



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:20 AM UTC

PDB ID : 6SGE / pdb_00006sge
Title : Crystal structure of Human RHOB-GTP in complex with nanobody B6
Authors : Soulie, S.; Gence, R.; Cabantous, S.; Lajoie-Mazenc, I.; Favre, G.; Pedelacq, J.D.
Deposited on : 2019-08-04
Resolution : 1.50 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

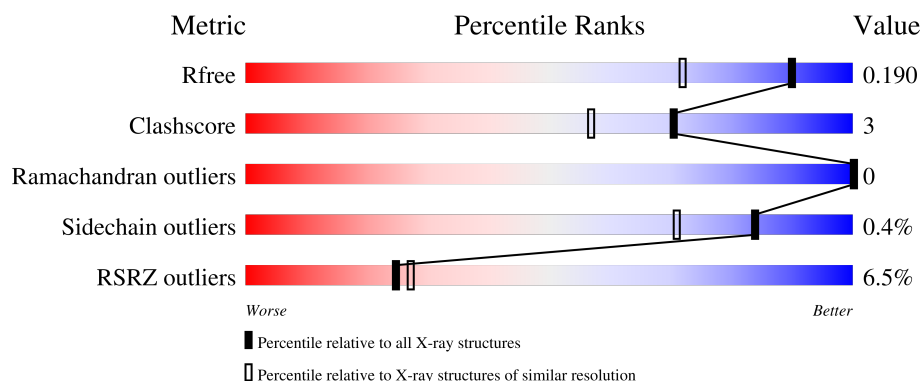
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	183	2% 91% 7% .
1	C	183	4% 96% . .
2	B	134	11% 78% 16% 6% .
2	D	134	10% 84% 16% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10405 atoms, of which 4783 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 Rho-related GTP-binding protein RhoB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	178	Total	C	H	N	O	S	0	2	0
			2838	900	1418	240	272	8			
1	C	182	Total	C	H	N	O	S	0	0	0
			2883	920	1433	245	277	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	LEU	GLN	engineered mutation	UNP P62745
C	63	LEU	GLN	engineered mutation	UNP P62745

- Molecule 2 is a protein called Nanobody B6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	126	Total	C	H	N	O	S	0	1	0
			1900	605	927	172	190	6			
2	D	134	Total	C	H	N	O	S	0	0	0
			2012	645	979	181	201	6			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP A0A4E0W6L3
B	5	GLN	LEU	conflict	UNP A0A4E0W6L3
B	6	ALA	GLU	conflict	UNP A0A4E0W6L3
B	11	PHE	LEU	conflict	UNP A0A4E0W6L3
B	27	TYR	VAL	conflict	UNP A0A4E0W6L3
B	28	GLY	ARG	conflict	UNP A0A4E0W6L3
B	29	SER	PHE	conflict	UNP A0A4E0W6L3
B	30	THR	SER	conflict	UNP A0A4E0W6L3
B	31	ILE	ASN	conflict	UNP A0A4E0W6L3
B	33	THR	VAL	conflict	UNP A0A4E0W6L3

Continued on next page...

Continued from previous page...

