



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:33 PM UTC

PDB ID : 7C41 / pdb_00007c41
Title : KRAS G12V and H-REV107 peptide complex
Authors : Han, C.W.; Jeong, M.S.; Jang, S.B.
Deposited on : 2020-05-14
Resolution : 2.28 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

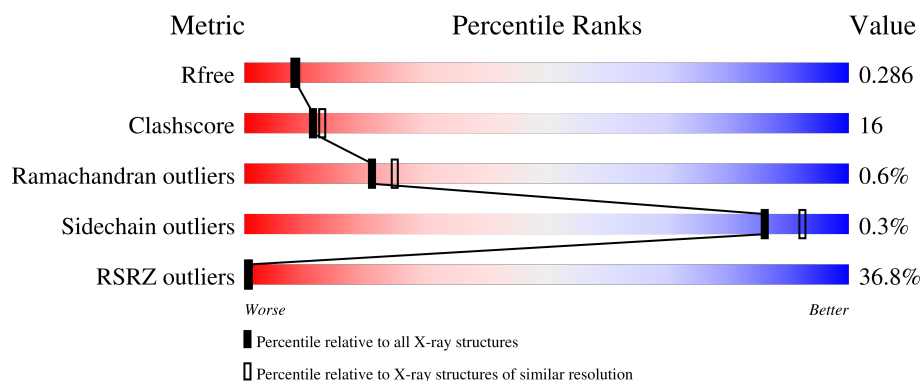
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	174	45% 66% 30% .
1	G	174	46% 72% 25% .
1	J	174	17% 74% 23% .
1	M	174	34% 73% 24% .
2	D	10	40% 10% 70% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5626 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 GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1337	840	227	263	7			
1	J	168	Total	C	N	O	S	0	0	0
			1337	840	227	263	7			
1	M	168	Total	C	N	O	S	0	0	0
			1337	840	227	263	7			
1	G	168	Total	C	N	O	S	0	0	0
			1337	840	227	263	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	VAL	GLY	engineered mutation	UNP P01116
A	169	HIS	-	expression tag	UNP P01116
A	170	HIS	-	expression tag	UNP P01116
A	171	HIS	-	expression tag	UNP P01116
A	172	HIS	-	expression tag	UNP P01116
A	173	HIS	-	expression tag	UNP P01116
A	174	HIS	-	expression tag	UNP P01116
J	12	VAL	GLY	engineered mutation	UNP P01116
J	169	HIS	-	expression tag	UNP P01116
J	170	HIS	-	expression tag	UNP P01116
J	171	HIS	-	expression tag	UNP P01116
J	172	HIS	-	expression tag	UNP P01116
J	173	HIS	-	expression tag	UNP P01116
J	174	HIS	-	expression tag	UNP P01116
M	12	VAL	GLY	engineered mutation	UNP P01116
M	169	HIS	-	expression tag	UNP P01116
M	170	HIS	-	expression tag	UNP P01116
M	171	HIS	-	expression tag	UNP P01116
M	172	HIS	-	expression tag	UNP P01116
M	173	HIS	-	expression tag	UNP P01116
M	174	HIS	-	expression tag	UNP P01116

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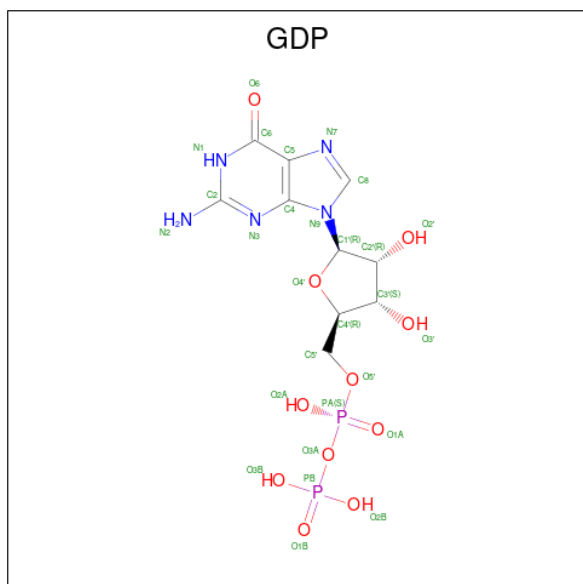
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Chain	Residue	Modelled	Actual	Comment	Reference
G	12	VAL	GLY	engineered mutation	UNP P01116
G	169	HIS	-	expression tag	UNP P01116
G	170	HIS	-	expression tag	UNP P01116
G	171	HIS	-	expression tag	UNP P01116
G	172	HIS	-	expression tag	UNP P01116
G	173	HIS	-	expression tag	UNP P01116
G	174	HIS	-	expression tag	UNP P01116

- Molecule 2 is a protein called HRAS-like suppressor 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	0	0	0
			79	51	11	17			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	J	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	M	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0

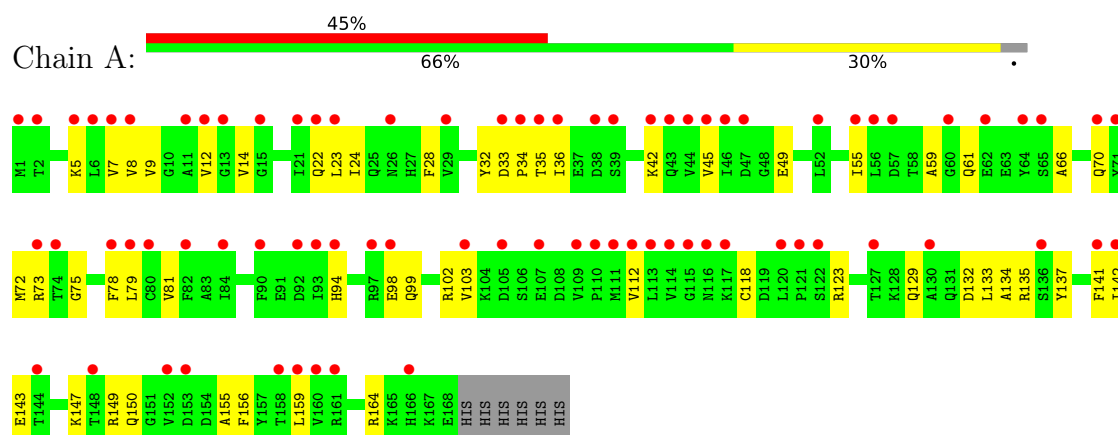
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total 19	O 19	0	0
5	D	1	Total 1	O 1	0	0
5	J	22	Total 22	O 22	0	0
5	M	26	Total 26	O 26	0	0
5	G	15	Total 15	O 15	0	0

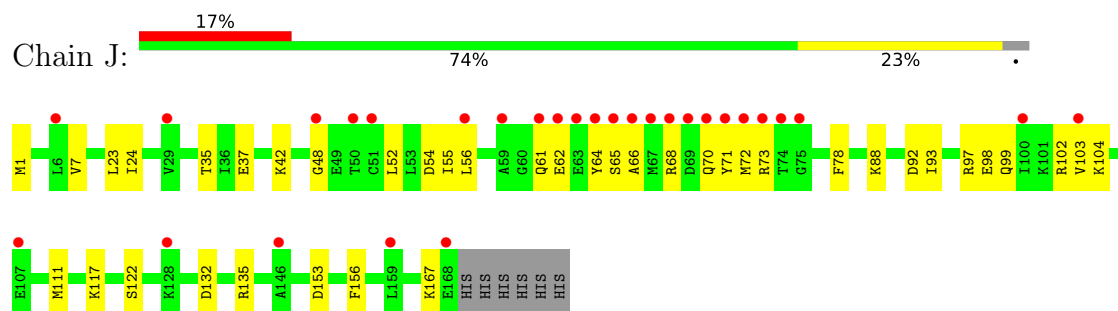
3 Residue-property plots

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.

