



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:08 PM UTC

PDB ID : 2W83 / pdb_00002w83
Title : Crystal structure of the ARF6 GTPase in complex with a specific effector, JIP4
Authors : Isabet, T.; Montagnac, G.; Regazzoni, K.; Raynal, B.; El Khadali, F.; Franco, M.; England, P.; Chavrier, P.; Houdusse, A.; Menetrey, J.
Deposited on : 2009-01-08
Resolution : 1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

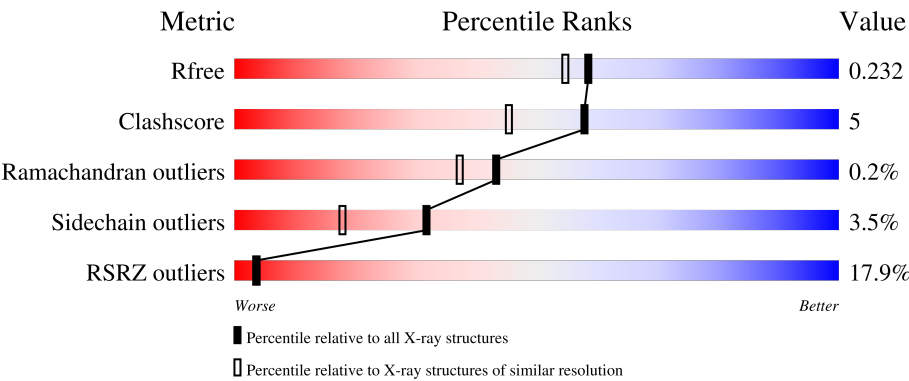
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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	165	4% 89% 7% ..
1	B	165	39% 82% 13% ..
1	E	165	4% 89% 8% ..
2	C	77	21% 82% .. 13%

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Mol	Chain	Length	Quality of chain
2	D	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DIO	A	1175	-	-	X	-
5	DIO	E	1175	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5359 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 ADP-RIBOSYLATION FACTOR 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	23	0	0
			1301	826	229	239	7			
1	B	161	Total	C	N	O	S	12	0	0
			1301	826	229	239	7			
1	E	162	Total	C	N	O	S	11	0	0
			1306	829	230	240	7			

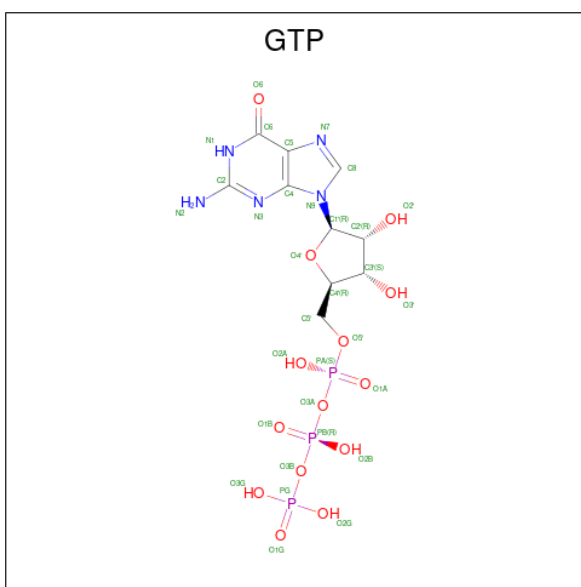
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	LEU	GLN	engineered mutation	UNP P62330
B	67	LEU	GLN	engineered mutation	UNP P62330
E	67	LEU	GLN	engineered mutation	UNP P62330

- Molecule 2 is a protein called C-JUN-AMINO-TERMINAL KINASE-INTERACTING PROTEIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	23	2	0
			539	337	87	111	4			
2	D	62	Total	C	N	O	S	30	1	0
			497	312	82	101	2			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

