Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 12:49 pm GMT

PDB ID	:	7QTM
Title	:	Transition state analogue of small G protein in complex with relevant GAP
Authors	:	Baumann, P.; Jin, Y.
Deposited on	:	2022-01-14
Resolution	:	2.25 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:

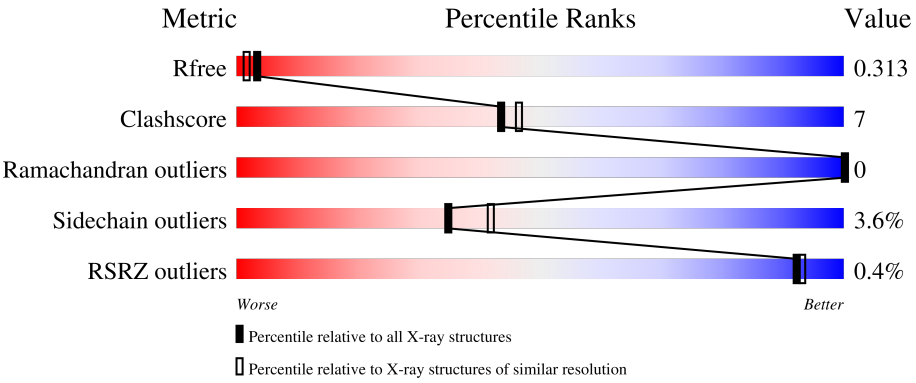
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	244	62% 14% • 23%
1	H	244	65% 12% 23%
2	B	192	% 73% 20% 7%
2	I	192	% 74% 18% • 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6084 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 Rho GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1513	981	254	276	2			
1	H	187	Total	C	N	O	S	0	1	0
			1513	981	254	276	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q07960
A	0	SER	-	expression tag	UNP Q07960
A	85	ALA	ARG	engineered mutation	UNP Q07960
H	-1	GLY	-	expression tag	UNP Q07960
H	0	SER	-	expression tag	UNP Q07960
H	85	ALA	ARG	engineered mutation	UNP Q07960

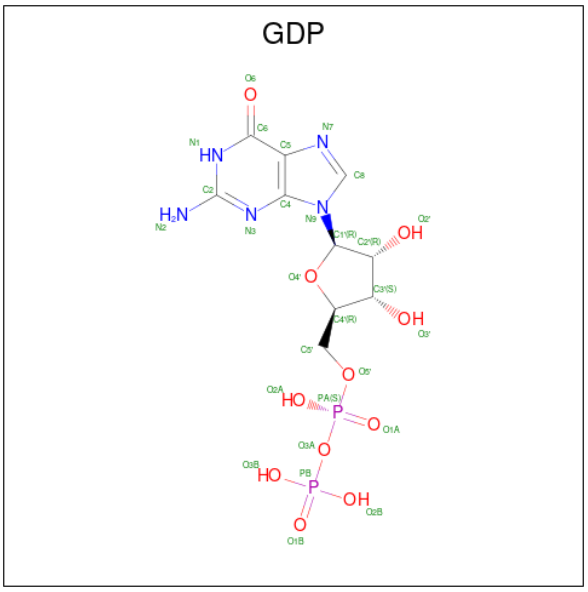
- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	178	Total	C	F	N	O	S	0	0	0
			1412	889	2	240	271	10			
2	I	178	Total	C	F	N	O	S	0	0	0
			1412	889	2	240	271	10			

There are 2 discrepancies between the modelled and reference sequences:

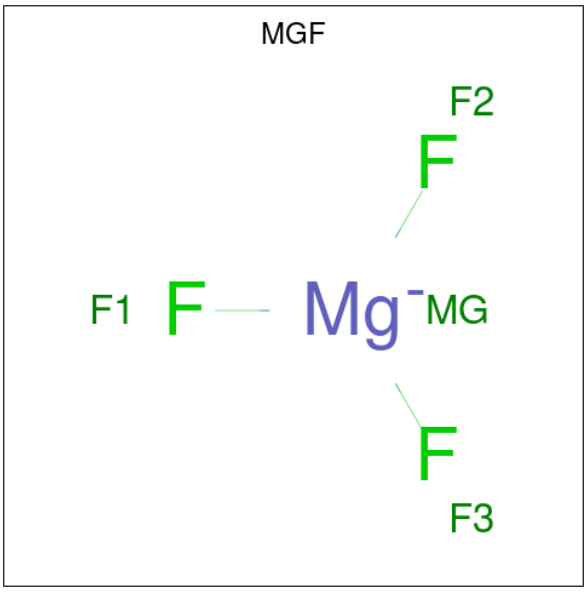
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	PHE	engineered mutation	UNP P61586
I	25	ASN	PHE	engineered mutation	UNP P61586

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: 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	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F_3Mg) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	F	Mg	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total F Mg 4 3 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	I	1	Total Mg 1 1	0	0

- Molecule 6 is water.

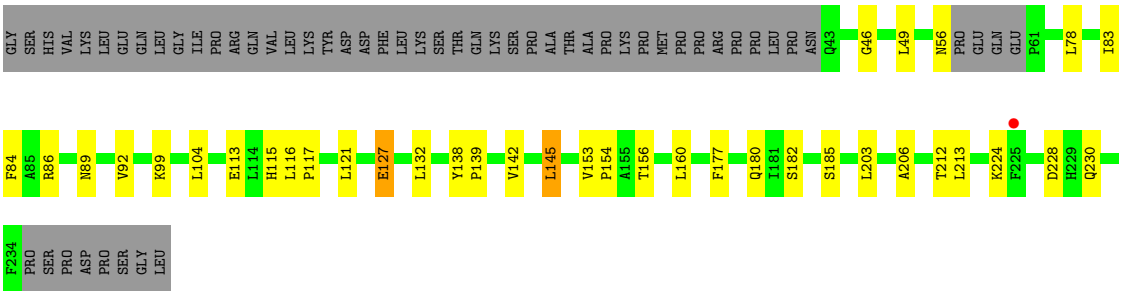
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	27	Total O 27 27	0	0
6	B	43	Total O 46 46	0	3
6	H	49	Total O 49 49	0	0
6	I	46	Total O 46 46	0	0

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.

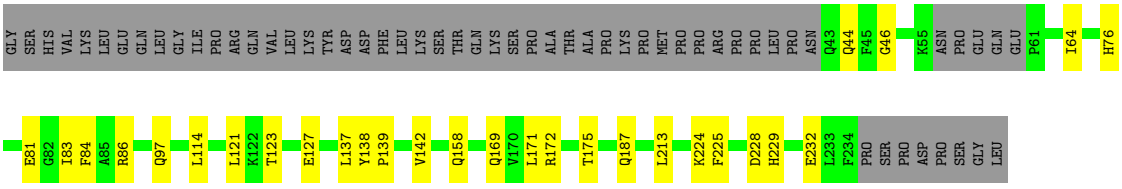
• Molecule 1: Rho GTPase-activating protein 1

Chain A:



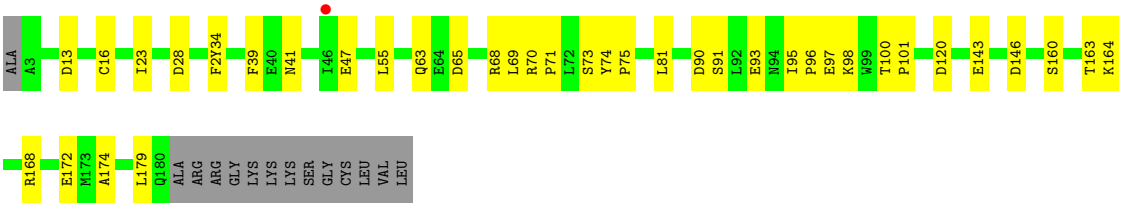
• Molecule 1: Rho GTPase-activating protein 1

