Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 05:22 PM EDT

PDB ID	:	4LNU
Title	:	Nucleotide-free kinesin motor domain in complex with tubulin and a DARPin
Authors	:	Cao, L.; Gigant, B.; Knossow, M.
Deposited on	:	2013-07-12
Resolution	:	2.19 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 (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:

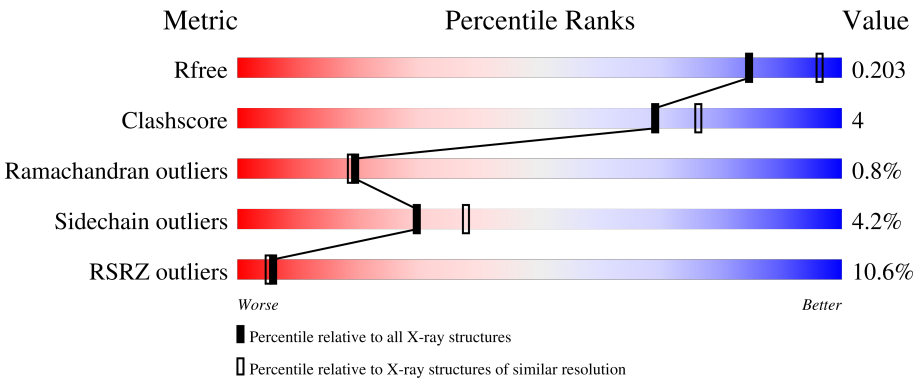
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	451	5%, 86%, 9%, • •
2	B	445	9%, 86%, 10%, • •
3	D	169	3%, 85%, 8%, 7%
4	K	325	23%, 80%, 14%, • 5%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11209 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	434	3410	2161	578	648	23	0	3	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3424	2145	585	668	26	0	5	0

- Molecule 3 is a protein called Designed ankyrin repeat protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	157	1170	737	201	229	3	0	0	0

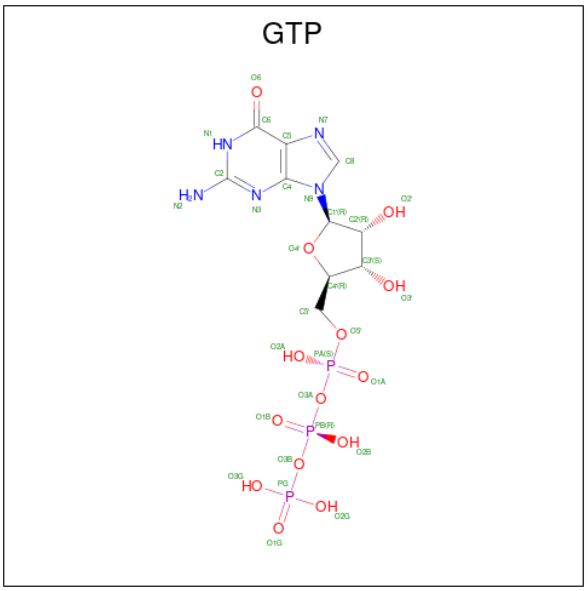
- Molecule 4 is a protein called Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	309	2420	1512	416	483	9	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	SER	CYS	engineered mutation	UNP P33176
K	65	ALA	CYS	engineered mutation	UNP P33176
K	168	ALA	CYS	engineered mutation	UNP P33176
K	174	SER	CYS	engineered mutation	UNP P33176
K	294	ALA	CYS	engineered mutation	UNP P33176

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

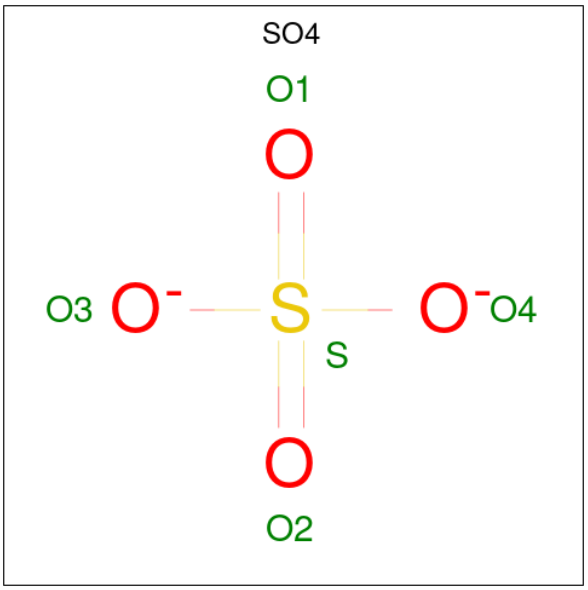


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

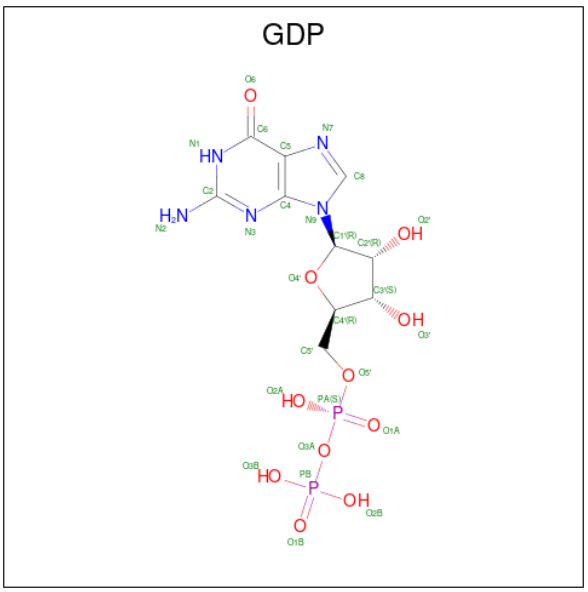
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