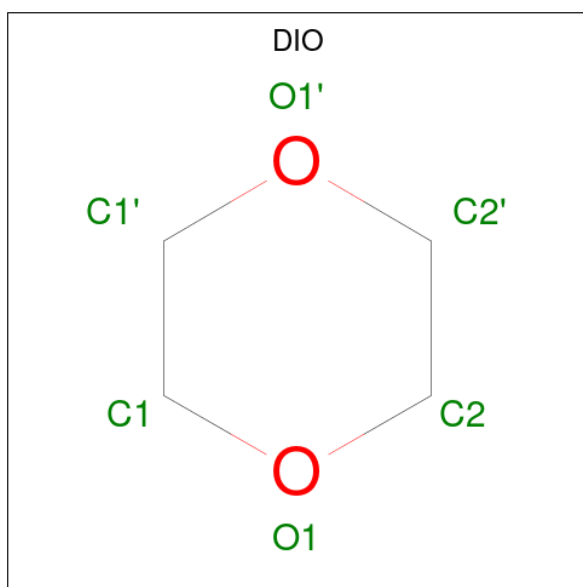


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

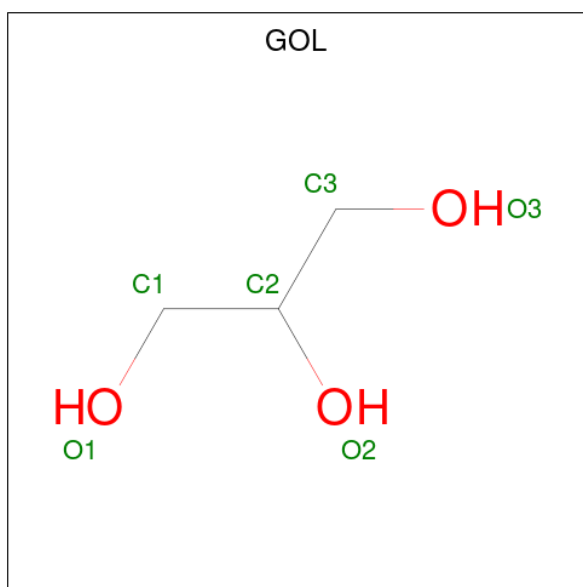
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	C	1	Total	C	O	0	0
			6	4	2		
5	C	1	Total	C	O	0	0
			6	4	2		
5	E	1	Total	C	O	0	0
			6	4	2		
5	E	1	Total	C	O	0	0
			6	4	2		
5	E	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

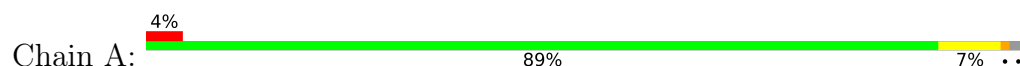
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	99	Total	O	0	0
			99	99		
7	B	29	Total	O	0	0
			29	29		
7	C	35	Total	O	0	0
			35	35		
7	D	21	Total	O	0	0
			21	21		
7	E	90	Total	O	0	0
			90	90		

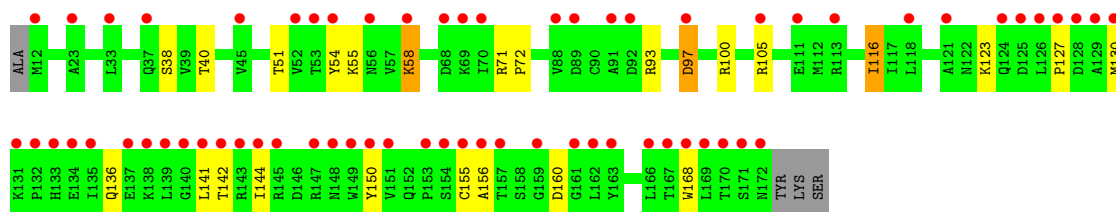
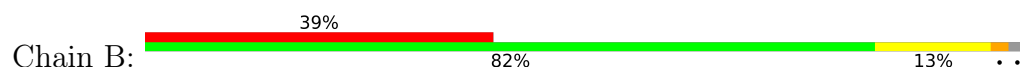
3 Residue-property plots [i](#)

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.

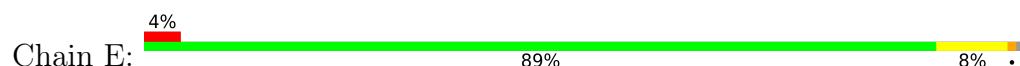
- Molecule 1: ADP-RIBOSYLATION FACTOR 6



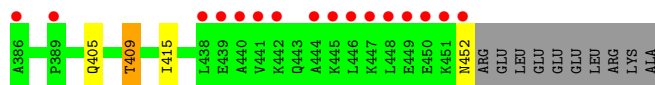
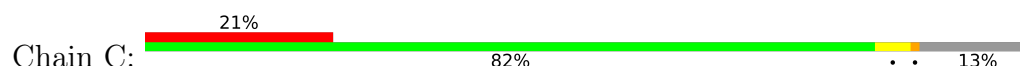
- Molecule 1: ADP-RIBOSYLATION FACTOR 6



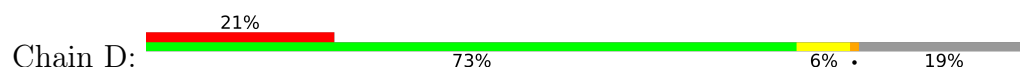
- Molecule 1: ADP-RIBOSYLATION FACTOR 6

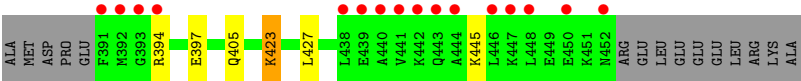


- Molecule 2: C-JUN-AMINO-TERMINAL KINASE-INTERACTING PROTEIN 4



- Molecule 2: C-JUN-AMINO-TERMINAL KINASE-INTERACTING PROTEIN 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.27Å 137.27Å 165.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	118.68 – 1.93 118.68 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.68-1.93) 99.9 (118.68-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.07 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.238 0.210 , 0.232	Depositor DCC
R_{free} test set	6987 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5359	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: DIO, GTP, MG, GOL

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	0.55	0/1326	0.76	0/1795
1	B	0.48	0/1326	0.78	0/1795
1	E	0.59	0/1331	0.74	0/1802
2	C	0.56	0/546	1.13	3/732 (0.4%)
2	D	0.64	0/500	0.95	1/670 (0.1%)
All	All	0.55	0/5029	0.82	4/6794 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	452	ASN	CA-CB-CG	15.56	128.16	112.60
2	C	452	ASN	CB-CG-ND2	8.52	129.18	116.40
2	C	452	ASN	CB-CG-OD1	-6.32	108.17	120.80
2	D	397	GLU	CA-CB-CG	5.28	124.67	114.10