Chain H:



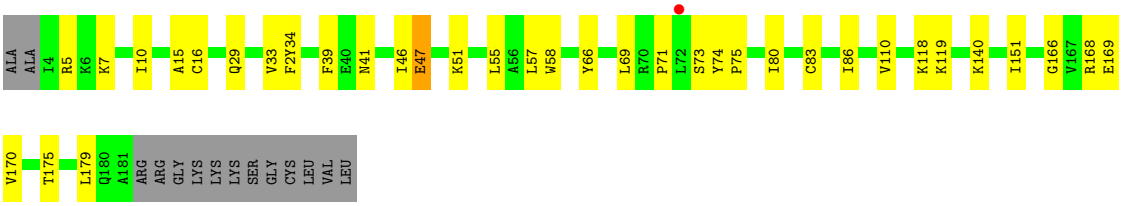
• Molecule 2: Transforming protein RhoA

Chain B:



• Molecule 2: Transforming protein RhoA

Chain I:


ALA ALA
T4
R5
K6
K7
I10
A15 C16
Q29
V33 F2Y34
F39
E40 N41
I46 E47
K51
L55
A56 L57 W58
Y66
L69
R70 P71 L72 S73 Y74 P75
I80
C83
I86
V110
K118 K119
K140
T151
G166
V167 R168 E169
V170
T175
L179
Q180 A181
ARG ARG GLY LYS LYS LYS SER GLY CYS LEU VAL LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.63Å 66.60Å 76.46Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	55.31 – 2.25 55.31 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.31-2.25) 99.8 (55.31-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.304 0.228 , 0.313	Depositor DCC
R_{free} test set	1683 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 19.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.147 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6084	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MGF, F2Y, GDP, 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	0.69	0/1547	0.80	0/2109
1	H	0.70	0/1547	0.77	0/2110
2	B	0.70	0/1423	0.85	0/1923
2	I	0.71	0/1423	0.85	0/1923
All	All	0.70	0/5940	0.82	0/8065

There are no bond length outliers.

There are no bond angle outliers.

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	1513	0	1524	25	0
1	H	1513	0	1524	16	0
2	B	1412	0	1397	21	0
2	I	1412	0	1397	21	0
3	B	28	0	12	0	0
3	I	28	0	12	0	0
4	B	4	0	0	0	0
4	I	4	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1	0	0	0	0
6	A	27	0	0	2	0
6	B	46	0	0	2	0
6	H	49	0	0	2	0
6	I	46	0	0	1	0
All	All	6084	0	5866	79	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 7.

All (79) 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)
2:I:7:LYS:HE3	2:I:58:TRP:CE2	2.15	0.82
2:I:39:PHE:HE2	2:I:73:SER:HG	1.40	0.66
1:A:206:ALA:HB3	1:A:212:THR:OG1	1.96	0.66
1:H:169:GLN:OE1	1:H:172:ARG:NH2	2.31	0.63
1:A:145:LEU:HD23	2:I:29:GLN:HE22	1.63	0.62
1:A:89:ASN:OD1	1:A:92:VAL:HG23	2.03	0.59
2:B:39:PHE:HE2	2:B:73:SER:HG	1.49	0.59
1:H:213:LEU:HD23	6:H:329:HOH:O	2.02	0.59
1:A:86:ARG:HD2	1:A:115:HIS:CE1	2.40	0.57
1:A:99:LYS:HG3	1:A:104:LEU:HB2	1.87	0.56
1:A:46:GLY:HA2	1:A:127:GLU:O	2.05	0.56
2:B:63:GLN:HB3	2:B:65:ASP:OD2	2.05	0.56
2:I:39:PHE:CE2	2:I:73:SER:OG	2.60	0.55
1:A:138:TYR:HB3	1:A:139:PRO:HD3	1.88	0.55
1:H:86:ARG:HD3	2:I:15:ALA:HB3	1.89	0.55
2:B:69:LEU:N	2:B:69:LEU:HD23	2.23	0.53
2:I:7:LYS:HE3	2:I:58:TRP:CZ2	2.43	0.53
1:A:145:LEU:HD23	2:I:29:GLN:NE2	2.24	0.51
2:I:74:TYR:N	2:I:75:PRO:CD	2.73	0.51
1:A:177:PHE:HA	1:A:180:GLN:OE1	2.11	0.51
2:B:93:GLU:OE2	2:B:97:GLU:OE2	2.29	0.51
2:B:93:GLU:O	2:B:96:PRO:HD2	2.11	0.51
2:I:15:ALA:O	2:I:118:LYS:NZ	2.36	0.51
1:H:137:LEU:HA	6:H:301:HOH:O	2.11	0.51
1:H:138:TYR:HB3	1:H:139:PRO:HD3	1.93	0.50
1:H:121:LEU:C	1:H:121:LEU:HD23	2.33	0.50
2:I:80:ILE:HD12	2:I:110:VAL:HG11	1.94	0.49
1:A:132:LEU:HD23	1:A:203:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ASP:OD2	2:B:91:SER:HA	2.12	0.49
2:B:41:ASN:HB3	6:B:324:HOH:O	2.12	0.49
1:H:46:GLY:HA2	1:H:127:GLU:O	2.13	0.48
1:H:123:THR:O	1:H:127:GLU:CG	2.62	0.48
1:H:224:LYS:NZ	1:H:228:ASP:OD2	2.47	0.48
2:B:168:ARG:O	2:B:172:GLU:HG3	2.13	0.48
1:H:171:LEU:O	1:H:175:THR:HG23	2.15	0.47
1:A:83:ILE:O	1:A:84:PHE:HB2	2.14	0.47
2:B:81:LEU:HD21	2:B:174:ALA:HB2	1.97	0.47
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.50	0.46
2:B:120:ASP:OD1	2:B:160:SER:OG	2.33	0.46
1:H:123:THR:O	1:H:127:GLU:HG2	2.15	0.46
2:B:68:ARG:NH1	6:B:320[C]:HOH:O	2.48	0.46
2:I:166:GLY:O	2:I:170:VAL:HG23	2.15	0.46
2:B:74:TYR:N	2:B:75:PRO:CD	2.79	0.46
2:I:47:GLU:HA	2:I:51:LYS:O	2.16	0.46
2:I:46:ILE:HD13	2:I:55:LEU:HD12	1.98	0.45
1:A:156:THR:O	1:A:160:LEU:HG	2.16	0.45
2:I:71:PRO:HA	2:I:74:TYR:CD2	2.51	0.45
2:I:80:ILE:HD12	2:I:110:VAL:CG1	2.46	0.45
2:I:55:LEU:HB3	2:I:57:LEU:HD21	1.99	0.45
1:H:44:GLN:OE1	1:H:64:ILE:HG22	2.17	0.45
1:A:121:LEU:C	1:A:121:LEU:HD23	2.38	0.44
2:B:100:THR:HB	2:B:101:PRO:HD3	1.99	0.44
2:I:86:ILE:HD13	2:I:119:LYS:HA	1.99	0.44
2:I:41:ASN:HB3	6:I:323:HOH:O	2.18	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.91	0.43
1:H:76:HIS:HB3	1:H:114:LEU:HD21	2.01	0.43
1:H:225:PHE:CE1	1:H:229:HIS:CD2	3.06	0.43
1:A:213:LEU:HD23	6:A:315:HOH:O	2.19	0.43
2:B:95:ILE:HB	2:B:96:PRO:HD3	2.01	0.43
1:A:224:LYS:NZ	1:A:228:ASP:OD2	2.49	0.42
1:A:153:VAL:HB	1:A:154:PRO:HD3	2.01	0.42
2:B:143:GLU:O	2:B:146:ASP:HB2	2.19	0.42
1:H:138:TYR:CZ	1:H:142:VAL:HG21	2.55	0.42
1:A:113:GLU:HG3	2:B:90:ASP:OD2	2.20	0.42
1:H:83:ILE:O	1:H:84:PHE:HB2	2.19	0.42
2:B:39:PHE:CE2	2:B:73:SER:OG	2.71	0.41
1:A:127:GLU:HB3	6:A:313:HOH:O	2.19	0.41
1:A:116:LEU:HB3	1:A:117:PRO:CD	2.51	0.41
2:B:55:LEU:HD23	2:B:55:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HG3	1:A:104:LEU:CB	2.49	0.41
1:A:182:SER:O	1:A:185:SER:HB3	2.20	0.41
2:I:10:ILE:HD11	2:I:83:CYS:SG	2.61	0.41
1:A:138:TYR:CZ	1:A:142:VAL:HG11	2.56	0.41
1:A:56:ASN:HD22	1:A:56:ASN:HA	1.75	0.41
1:A:86:ARG:HB2	1:A:115:HIS:CE1	2.56	0.41
2:B:163:THR:O	2:B:164:LYS:HB2	2.20	0.40
2:I:175:THR:O	2:I:179:LEU:HG	2.21	0.40
2:B:70:ARG:HB3	2:B:71:PRO:HD3	2.03	0.40
2:I:66:TYR:HD1	2:I:69:LEU:HD12	1.86	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	184/244 (75%)	176 (96%)	8 (4%)	0	100	100
1	H	184/244 (75%)	177 (96%)	7 (4%)	0	100	100
2	B	175/192 (91%)	164 (94%)	11 (6%)	0	100	100
2	I	175/192 (91%)	162 (93%)	13 (7%)	0	100	100
All	All	718/872 (82%)	679 (95%)	39 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	168/219 (77%)	164 (98%)	4 (2%)	49	58
1	H	168/219 (77%)	163 (97%)	5 (3%)	41	50
2	B	155/165 (94%)	149 (96%)	6 (4%)	32	38
2	I	155/165 (94%)	147 (95%)	8 (5%)	23	24
All	All	646/768 (84%)	623 (96%)	23 (4%)	35	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	127	GLU
1	A	145	LEU
1	A	230	GLN
2	B	16	CYS
2	B	23	ILE
2	B	28	ASP
2	B	47	GLU
2	B	98	LYS
2	B	179	LEU
1	H	81	GLU
1	H	97	GLN
1	H	158	GLN
1	H	187	GLN
1	H	232	GLU
2	I	5	ARG
2	I	16	CYS
2	I	33	VAL
2	I	47	GLU
2	I	140	LYS
2	I	151	ILE
2	I	168	ARG
2	I	169	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	56	ASN