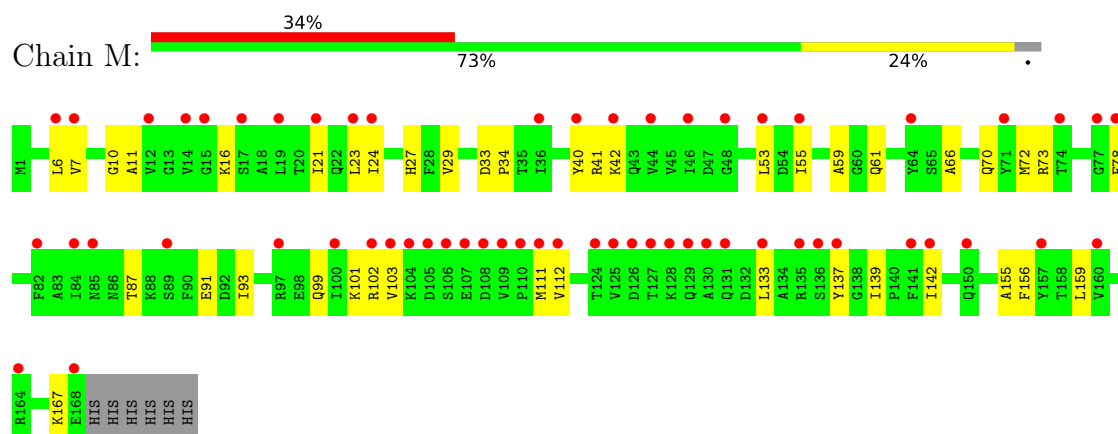
• Molecule 1: GTPase KRas



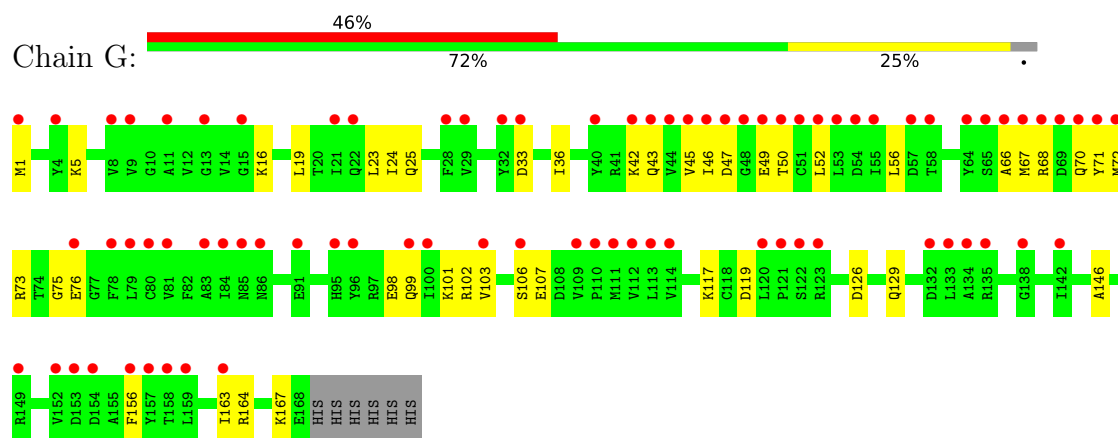
• Molecule 1: GTPase KRas



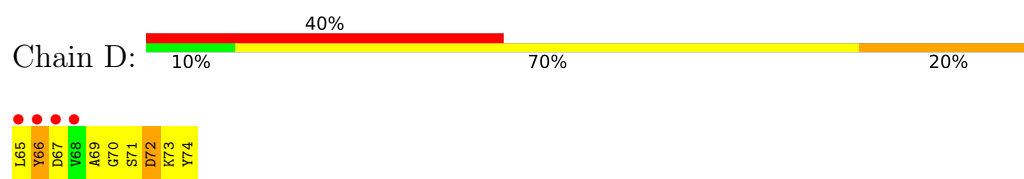
• Molecule 1: GTPase KRas



- Molecule 1: GTPase KRas



- Molecule 2: HRAS-like suppressor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.91Å 84.34Å 84.33Å 59.98° 89.96° 89.97°	Depositor
Resolution (Å)	36.52 – 2.28 36.52 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.52-2.28) 99.9 (36.52-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.260 , 0.283 0.261 , 0.286	Depositor DCC
R_{free} test set	2145 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,k-l,k 0.000 for h,l,-k+l 0.040 for h,-l,k-l 0.040 for h,-k+l,-k 0.026 for h,-k,-l 0.000 for -h,-l,-k 0.000 for -h,-k+l,l 0.000 for -h,-k,-k+l 0.000 for -h,k,k-l 0.000 for -h,l,k 0.000 for -h,k-l,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5626	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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, 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	0.34	0/1358	0.53	0/1833
1	G	0.34	0/1358	0.56	0/1833
1	J	0.47	0/1358	0.61	0/1833
1	M	0.37	0/1358	0.55	0/1833
2	D	0.48	0/80	1.25	2/107 (1.9%)
All	All	0.39	0/5512	0.58	2/7439 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	66	TYR	CA-C-N	5.66	129.74	120.63
2	D	66	TYR	C-N-CA	5.66	129.74	120.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	72	ASP	Peptide

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	1337	0	1318	67	0
1	G	1337	0	1318	46	0
1	J	1337	0	1318	39	0
1	M	1337	0	1318	30	0
2	D	79	0	71	33	0
3	A	28	0	12	6	0
3	G	28	0	12	3	0
3	J	28	0	12	2	0
3	M	28	0	12	0	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
4	M	1	0	0	0	0
5	A	19	0	0	5	0
5	D	1	0	0	0	0
5	G	15	0	0	2	0
5	J	22	0	0	6	0
5	M	26	0	0	2	0
All	All	5626	0	5391	177	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 16.