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	1301	0	1308	12	0
1	B	1301	0	1308	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1306	0	1313	14	0
2	C	539	0	559	2	0
2	D	497	0	524	1	0
3	A	32	0	12	0	0
3	B	32	0	12	2	0
3	E	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	6	0	8	4	0
5	C	12	0	16	3	0
5	E	18	0	24	10	0
6	A	6	0	8	0	0
7	A	99	0	0	0	0
7	B	29	0	0	0	0
7	C	35	0	0	0	0
7	D	21	0	0	0	0
7	E	90	0	0	0	0
All	All	5359	0	5104	45	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 5.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:HG11	1:A:170:THR:HG22	1.41	1.02
1:A:132:PRO:HB2	5:E:1175:DIO:H2'1	1.54	0.88
1:B:93:ARG:HG2	1:B:130:MET:HE3	1.57	0.84
1:B:51:THR:HG21	1:B:58:LYS:NZ	1.94	0.81
1:A:70:ILE:HG22	5:C:1453:DIO:H21	1.67	0.75
1:B:51:THR:HG21	1:B:58:LYS:HZ3	1.51	0.75
1:E:35:LEU:HD23	5:E:1176:DIO:H12	1.72	0.71
1:A:57:VAL:CG1	1:A:170:THR:HG22	2.20	0.68
2:C:405:GLN:O	2:C:409:THR:HG23	1.97	0.64
1:E:132:PRO:HB2	5:E:1175:DIO:H2'2	1.80	0.63
1:E:34:LYS:HE3	5:E:1176:DIO:H11	1.80	0.62
2:C:415:ILE:HD13	5:C:1453:DIO:H22	1.81	0.62
1:E:70:ILE:HA	5:E:1177:DIO:H2'2	1.85	0.59
1:B:51:THR:HG21	1:B:58:LYS:HZ2	1.69	0.55
1:B:136:GLN:HE21	1:B:142:THR:HG22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LEU:HD11	5:E:1177:DIO:H2'1	1.89	0.55
5:A:1175:DIO:H21	1:E:136:GLN:HB2	1.88	0.54
1:E:131:LYS:HD2	5:E:1175:DIO:H12	1.88	0.54
1:E:57:VAL:CG1	1:E:170:THR:HG22	2.38	0.53
1:E:57:VAL:HG11	1:E:170:THR:HG22	1.91	0.51
1:E:166:LEU:O	1:E:170:THR:HG23	2.11	0.50
1:B:155:CYS:HB3	1:B:160:ASP:HB2	1.94	0.49
1:A:133:HIS:ND1	5:E:1175:DIO:H21	2.29	0.48
1:A:72:PRO:HB2	5:C:1454:DIO:H2'2	1.95	0.47
1:B:97:ASP:OD1	1:B:100:ARG:NH1	2.48	0.47
1:A:133:HIS:HA	5:A:1175:DIO:C1'	2.46	0.46
1:B:54:TYR:CE2	1:B:55:LYS:HE2	2.51	0.45
2:D:423:LYS:HE3	2:D:427:LEU:HG	1.99	0.44
1:B:51:THR:CG2	1:B:58:LYS:HG3	2.48	0.44
5:A:1175:DIO:H21	1:E:136:GLN:CB	2.48	0.44
1:B:141:LEU:HA	1:B:144:ILE:HD12	1.99	0.43
1:B:54:TYR:O	1:B:55:LYS:HB2	2.18	0.43
1:A:166:LEU:O	1:A:170:THR:HG23	2.18	0.43
1:A:135:ILE:HA	1:A:135:ILE:HD12	1.79	0.43
1:B:150:TYR:HB2	1:B:168:TRP:CE2	2.54	0.43
1:A:131:LYS:HB3	5:E:1175:DIO:H22	2.02	0.42
1:E:96:ILE:HG21	1:E:138:LYS:HD3	2.01	0.42
1:B:116:ILE:HG23	1:B:168:TRP:CZ3	2.54	0.42
1:B:71:ARG:N	1:B:72:PRO:CD	2.83	0.41
1:E:73:LEU:CD1	5:E:1177:DIO:H2'1	2.50	0.41
1:A:19:LEU:C	1:A:26:LYS:HD3	2.45	0.41
1:A:57:VAL:HG13	1:A:59:PHE:CE1	2.56	0.41
5:A:1175:DIO:C2	1:E:136:GLN:HG3	2.51	0.40
1:B:123:LYS:HG2	3:B:1173:GTP:C6	2.56	0.40
1:B:156:ALA:HB3	3:B:1173:GTP:N7	2.37	0.40

There are no symmetry-related clashes.

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	159/165 (96%)	158 (99%)	1 (1%)	0	100	100
1	B	159/165 (96%)	155 (98%)	3 (2%)	1 (1%)	21	11
1	E	160/165 (97%)	160 (100%)	0	0	100	100
2	C	67/77 (87%)	67 (100%)	0	0	100	100
2	D	61/77 (79%)	61 (100%)	0	0	100	100
All	All	606/649 (93%)	601 (99%)	4 (1%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	PRO

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	141/144 (98%)	137 (97%)	4 (3%)	38	25
1	B	141/144 (98%)	135 (96%)	6 (4%)	26	13
1	E	141/144 (98%)	137 (97%)	4 (3%)	38	25
2	C	62/69 (90%)	61 (98%)	1 (2%)	55	46
2	D	57/69 (83%)	53 (93%)	4 (7%)	14	3
All	All	542/570 (95%)	523 (96%)	19 (4%)	32	18

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	40	THR
1	A	57	VAL
1	A	135	ILE