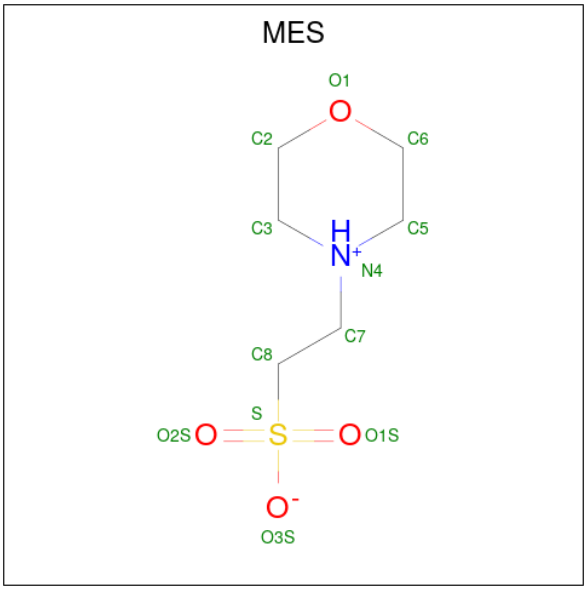
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	K	1	5	4	1	0	0
			Total	O	S		
7	K	1	5	4	1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



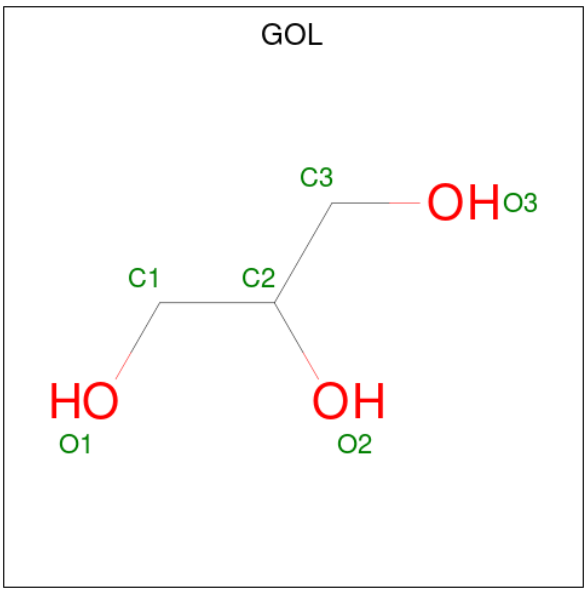
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	B	1	6	3	3	0	0
			Total	C	O		
10	B	1	6	3	3	0	0
			Total	C	O		
10	D	1	6	3	3	0	0
			Total	C	O		
10	K	1	6	3	3	0	0

- Molecule 11 is water.

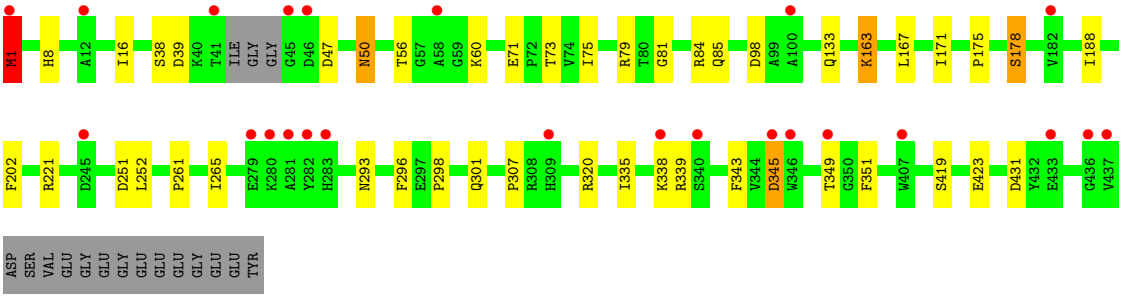
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	262	262	262	0	0
			Total	O		
11	B	219	219	219	0	1
			Total	O		
11	D	99	99	99	0	0
			Total	O		
11	K	53	53	53	0	0

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.

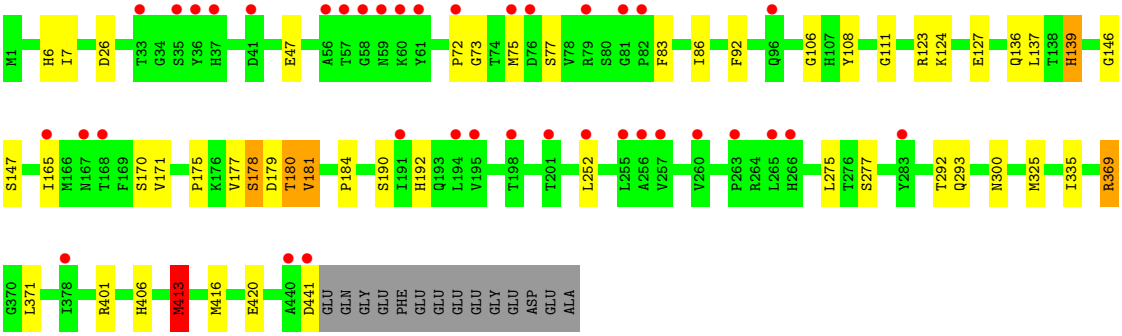
• Molecule 1: Tubulin alpha chain

Chain A:



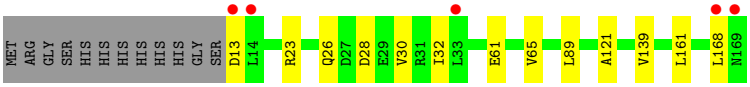
• Molecule 2: Tubulin beta chain

Chain B:



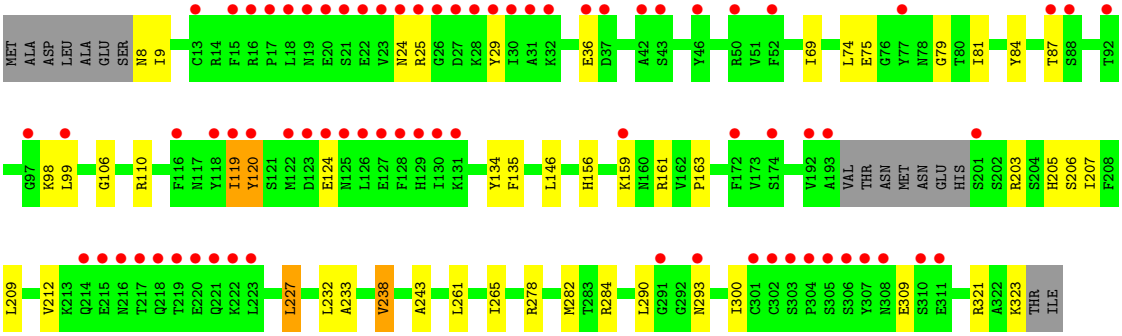
• Molecule 3: Designed ankyrin repeat protein (DARPIN) D1

Chain D:



• Molecule 4: Kinesin-1 heavy chain

Chain K:


MET
ALA
ASP
LEU
ALA
GLU
SER
N8
I9
C13
R14
F15
R16
P17
L18
N19
E20
S21
E22
V23
N24
R25
G26
D27
K28
Y29
I30
A31
K32
E36
D37
A42
S43
Y46
R50
V51
F52
I69
L74
E75
G76
Y77
N78
G79
T80
I81
Y84
T87
S88
T92
G97
K98
L99
G106
R110
F116
N117
Y118
I119
Y120
S121
M122
D123
E124
M125
L126
E127
F128
H129
I130
K131
Y134
F135
L146
H156
K159
N160
R161
V162
P163
F172
V173
S174
V192
A193
VAL
THR
ASN
MET
ASN
GLU
HIS
S201
S202
R203
S204
H205
S206
I207
F208
L209
V212
K213
Q214
E215
M216
T217
Q218
T219
E220
Q221
K222
L223
L227
L232
A233
V238
A243
L261
I265
R278
M282
T283
R284
L290
G291
G292
N293
I300
C301
C302
S303
P304
S305
S306
Y307
N308
E309
S310
E311
R321
A322
K323
THR
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.40Å 83.01Å 83.31Å 116.16° 105.08° 97.57°	Depositor
Resolution (Å)	43.45 – 2.19 43.45 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.45-2.19) 92.0 (43.45-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.155 , 0.195 0.162 , 0.203	Depositor DCC
R_{free} test set	3882 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11209	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.12% 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: SO4, GTP, MES, GDP, GOL, 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	0.53	0/3495	0.71	2/4744 (0.0%)
2	B	0.53	0/3510	0.70	3/4754 (0.1%)
3	D	0.52	0/1186	0.74	0/1612
4	K	0.45	0/2457	0.69	0/3309
All	All	0.51	0/10648	0.71	5/14419 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	177	VAL	C-N-CA	5.38	135.15	121.70
2	B	178[A]	SER	N-CA-C	5.29	125.30	111.00
2	B	178[B]	SER	N-CA-C	5.29	125.30	111.00
1	A	1[A]	MET	C-N-CA	5.21	134.71	121.70
1	A	1[B]	MET	C-N-CA	5.21	134.71	121.70

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	3410	0	3323	30	0
2	B	3424	0	3292	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1170	0	1173	8	0
4	K	2420	0	2397	16	1
5	A	32	0	12	0	0
6	A	1	0	0	0	0
7	A	15	0	0	0	0
7	B	30	0	0	0	0
7	K	10	0	0	0	0
8	B	28	0	12	0	0
9	B	12	0	13	1	0
10	B	12	0	16	1	0
10	D	6	0	8	1	0
10	K	6	0	8	0	0
11	A	262	0	0	3	1
11	B	219	0	0	1	0
11	D	99	0	0	0	0
11	K	53	0	0	1	0
All	All	11209	0	10254	77	1

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 4.