All (177) 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:M:41:ARG:O	1:M:42:LYS:HD2	1.72	0.89
1:M:24:ILE:HG23	1:M:42:LYS:HD3	1.58	0.85
1:J:62:GLU:HB2	1:G:43:GLN:HE21	1.43	0.83
1:A:12:VAL:HG12	2:D:74:TYR:CD1	2.15	0.82
1:G:66:ALA:O	1:G:70:GLN:NE2	2.13	0.81
1:G:67:MET:HE3	1:G:71:TYR:HE1	1.46	0.80
1:G:67:MET:HE3	1:G:71:TYR:CE1	2.16	0.79
1:A:34:PRO:HG3	2:D:70:GLY:HA3	1.65	0.78
1:G:50:THR:OG1	5:G:301:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:54:ASP:OD1	1:J:71:TYR:OH	2.06	0.73
1:J:62:GLU:HB2	1:G:43:GLN:NE2	2.03	0.73
1:A:66:ALA:O	1:A:70:GLN:HG2	1.89	0.73
1:A:70:GLN:HA	1:A:73:ARG:HD3	1.71	0.72
1:M:91:GLU:O	5:M:301:HOH:O	2.08	0.71
1:G:16:LYS:N	3:G:201:GDP:O3B	2.25	0.70
1:A:61:GLN:HE21	2:D:65:LEU:N	1.88	0.70
1:A:35:THR:HA	2:D:67:ASP:CG	2.19	0.68
1:J:167:LYS:NZ	5:J:303:HOH:O	2.26	0.68
1:J:97:ARG:HG3	1:J:111:MET:HE1	1.76	0.67
1:A:34:PRO:C	2:D:67:ASP:HA	2.20	0.67
1:M:24:ILE:HD11	1:M:55:ILE:HD12	1.77	0.67
1:G:5:LYS:HG2	1:G:75:GLY:HA2	1.78	0.65
1:A:8:VAL:HG22	1:A:79:LEU:HD12	1.79	0.65
1:J:99:GLN:O	1:J:103:VAL:HG23	1.97	0.65
3:A:201:GDP:O2A	5:A:301:HOH:O	2.14	0.65
1:J:62:GLU:HA	1:G:50:THR:HG21	1.78	0.64
1:A:5:LYS:HG2	1:A:75:GLY:HA2	1.79	0.64
1:A:123:ARG:NH2	1:A:143:GLU:OE2	2.29	0.64
1:A:12:VAL:CG2	2:D:66:TYR:HA	2.28	0.63
1:J:71:TYR:O	5:J:301:HOH:O	2.15	0.63
1:J:24:ILE:HD11	1:J:55:ILE:HD12	1.81	0.63
1:J:64:TYR:CD1	1:G:1:MET:HB3	2.34	0.63
1:G:101:LYS:HE3	1:G:107:GLU:HG3	1.81	0.62
1:A:12:VAL:HG11	2:D:69:ALA:HB3	1.81	0.62
1:A:59:ALA:O	2:D:66:TYR:HB3	2.00	0.62
1:J:102:ARG:HB2	1:G:47:ASP:CG	2.26	0.61
1:A:35:THR:HG22	2:D:67:ASP:HB3	1.82	0.61
1:J:65:SER:H	1:G:1:MET:HB2	1.65	0.61
1:M:112:VAL:CG1	1:M:142:ILE:HD12	2.29	0.61
1:M:111:MET:HE2	1:M:139:ILE:HD13	1.83	0.60
1:A:79:LEU:HD23	1:A:112:VAL:HB	1.82	0.60
1:G:98:GLU:O	1:G:102:ARG:HG3	2.02	0.60
1:A:9:VAL:O	1:A:81:VAL:HG22	2.02	0.59
1:A:12:VAL:HG12	2:D:74:TYR:CE1	2.37	0.58
1:A:14:VAL:HG21	1:A:81:VAL:HG23	1.83	0.58
1:J:132:ASP:CG	1:J:135:ARG:HH21	2.11	0.58
1:M:99:GLN:O	1:M:103:VAL:HG23	2.03	0.58
1:G:24:ILE:HA	1:G:42:LYS:HD2	1.86	0.58
1:A:118:CYS:SG	1:A:143:GLU:HB3	2.44	0.57
1:A:35:THR:HA	2:D:67:ASP:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:72:MET:HB3	1:M:103:VAL:HG11	1.87	0.57
1:A:12:VAL:HG21	2:D:70:GLY:H	1.69	0.57
1:M:11:ALA:O	1:M:16:LYS:NZ	2.38	0.57
1:J:66:ALA:HA	1:G:1:MET:H2	1.70	0.56
1:M:112:VAL:HG11	1:M:142:ILE:HD12	1.86	0.56
1:G:24:ILE:HG22	1:G:25:GLN:HG3	1.87	0.56
3:A:201:GDP:C5'	2:D:71:SER:HA	2.35	0.56
1:G:46:ILE:HB	1:G:164:ARG:HH22	1.70	0.56
1:A:72:MET:HB3	1:A:103:VAL:HG11	1.88	0.56
1:A:129:GLN:O	5:A:302:HOH:O	2.18	0.55
1:A:99:GLN:O	1:A:103:VAL:HG23	2.06	0.55
1:J:88:LYS:NZ	1:J:92:ASP:OD1	2.39	0.55
1:G:1:MET:HE2	1:G:50:THR:O	2.06	0.55
1:M:10:GLY:O	5:M:302:HOH:O	2.18	0.54
1:M:27:HIS:HE1	1:M:29:VAL:HG22	1.71	0.54
1:G:1:MET:HG2	1:G:52:LEU:HD12	1.89	0.53
1:G:70:GLN:OE1	1:G:73:ARG:NH1	2.40	0.53
1:M:27:HIS:CE1	1:M:29:VAL:HG22	2.44	0.53
3:A:201:GDP:H5'	2:D:71:SER:HA	1.91	0.53
1:J:153:ASP:OD2	5:J:302:HOH:O	2.19	0.53
1:M:142:ILE:HD13	1:M:155:ALA:HA	1.90	0.53
1:A:36:ILE:O	2:D:66:TYR:HE2	1.92	0.53
1:A:28:PHE:CE2	1:A:147:LYS:HG3	2.45	0.52
1:J:62:GLU:O	1:G:43:GLN:NE2	2.43	0.52
1:G:70:GLN:HA	1:G:73:ARG:NH1	2.24	0.52
1:A:22:GLN:CD	1:A:149:ARG:HG3	2.34	0.52
1:G:99:GLN:O	1:G:103:VAL:HG23	2.09	0.52
1:A:59:ALA:HA	2:D:66:TYR:HD2	1.74	0.52
1:A:34:PRO:O	2:D:67:ASP:HA	2.09	0.51
1:J:68:ARG:O	1:J:71:TYR:N	2.40	0.51
1:A:28:PHE:HD1	5:A:309:HOH:O	1.91	0.51
1:J:37:GLU:OE2	1:J:68:ARG:NE	2.44	0.51
1:A:59:ALA:HA	2:D:66:TYR:CD2	2.46	0.51
1:M:41:ARG:HA	1:M:53:LEU:O	2.11	0.51
1:G:76:GLU:HB2	1:G:163:ILE:HD13	1.93	0.50
1:A:98:GLU:O	1:A:102:ARG:HG3	2.11	0.50
1:G:72:MET:HB3	1:G:103:VAL:HG11	1.93	0.50
1:M:59:ALA:O	1:M:61:GLN:NE2	2.36	0.50
1:A:32:TYR:HD2	2:D:66:TYR:OH	1.95	0.50
1:J:72:MET:HA	5:J:301:HOH:O	2.11	0.50
1:G:56:LEU:HB2	1:G:71:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:OE1	1:A:164:ARG:NH2	2.44	0.49
1:A:14:VAL:CG2	1:A:81:VAL:HG23	2.42	0.49
1:A:70:GLN:OE1	1:A:73:ARG:NH1	2.46	0.49
1:J:7:VAL:HB	1:J:78:PHE:CD2	2.47	0.49
1:M:23:LEU:HD22	1:M:156:PHE:CD2	2.47	0.48
1:G:117:LYS:HG2	3:G:201:GDP:C6	2.48	0.48
1:A:129:GLN:HG3	5:A:312:HOH:O	2.14	0.48
1:G:45:VAL:HA	1:G:49:GLU:O	2.13	0.48
1:G:167:LYS:NZ	5:G:304:HOH:O	2.46	0.48
1:A:34:PRO:O	2:D:66:TYR:CD2	2.66	0.47
1:A:59:ALA:CB	2:D:66:TYR:HD2	2.27	0.47
1:J:104:LYS:HB3	5:J:322:HOH:O	2.15	0.47
1:A:33:ASP:N	5:A:304:HOH:O	2.48	0.46
1:G:19:LEU:HD23	1:G:146:ALA:HB2	1.96	0.46
1:A:33:ASP:HB3	1:A:36:ILE:HG13	1.97	0.46
1:J:24:ILE:HA	1:J:42:LYS:HD2	1.98	0.46
1:J:23:LEU:HD22	1:J:156:PHE:CG	2.51	0.46
1:M:23:LEU:HD22	1:M:156:PHE:CG	2.49	0.46
1:M:99:GLN:HG3	1:M:102:ARG:HH12	1.81	0.46
1:G:1:MET:HE2	1:G:50:THR:C	2.41	0.46
1:M:24:ILE:HG21	1:M:40:TYR:HD2	1.81	0.46
1:A:134:ALA:HB2	1:A:141:PHE:HB2	1.98	0.46
1:M:7:VAL:HB	1:M:78:PHE:CD2	2.51	0.46
1:A:34:PRO:HA	2:D:66:TYR:CE1	2.51	0.45
1:G:119:ASP:OD2	3:G:201:GDP:N2	2.43	0.45
1:A:34:PRO:HB2	2:D:67:ASP:O	2.17	0.45
1:A:34:PRO:HB3	2:D:66:TYR:O	2.16	0.45
1:J:35:THR:HB	1:J:61:GLN:HG3	1.98	0.45
1:A:24:ILE:HD11	1:A:55:ILE:HD12	1.98	0.45
1:A:35:THR:HG22	2:D:67:ASP:CB	2.46	0.45
1:A:45:VAL:HA	1:A:49:GLU:O	2.17	0.44
1:J:98:GLU:O	1:J:102:ARG:HG3	2.16	0.44
1:M:66:ALA:O	1:M:70:GLN:HG2	2.16	0.44
1:G:1:MET:SD	1:G:43:GLN:OE1	2.75	0.44
1:A:94:HIS:O	1:A:98:GLU:HG2	2.17	0.44
1:A:32:TYR:CD2	2:D:66:TYR:OH	2.71	0.44
1:A:28:PHE:HE1	3:A:201:GDP:C8	2.36	0.44
1:J:56:LEU:HB2	1:J:71:TYR:CD1	2.53	0.44
1:A:12:VAL:CG2	2:D:70:GLY:H	2.30	0.43
1:G:126:ASP:OD1	1:G:129:GLN:HB2	2.17	0.43
1:A:7:VAL:HB	1:A:78:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LEU:HD22	1:J:156:PHE:CD2	2.53	0.43
3:J:201:GDP:H5''	5:J:305:HOH:O	2.18	0.43
1:J:65:SER:HB3	1:J:68:ARG:HB3	1.99	0.43
1:J:93:ILE:HD13	1:J:93:ILE:HA	1.90	0.43
1:G:70:GLN:HA	1:G:73:ARG:HH12	1.83	0.43
1:A:22:GLN:CG	1:A:149:ARG:HG3	2.47	0.43
1:A:59:ALA:CA	2:D:66:TYR:HD2	2.32	0.43
1:J:70:GLN:OE1	1:J:73:ARG:NH2	2.45	0.43
1:G:33:ASP:HB3	1:G:36:ILE:HG13	2.01	0.43
1:A:12:VAL:H	2:D:74:TYR:HE1	1.65	0.43
1:J:117:LYS:HG2	3:J:201:GDP:C6	2.54	0.43
1:G:23:LEU:O	1:G:42:LYS:NZ	2.48	0.43
1:A:142:ILE:HD13	1:A:155:ALA:HA	2.01	0.42
1:J:73:ARG:O	1:J:104:LYS:NZ	2.51	0.42
1:M:6:LEU:HD13	1:M:159:LEU:HD23	2.01	0.42
1:A:103:VAL:HG13	1:J:48:GLY:HA3	2.00	0.42
1:J:1:M:1:MET:SD	1:J:52:LEU:HG	2.59	0.42
1:J:99:GLN:HG2	1:G:47:ASP:HA	2.02	0.42
1:G:67:MET:HA	1:G:70:GLN:HB2	2.00	0.42
1:M:21:ILE:HG21	1:M:29:VAL:CG2	2.49	0.42
1:A:12:VAL:HG23	2:D:66:TYR:HA	2.01	0.42
1:A:132:ASP:OD1	1:A:135:ARG:NH2	2.49	0.42
1:J:65:SER:HB2	1:J:68:ARG:NH1	2.34	0.42
1:M:93:ILE:HD13	1:M:93:ILE:HA	1.94	0.42
1:M:133:LEU:HD11	1:M:137:TYR:CZ	2.55	0.42
1:M:21:ILE:HD13	1:M:29:VAL:HG21	2.01	0.42
1:A:61:GLN:HG3	2:D:67:ASP:CG	2.45	0.41
1:A:134:ALA:CB	1:A:141:PHE:HB2	2.50	0.41
1:M:101:LYS:HB2	1:M:101:LYS:HE3	1.63	0.41
1:A:23:LEU:HD22	1:A:156:PHE:CD2	2.56	0.41
1:J:68:ARG:NH1	1:G:50:THR:HB	2.35	0.41
1:A:5:LYS:HB2	1:A:5:LYS:HE2	1.61	0.41
3:A:201:GDP:H5''	2:D:71:SER:HA	2.01	0.41
1:A:133:LEU:HD11	1:A:137:TYR:CZ	2.56	0.41
1:A:112:VAL:HG23	1:A:159:LEU:HD13	2.03	0.41
3:A:201:GDP:O1B	2:D:66:TYR:CE1	2.74	0.41
1:M:87:THR:O	1:M:91:GLU:HG3	2.21	0.41
1:G:70:GLN:HG3	1:G:73:ARG:HH12	1.86	0.41
1:J:37:GLU:OE2	1:J:68:ARG:HB2	2.20	0.40
1:G:23:LEU:HD22	1:G:156:PHE:CG	2.57	0.40
1:G:101:LYS:HG2	1:G:106:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HA	1:A:42:LYS:HD2	2.03	0.40
1:M:33:ASP:HA	1:M:34:PRO:HD2	1.92	0.40
1:G:68:ARG:O	1:G:72:MET:HG2	2.21	0.40
1:G:70:GLN:CG	1:G:73:ARG:HH12	2.35	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	166/174 (95%)	161 (97%)	5 (3%)	0	100	100
1	G	166/174 (95%)	164 (99%)	2 (1%)	0	100	100
1	J	166/174 (95%)	163 (98%)	2 (1%)	1 (1%)	21	25
1	M	166/174 (95%)	161 (97%)	4 (2%)	1 (1%)	21	25
2	D	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
All	All	672/706 (95%)	653 (97%)	15 (2%)	4 (1%)	21	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	122	SER
2	D	72	ASP
2	D	73	LYS
1	M	167	LYS