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Mol	Chain	Res	Type
1	B	38	SER
1	B	40	THR
1	B	58	LYS
1	B	97	ASP
1	B	105	ARG
1	B	116	ILE
2	C	409	THR
2	D	394	ARG
2	D	405	GLN
2	D	423	LYS
2	D	445	LYS
1	E	57	VAL
1	E	137	GLU
1	E	143	ARG
1	E	148	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	122	ASN
1	B	136	GLN
1	B	152	GLN
2	C	411	ASN
1	E	108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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$
5	DIO	E	1175	-	6,6,6	0.51	0	6,6,6	0.65	0
5	DIO	C	1453	-	6,6,6	0.53	0	6,6,6	0.62	0
3	GTP	E	1173	4	33,34,34	1.06	2 (6%)	50,54,54	1.47	11 (22%)
3	GTP	B	1173	4	33,34,34	0.92	1 (3%)	50,54,54	1.60	11 (22%)
5	DIO	E	1176	-	6,6,6	0.52	0	6,6,6	0.56	0
6	GOL	A	1176	-	5,5,5	0.31	0	5,5,5	0.36	0
5	DIO	E	1177	-	6,6,6	0.52	0	6,6,6	0.62	0
3	GTP	A	1173	4	33,34,34	0.97	2 (6%)	50,54,54	1.50	10 (20%)
5	DIO	C	1454	-	6,6,6	0.54	0	6,6,6	0.67	0
5	DIO	A	1175	-	6,6,6	0.53	0	6,6,6	0.71	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	DIO	E	1175	-	-	-	0/1/1/1
5	DIO	C	1453	-	-	-	0/1/1/1
3	GTP	E	1173	4	-	2/22/38/38	0/3/3/3
3	GTP	B	1173	4	-	2/22/38/38	0/3/3/3
6	GOL	A	1176	-	-	0/4/4/4	-
5	DIO	E	1176	-	-	-	0/1/1/1
5	DIO	E	1177	-	-	-	0/1/1/1
3	GTP	A	1173	4	-	2/22/38/38	0/3/3/3
5	DIO	C	1454	-	-	-	0/1/1/1
5	DIO	A	1175	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1173	GTP	PB-O3B	2.78	1.62	1.59
3	E	1173	GTP	PA-O3A	2.74	1.62	1.59
3	A	1173	GTP	C2-N3	2.55	1.39	1.33
3	A	1173	GTP	PB-O3A	2.39	1.62	1.59
3	B	1173	GTP	C2-N3	2.19	1.38	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1173	GTP	C5-C4-N3	-4.79	120.76	128.39
3	B	1173	GTP	C2-N3-C4	4.70	120.40	112.30
3	E	1173	GTP	C2-N3-C4	4.36	119.80	112.30
3	A	1173	GTP	C5-C4-N3	-4.32	121.51	128.39
3	A	1173	GTP	C2-N3-C4	4.16	119.46	112.30
3	E	1173	GTP	C5-C4-N3	-3.95	122.10	128.39
3	A	1173	GTP	N9-C8-N7	-2.79	108.23	113.40
3	E	1173	GTP	N9-C8-N7	-2.77	108.27	113.40
3	B	1173	GTP	C2-N1-C6	-2.76	120.10	125.11
3	A	1173	GTP	N9-C4-N3	2.73	131.42	125.95
3	B	1173	GTP	N9-C8-N7	-2.67	108.44	113.40
3	B	1173	GTP	N9-C4-N3	2.67	131.29	125.95
3	B	1173	GTP	C8-N7-C5	2.62	108.93	104.26
3	A	1173	GTP	C2-N1-C6	-2.52	120.54	125.11
3	A	1173	GTP	C8-N7-C5	2.50	108.72	104.26
3	B	1173	GTP	C5-C6-N1	2.47	119.54	113.25
3	A	1173	GTP	C5-C6-N1	2.43	119.45	113.25
3	E	1173	GTP	C8-N7-C5	2.34	108.43	104.26
3	B	1173	GTP	O6-C6-C5	-2.33	120.39	126.53
3	E	1173	GTP	C5-C6-N1	2.32	119.16	113.25
3	E	1173	GTP	C6-C5-N7	2.24	134.36	130.29
3	B	1173	GTP	O2B-PB-O3B	2.21	113.24	107.27
3	E	1173	GTP	C2-N1-C6	-2.20	121.11	125.11
3	A	1173	GTP	O2B-PB-O3B	2.17	113.13	107.27
3	B	1173	GTP	N2-C2-N1	2.13	121.26	116.76
3	E	1173	GTP	N9-C4-N3	2.11	130.18	125.95
3	E	1173	GTP	C4-C5-N7	-2.11	107.33	110.67
3	E	1173	GTP	N1-C2-N3	-2.08	119.52	123.32
3	B	1173	GTP	C4-C5-N7	-2.07	107.39	110.67
3	E	1173	GTP	N2-C2-N1	2.03	121.04	116.76
3	A	1173	GTP	O6-C6-C5	-2.02	121.20	126.53
3	A	1173	GTP	O2B-PB-O3A	2.02	112.73	107.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1173	GTP	PA-O3A-PB-O2B
3	A	1173	GTP	PA-O3A-PB-O2B
3	E	1173	GTP	PA-O3A-PB-O2B
3	A	1173	GTP	PA-O3A-PB-O1B
3	B	1173	GTP	PA-O3A-PB-O1B
3	E	1173	GTP	PA-O3A-PB-O1B