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Mol	Chain	Res	Type
1	A	74	GLN
1	A	230	GLN
1	H	50	GLN
1	H	97	GLN
1	H	110	GLN
1	H	184	HIS
1	H	187	GLN
2	I	29	GLN
2	I	149	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	F2Y	B	34	2	13,14,15	0.34	0	16,19,21	1.48	4 (25%)
2	F2Y	I	34	2	13,14,15	0.47	0	16,19,21	1.34	3 (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
2	F2Y	B	34	2	-	0/5/6/8	0/1/1/1
2	F2Y	I	34	2	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	34	F2Y	CD1-CE1-CZ	-3.07	121.39	123.79
2	B	34	F2Y	F1-CE1-CZ	2.85	119.24	117.13
2	B	34	F2Y	F2-CE2-CZ	2.84	119.24	117.13
2	I	34	F2Y	F2-CE2-CZ	2.83	119.23	117.13
2	B	34	F2Y	CD1-CE1-CZ	-2.76	121.63	123.79
2	B	34	F2Y	CD2-CE2-CZ	-2.30	121.99	123.79
2	I	34	F2Y	CD2-CE2-CZ	-2.29	121.99	123.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	MGF	B	202	6,3	0,3,3	-	-	-		
3	GDP	B	201	5,4	24,30,30	1.51	3 (12%)	30,47,47	1.52	5 (16%)
4	MGF	I	202	6,3	0,3,3	-	-	-		
3	GDP	I	201	5,4	24,30,30	1.34	3 (12%)	30,47,47	1.51	6 (20%)

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	B	201	5,4	-	4/12/32/32	0/3/3/3
3	GDP	I	201	5,4	-	6/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	GDP	C6-N1	-4.56	1.31	1.37
3	I	201	GDP	C6-N1	-3.11	1.33	1.37
3	I	201	GDP	C2-N3	2.96	1.40	1.33
3	B	201	GDP	C2-N3	2.54	1.39	1.33
3	B	201	GDP	C5-C6	-2.51	1.42	1.47
3	I	201	GDP	C5-C6	-2.27	1.42	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	GDP	PA-O3A-PB	-3.57	120.58	132.83
3	I	201	GDP	PA-O3A-PB	-3.56	120.59	132.83
3	B	201	GDP	C5-C6-N1	3.38	119.92	113.95
3	I	201	GDP	C5-C6-N1	3.38	119.92	113.95
3	B	201	GDP	C2-N1-C6	-2.74	120.05	125.10
3	I	201	GDP	C2-N1-C6	-2.73	120.06	125.10
3	I	201	GDP	C8-N7-C5	2.62	107.99	102.99
3	B	201	GDP	C8-N7-C5	2.60	107.95	102.99
3	I	201	GDP	O6-C6-C5	-2.21	120.05	124.37
3	B	201	GDP	O6-C6-C5	-2.19	120.10	124.37
3	I	201	GDP	C2'-C3'-C4'	2.06	106.64	102.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	GDP	PA-O3A-PB-O2B
3	B	201	GDP	C5'-O5'-PA-O3A
3	I	201	GDP	C5'-O5'-PA-O3A
3	I	201	GDP	C5'-O5'-PA-O1A
3	I	201	GDP	C5'-O5'-PA-O2A
3	I	201	GDP	PA-O3A-PB-O1B
3	B	201	GDP	PA-O3A-PB-O3B
3	I	201	GDP	PA-O3A-PB-O2B

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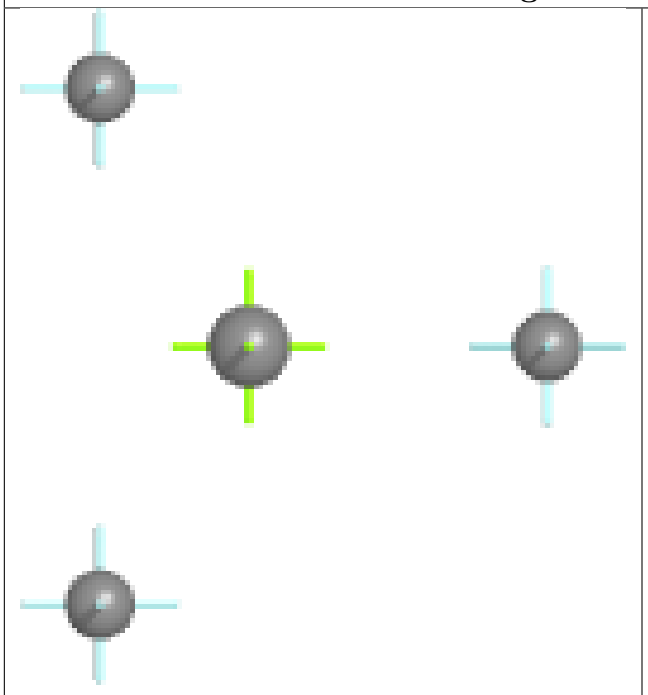
Mol	Chain	Res	Type	Atoms
3	I	201	GDP	PA-O3A-PB-O3B
3	B	201	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