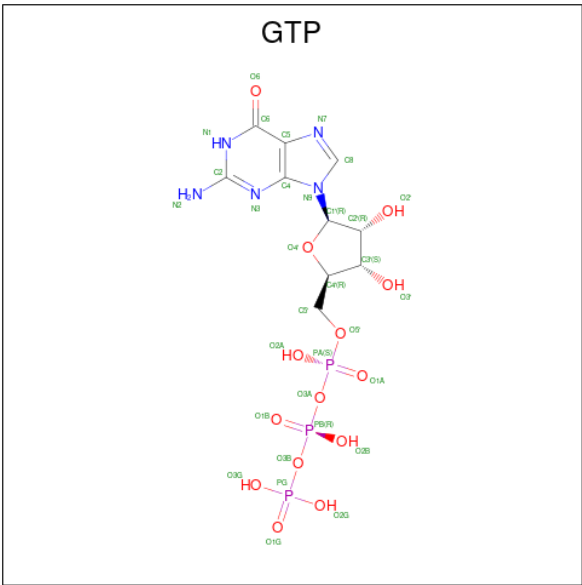
Chain	Residue	Modelled	Actual	Comment	Reference
B	35	GLY	ALA	conflict	UNP A0A4E0W6L3
B	37	PHE	VAL	conflict	UNP A0A4E0W6L3
B	44	GLU	GLY	conflict	UNP A0A4E0W6L3
B	45	ARG	LEU	conflict	UNP A0A4E0W6L3
B	47	PHE	TRP	conflict	UNP A0A4E0W6L3
B	49	SER	-	insertion	UNP A0A4E0W6L3
B	50	ALA	GLY	conflict	UNP A0A4E0W6L3
B	52	SER	GLU	conflict	UNP A0A4E0W6L3
B	53	ARG	LYS	conflict	UNP A0A4E0W6L3
B	54	ALA	MET	conflict	UNP A0A4E0W6L3
B	55	PRO	ASN	conflict	UNP A0A4E0W6L3
B	56	GLY	ASP	conflict	UNP A0A4E0W6L3
B	57	PRO	GLY	conflict	UNP A0A4E0W6L3
B	59	GLN	THR	conflict	UNP A0A4E0W6L3
B	80	VAL	LEU	conflict	UNP A0A4E0W6L3
B	94	THR	VAL	conflict	UNP A0A4E0W6L3
B	99	PRO	SER	conflict	UNP A0A4E0W6L3
B	100	ILE	TRP	conflict	UNP A0A4E0W6L3
B	101	ASN	GLY	conflict	UNP A0A4E0W6L3
B	102	ASN	HIS	conflict	UNP A0A4E0W6L3
B	103	ARG	SER	conflict	UNP A0A4E0W6L3
B	104	THR	ARG	conflict	UNP A0A4E0W6L3
B	105	MET	ARG	conflict	UNP A0A4E0W6L3
B	107	ASP	GLN	conflict	UNP A0A4E0W6L3
B	109	MET	LYS	conflict	UNP A0A4E0W6L3
B	111	LEU	-	insertion	UNP A0A4E0W6L3
B	112	TRP	-	insertion	UNP A0A4E0W6L3
B	114	TYR	SER	conflict	UNP A0A4E0W6L3
B	120	GLN	LEU	conflict	UNP A0A4E0W6L3
B	129	GLU	-	expression tag	UNP A0A4E0W6L3
B	130	ASN	-	expression tag	UNP A0A4E0W6L3
B	131	LEU	-	expression tag	UNP A0A4E0W6L3
B	132	TYR	-	expression tag	UNP A0A4E0W6L3
B	133	PHE	-	expression tag	UNP A0A4E0W6L3
B	134	GLN	-	expression tag	UNP A0A4E0W6L3
D	1	ALA	-	expression tag	UNP A0A4E0W6L3
D	5	GLN	LEU	conflict	UNP A0A4E0W6L3
D	6	ALA	GLU	conflict	UNP A0A4E0W6L3
D	11	PHE	LEU	conflict	UNP A0A4E0W6L3
D	27	TYR	VAL	conflict	UNP A0A4E0W6L3
D	28	GLY	ARG	conflict	UNP A0A4E0W6L3
D	29	SER	PHE	conflict	UNP A0A4E0W6L3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	THR	SER	conflict	UNP A0A4E0W6L3
D	31	ILE	ASN	conflict	UNP A0A4E0W6L3
D	33	THR	VAL	conflict	UNP A0A4E0W6L3
D	35	GLY	ALA	conflict	UNP A0A4E0W6L3
D	37	PHE	VAL	conflict	UNP A0A4E0W6L3
D	44	GLU	GLY	conflict	UNP A0A4E0W6L3
D	45	ARG	LEU	conflict	UNP A0A4E0W6L3
D	47	PHE	TRP	conflict	UNP A0A4E0W6L3
D	49	SER	-	insertion	UNP A0A4E0W6L3
D	50	ALA	GLY	conflict	UNP A0A4E0W6L3
D	52	SER	GLU	conflict	UNP A0A4E0W6L3
D	53	ARG	LYS	conflict	UNP A0A4E0W6L3
D	54	ALA	MET	conflict	UNP A0A4E0W6L3
D	55	PRO	ASN	conflict	UNP A0A4E0W6L3
D	56	GLY	ASP	conflict	UNP A0A4E0W6L3
D	57	PRO	GLY	conflict	UNP A0A4E0W6L3
D	59	GLN	THR	conflict	UNP A0A4E0W6L3
D	80	VAL	LEU	conflict	UNP A0A4E0W6L3
D	94	THR	VAL	conflict	UNP A0A4E0W6L3
D	99	PRO	SER	conflict	UNP A0A4E0W6L3
D	100	ILE	TRP	conflict	UNP A0A4E0W6L3
D	101	ASN	GLY	conflict	UNP A0A4E0W6L3
D	102	ASN	HIS	conflict	UNP A0A4E0W6L3
D	103	ARG	SER	conflict	UNP A0A4E0W6L3
D	104	THR	ARG	conflict	UNP A0A4E0W6L3
D	105	MET	ARG	conflict	UNP A0A4E0W6L3
D	107	ASP	GLN	conflict	UNP A0A4E0W6L3
D	109	MET	LYS	conflict	UNP A0A4E0W6L3
D	111	LEU	-	insertion	UNP A0A4E0W6L3
D	112	TRP	-	insertion	UNP A0A4E0W6L3
D	114	TYR	SER	conflict	UNP A0A4E0W6L3
D	120	GLN	LEU	conflict	UNP A0A4E0W6L3
D	129	GLU	-	expression tag	UNP A0A4E0W6L3
D	130	ASN	-	expression tag	UNP A0A4E0W6L3
D	131	LEU	-	expression tag	UNP A0A4E0W6L3
D	132	TYR	-	expression tag	UNP A0A4E0W6L3
D	133	PHE	-	expression tag	UNP A0A4E0W6L3
D	134	GLN	-	expression tag	UNP A0A4E0W6L3

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			45	10	13	5	14	3		
3	C	1	Total	C	H	N	O	P	0	0
			45	10	13	5	14	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

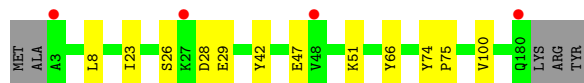
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	208	Total	O	0	0
			208	208		
5	B	128	Total	O	0	0
			128	128		
5	C	207	Total	O	0	0
			207	207		
5	D	135	Total	O	0	0
			135	135		

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.

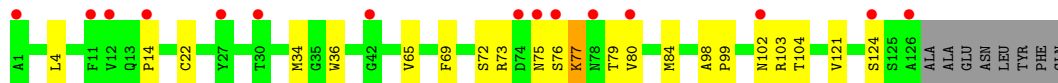
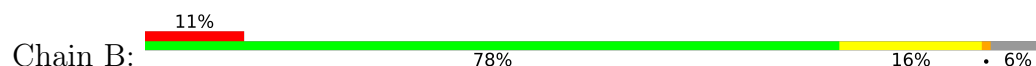
- Molecule 1: Rho-related GTP-binding protein RhoB



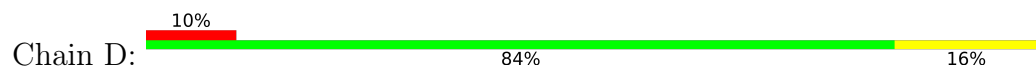
- Molecule 1: Rho-related GTP-binding protein RhoB



- Molecule 2: Nanobody B6



- Molecule 2: Nanobody B6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.84Å 70.23Å 71.21Å 90.00° 107.68° 90.00°	Depositor
Resolution (Å)	47.17 – 1.50 47.17 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.17-1.50) 95.0 (47.17-1.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.161 , 0.188 0.166 , 0.190	Depositor DCC
R_{free} test set	1992 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10405	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP

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	0.74	2/1456 (0.1%)	0.84	0/1976
1	C	0.85	4/1478 (0.3%)	0.88	0/2005
2	B	1.10	8/995 (0.8%)	0.96	2/1348 (0.1%)
2	D	0.90	6/1057 (0.6%)	0.84	2/1432 (0.1%)
All	All	0.89	20/4986 (0.4%)	0.88	4/6761 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	76	SER	CA-C	9.05	1.63	1.52
1	C	100	VAL	CA-CB	6.96	1.58	1.54
2	B	103	ARG	CZ-NH2	6.88	1.42	1.33
2	B	73	ARG	CZ-NH1	6.67	1.42	1.32
2	D	73	ARG	CZ-NH2	6.65	1.42	1.33
1	C	70	ARG	CA-CB	6.62	1.61	1.53
2	D	73	ARG	CZ-NH1	6.61	1.42	1.32
1	C	70	ARG	CZ-NH2	6.56	1.42	1.33
1	C	70	ARG	CZ-NH1	6.54	1.42	1.32
2	B	103	ARG	CZ-NH1	6.48	1.41	1.32
1	A	100	VAL	CA-CB	-6.47	1.50	1.54
2	B	73	ARG	CZ-NH2	6.43	1.41	1.33
2	B	76	SER	N-CA	6.02	1.53	1.46
2	D	109	MET	CG-SD	-5.46	1.67	1.80
2	D	75	ASN	CA-C	5.30	1.60	1.52
2	B	79	THR	CA-C	5.15	1.58	1.52
1	A	26	SER	CA-C	5.12	1.59	1.52
2	D	77	LYS	CA-C	5.12	1.57	1.52
2	B	102	ASN	CA-C	5.09	1.59	1.52
2	D	79	THR	CA-C	5.01	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	SER	CA-C-O	-5.96	115.08	121.45
2	D	72	SER	CA-C-O	-5.86	115.01	121.33
2	B	77	LYS	N-CA-C	5.39	119.83	112.88
2	D	113	ASN	N-CA-C	-5.03	107.14	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1420	1418	1408	9	0
1	C	1450	1433	1447	3	0
2	B	973	927	926	11	0
2	D	1033	979	979	11	0
3	A	32	13	11	0	0
3	C	32	13	11	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	208	0	0	1	0
5	B	128	0	0	0	0
5	C	207	0	0	1	0
5	D	135	0	0	2	0
All	All	5622	4783	4782	33	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 3.

All (33) 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:23:ILE:HD11	1:A:42:TYR:CZ	2.13	0.83
1:A:23:ILE:HD11	1:A:42:TYR:CE1	2.21	0.75
2:D:20:LEU:HG	2:D:84:MET:HE2	1.70	0.71
1:A:66:TYR:OH	2:D:102:ASN:OD1	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ASN:N	5:D:203:HOH:O	2.33	0.60
2:B:99:PRO:O	2:B:104[A]:THR:HG21	2.05	0.56
2:B:84:MET:HE1	2:B:121:VAL:HG21	1.89	0.55
2:B:14:PRO:HD3	2:B:124:SER:O	2.07	0.54
1:C:140:ARG:HD3	5:C:478:HOH:O	2.08	0.54
2:B:34:MET:HG2	2:B:80:VAL:HG21	1.91	0.52
2:D:34:MET:C	2:D:34:MET:SD	2.94	0.50
2:B:34:MET:C	2:B:34:MET:SD	2.95	0.50
2:B:75:ASN:O	2:B:75:ASN:OD1	2.30	0.49
1:A:28:ASP:OD2	5:A:301:HOH:O	2.20	0.49
1:C:23:ILE:HD11	1:C:42:TYR:CZ	2.48	0.48
2:B:98:ALA:HB1	2:B:99:PRO:HD2	1.95	0.47
1:A:8:LEU:C	1:A:8:LEU:HD23	2.42	0.45
2:D:12:VAL:HG11	2:D:87:LEU:HD13	1.99	0.44
2:D:22:CYS:HB2	2:D:36:TRP:CZ2	2.53	0.43
1:A:23:ILE:CD1	1:A:42:TYR:CE1	2.98	0.43
2:D:74:ASP:HB3	5:D:203:HOH:O	2.18	0.43
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.60	0.42
1:A:23:ILE:HG22	1:A:29:GLU:O	2.19	0.42
2:D:1:ALA:HB3	2:D:27:TYR:O	2.20	0.42
1:A:74:TYR:N	1:A:75:PRO:CD	2.83	0.42
2:B:65:VAL:HB	2:B:69:PHE:CG	2.56	0.41
2:B:22:CYS:HB2	2:B:36:TRP:CZ2	2.56	0.41
2:D:77:LYS:HE3	2:D:77:LYS:HB3	1.89	0.41
1:C:137:GLU:OE1	1:C:140:ARG:NH2	2.54	0.41
2:D:4:LEU:HB3	2:D:22:CYS:SG	2.60	0.41
1:A:47:GLU:HA	1:A:51:LYS:O	2.20	0.41
2:B:14:PRO:HD3	2:B:124:SER:C	2.46	0.40
2:D:13:GLN:NE2	2:D:125:SER:O	2.54	0.40

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	178/183 (97%)	174 (98%)	4 (2%)	0	100	100
1	C	180/183 (98%)	175 (97%)	5 (3%)	0	100	100
2	B	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
2	D	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
All	All	615/634 (97%)	598 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/161 (98%)	158 (100%)	0	100	100
1	C	160/161 (99%)	160 (100%)	0	100	100
2	B	102/107 (95%)	101 (99%)	1 (1%)	68	45
2	D	107/107 (100%)	106 (99%)	1 (1%)	70	49
All	All	527/536 (98%)	525 (100%)	2 (0%)	84	71

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	77	LYS
2	D	77	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	C	52	GLN
2	D	78	ASN
2	D	83	GLN
2	D	85	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	117	GLN
2	D	134	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	GTP	A	201	4	33,34,34	2.87	13 (39%)	50,54,54	1.48	7 (14%)
3	GTP	C	201	4	33,34,34	2.89	13 (39%)	50,54,54	1.68	9 (18%)