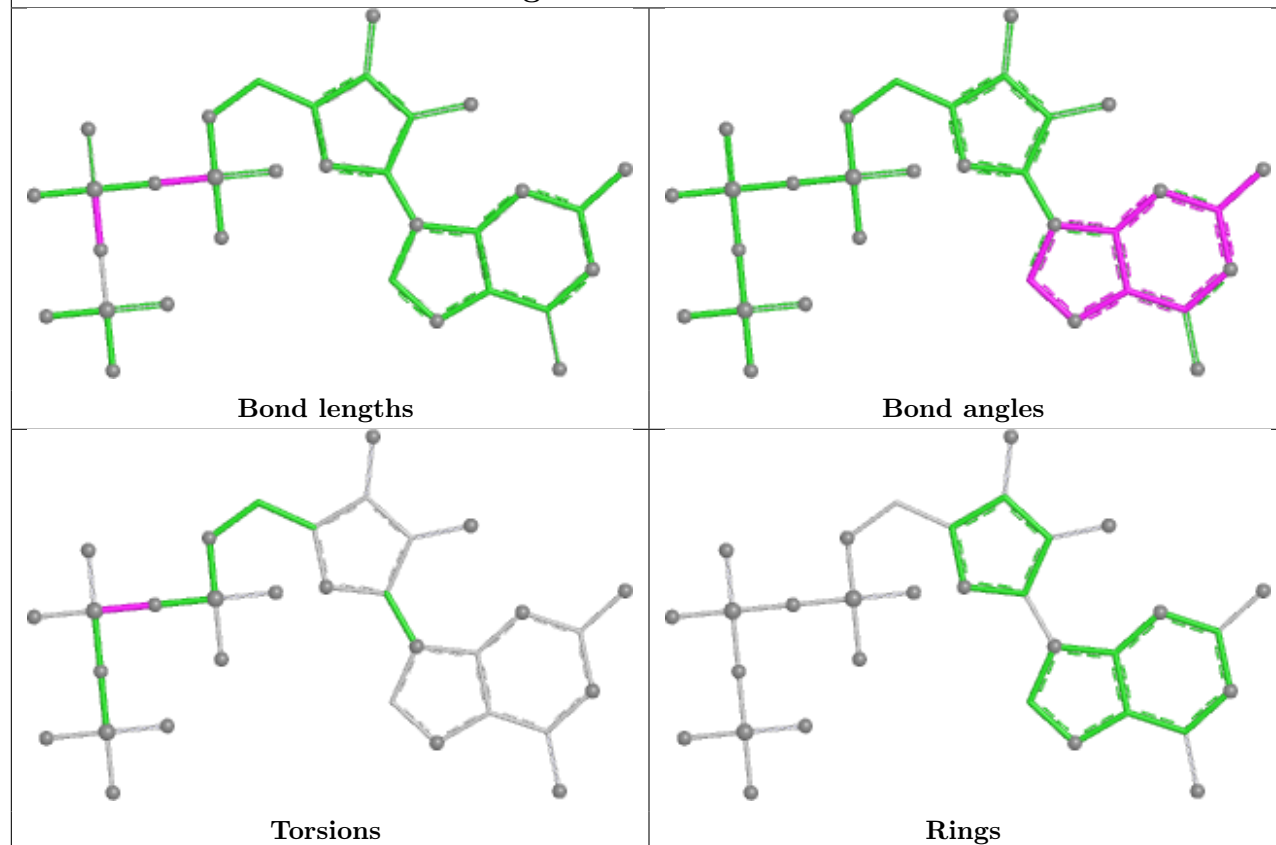
There are no ring outliers.

7 monomers are involved in 19 short contacts:

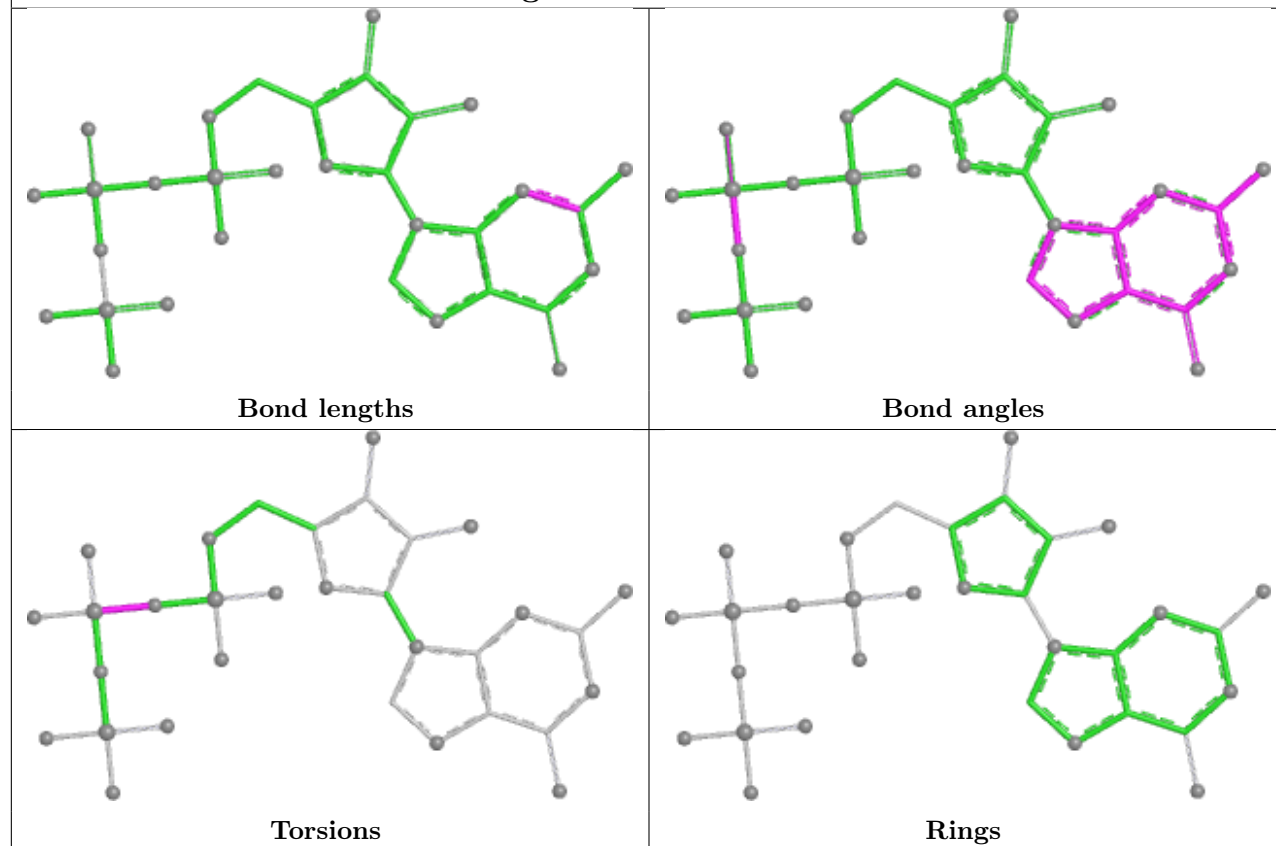
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1175	DIO	5	0
5	C	1453	DIO	2	0
3	B	1173	GTP	2	0
5	E	1176	DIO	2	0
5	E	1177	DIO	3	0
5	C	1454	DIO	1	0
5	A	1175	DIO	4	0

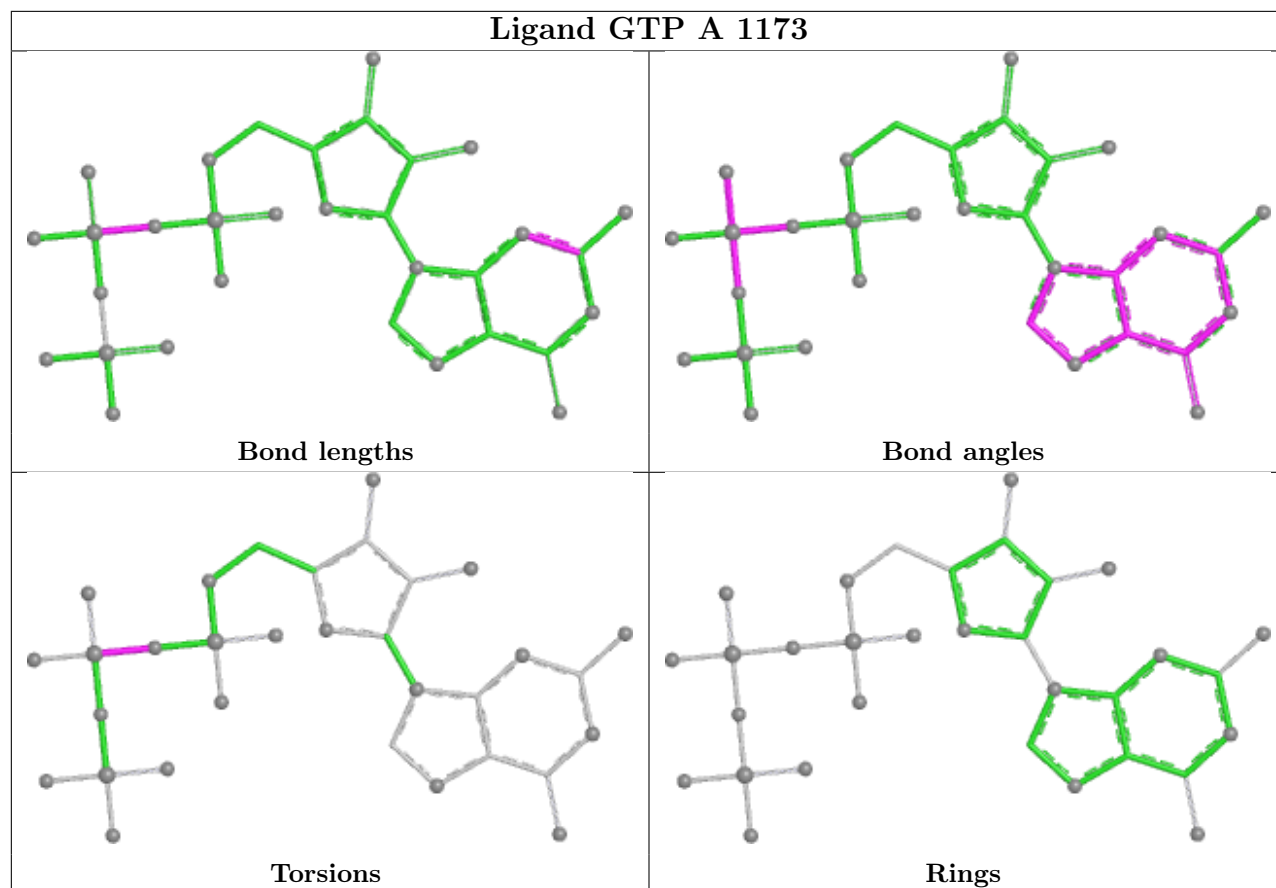
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand GTP E 1173



