



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:46 PM UTC

PDB ID : 5HPY / pdb_00005hpy
Title : Crystal Structure of RhoA.GDP.MgF3-in complex with human Myosin 9b RhoGAP domain
Authors : Yi, F.S.; Ren, J.Q.; Feng, W.
Deposited on : 2016-01-21
Resolution : 2.40 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

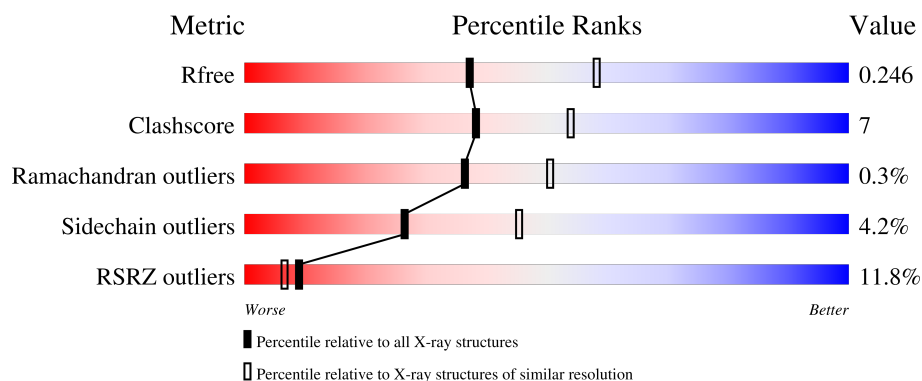
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	232	 13% 68% 11% • 17%
1	D	232	 13% 64% 18% 18%
2	B	185	 6% 78% 16% • •
2	F	185	 8% 78% 16% • •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5968 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 Unconventional myosin-IXb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1501	966	257	269	9			
1	D	190	Total	C	N	O	S	0	0	0
			1496	964	254	267	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLY	-	expression tag	UNP Q13459
A	186	PRO	-	expression tag	UNP Q13459
A	187	GLY	-	expression tag	UNP Q13459
A	188	SER	-	expression tag	UNP Q13459
A	189	GLU	-	expression tag	UNP Q13459
A	190	PHE	-	expression tag	UNP Q13459
D	185	GLY	-	expression tag	UNP Q13459
D	186	PRO	-	expression tag	UNP Q13459
D	187	GLY	-	expression tag	UNP Q13459
D	188	SER	-	expression tag	UNP Q13459
D	189	GLU	-	expression tag	UNP Q13459
D	190	PHE	-	expression tag	UNP Q13459

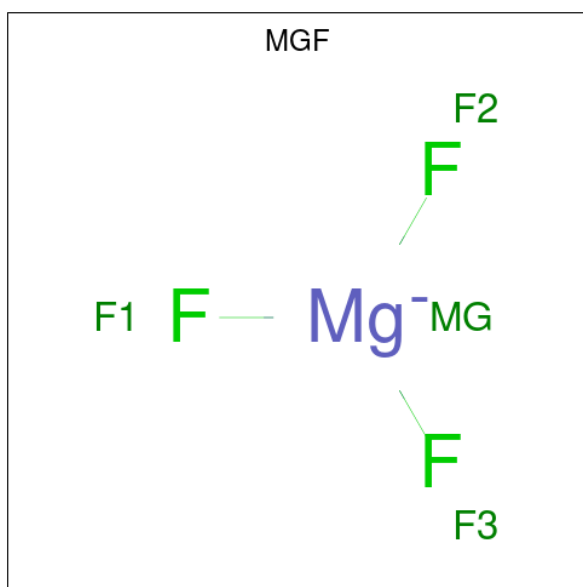
- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	1	0
			1398	884	234	270	10			
2	F	178	Total	C	N	O	S	0	0	0
			1370	866	229	265	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P61586
B	-2	PRO	-	expression tag	UNP P61586
B	-1	GLY	-	expression tag	UNP P61586
B	0	SER	-	expression tag	UNP P61586
B	1	GLU	-	expression tag	UNP P61586
B	2	PHE	-	expression tag	UNP P61586
B	25	ASN	PHE	engineered mutation	UNP P61586
F	-3	GLY	-	expression tag	UNP P61586
F	-2	PRO	-	expression tag	UNP P61586
F	-1	GLY	-	expression tag	UNP P61586
F	0	SER	-	expression tag	UNP P61586
F	1	GLU	-	expression tag	UNP P61586
F	2	PHE	-	expression tag	UNP P61586
F	25	ASN	PHE	engineered mutation	UNP P61586

- Molecule 3 is TRIFLUOROMAGNESATE (CCD ID: MGF) (formula: F₃Mg).