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
3	GTP	A	201	4	-	2/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	C	201	4	-	2/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	GTP	C2'-C3'	-8.62	1.30	1.53
3	A	201	GTP	C2'-C3'	-7.73	1.32	1.53
3	A	201	GTP	PB-O3B	7.09	1.67	1.59
3	C	201	GTP	PB-O3B	6.40	1.66	1.59
3	A	201	GTP	PG-O3G	5.58	1.75	1.54
3	C	201	GTP	PG-O3G	5.45	1.75	1.54
3	C	201	GTP	C3'-C4'	4.99	1.65	1.53
3	A	201	GTP	PA-O3A	4.03	1.63	1.59
3	A	201	GTP	C4-N3	3.84	1.43	1.34
3	A	201	GTP	O4'-C1'	3.83	1.50	1.42
3	C	201	GTP	C1'-N9	-3.72	1.37	1.47
3	C	201	GTP	C2-N3	3.64	1.42	1.33
3	A	201	GTP	C3'-C4'	3.62	1.62	1.53
3	C	201	GTP	C4-N3	3.61	1.42	1.34
3	A	201	GTP	C2-N3	3.45	1.41	1.33
3	A	201	GTP	C1'-N9	-3.44	1.37	1.47
3	C	201	GTP	O4'-C1'	3.38	1.49	1.42
3	A	201	GTP	C8-N9	-3.05	1.30	1.37
3	C	201	GTP	O2'-C2'	2.99	1.50	1.43
3	A	201	GTP	C5-N7	-2.96	1.33	1.39
3	A	201	GTP	O6-C6	-2.72	1.18	1.23
3	C	201	GTP	C5-N7	-2.52	1.34	1.39
3	C	201	GTP	C2-N2	2.44	1.39	1.34
3	A	201	GTP	O2'-C2'	2.33	1.48	1.43
3	C	201	GTP	C8-N9	-2.30	1.32	1.37
3	C	201	GTP	PA-O3A	2.18	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	GTP	C3'-C2'-C1'	6.11	113.02	101.46
3	A	201	GTP	C3'-C2'-C1'	5.07	111.06	101.46
3	A	201	GTP	O4'-C1'-C2'	-4.47	97.05	106.62
3	C	201	GTP	O4'-C1'-C2'	-3.76	98.57	106.62
3	C	201	GTP	N2-C2-N1	3.60	124.35	116.76
3	A	201	GTP	O3'-C3'-C4'	-2.99	102.48	111.08
3	C	201	GTP	C1'-N9-C4	-2.88	117.97	126.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	GTP	O3'-C3'-C2'	2.61	120.20	111.82
3	C	201	GTP	C5-C4-N3	-2.60	124.26	128.39
3	C	201	GTP	C1'-N9-C8	2.52	133.88	126.73
3	C	201	GTP	C2-N3-C4	2.27	116.21	112.30
3	C	201	GTP	O3'-C3'-C4'	-2.18	104.83	111.08
3	A	201	GTP	O3G-PG-O3B	-2.12	97.53	104.64
3	A	201	GTP	N2-C2-N1	2.06	121.10	116.76
3	A	201	GTP	C1'-N9-C4	-2.05	120.44	126.49
3	C	201	GTP	N9-C4-N3	2.01	129.98	125.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

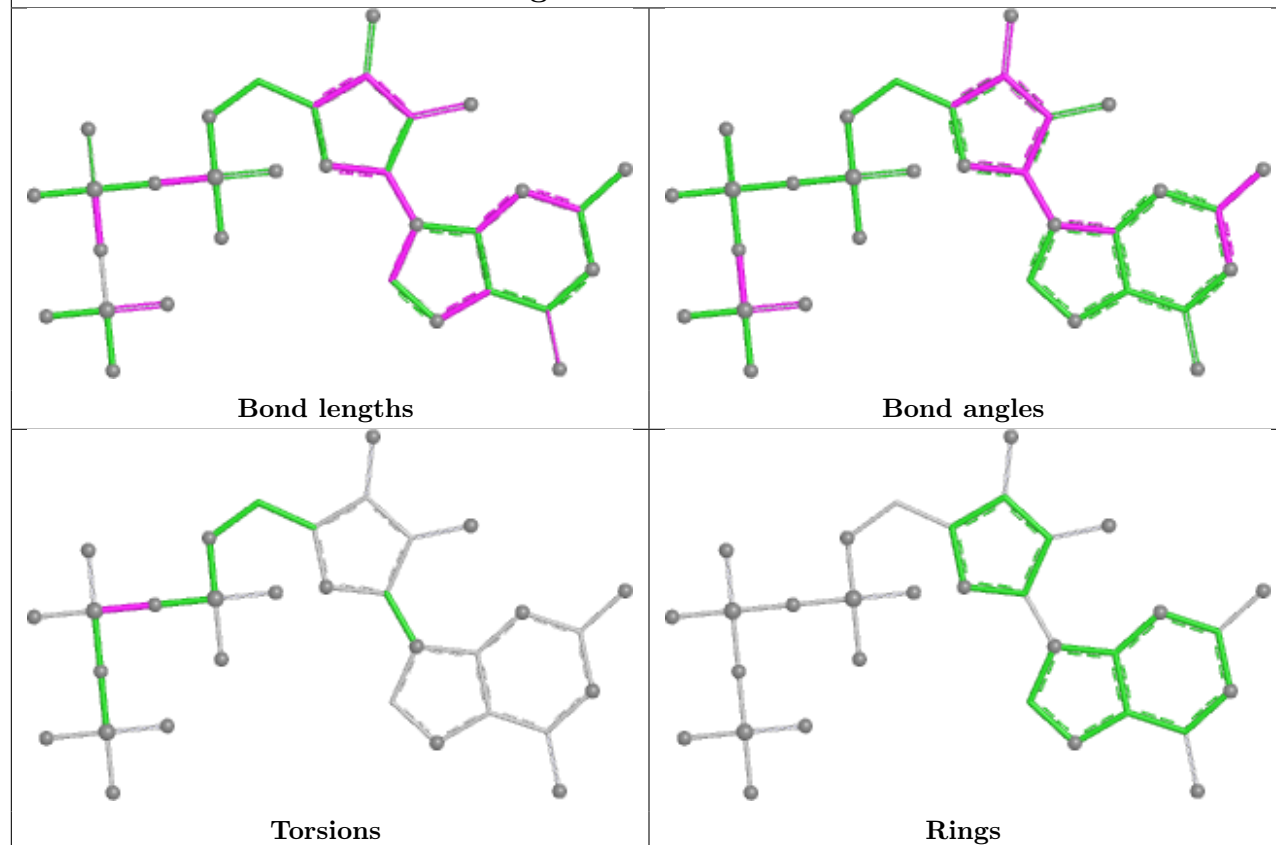
Mol	Chain	Res	Type	Atoms
3	A	201	GTP	PA-O3A-PB-O2B
3	C	201	GTP	PA-O3A-PB-O2B
3	A	201	GTP	PA-O3A-PB-O1B
3	C	201	GTP	PA-O3A-PB-O1B

There are no ring outliers.