Ligand GTP B 1173





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	161/165 (97%)	0.05	6 (3%) 45 51	11, 23, 33, 45	4 (2%)
1	B	161/165 (97%)	1.73	65 (40%) 0 0	26, 43, 59, 63	2 (1%)
1	E	162/165 (98%)	0.04	7 (4%) 40 44	14, 22, 31, 39	2 (1%)
2	C	67/77 (87%)	0.93	16 (23%) 2 1	13, 24, 59, 67	8 (11%)
2	D	62/77 (80%)	1.15	16 (25%) 1 1	15, 27, 66, 75	8 (12%)
All	All	613/649 (94%)	0.70	110 (17%) 3 4	11, 26, 56, 75	24 (3%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	391	PHE	8.5
2	C	452	ASN	5.6
1	A	12	MET	5.2
2	D	450	GLU	5.0
2	D	446	LEU	4.9
2	C	446	LEU	4.8
1	B	12	MET	4.6
1	B	144	ILE	4.6
1	A	37	GLN	4.4
2	C	450	GLU	4.3
1	B	143	ARG	4.3
2	C	447	LYS	4.2
2	C	448	LEU	4.2
1	B	88	VAL	4.1
2	D	448	LEU	4.1
2	D	452	ASN	4.0
1	B	154	SER	4.0
1	B	126	LEU	3.9
1	B	127	PRO	3.9
2	C	451	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	133	HIS	3.8
1	B	91	ALA	3.7
1	E	128	ASP	3.7
1	B	54	TYR	3.6
2	C	441	VAL	3.5
1	B	129	ALA	3.5
2	C	440	ALA	3.5
1	B	171	SER	3.5
1	B	135	ILE	3.4
1	B	58	LYS	3.4
2	D	392	MET	3.4
1	B	155	CYS	3.4
1	B	161	GLY	3.3
2	D	439	GLU	3.3
2	D	440	ALA	3.3
1	B	149	TRP	3.2
2	C	386	ALA	3.2
1	B	130	MET	3.2
1	B	56	ASN	3.1
1	B	170	THR	3.1
1	B	132	PRO	3.1
1	B	97	ASP	3.1
1	B	151	VAL	3.1
2	C	438	LEU	3.1
1	B	167	THR	3.1
1	B	166	LEU	3.0
1	B	53	THR	3.0
1	B	125	ASP	3.0
2	D	447	LYS	3.0
1	B	169	LEU	2.9
1	E	101	GLN	2.9
2	C	444	ALA	2.9
1	B	147	ARG	2.9
1	B	156	ALA	2.9
1	B	145	ARG	2.9
1	B	148	ASN	2.9
1	B	138	LYS	2.8
1	B	105	ARG	2.8
1	B	140	GLY	2.7
1	B	68	ASP	2.7
1	A	111	GLU	2.7
1	B	141	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	162	LEU	2.7
2	D	438	LEU	2.7
2	C	439	GLU	2.7
2	C	442	LYS	2.7
1	B	92	ASP	2.6
1	B	139	LEU	2.6
1	B	121	ALA	2.6
1	B	33	LEU	2.6
1	B	118	LEU	2.6
1	B	168	TRP	2.6
1	B	128	ASP	2.6
1	B	134	GLU	2.6
1	B	137	GLU	2.6
1	B	153	PRO	2.5
1	B	124	GLN	2.5
1	E	12	MET	2.5
1	E	11	ALA	2.5
2	D	444	ALA	2.5
1	B	131	LYS	2.5
2	C	445	LYS	2.5
2	D	393	GLY	2.5
1	A	56	ASN	2.5
1	B	52	VAL	2.4
1	B	172	ASN	2.4
2	C	449	GLU	2.4
1	B	150	TYR	2.4
1	B	89	ASP	2.4
1	E	45	VAL	2.4
1	B	157	THR	2.4
1	B	45	VAL	2.4
1	B	163	TYR	2.3
2	D	442	LYS	2.3
2	D	441	VAL	2.3
1	E	148	ASN	2.3
1	A	53	THR	2.3
1	B	142	THR	2.3
1	B	111	GLU	2.2
1	B	70	ILE	2.2
2	D	443	GLN	2.2
1	A	146	ASP	2.2
1	B	159	GLY	2.2
1	B	23	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	69	LYS	2.1
2	C	389	PRO	2.1
1	E	145	ARG	2.1
1	B	37	GLN	2.1
1	B	113	ARG	2.0
2	D	394	ARG	2.0

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](#)