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	147/155 (95%)	146 (99%)	1 (1%)	76	86
1	G	147/155 (95%)	147 (100%)	0	100	100
1	J	147/155 (95%)	147 (100%)	0	100	100
1	M	147/155 (95%)	146 (99%)	1 (1%)	76	86
2	D	8/8 (100%)	8 (100%)	0	100	100
All	All	596/628 (95%)	594 (100%)	2 (0%)	86	92

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

Mol	Chain	Res	Type
1	A	150	GLN
1	M	73	ARG

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	86	ASN
1	J	43	GLN
1	J	99	GLN
1	G	43	GLN
1	G	95	HIS
1	G	131	GLN
1	G	166	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	M	201	4	29,30,30	1.12	2 (6%)	45,47,47	1.99	8 (17%)
3	GDP	G	201	-	29,30,30	1.42	5 (17%)	45,47,47	1.91	9 (20%)
3	GDP	J	201	4	29,30,30	1.33	3 (10%)	45,47,47	2.17	11 (24%)
3	GDP	A	201	4	29,30,30	1.22	4 (13%)	45,47,47	2.06	14 (31%)

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	GDP	M	201	4	-	0/16/32/32	0/3/3/3
3	GDP	G	201	-	-	5/16/32/32	0/3/3/3
3	GDP	J	201	4	-	5/16/32/32	0/3/3/3
3	GDP	A	201	4	-	6/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	201	GDP	C5-C4	3.60	1.48	1.38
3	G	201	GDP	PA-O3A	3.40	1.63	1.59
3	J	201	GDP	C6-N1	-3.40	1.32	1.38
3	J	201	GDP	PA-O3A	-3.10	1.56	1.59
3	M	201	GDP	C5-C4	2.95	1.46	1.38
3	A	201	GDP	C5-C4	2.91	1.46	1.38
3	J	201	GDP	C5-C4	2.87	1.46	1.38
3	A	201	GDP	C6-N1	-2.67	1.33	1.38
3	A	201	GDP	C5-N7	-2.64	1.33	1.39
3	G	201	GDP	C6-N1	-2.43	1.34	1.38
3	M	201	GDP	C5-N7	-2.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	201	GDP	C5-N7	-2.04	1.35	1.39
3	A	201	GDP	C4-N9	-2.02	1.32	1.38
3	G	201	GDP	C2-N3	2.00	1.38	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201	GDP	C5-C4-N3	-6.36	118.26	128.39
3	J	201	GDP	C5-C4-N3	-6.33	118.31	128.39
3	M	201	GDP	C5-C4-N3	-6.32	118.33	128.39
3	J	201	GDP	C2-N3-C4	5.68	122.08	112.30
3	M	201	GDP	C2-N3-C4	5.37	121.56	112.30
3	A	201	GDP	N9-C4-N3	5.26	136.47	125.95
3	A	201	GDP	C5-C4-N3	-5.09	120.29	128.39
3	J	201	GDP	N9-C4-N3	5.07	136.10	125.95
3	M	201	GDP	N9-C4-N3	4.94	135.83	125.95
3	G	201	GDP	C2-N3-C4	4.92	120.77	112.30
3	G	201	GDP	N9-C4-N3	4.86	135.66	125.95
3	A	201	GDP	O4'-C1'-N9	-4.33	98.55	108.36
3	A	201	GDP	C2-N3-C4	4.03	119.23	112.30
3	J	201	GDP	C6-C5-N7	3.81	137.22	130.29
3	A	201	GDP	O2A-PA-O3A	3.69	117.25	107.27
3	J	201	GDP	O4'-C1'-N9	3.50	116.28	108.36
3	A	201	GDP	O6-C6-C5	-3.45	117.43	126.53
3	M	201	GDP	O6-C6-C5	-3.30	117.81	126.53
3	J	201	GDP	C5'-C4'-C3'	-3.17	103.81	115.21
3	J	201	GDP	C5-C6-N1	2.85	120.50	113.25
3	G	201	GDP	O2B-PB-O3A	2.81	114.05	104.64
3	M	201	GDP	C6-C5-N7	2.80	135.38	130.29
3	G	201	GDP	C6-C5-N7	2.78	135.34	130.29
3	J	201	GDP	C2'-C1'-N9	-2.71	105.72	113.25
3	G	201	GDP	O4'-C1'-C2'	-2.70	100.83	106.62
3	G	201	GDP	O2'-C2'-C1'	2.69	119.36	110.10
3	A	201	GDP	C8-N9-C4	2.60	110.91	106.03
3	G	201	GDP	O2A-PA-O5'	2.55	119.14	107.57
3	M	201	GDP	C4-C5-N7	-2.53	106.65	110.67
3	A	201	GDP	O6-C6-N1	2.42	124.66	120.11
3	J	201	GDP	C6-C5-C4	-2.32	115.34	118.83
3	A	201	GDP	C6-C5-N7	2.28	134.43	130.29
3	A	201	GDP	O5'-C5'-C4'	2.24	116.63	108.99
3	M	201	GDP	O4'-C1'-N9	2.18	113.29	108.36
3	A	201	GDP	O2B-PB-O3A	2.15	111.85	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201	GDP	C4-C5-N7	-2.15	107.27	110.67
3	J	201	GDP	C2'-C3'-C4'	2.15	106.76	102.61
3	A	201	GDP	C3'-C2'-C1'	-2.14	97.42	101.46
3	M	201	GDP	O6-C6-N1	2.05	123.98	120.11
3	A	201	GDP	O4'-C1'-C2'	-2.05	102.23	106.62
3	J	201	GDP	C4-C5-N7	-2.04	107.44	110.67
3	A	201	GDP	O3'-C3'-C4'	-2.00	105.33	111.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GDP	C5'-O5'-PA-O3A
3	A	201	GDP	C5'-O5'-PA-O2A
3	J	201	GDP	C5'-O5'-PA-O3A
3	J	201	GDP	C5'-O5'-PA-O1A
3	J	201	GDP	C5'-O5'-PA-O2A
3	G	201	GDP	C5'-O5'-PA-O3A
3	G	201	GDP	C5'-O5'-PA-O1A
3	G	201	GDP	C5'-O5'-PA-O2A
3	J	201	GDP	O4'-C4'-C5'-O5'
3	J	201	GDP	C3'-C4'-C5'-O5'
3	A	201	GDP	C3'-C4'-C5'-O5'
3	G	201	GDP	O4'-C4'-C5'-O5'
3	A	201	GDP	O4'-C4'-C5'-O5'
3	A	201	GDP	C5'-O5'-PA-O1A
3	G	201	GDP	C3'-C4'-C5'-O5'
3	A	201	GDP	C4'-C5'-O5'-PA

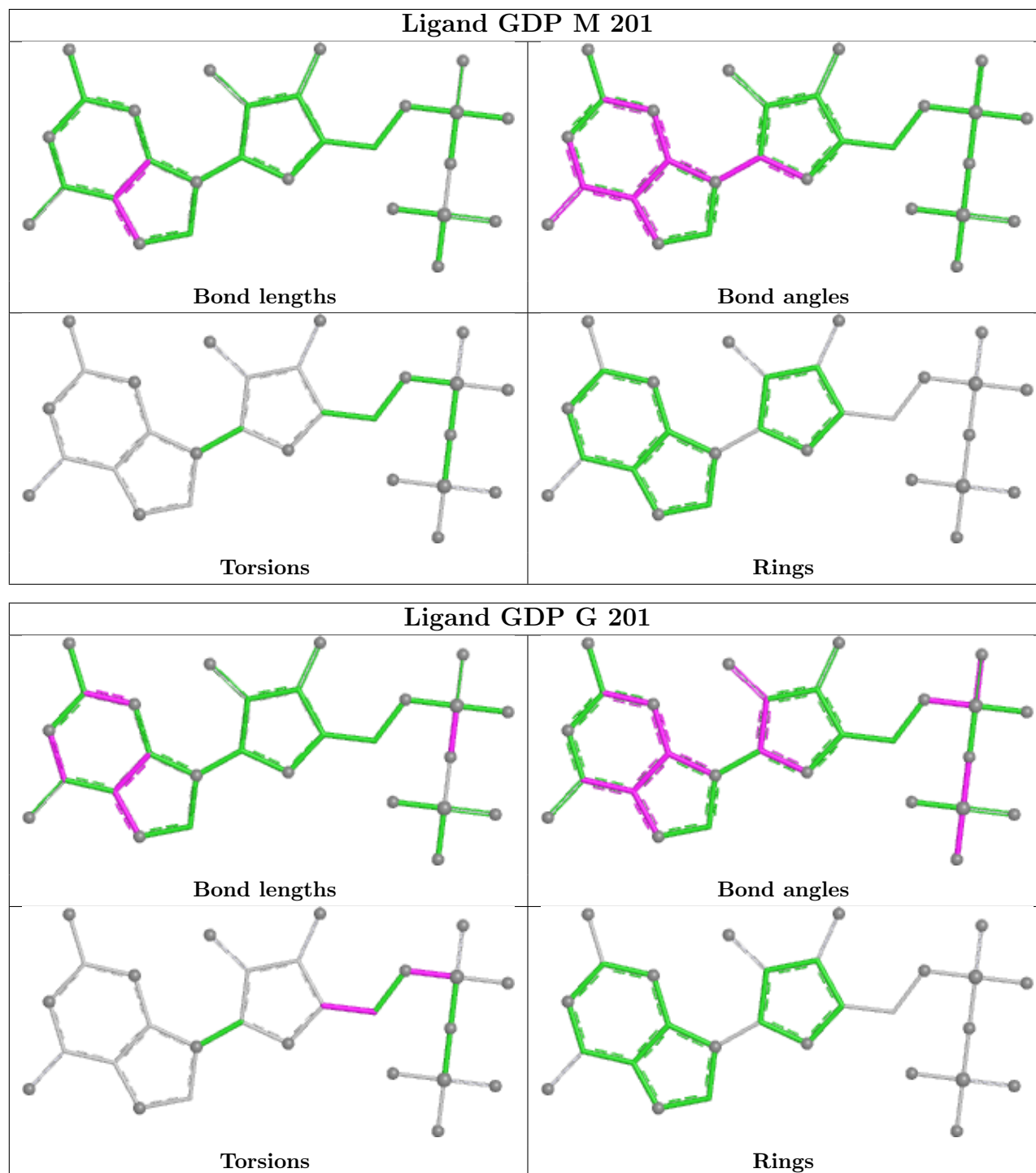
There are no ring outliers.