All (77) 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:71:GLU:OE2	1:A:73:THR:HB	1.63	0.98
2:B:6:HIS:HD2	2:B:136:GLN:HE21	1.20	0.87
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.58	0.84
1:A:133:GLN:HE22	1:A:252:LEU:H	1.34	0.74
2:B:192:HIS:HD2	11:B:767:HOH:O	1.75	0.70
1:A:133:GLN:NE2	1:A:252:LEU:H	1.92	0.67
2:B:292:THR:HG22	2:B:335:ILE:HG13	1.79	0.65
1:A:1[A]:MET:HG3	1:A:50:ASN:HB3	1.82	0.62
2:B:6:HIS:CD2	2:B:136:GLN:HE21	2.10	0.62
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.82	0.61
4:K:205:HIS:HD2	4:K:233:ALA:H	1.50	0.59
2:B:75:MET:HG3	2:B:92:PHE:CD2	2.38	0.59
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.82	0.59
4:K:238:VAL:HG22	4:K:243:ALA:HB3	1.85	0.58
4:K:205:HIS:CD2	4:K:233:ALA:H	2.22	0.58
2:B:106:GLY:O	2:B:111:GLY:HA3	2.04	0.58
2:B:124:LYS:HB3	10:B:504:GOL:H12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:O	2:B:127:GLU:HG2	2.06	0.56
1:A:261:PRO:HD2	11:A:845:HOH:O	2.05	0.56
1:A:133:GLN:NE2	1:A:251:ASP:HB2	2.21	0.56
2:B:175:PRO:HA	2:B:178[A]:SER:HB3	1.87	0.56
3:D:61:GLU:O	3:D:65:VAL:HG23	2.07	0.54
3:D:61:GLU:CD	3:D:61:GLU:H	2.12	0.52
1:A:8:HIS:HE1	11:A:768:HOH:O	1.91	0.52
4:K:84:TYR:HB3	4:K:300:ILE:HG22	1.92	0.52
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.92	0.52
4:K:278:ARG:NH2	11:K:506:HOH:O	2.30	0.49
2:B:406[B]:HIS:CD2	3:D:23:ARG:HH22	2.30	0.49
2:B:420:GLU:OE1	4:K:156:HIS:HD2	1.96	0.49
3:D:121:ALA:HB1	3:D:161:LEU:HD21	1.96	0.48
4:K:261:LEU:HG	4:K:265:ILE:HD11	1.96	0.48
2:B:6:HIS:HD2	2:B:136:GLN:NE2	2.00	0.47
4:K:74:LEU:HD23	4:K:212:VAL:HG11	1.97	0.47
3:D:23:ARG:NH1	10:D:201:GOL:O2	2.48	0.47
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.30	0.47
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.96	0.47
3:D:28:ASP:O	3:D:32:ILE:HG12	2.16	0.46
2:B:165:ILE:HD13	9:B:502:MES:H82	1.98	0.46
2:B:401:ARG:HD3	3:D:89:LEU:HD22	1.96	0.46
1:A:16:ILE:HD13	1:A:171:ILE:CD1	2.46	0.45
2:B:75:MET:HG3	2:B:92:PHE:HD2	1.79	0.45
2:B:139:HIS:HD2	2:B:146:GLY:O	1.99	0.45
4:K:278:ARG:HG2	4:K:284:ARG:HD2	1.97	0.45
1:A:175:PRO:HA	1:A:178:SER:HB2	1.99	0.45
1:A:293:ASN:HA	1:A:335:ILE:HD11	1.99	0.45
1:A:47:ASP:O	1:A:50:ASN:HB2	2.17	0.45
2:B:83:PHE:O	2:B:86:ILE:HG22	2.17	0.44
1:A:338:LYS:HE2	1:A:339:ARG:HG2	2.00	0.44
1:A:163:LYS:HE3	1:A:163:LYS:H	1.83	0.44
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.00	0.44
4:K:81:ILE:HD12	4:K:227:LEU:HD21	1.99	0.44
1:A:419:SER:O	1:A:423[A]:GLU:HG3	2.18	0.44
1:A:60:LYS:NZ	1:A:85:GLN:O	2.49	0.43
4:K:207:ILE:HD11	4:K:282:MET:HG3	2.00	0.43
1:A:296:PHE:HZ	1:A:351:PHE:HE2	1.64	0.43
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.01	0.43
1:A:133:GLN:HE22	1:A:252:LEU:N	2.09	0.43
1:A:75:ILE:O	1:A:79:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:HB2	2:B:190:SER:OG	2.19	0.43
2:B:108:TYR:CE1	2:B:413:MET:HG3	2.54	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
2:B:139:HIS:HE1	2:B:170:SER:OG	2.02	0.42
4:K:156:HIS:O	4:K:163:PRO:HA	2.20	0.42
1:A:301:GLN:HE22	1:A:307:PRO:CD	2.32	0.42
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.20	0.42
1:A:81:GLY:O	1:A:84:ARG:HD3	2.20	0.41
1:A:301:GLN:HE22	1:A:307:PRO:HD3	1.85	0.41
3:D:26:GLN:O	3:D:30:VAL:HG23	2.21	0.41
1:A:167[A]:LEU:HD13	1:A:252:LEU:HD22	2.03	0.41
4:K:106:GLY:O	4:K:110:ARG:HD2	2.21	0.41
1:A:320:ARG:HB2	11:A:725:HOH:O	2.21	0.41
4:K:205:HIS:HD2	4:K:232:LEU:HA	1.86	0.41
1:A:167[B]:LEU:HD13	1:A:202:PHE:HE1	1.86	0.41
2:B:181:VAL:O	2:B:184:PRO:HD2	2.21	0.40
4:K:69:ILE:HG23	4:K:79:GLY:HA3	2.03	0.40
4:K:119:ILE:O	4:K:120:TYR:HB3	2.21	0.40

All (1) 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)
4:K:120:TYR:OH	11:A:861:HOH:O[1_454]	2.13	0.07