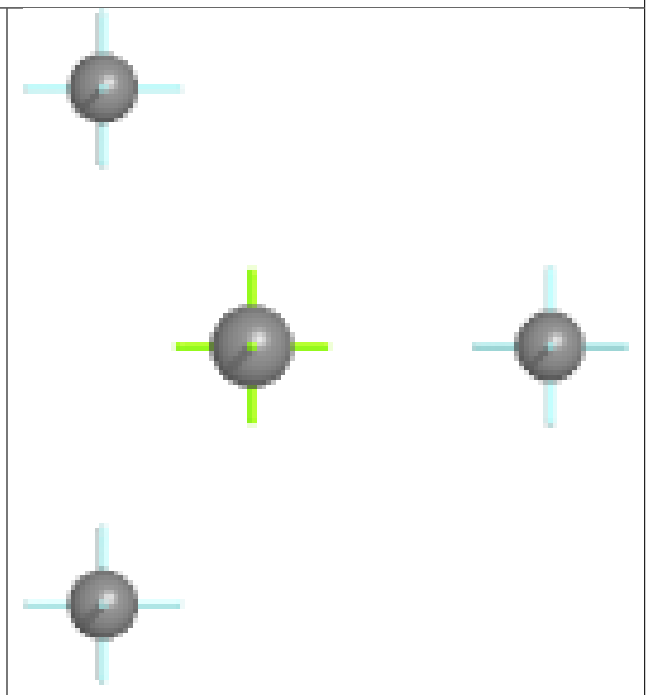
No monomer is involved in short contacts.

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 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.