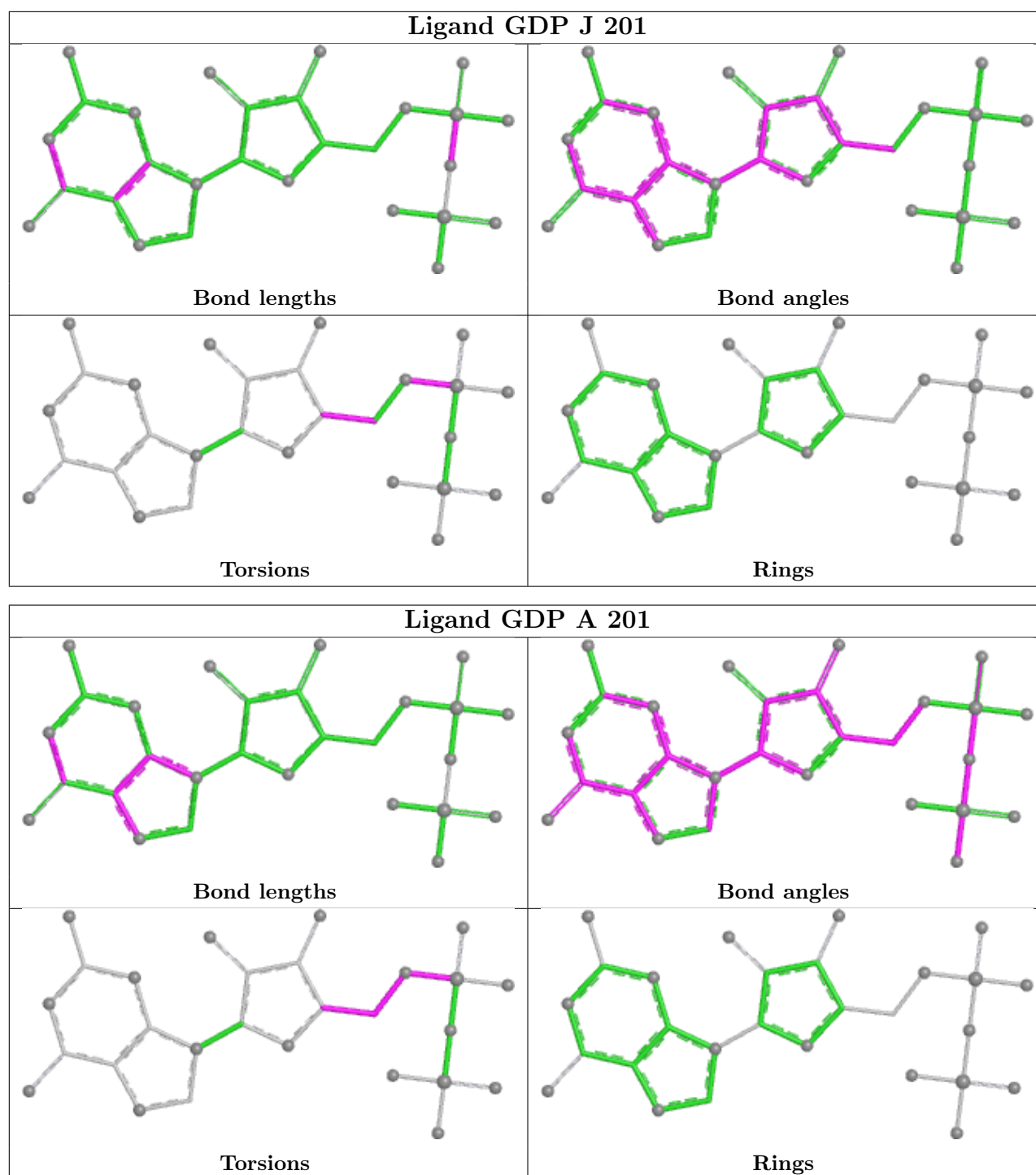
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	201	GDP	3	0
3	J	201	GDP	2	0
3	A	201	GDP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	168/174 (96%)	2.12	79 (47%) 0 0	20, 34, 45, 70	0
1	G	168/174 (96%)	2.07	80 (47%) 0 0	17, 34, 47, 53	0
1	J	168/174 (96%)	1.36	29 (17%) 4 4	7, 19, 60, 98	0
1	M	168/174 (96%)	1.76	59 (35%) 1 1	17, 30, 44, 55	0
2	D	10/10 (100%)	2.34	4 (40%) 1 0	26, 33, 37, 44	0
All	All	682/706 (96%)	1.84	251 (36%) 1 0	7, 30, 46, 98	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	66	ALA	10.3
1	A	1	MET	8.8
1	J	67	MET	8.4
1	A	127	THR	8.0
1	A	52	LEU	7.1
1	J	69	ASP	6.8
1	G	152	VAL	6.7
1	J	103	VAL	6.4
1	G	112	VAL	6.0
1	J	70	GLN	6.0
1	A	35	THR	5.8
1	J	64	TYR	5.5
1	J	65	SER	5.4
1	J	71	TYR	5.3
1	J	63	GLU	5.1
1	J	62	GLU	5.0
1	J	72	MET	4.8
1	M	124	THR	4.7
1	G	68	ARG	4.7
1	G	43	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	153	ASP	4.6
1	A	42	LYS	4.6
1	G	114	VAL	4.5
1	A	22	GLN	4.5
1	A	109	VAL	4.5
1	A	65	SER	4.4
2	D	66	TYR	4.4
1	M	15	GLY	4.4
1	G	1	MET	4.4
1	J	74	THR	4.4
1	G	55	ILE	4.4
1	G	95	HIS	4.3
1	M	77	GLY	4.3
1	A	23	LEU	4.2
1	G	50	THR	4.2
1	A	78	PHE	4.1
1	M	127	THR	4.1
1	G	29	VAL	4.0
1	A	97	ARG	3.9
2	D	67	ASP	3.9
1	G	64	TYR	3.9
2	D	68	VAL	3.9
1	J	75	GLY	3.9
1	M	130	ALA	3.8
1	G	71	TYR	3.8
1	M	74	THR	3.8
1	M	82	PHE	3.8
1	M	137	TYR	3.7
1	A	7	VAL	3.7
1	G	40	TYR	3.7
1	A	161	ARG	3.7
1	M	71	TYR	3.7
1	G	32	TYR	3.7
1	A	110	PRO	3.7
1	G	76	GLU	3.6
1	G	48	GLY	3.6
1	G	66	ALA	3.6
1	A	73	ARG	3.6
1	M	14	VAL	3.6
1	G	113	LEU	3.6
1	M	168	GLU	3.6
1	M	19	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	133	LEU	3.6
1	M	106	SER	3.5
1	A	79	LEU	3.5
2	D	65	LEU	3.5
1	G	86	ASN	3.5
1	A	33	ASP	3.5
1	M	103	VAL	3.5
1	A	111	MET	3.4
1	M	125	VAL	3.4
1	G	28	PHE	3.4
1	G	54	ASP	3.4
1	G	84	ILE	3.4
1	M	40	TYR	3.4
1	G	45	VAL	3.4
1	A	60	GLY	3.3
1	A	142	ILE	3.3
1	A	71	TYR	3.3
1	G	67	MET	3.3
1	A	80	CYS	3.3
1	A	158	THR	3.3
1	A	12	VAL	3.3
1	G	103	VAL	3.3
1	M	100	ILE	3.2
1	M	48	GLY	3.2
1	G	58	THR	3.2
1	A	29	VAL	3.2
1	G	52	LEU	3.2
1	J	73	ARG	3.2
1	M	17	SER	3.2
1	M	136	SER	3.2
1	A	45	VAL	3.2
1	G	159	LEU	3.2
1	A	13	GLY	3.1
1	M	150	GLN	3.1
1	M	104	LYS	3.1
1	G	122	SER	3.1
1	A	38	ASP	3.1
1	M	133	LEU	3.1
1	A	152	VAL	3.1
1	G	110	PRO	3.1
1	M	157	TYR	3.0
1	G	42	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	3.0
1	A	70	GLN	3.0
1	J	50	THR	3.0
1	A	43	GLN	3.0
1	A	62	GLU	3.0
1	A	107	GLU	3.0
1	A	103	VAL	3.0
1	J	61	GLN	3.0
1	A	64	TYR	3.0
1	J	68	ARG	3.0
1	M	164	ARG	3.0
1	A	47	ASP	3.0
1	A	113	LEU	2.9
1	G	96	TYR	2.9
1	M	89	SER	2.9
1	A	114	VAL	2.9
1	M	97	ARG	2.9
1	G	51	CYS	2.9
1	M	142	ILE	2.9
1	G	11	ALA	2.9
1	A	8	VAL	2.9
1	G	157	TYR	2.8
1	J	51	CYS	2.8
1	G	85	ASN	2.8
1	G	65	SER	2.8
1	G	138	GLY	2.8
1	J	146	ALA	2.8
1	A	56	LEU	2.8
1	A	93	ILE	2.8
1	G	57	ASP	2.8
1	A	120	LEU	2.8
1	J	56	LEU	2.8
1	M	53	LEU	2.8
1	A	141	PHE	2.8
1	G	99	GLN	2.7
1	G	33	ASP	2.7
1	G	158	THR	2.7
1	A	136	SER	2.7
1	A	112	VAL	2.7
1	M	109	VAL	2.7
1	G	132	ASP	2.7
1	A	15	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	21	ILE	2.7
1	A	121	PRO	2.7
1	G	79	LEU	2.7
1	G	22	GLN	2.7
1	M	78	PHE	2.7
1	A	160	VAL	2.7
1	A	2	THR	2.7
1	M	129	GLN	2.6
1	G	49	GLU	2.6
1	M	7	VAL	2.6
1	A	74	THR	2.6
1	G	111	MET	2.6
1	G	53	LEU	2.6
1	A	117	LYS	2.6
1	A	46	ILE	2.6
1	G	135	ARG	2.6
1	A	36	ILE	2.6
1	G	70	GLN	2.6
1	M	141	PHE	2.6
1	J	29	VAL	2.6
1	J	100	ILE	2.6
1	M	64	TYR	2.6
1	A	94	HIS	2.6
1	J	107	GLU	2.5
1	G	83	ALA	2.5
1	G	47	ASP	2.5
1	G	121	PRO	2.5
1	M	84	ILE	2.5
1	M	23	LEU	2.5
1	G	46	ILE	2.5
1	A	98	GLU	2.5
1	G	120	LEU	2.5
1	G	81	VAL	2.5
1	M	42	LYS	2.5
1	G	123	ARG	2.4
1	M	36	ILE	2.4
1	A	92	ASP	2.4
1	M	131	GLN	2.4
1	G	91	GLU	2.4
1	A	55	ILE	2.4
1	M	112	VAL	2.4
1	A	11	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	2.4
1	A	90	PHE	2.4
1	M	160	VAL	2.4
1	J	168	GLU	2.4
1	M	111	MET	2.3
1	G	72	MET	2.3
1	G	100	ILE	2.3
1	G	80	CYS	2.3
1	A	115	GLY	2.3
1	J	48	GLY	2.3
1	J	59	ALA	2.3
1	G	156	PHE	2.3
1	A	148	THR	2.3
1	A	5	LYS	2.3
1	A	159	LEU	2.2
1	A	26	ASN	2.2
1	A	116	ASN	2.2
1	A	153	ASP	2.2
1	G	69	ASP	2.2
1	A	34	PRO	2.2
1	M	107	GLU	2.2
1	A	6	LEU	2.2
1	A	57	ASP	2.2
1	M	135	ARG	2.2
1	M	44	VAL	2.2
1	M	102	ARG	2.2
1	M	110	PRO	2.2
1	A	39	SER	2.2
1	J	159	LEU	2.2
1	M	55	ILE	2.2
1	G	142	ILE	2.2
1	G	163	ILE	2.2
1	M	126	ASP	2.2
1	G	8	VAL	2.2
1	M	128	LYS	2.2
1	G	134	ALA	2.2
1	M	21	ILE	2.1
1	M	46	ILE	2.1
1	M	105	ASP	2.1
1	G	109	VAL	2.1
1	G	78	PHE	2.1
1	M	85	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	166	HIS	2.1
1	A	144	THR	2.1
1	J	6	LEU	2.1
1	M	108	ASP	2.1
1	G	13	GLY	2.1
1	G	15	GLY	2.1
1	G	106	SER	2.1
1	A	105	ASP	2.1
1	M	12	VAL	2.1
1	G	9	VAL	2.1
1	G	44	VAL	2.1
1	A	122	SER	2.0
1	A	130	ALA	2.0
1	M	6	LEU	2.0
1	A	84	ILE	2.0
1	G	21	ILE	2.0
1	G	4	TYR	2.0
1	G	149	ARG	2.0
1	G	154	ASP	2.0
1	M	24	ILE	2.0
1	J	128	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