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	432/451 (96%)	412 (95%)	17 (4%)	3 (1%)	22 22
2	B	434/445 (98%)	420 (97%)	8 (2%)	6 (1%)	11 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	155/169 (92%)	154 (99%)	0	1 (1%)	25	26
4	K	305/325 (94%)	289 (95%)	15 (5%)	1 (0%)	41	46
All	All	1326/1390 (95%)	1275 (96%)	40 (3%)	11 (1%)	19	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	345	ASP
2	B	181	VAL
3	D	168	LEU
4	K	99	LEU
2	B	73	GLY
2	B	180[A]	THR
2	B	180[B]	THR
2	B	413	MET
1	A	56	THR
2	B	72	PRO

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	368/379 (97%)	360 (98%)	8 (2%)	52	65
2	B	379/385 (98%)	366 (97%)	13 (3%)	37	47
3	D	122/132 (92%)	120 (98%)	2 (2%)	62	76
4	K	271/286 (95%)	244 (90%)	27 (10%)	7	7
All	All	1140/1182 (96%)	1090 (96%)	50 (4%)	30	35

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET

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Mol	Chain	Res	Type
1	A	1[B]	MET
1	A	39	ASP
1	A	50	ASN
1	A	163	LYS
1	A	178	SER
1	A	188	ILE
1	A	345	ASP
2	B	47	GLU
2	B	77	SER
2	B	139	HIS
2	B	171	VAL
2	B	180[A]	THR
2	B	180[B]	THR
2	B	277	SER
2	B	293	GLN
2	B	369	ARG
2	B	371	LEU
2	B	413	MET
2	B	416	MET
2	B	441	ASP
3	D	13	ASP
3	D	139	VAL
4	K	8	ASN
4	K	9	ILE
4	K	24	ASN
4	K	25	ARG
4	K	29	TYR
4	K	36	GLU
4	K	75	GLU
4	K	87	THR
4	K	98	LYS
4	K	119	ILE
4	K	120	TYR
4	K	124	GLU
4	K	134	TYR
4	K	135	PHE
4	K	146	LEU
4	K	159	LYS
4	K	161	ARG
4	K	203	ARG
4	K	206	SER
4	K	209	LEU

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Mol	Chain	Res	Type
4	K	227	LEU
4	K	238	VAL
4	K	290	LEU
4	K	293	ASN
4	K	309	GLU
4	K	321	ARG
4	K	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	107	HIS
1	A	133	GLN
1	A	139	HIS
1	A	216	ASN
1	A	285	GLN
1	A	301	GLN
1	A	309	HIS
2	B	6	HIS
2	B	139	HIS
2	B	247	GLN
2	B	282	GLN
2	B	394	GLN
4	K	156	HIS
4	K	205	HIS

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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
7	SO4	K	403	-	4,4,4	0.17	0	6,6,6	0.16	0
7	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.06	0
10	GOL	K	401	-	5,5,5	0.05	0	5,5,5	0.22	0
8	GDP	B	501	-	24,30,30	0.68	0	30,47,47	0.97	2 (6%)
7	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.21	0
7	SO4	B	509	-	4,4,4	0.15	0	6,6,6	0.12	0
10	GOL	B	504	-	5,5,5	0.06	0	5,5,5	0.20	0
10	GOL	B	503	-	5,5,5	0.04	0	5,5,5	0.26	0
10	GOL	D	201	-	5,5,5	0.13	0	5,5,5	0.38	0
7	SO4	B	510	-	4,4,4	0.12	0	6,6,6	0.16	0
7	SO4	B	508	-	4,4,4	0.14	0	6,6,6	0.09	0
7	SO4	K	402	-	4,4,4	0.18	0	6,6,6	0.13	0
7	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.08	0
9	MES	B	502	-	12,12,12	0.88	0	14,16,16	0.49	0
5	GTP	A	501	6	26,34,34	0.87	2 (7%)	32,54,54	0.64	0
7	SO4	B	507	-	4,4,4	0.14	0	6,6,6	0.12	0
7	SO4	B	505	-	4,4,4	0.12	0	6,6,6	0.11	0
7	SO4	B	506	-	4,4,4	0.12	0	6,6,6	0.12	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
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
10	GOL	B	504	-	-	2/4/4/4	-
10	GOL	B	503	-	-	1/4/4/4	-
10	GOL	D	201	-	-	0/4/4/4	-
9	MES	B	502	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	GOL	K	401	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C5-C6	-2.25	1.42	1.47
5	A	501	GTP	C8-N7	-2.12	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	O5'-PA-O1A	2.28	117.98	109.07
8	B	501	GDP	PA-O5'-C5'	2.17	134.38	121.68

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
10	B	503	GOL	C1-C2-C3-O3
10	B	504	GOL	O1-C1-C2-C3
8	B	501	GDP	C3'-C4'-C5'-O5'
8	B	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
8	B	501	GDP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
10	B	504	GOL	O1-C1-C2-O2

There are no ring outliers.