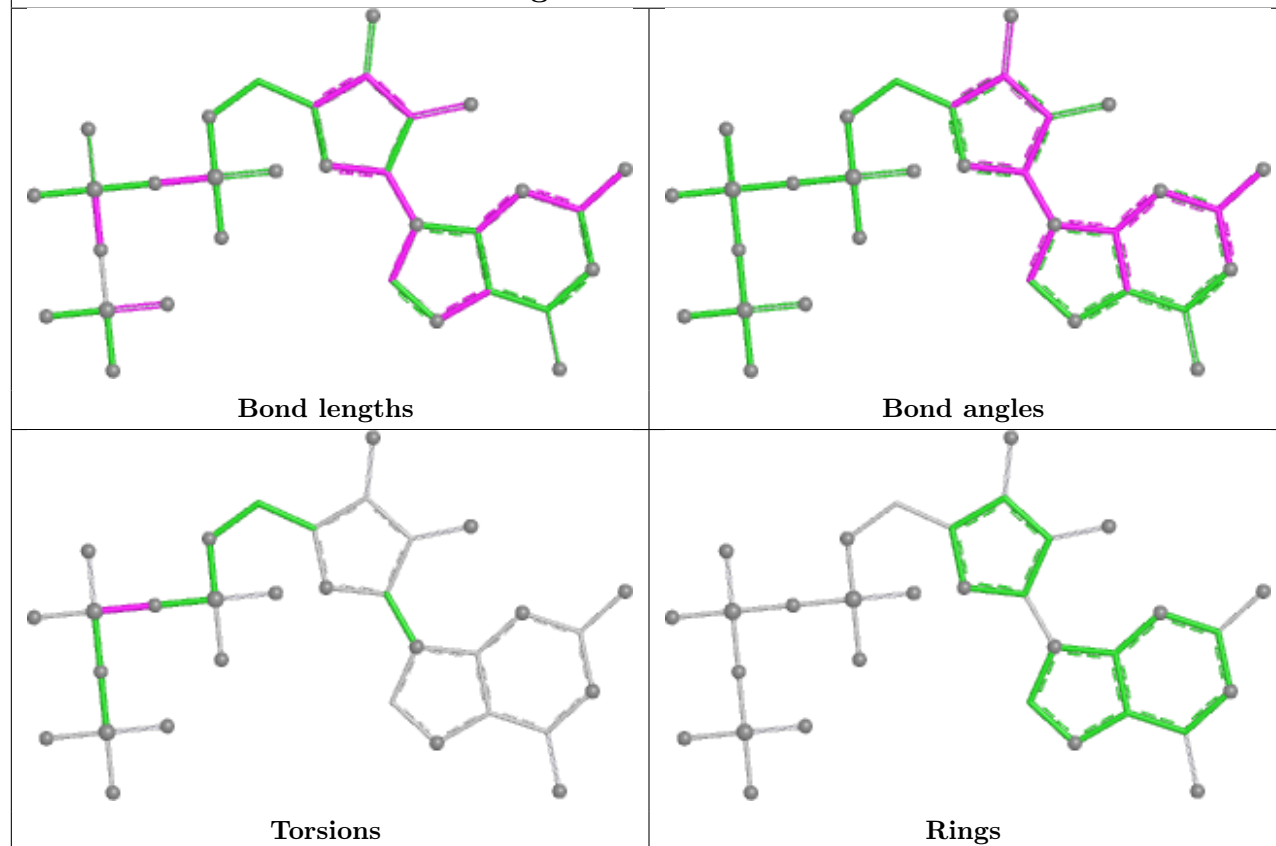
No monomer is involved in short contacts.

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 A 201



Ligand GTP C 201



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	178/183 (97%)	-0.21	4 (2%) 62 66	14, 24, 50, 74	1 (0%)
1	C	182/183 (99%)	-0.13	7 (3%) 44 48	15, 24, 49, 73	0
2	B	126/134 (94%)	0.65	15 (11%) 9 9	13, 36, 72, 96	1 (0%)
2	D	134/134 (100%)	0.56	14 (10%) 11 12	22, 39, 75, 110	0
All	All	620/634 (97%)	0.16	40 (6%) 25 27	13, 29, 59, 110	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	4.9
2	D	27	TYR	4.8
2	B	11	PHE	4.6
1	C	33	VAL	4.3
1	A	3	ALA	3.9
2	B	126	ALA	3.9
1	C	183	TYR	3.8
1	C	3	ALA	3.6
2	D	1	ALA	3.4
2	D	30	THR	3.3
2	B	12	VAL	3.3
2	D	107	ASP	3.2
2	B	27	TYR	3.2
2	B	76	SER	3.1
2	B	102	ASN	3.0
2	B	42	GLY	3.0
2	D	76	SER	2.9
2	B	1	ALA	2.9
2	B	75	ASN	2.9
2	B	80	VAL	2.7
1	C	32	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	124	SER	2.6
2	D	25	SER	2.6
2	D	102	ASN	2.5
2	B	74	ASP	2.5
1	A	180	GLN	2.4
1	C	123	SER	2.3
2	D	77	LYS	2.3
1	A	27	LYS	2.2
2	D	29	SER	2.2
1	A	48	VAL	2.2
1	C	43	VAL	2.2
2	B	30	THR	2.2
2	D	133	PHE	2.2
2	B	78	ASN	2.1
2	B	14	PRO	2.1
2	D	12	VAL	2.0
2	D	80	VAL	2.0
2	D	134	GLN	2.0
2	D	42	GLY	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.