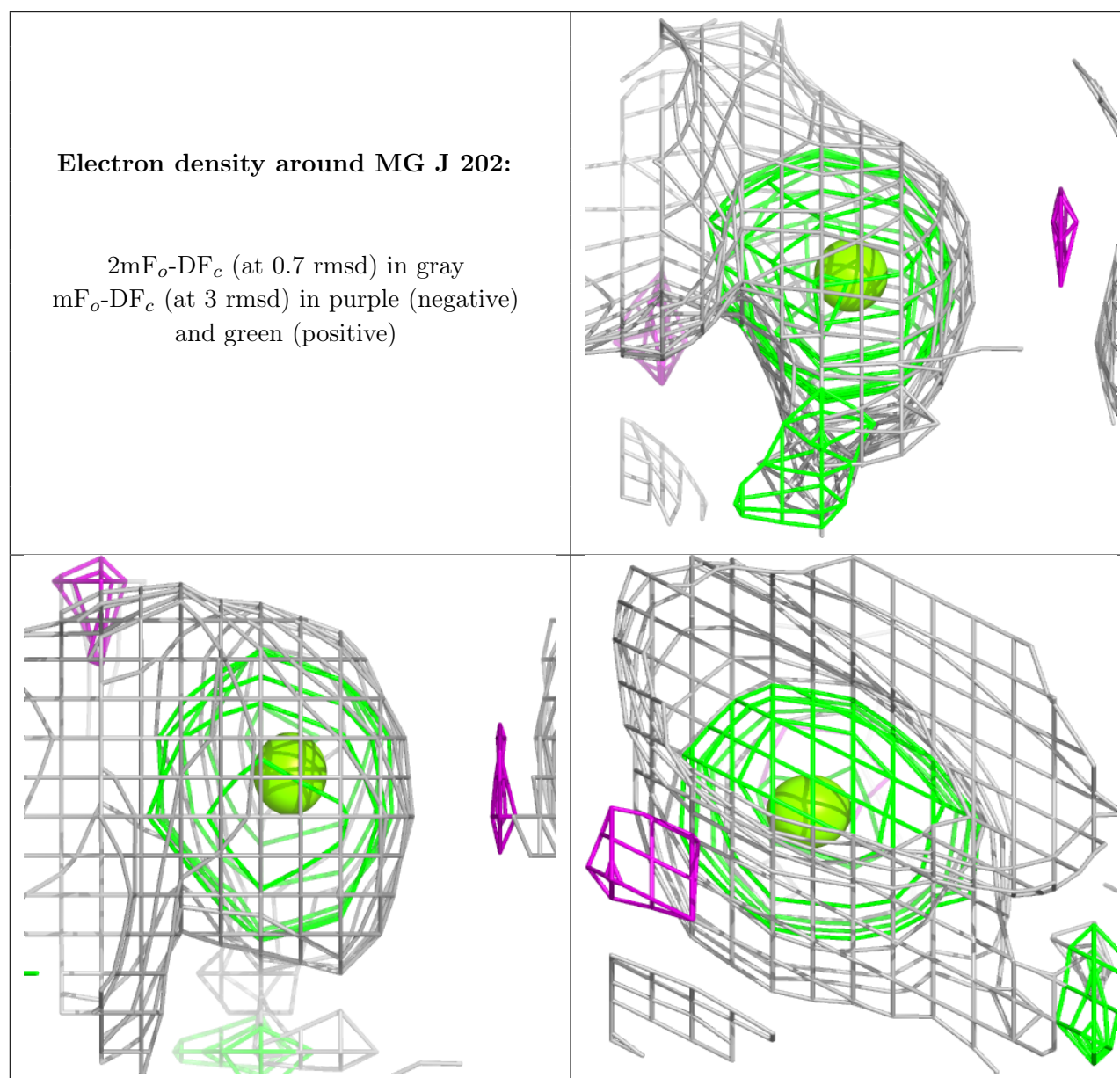
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	J	202	1/1	0.87	0.48	58,58,58,58	0
3	GDP	A	201	28/28	0.88	0.13	17,21,27,28	0