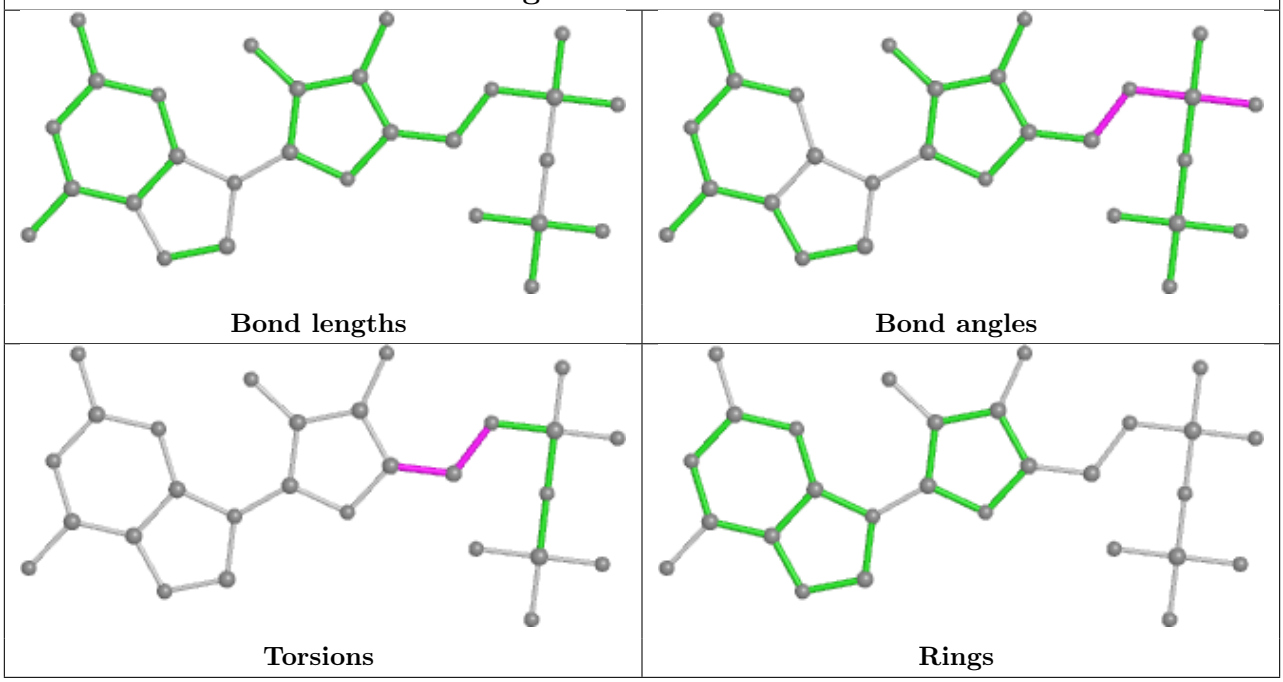
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	GOL	1	0
10	D	201	GOL	1	0
9	B	502	MES	1	0

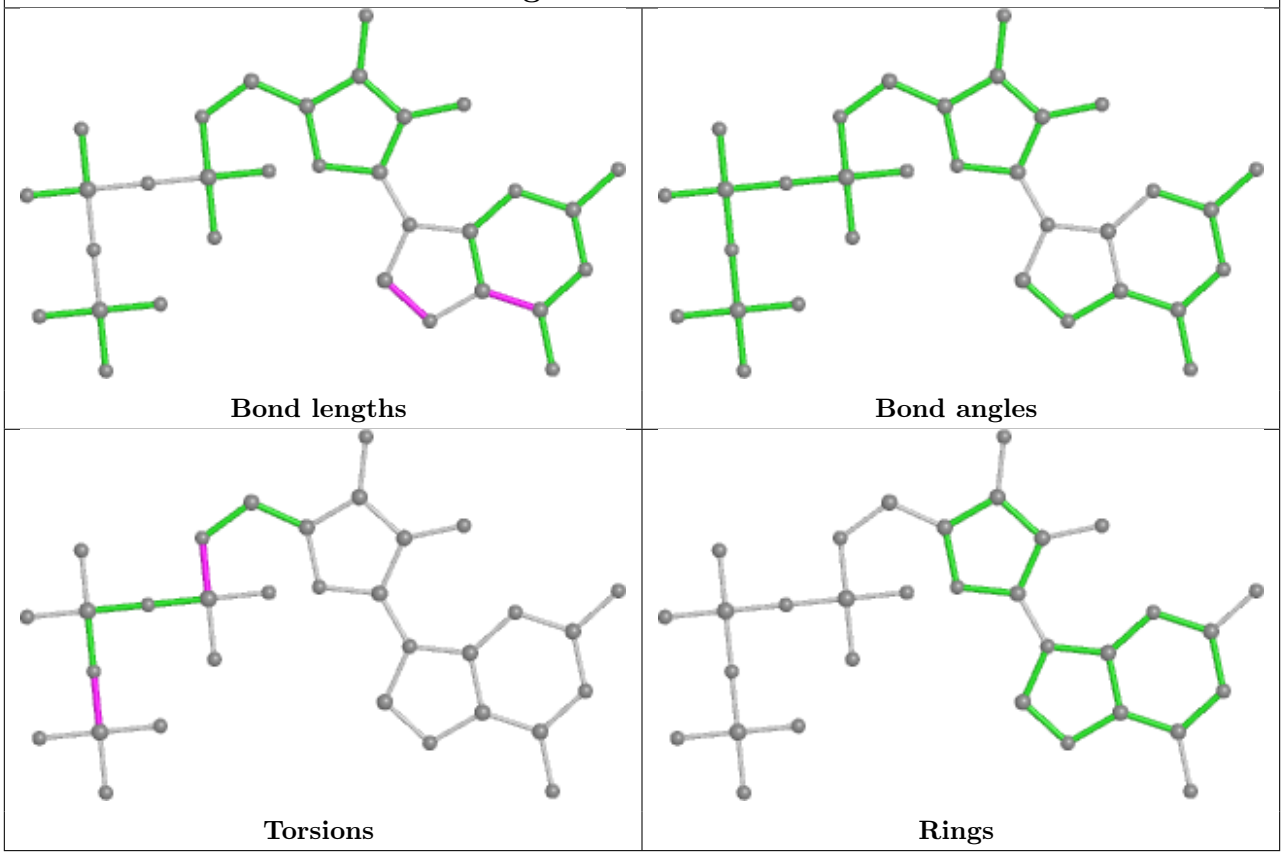
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 B 501