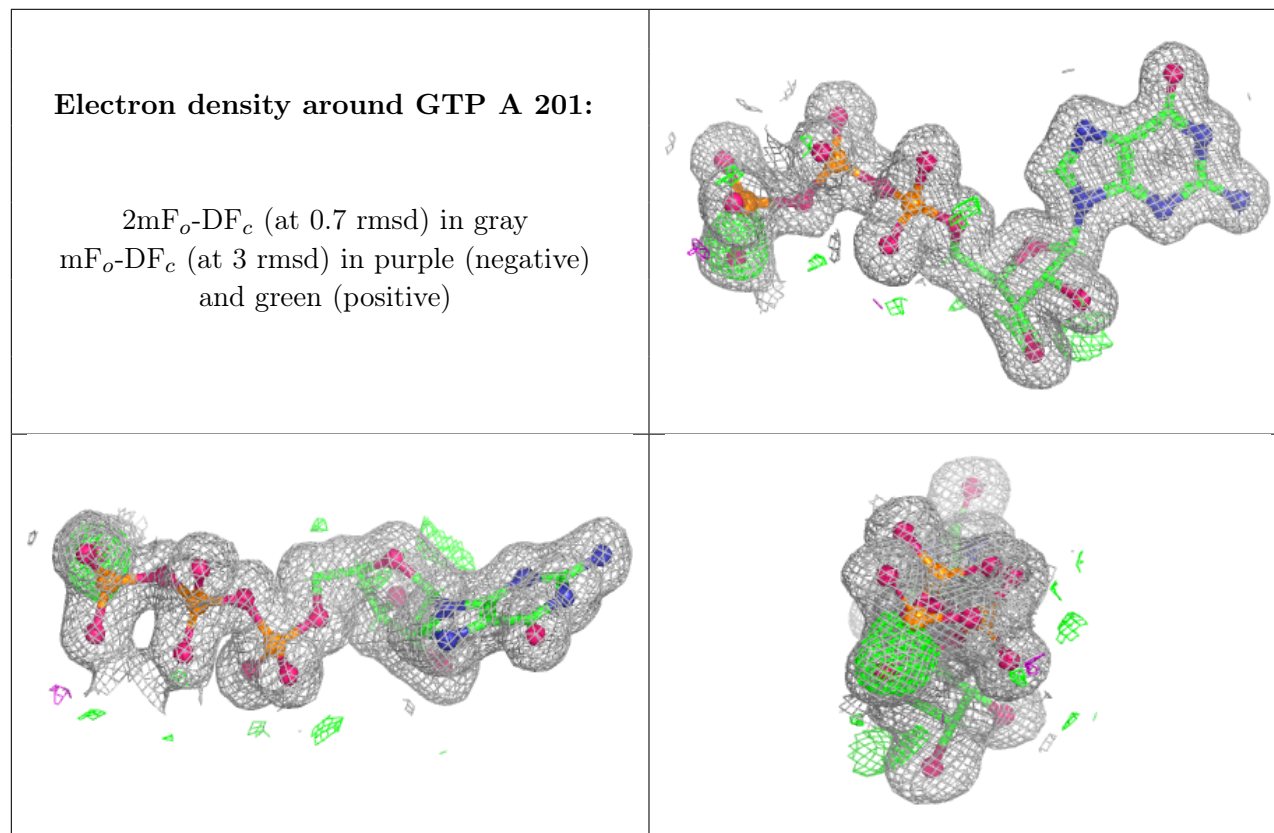
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTP	A	201	32/32	0.98	0.05	13,17,23,25	0
3	GTP	C	201	32/32	0.98	0.04	13,18,24,28	0
4	MG	A	202	1/1	0.99	0.03	15,15,15,15	0
4	MG	A	203	1/1	0.99	0.05	24,24,24,24	0

Continued on next page...

Continued from previous page...

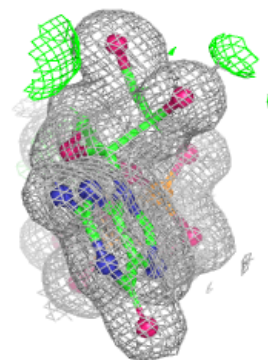
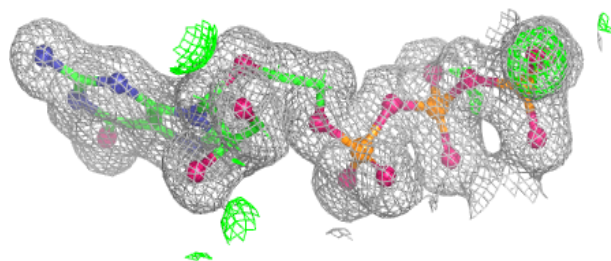
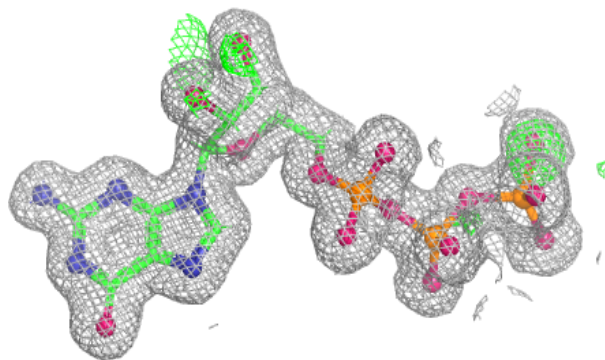
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	202	1/1	0.99	0.03	14,14,14,14	0
4	MG	C	203	1/1	0.99	0.03	23,23,23,23	0

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.



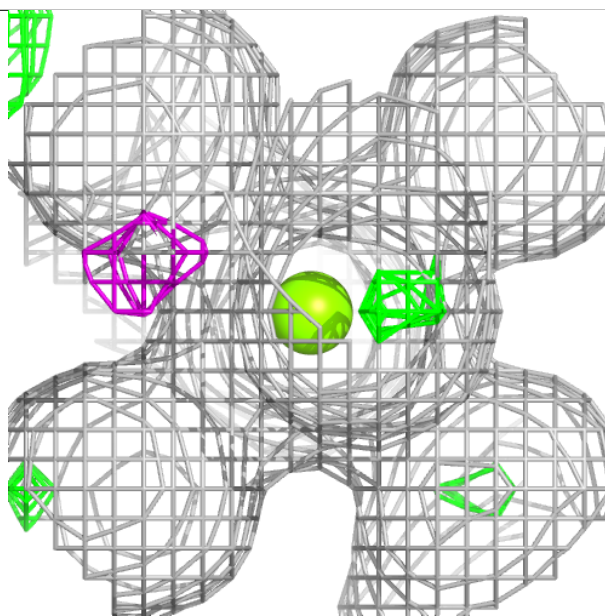
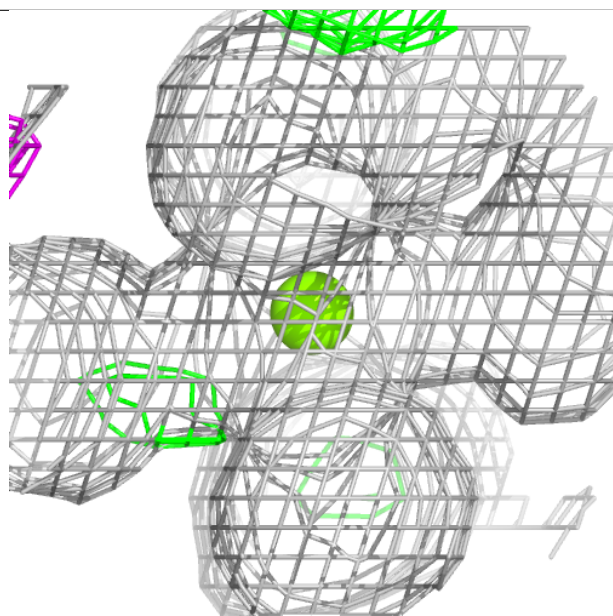
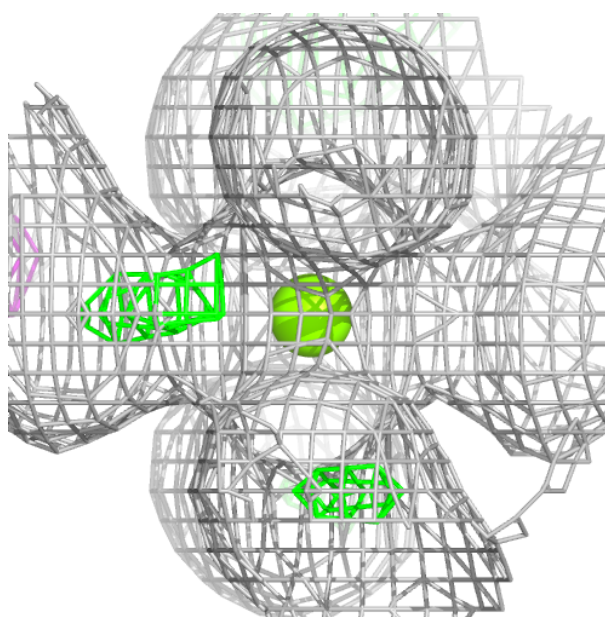
Electron density around GTP C 201:

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



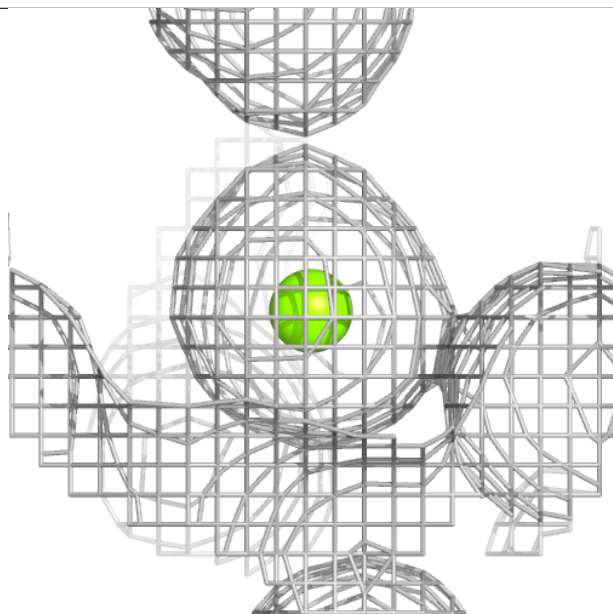
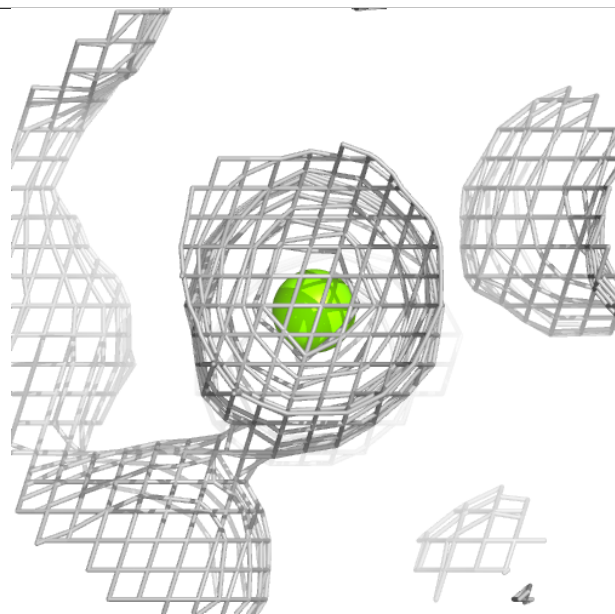
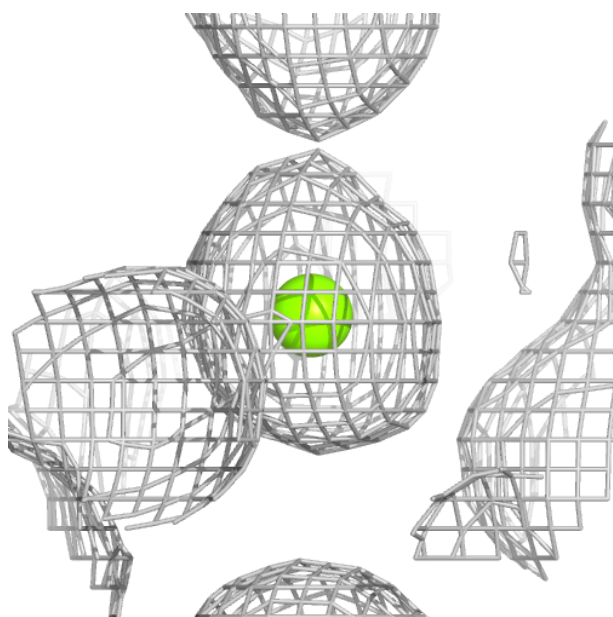
Electron density around MG A 202:

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



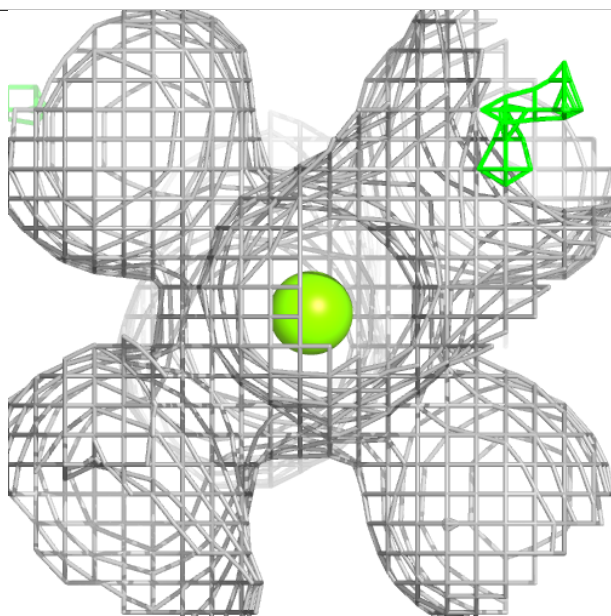
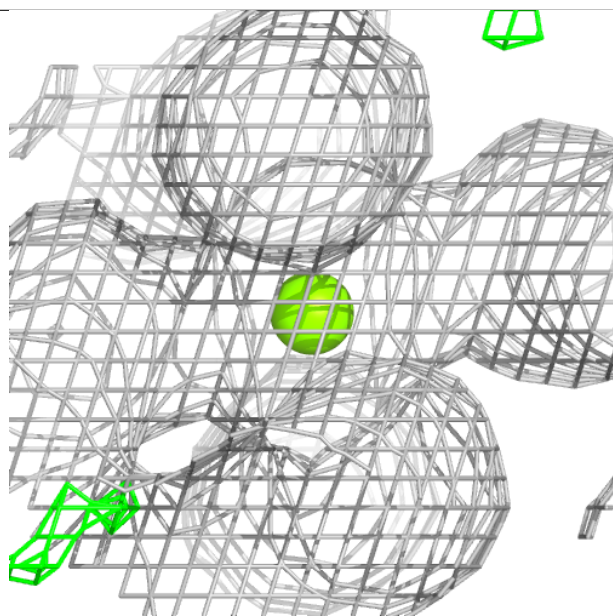
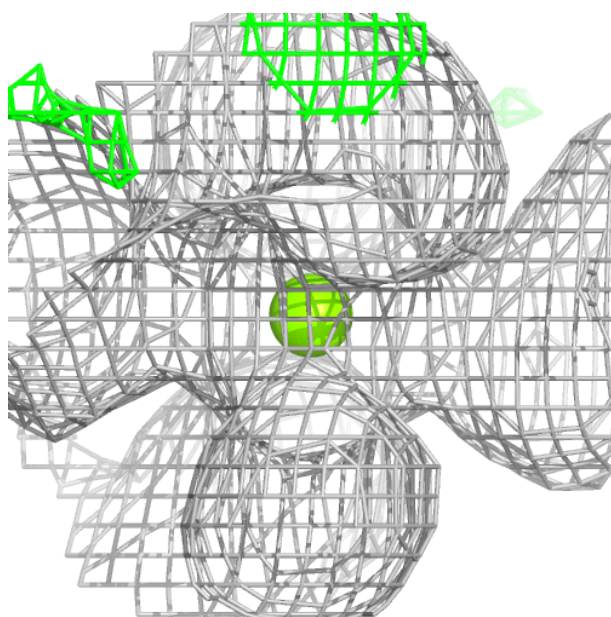
Electron density around MG A 203:

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



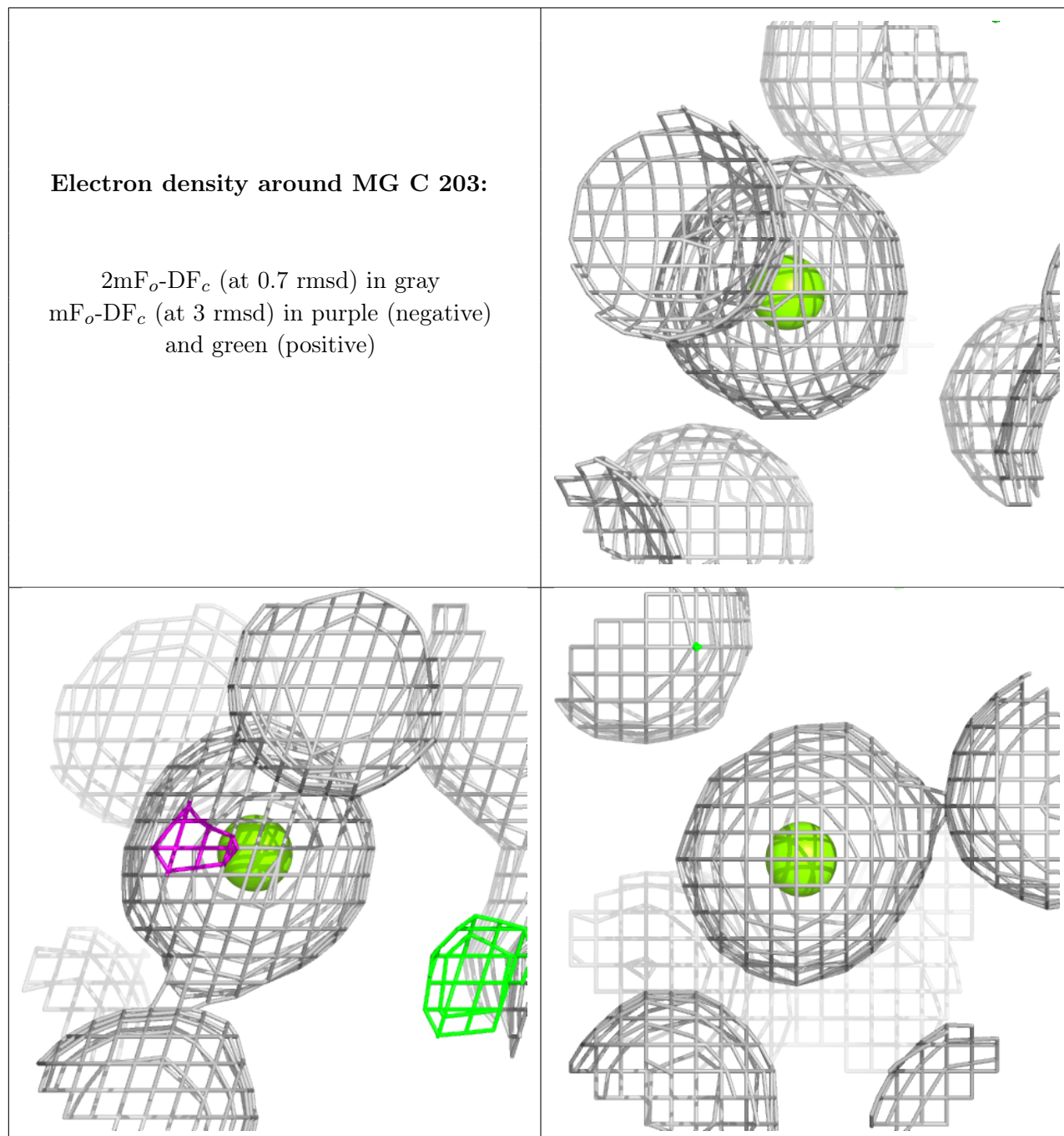
Electron density around MG C 202:

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



Electron density around MG C 203:

$2mF_o-DF_c$ (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.