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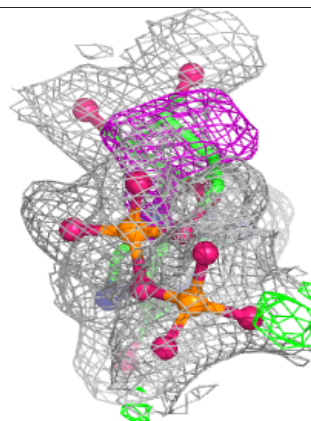
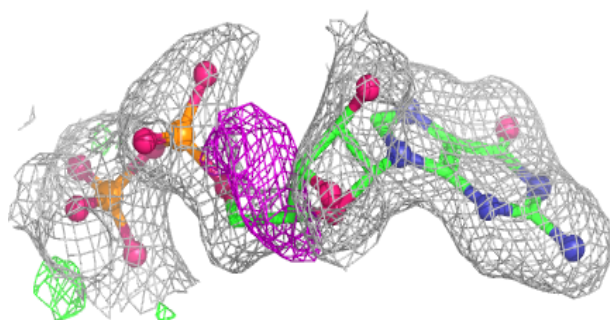
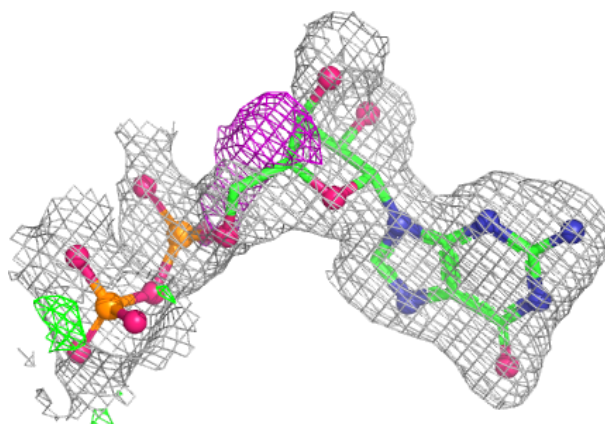
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDP	G	201	28/28	0.93	0.10	13,23,28,29	0
4	MG	A	202	1/1	0.95	0.05	16,16,16,16	0
3	GDP	M	201	28/28	0.95	0.10	10,19,22,24	0
4	MG	M	202	1/1	0.95	0.05	16,16,16,16	0
3	GDP	J	201	28/28	0.97	0.08	3,11,15,21	0
4	MG	G	202	1/1	0.97	0.05	17,17,17,17	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.



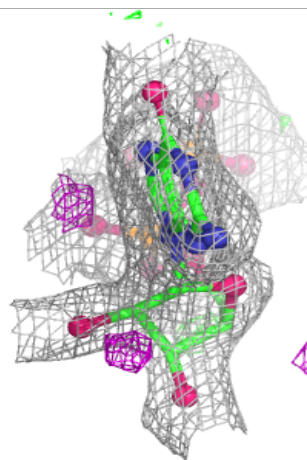
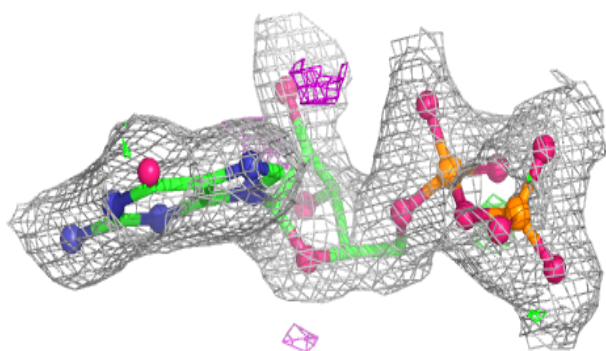
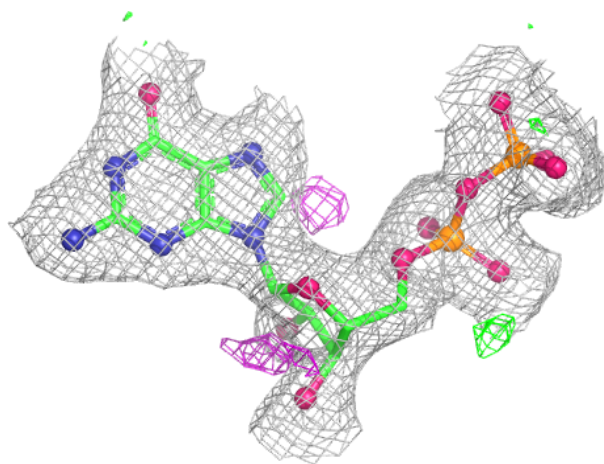
Electron density around GDP A 201:

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



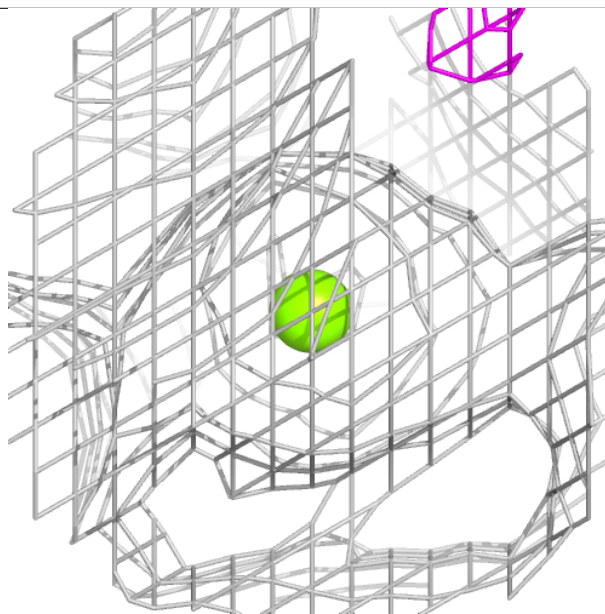
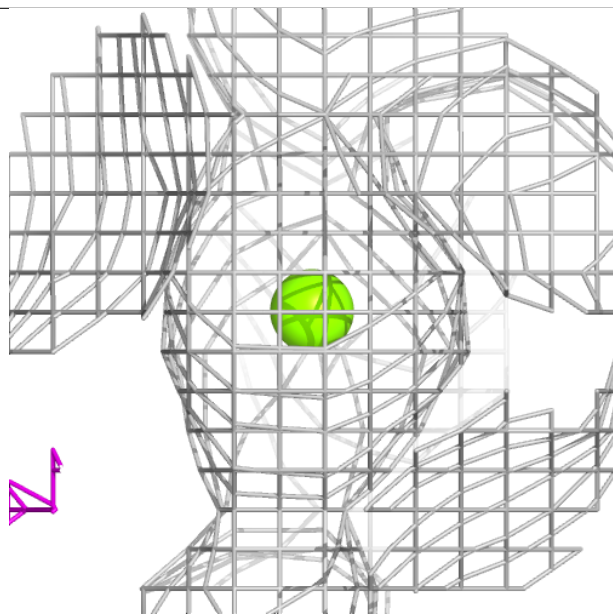
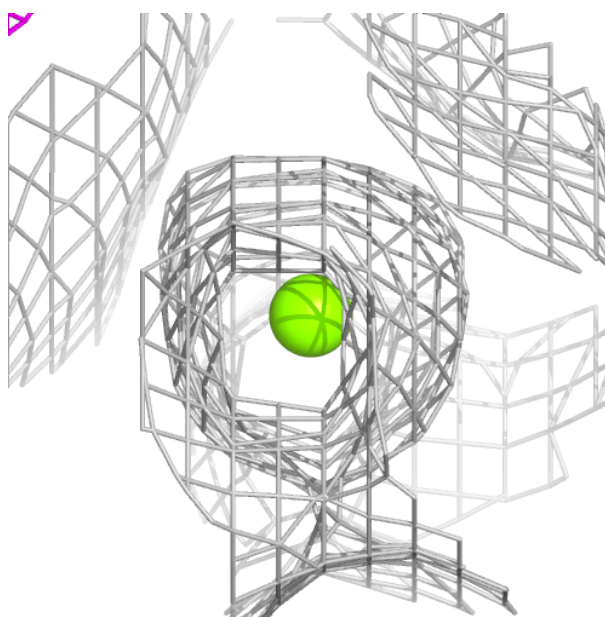
Electron density around GDP G 201:

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



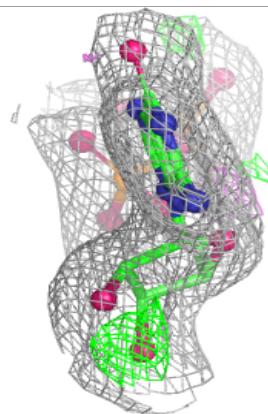
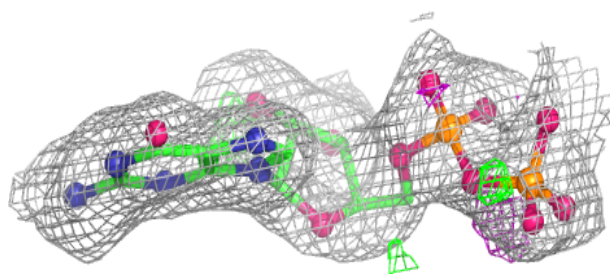
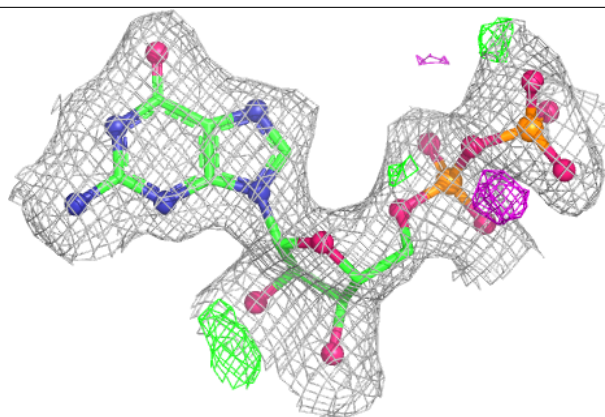
Electron density around MG A 202:

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



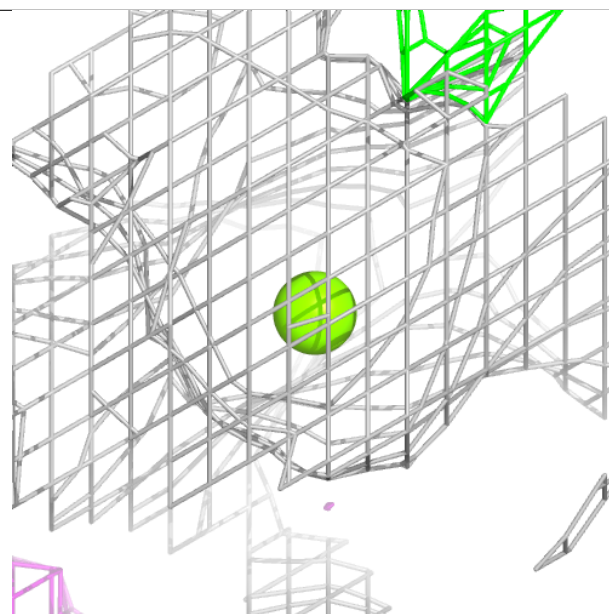
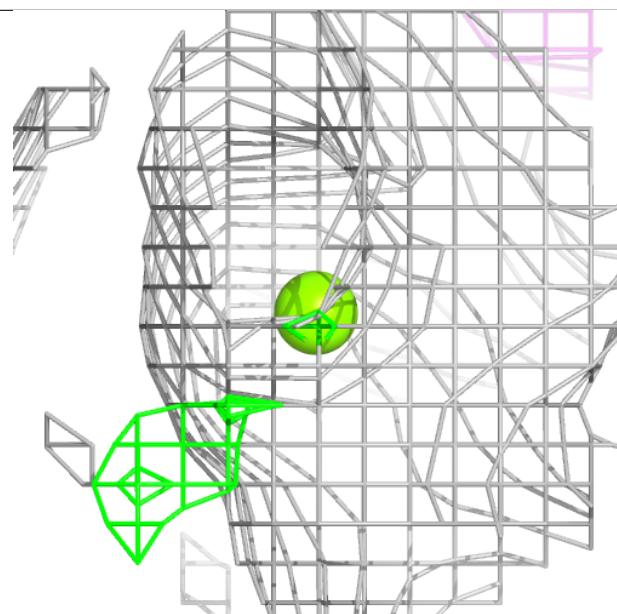
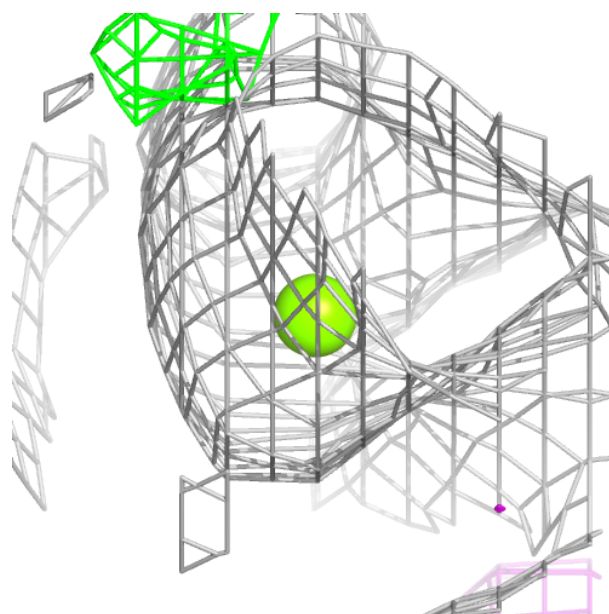
Electron density around GDP M 201:

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



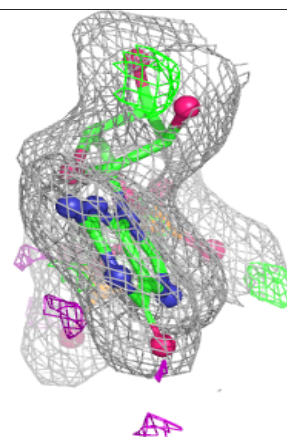
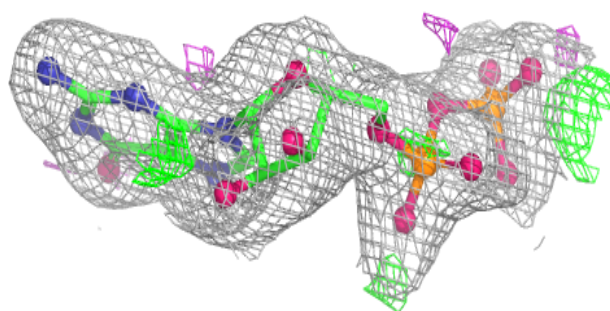
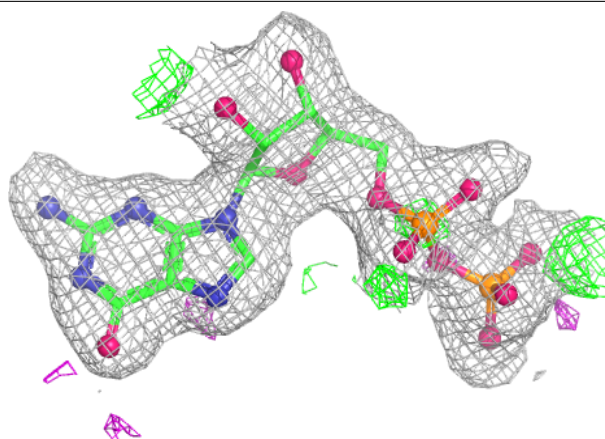
Electron density around MG M 202:

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



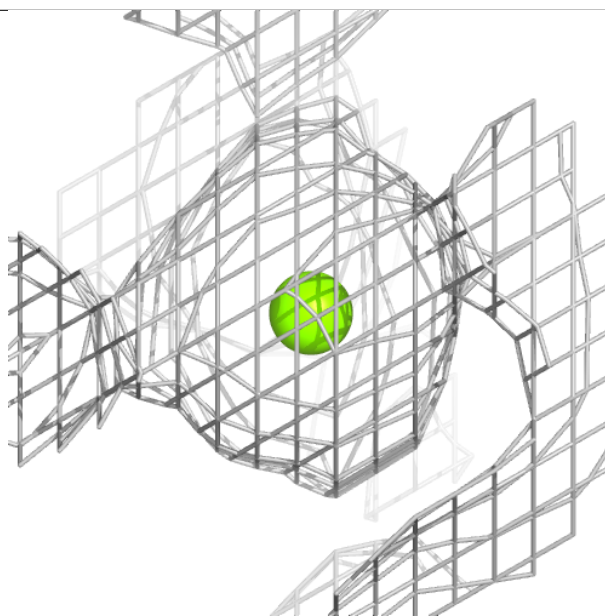
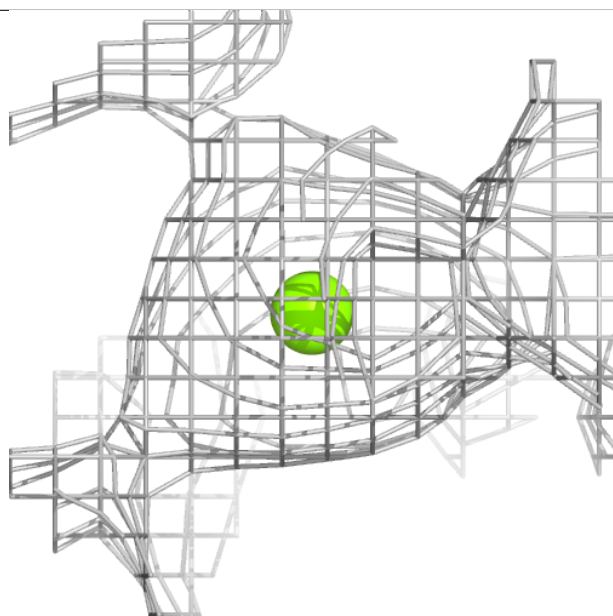
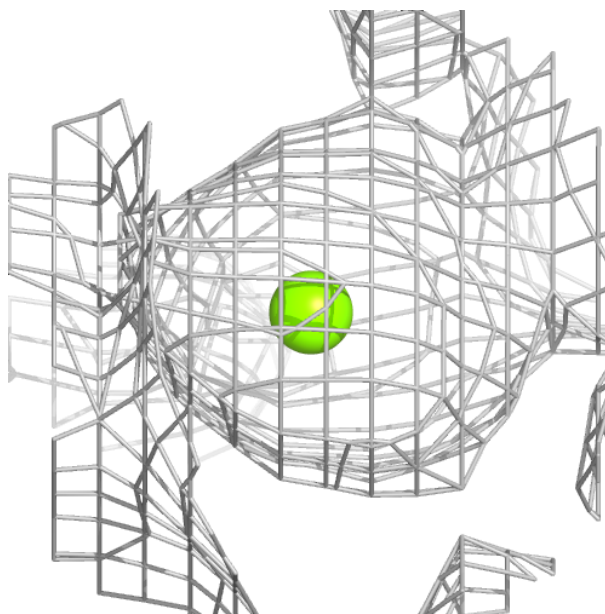
Electron density around GDP J 201:

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



Electron density around MG G 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.