Ligand GTP A 501



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	434/451 (96%)	0.33	24 (5%) 25 24	27, 44, 90, 114	0
2	B	431/445 (96%)	0.41	38 (8%) 10 8	27, 45, 78, 120	5 (1%)
3	D	157/169 (92%)	-0.08	5 (3%) 47 45	30, 46, 90, 124	0
4	K	309/325 (95%)	1.20	74 (23%) 0 0	34, 84, 153, 186	0
All	All	1331/1390 (95%)	0.51	141 (10%) 6 5	27, 50, 119, 186	5 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	21	SER	11.1
4	K	99	LEU	9.9
4	K	218	GLN	9.5
4	K	31	ALA	8.5
4	K	307	TYR	8.2
1	A	346	TRP	7.9
4	K	29	TYR	7.8
1	A	437	VAL	7.8
4	K	20	GLU	7.4
4	K	22	GLU	7.1
4	K	30	ILE	6.8
4	K	215	GLU	6.7
2	B	57	THR	6.6
4	K	28	LYS	6.5
1	A	281	ALA	6.4
4	K	120	TYR	6.2
1	A	282	TYR	6.1
4	K	24	ASN	6.0
4	K	19	ASN	5.6
4	K	125	ASN	5.6
2	B	59	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
4	K	293	ASN	5.5
4	K	223	LEU	5.5
2	B	441	ASP	5.4
4	K	27	ASP	5.4
1	A	345	ASP	5.4
4	K	126	LEU	5.3
4	K	216	ASN	5.3
4	K	219	THR	5.3
4	K	17	PRO	5.3
1	A	45	GLY	5.3
1	A	349	THR	5.2
4	K	201	SER	5.2
4	K	18	LEU	5.1
4	K	217	THR	5.1
4	K	88	SER	4.7
1	A	436	GLY	4.6
4	K	306	SER	4.5
2	B	37	HIS	4.5
4	K	15	PHE	4.5
4	K	25	ARG	4.4
4	K	130	ILE	4.4
2	B	33	THR	4.4
4	K	302	CYS	4.3
4	K	304	PRO	4.3
1	A	309	HIS	4.2
4	K	23	VAL	4.2
4	K	124	GLU	4.1
4	K	13	CYS	4.1
4	K	26	GLY	4.0
4	K	52	PHE	3.9
2	B	440	ALA	3.9
4	K	221	GLN	3.9
2	B	72	PRO	3.8
4	K	308	ASN	3.8
4	K	16	ARG	3.8
2	B	260	VAL	3.8
4	K	305	SER	3.7
4	K	43	SER	3.7
2	B	75	MET	3.7
3	D	169	ASN	3.6
4	K	127	GLU	3.6
4	K	220	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
4	K	222	LYS	3.6
2	B	60	LYS	3.6
4	K	159	LYS	3.6
2	B	56	ALA	3.5
4	K	174	SER	3.5
4	K	97	GLY	3.5
4	K	87	THR	3.4
4	K	36	GLU	3.4
2	B	255	LEU	3.4
1	A	46	ASP	3.3
1	A	280	LYS	3.3
1	A	433	GLU	3.2
4	K	129	HIS	3.2
4	K	116	PHE	3.2
2	B	165	ILE	3.1
4	K	311	GLU	3.1
1	A	245	ASP	3.1
2	B	252	LEU	3.1
4	K	122	MET	3.1
3	D	168	LEU	3.1
4	K	192	VAL	3.1
4	K	46	TYR	3.0
4	K	37	ASP	3.0
2	B	58	GLY	3.0
2	B	194	LEU	3.0
2	B	82	PRO	3.0
4	K	214	GLN	3.0
2	B	36	TYR	2.9
2	B	283	TYR	2.9
4	K	77	TYR	2.9
3	D	33	LEU	2.9
4	K	42	ALA	2.9
1	A	407	TRP	2.9
2	B	257	VAL	2.8
4	K	92	THR	2.8
3	D	13	ASP	2.8
4	K	123	ASP	2.8
1	A	1[A]	MET	2.8
4	K	32	LYS	2.7
2	B	198	THR	2.7
4	K	131	LYS	2.7
1	A	338	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	340	SER	2.7
2	B	35	SER	2.6
4	K	291	GLY	2.6
4	K	301	CYS	2.6
2	B	61	TYR	2.5
4	K	193	ALA	2.5
1	A	279	GLU	2.5
4	K	128	PHE	2.5
2	B	96	GLN	2.5
4	K	310	SER	2.4
2	B	81	GLY	2.4
4	K	172	PHE	2.4
2	B	265	LEU	2.4
4	K	303	SER	2.4
1	A	12	ALA	2.4
2	B	256	ALA	2.4
1	A	41	THR	2.3
2	B	378	ILE	2.3
2	B	168	THR	2.3
4	K	50	ARG	2.3
4	K	119	ILE	2.3
2	B	41	ASP	2.2
2	B	79	ARG	2.2
1	A	182	VAL	2.2
2	B	167	ASN	2.2
2	B	263	PRO	2.2
1	A	283	HIS	2.2
3	D	14	LEU	2.1
1	A	58	ALA	2.0
1	A	100	ALA	2.0
2	B	195	VAL	2.0
2	B	266	HIS	2.0
4	K	118	TYR	2.0
2	B	76	ASP	2.0
2	B	191	ILE	2.0
2	B	201	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

