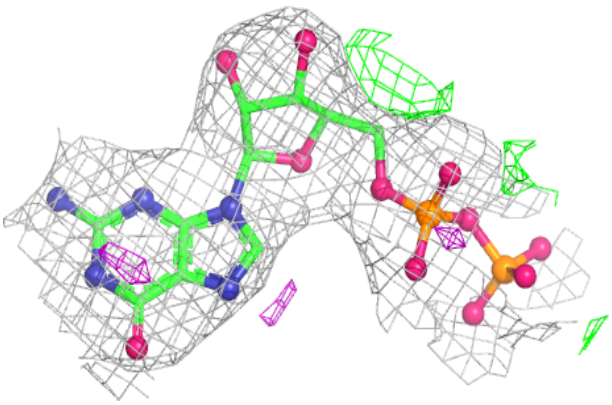
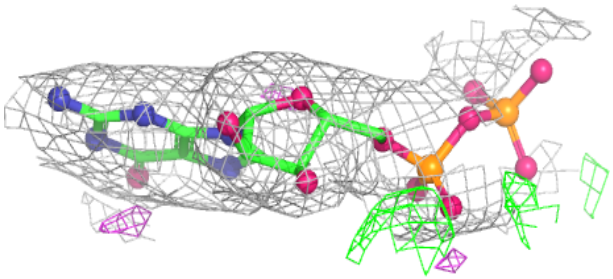
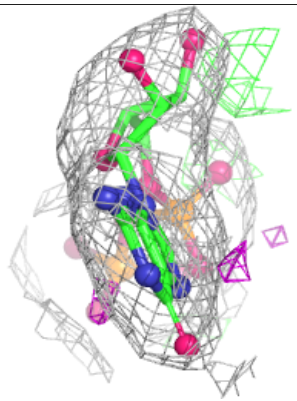
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

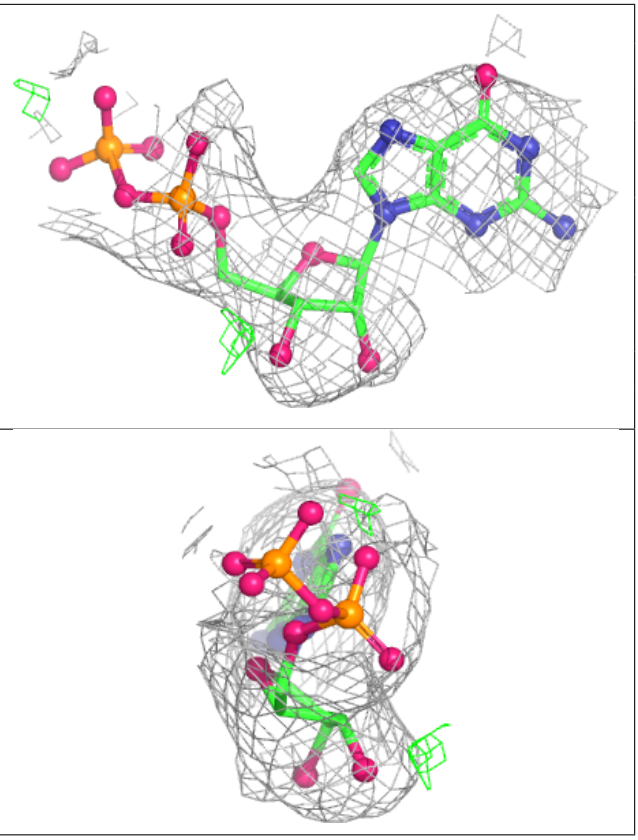






Electron density around GDP D 202:

$2mF_o$-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.