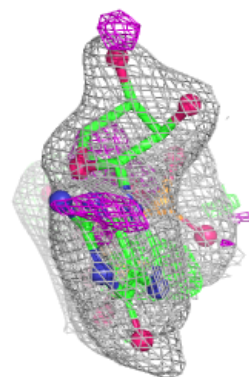
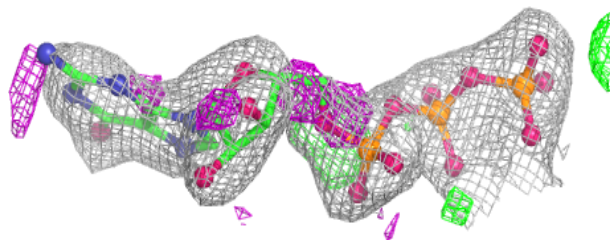
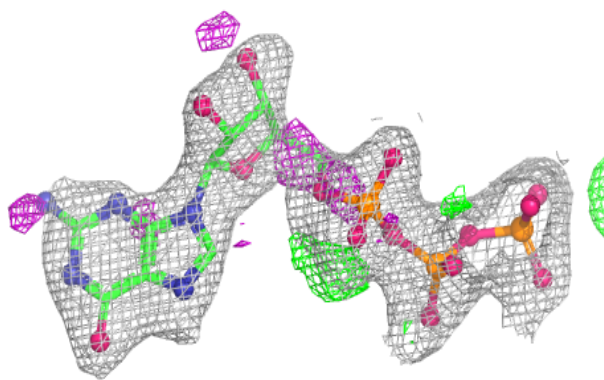
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DIO	C	1453	6/6	0.78	0.15	39,39,41,41	0
5	DIO	E	1175	6/6	0.78	0.23	42,43,44,44	0
5	DIO	E	1176	6/6	0.86	0.16	30,32,33,34	0
5	DIO	C	1454	6/6	0.88	0.12	36,36,37,37	0
5	DIO	E	1177	6/6	0.88	0.15	43,43,44,44	0
5	DIO	A	1175	6/6	0.89	0.11	29,30,30,31	0
6	GOL	A	1176	6/6	0.90	0.16	25,33,34,36	0
3	GTP	B	1173	32/32	0.94	0.10	32,38,42,42	0
4	MG	B	1174	1/1	0.97	0.04	30,30,30,30	0
4	MG	E	1174	1/1	0.99	0.01	17,17,17,17	0
3	GTP	E	1173	32/32	0.99	0.04	15,19,20,22	0
4	MG	A	1174	1/1	0.99	0.02	17,17,17,17	0
3	GTP	A	1173	32/32	0.99	0.04	15,20,21,21	0

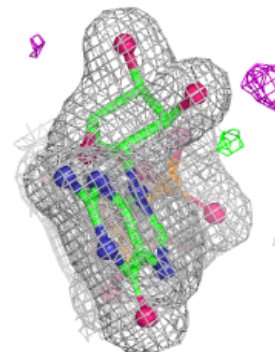
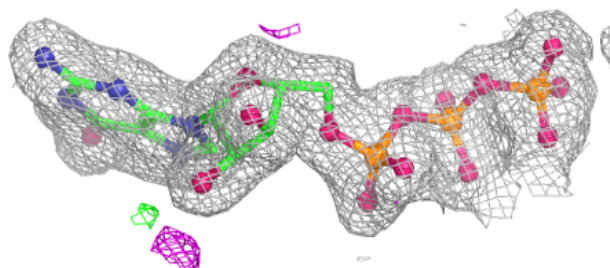
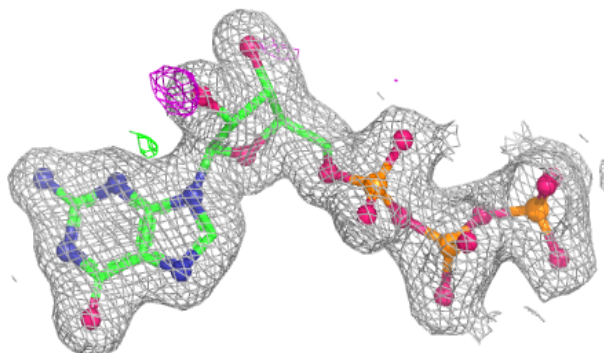
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP B 1173:

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

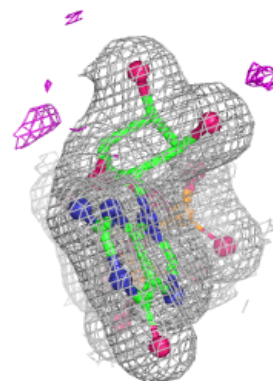
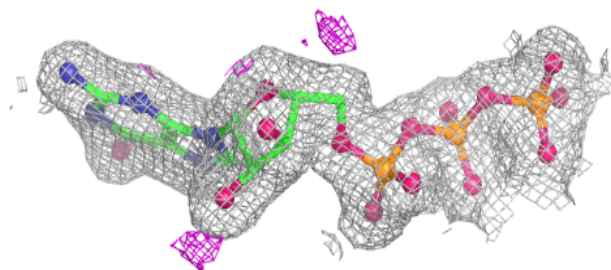
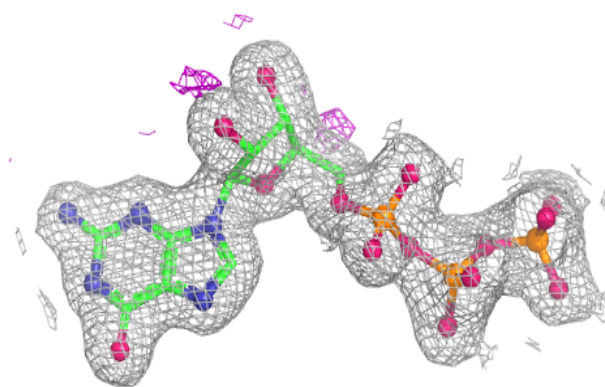
**Electron density around GTP E 1173:**

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



Electron density around GTP A 1173:

$2mF_o-DF_c$ (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.