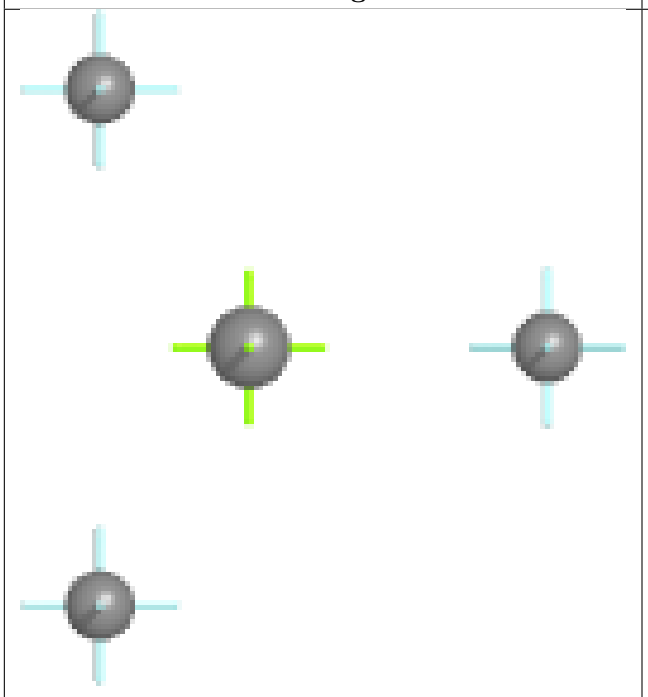
Ligand MGF B 202



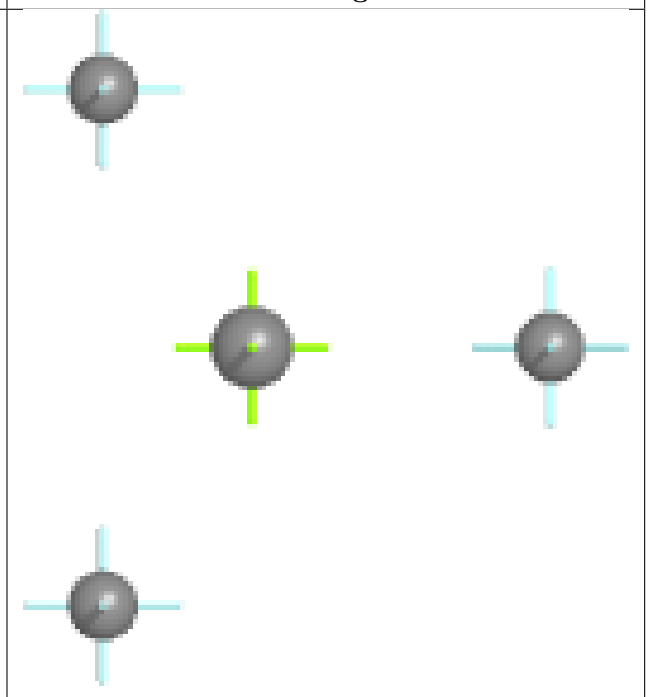
Bond lengths



Bond angles

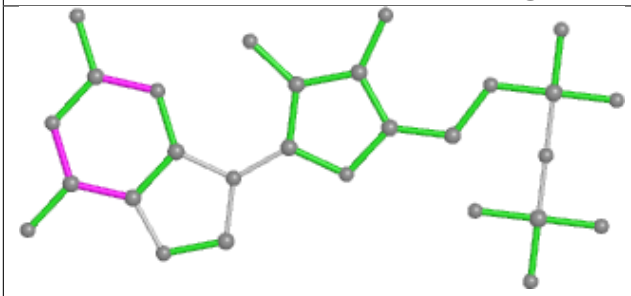


Torsions

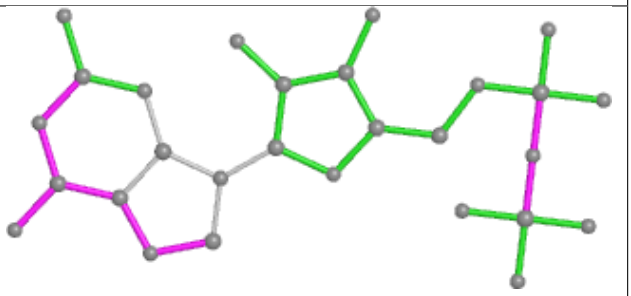


Rings

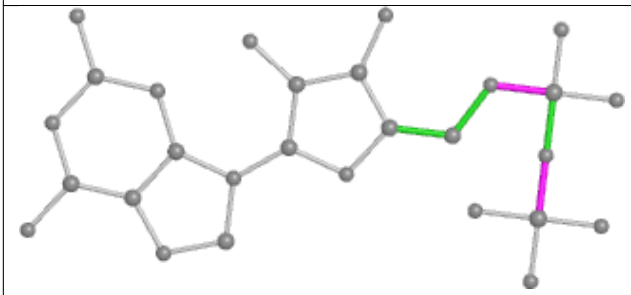
Ligand GDP B 201



Bond lengths



Bond angles



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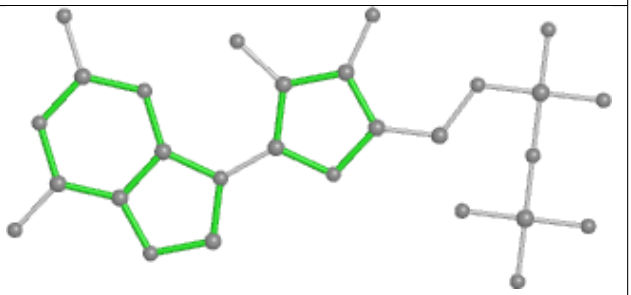
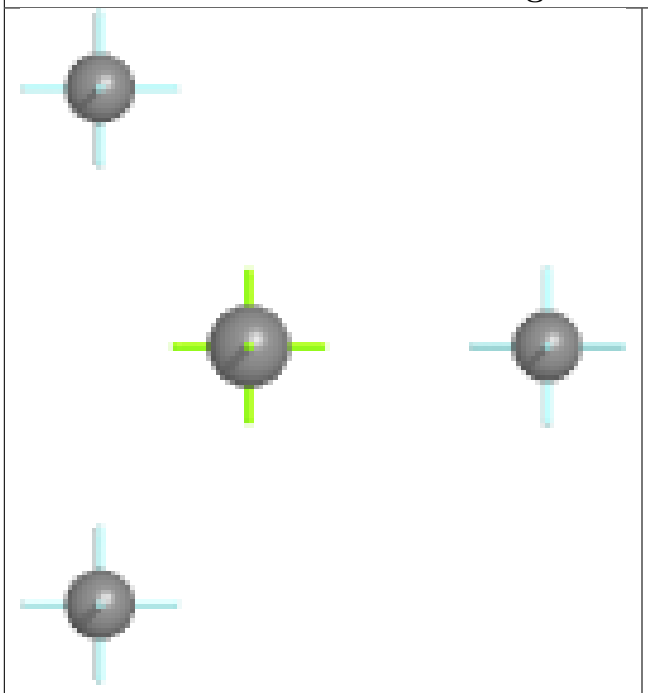
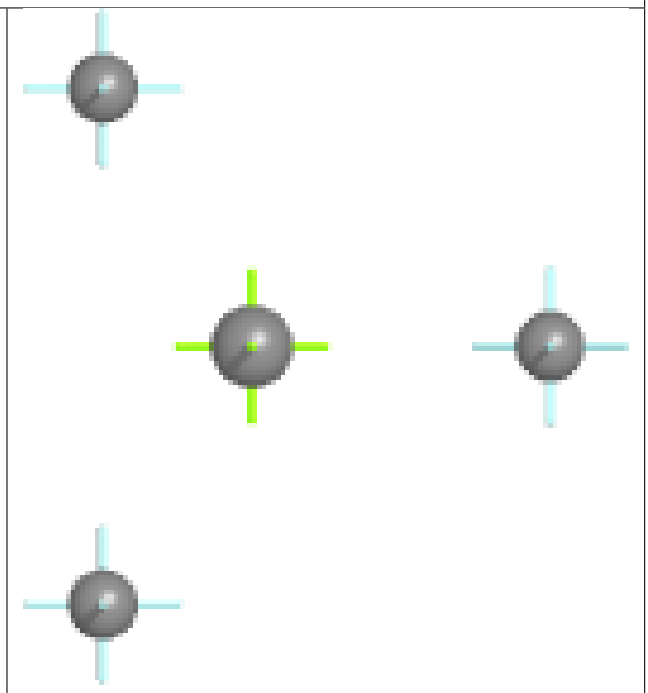


Rings

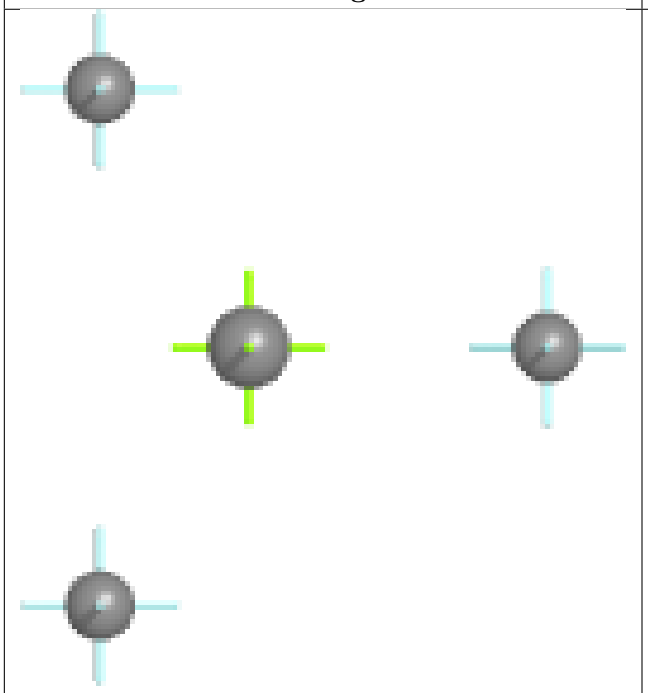
Ligand MGF I 202



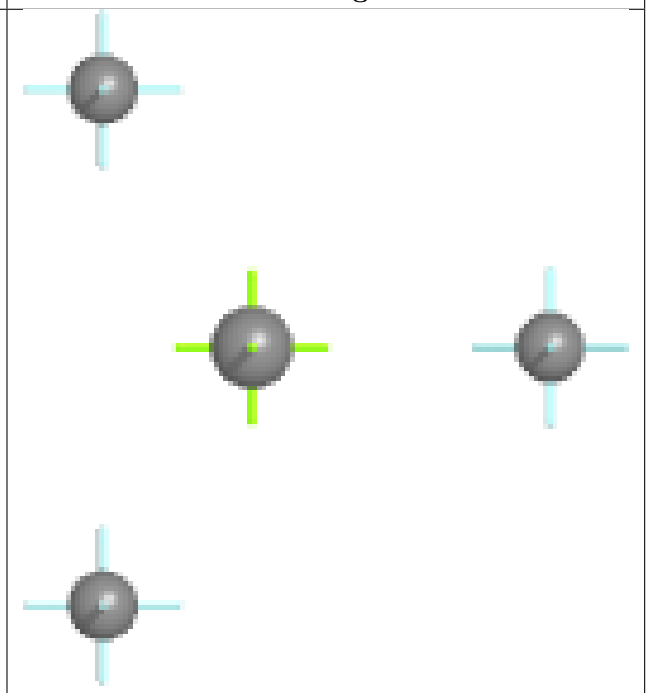
Bond lengths



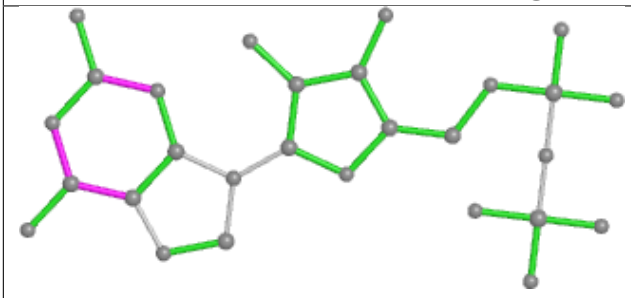
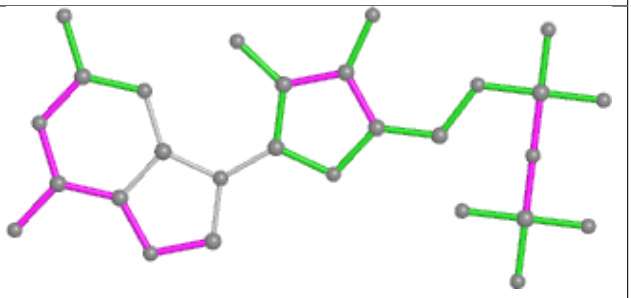
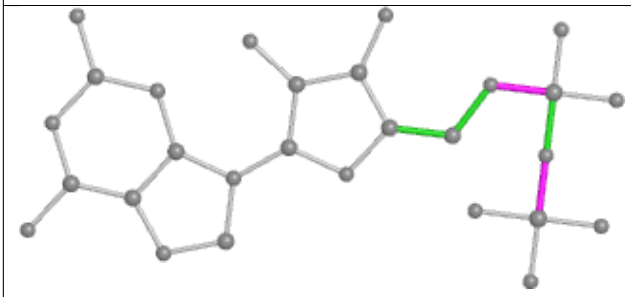
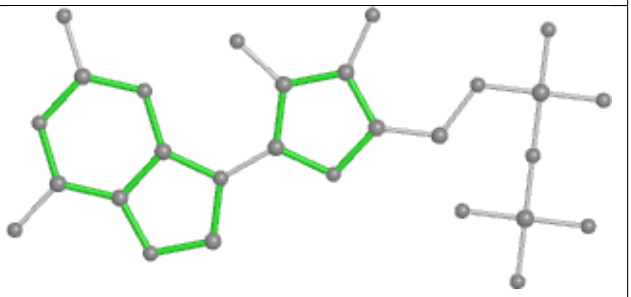
Bond angles