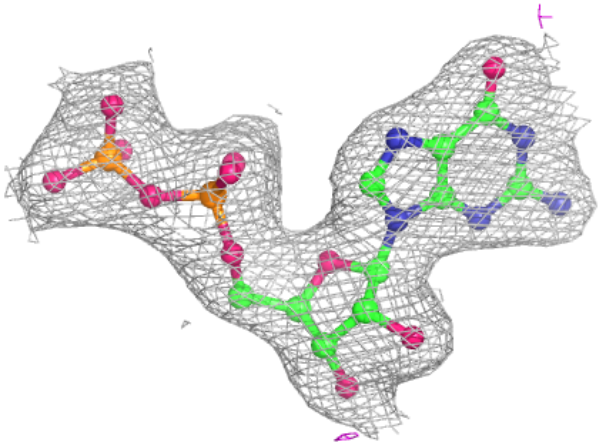
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

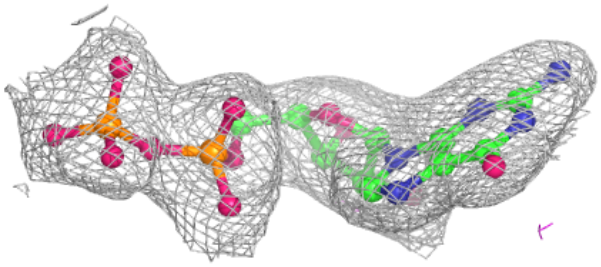
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	K	403	5/5	0.69	0.38	143,143,144,145	0
7	SO4	B	508	5/5	0.73	0.22	146,147,147,147	0
7	SO4	K	402	5/5	0.81	0.18	134,134,135,135	0
10	GOL	K	401	6/6	0.82	0.34	71,76,77,78	0
10	GOL	B	504	6/6	0.83	0.29	92,94,95,95	0
7	SO4	A	503	5/5	0.85	0.20	134,134,135,136	0
7	SO4	B	510	5/5	0.86	0.28	126,126,126,127	0
10	GOL	D	201	6/6	0.87	0.21	59,65,66,66	0
6	MG	A	502	1/1	0.89	0.21	36,36,36,36	0
10	GOL	B	503	6/6	0.90	0.26	85,86,87,87	0
7	SO4	A	505	5/5	0.92	0.28	106,109,109,111	0
7	SO4	B	507	5/5	0.92	0.15	121,121,121,122	0
7	SO4	B	505	5/5	0.95	0.25	122,122,123,124	0
7	SO4	B	509	5/5	0.96	0.14	99,99,100,101	0
7	SO4	A	504	5/5	0.96	0.09	106,107,108,108	0
8	GDP	B	501	28/28	0.98	0.10	33,36,45,46	0
9	MES	B	502	12/12	0.98	0.25	44,46,46,47	0
7	SO4	B	506	5/5	0.98	0.06	109,109,110,110	0
5	GTP	A	501	32/32	0.99	0.16	26,31,33,36	0

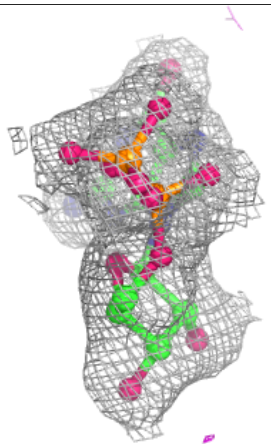
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 501:

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

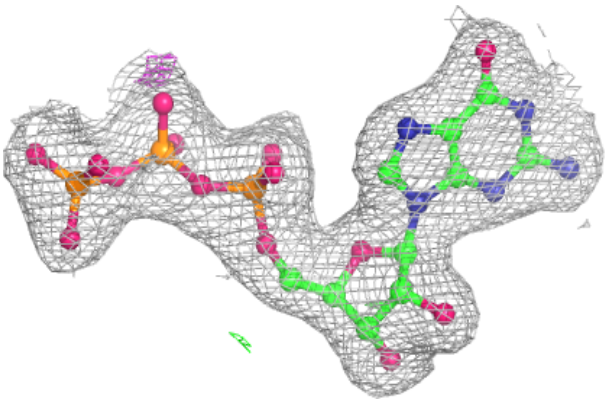


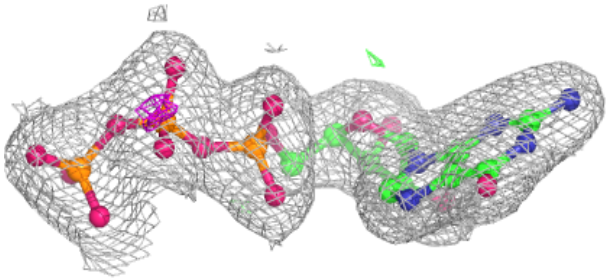


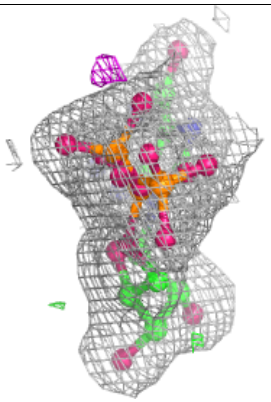


Electron density around GTP A 501:

$2mF_o$-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.