Torsions



Rings

Ligand GDP I 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	188/244 (77%)	-0.27	1 (0%) 91 91	27, 38, 60, 90	0
1	H	187/244 (76%)	-0.32	0 100 100	26, 39, 63, 78	0
2	B	177/192 (92%)	-0.25	1 (0%) 89 89	27, 38, 67, 78	0
2	I	177/192 (92%)	-0.23	1 (0%) 89 89	27, 40, 74, 87	2 (1%)
All	All	729/872 (83%)	-0.27	3 (0%) 92 93	26, 39, 67, 90	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	PHE	2.3
2	B	46	ILE	2.3
2	I	72	LEU	2.0

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

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, 95^{th} 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
2	F2Y	I	34	14/15	0.91	0.14	40,43,46,57	0
2	F2Y	B	34	14/15	0.93	0.11	36,41,47,54	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

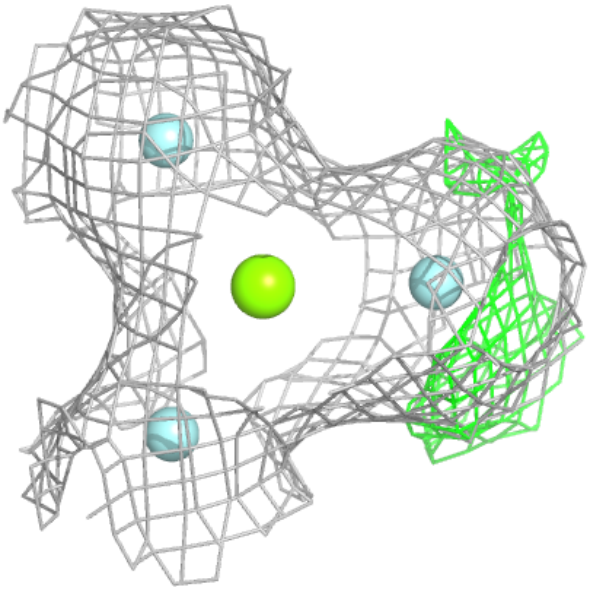
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

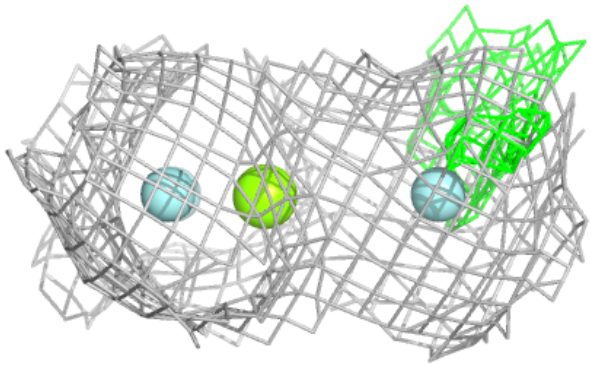
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MGF	I	202	4/4	0.96	0.10	20,22,26,29	0
4	MGF	B	202	4/4	0.97	0.08	22,23,25,27	0
3	GDP	B	201	28/28	0.97	0.11	26,33,37,40	0
5	MG	I	203	1/1	0.97	0.09	30,30,30,30	0
5	MG	B	203	1/1	0.98	0.06	32,32,32,32	0
3	GDP	I	201	28/28	0.98	0.10	23,37,40,47	0

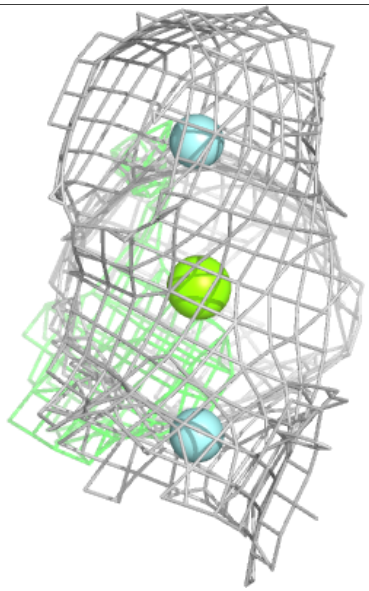
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGF I 202:

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

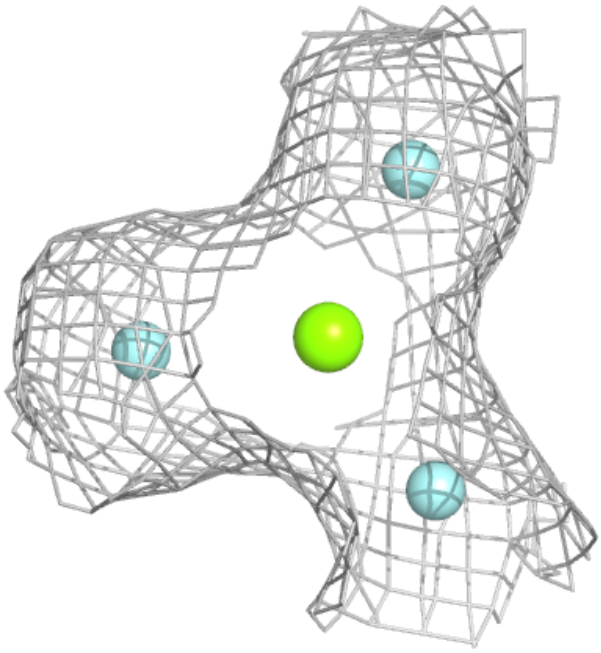


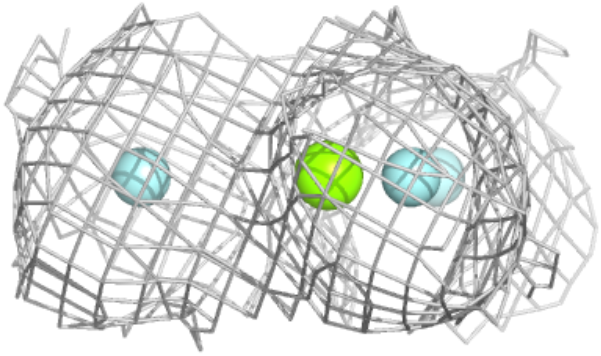


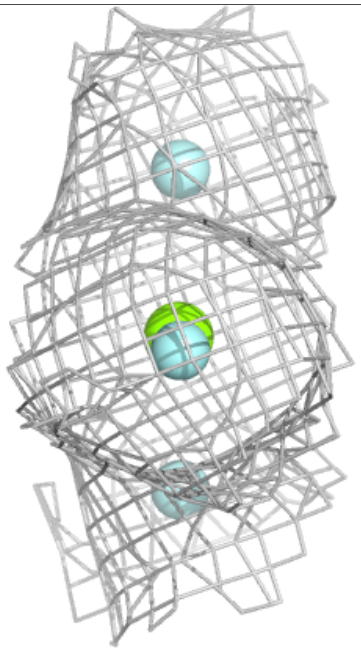


Electron density around MGF B 202:

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

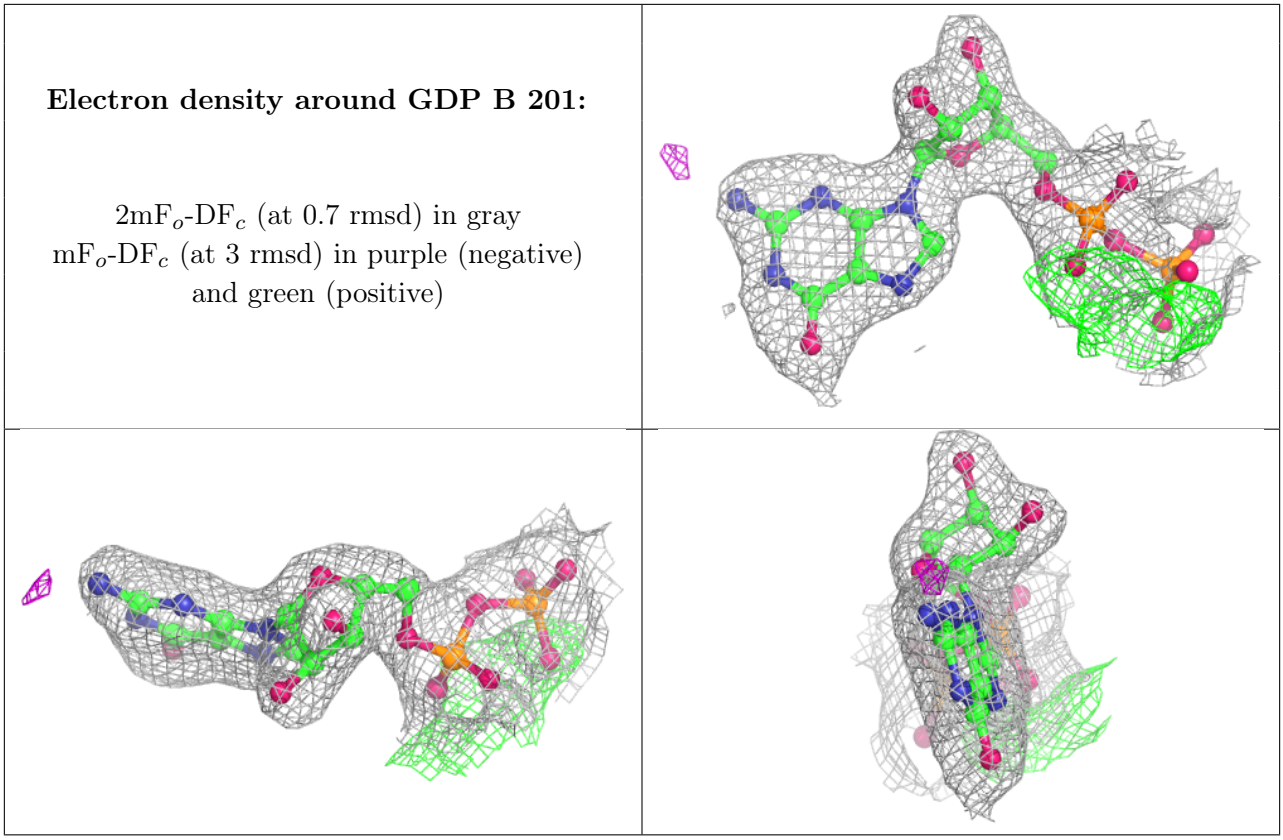






Electron density around GDP B 201:

$2mF_o$-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 I 203:

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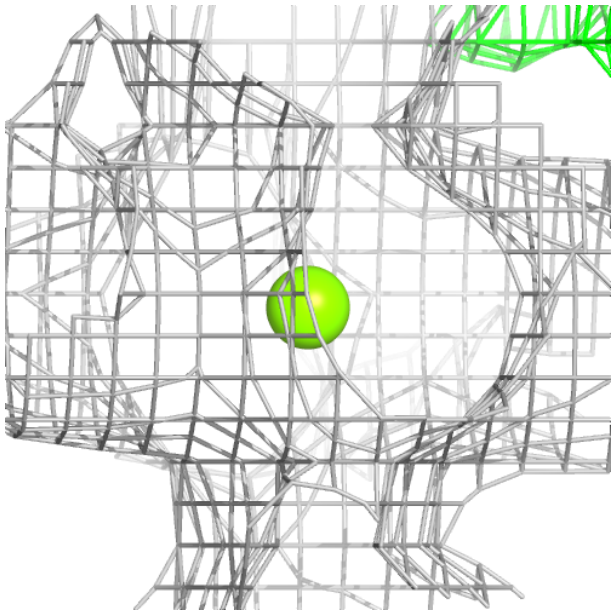
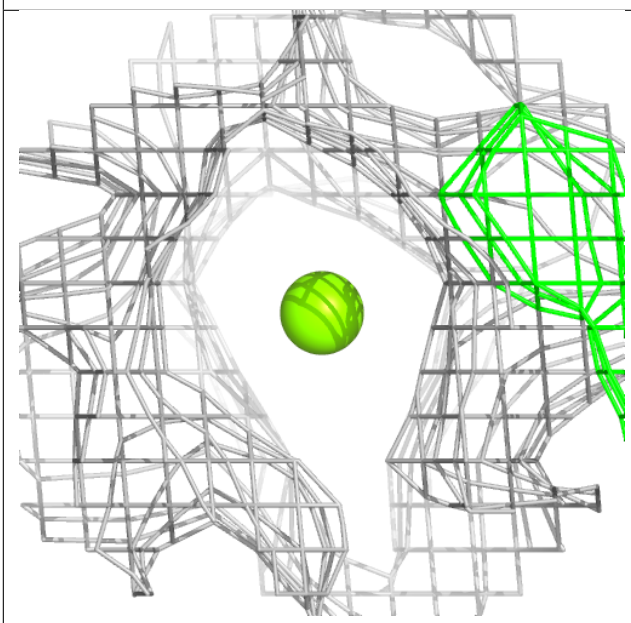
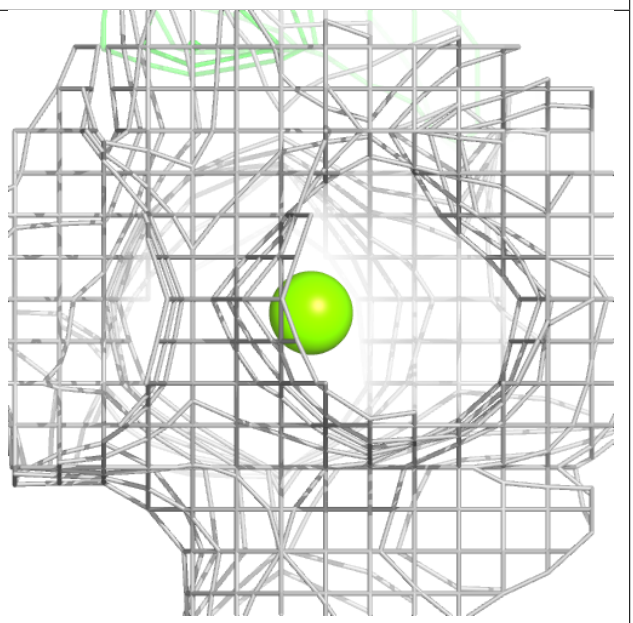
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around MG B 203:

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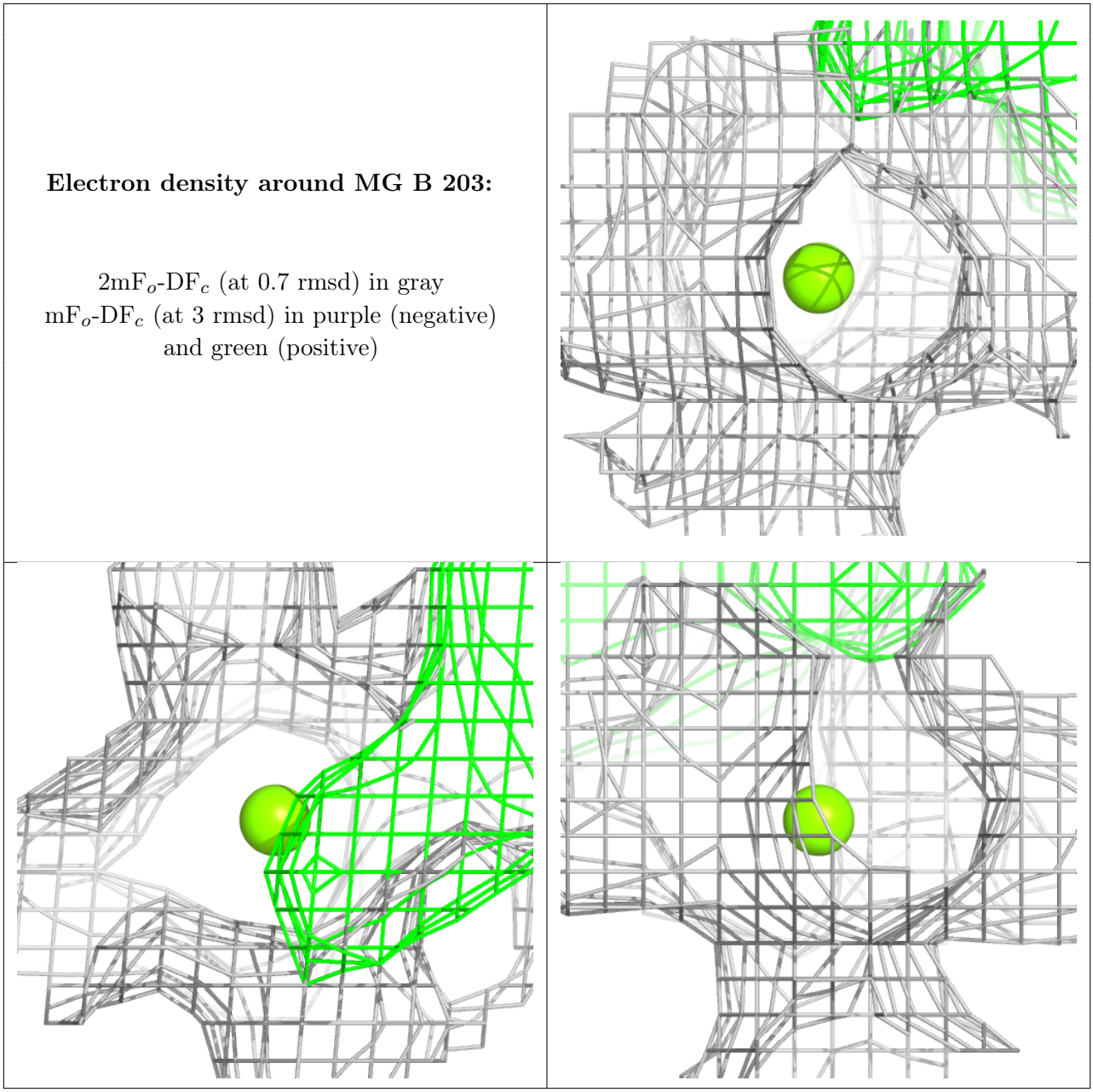
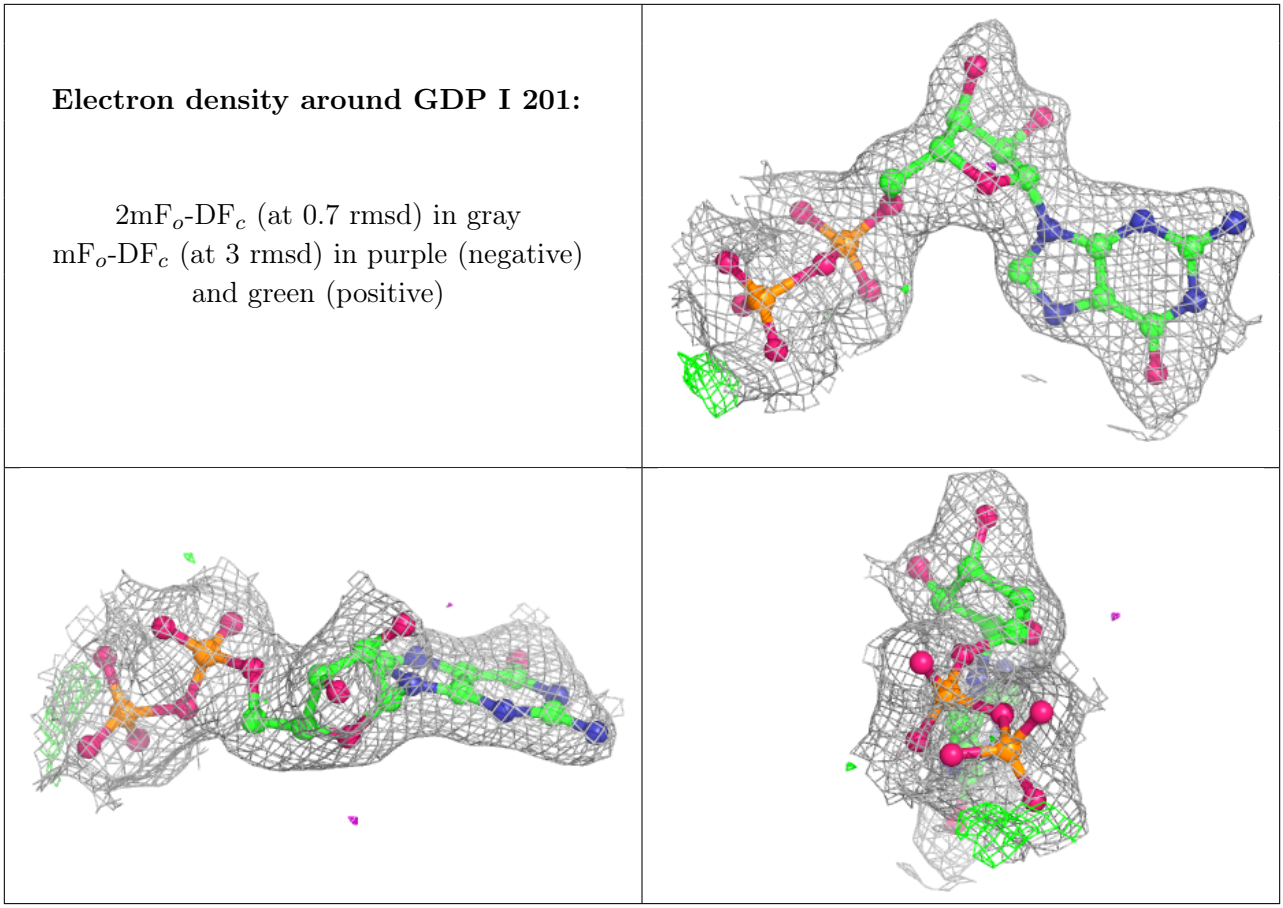
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GDP I 201:

$2mF_o$-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

There are no such residues in this entry.