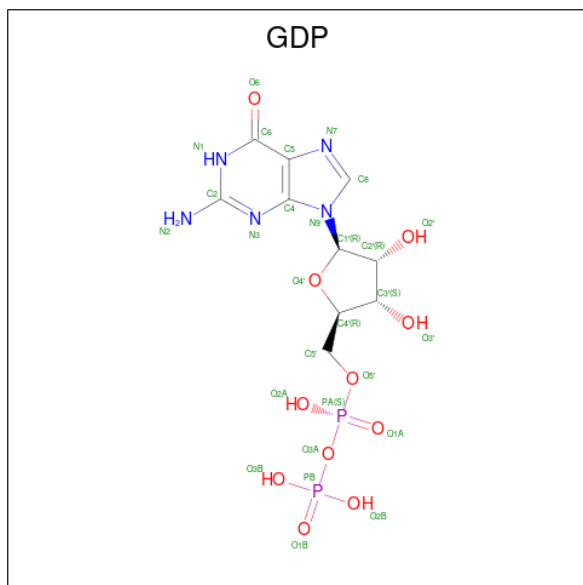


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	F	Mg	0	0
			4	3	1		
3	F	1	Total	F	Mg	0	0
			4	3	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	F	2	Total Mg 2 2	0	0

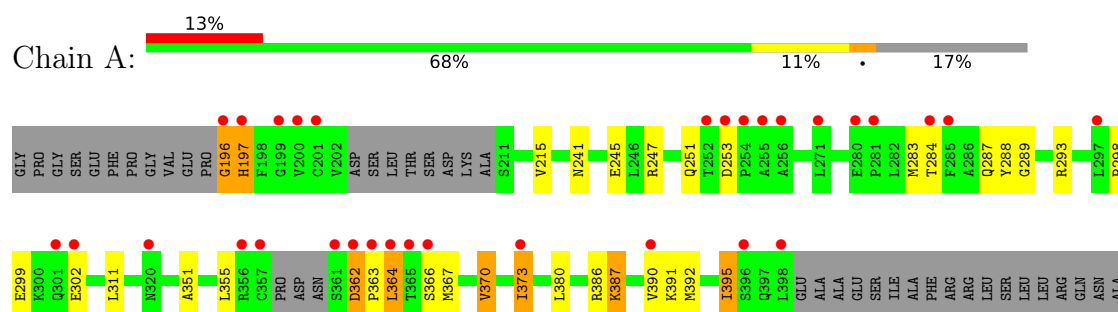
- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



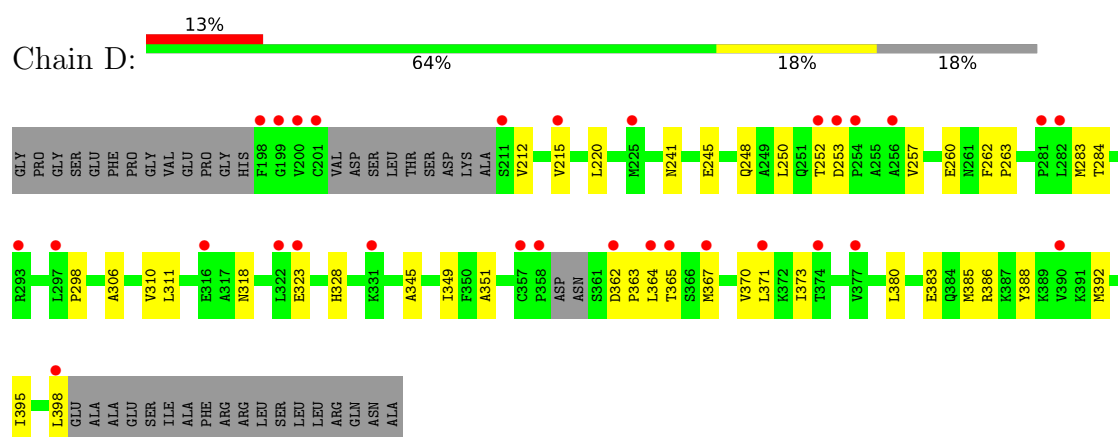
3 Residue-property plots [i](#)

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.

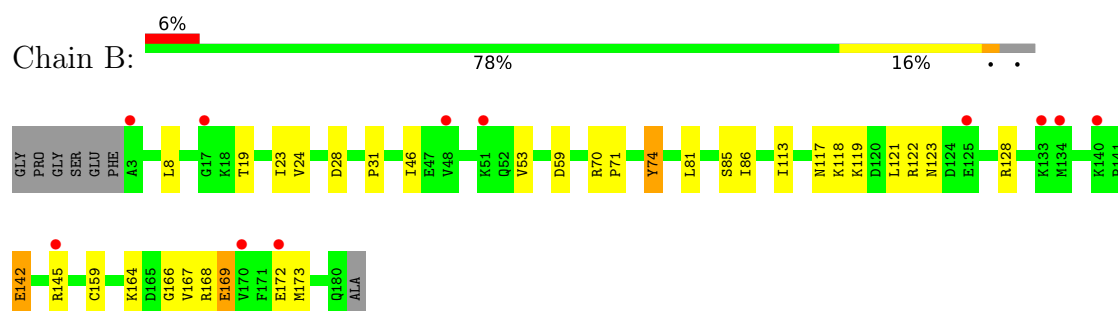
• Molecule 1: Unconventional myosin-IXb



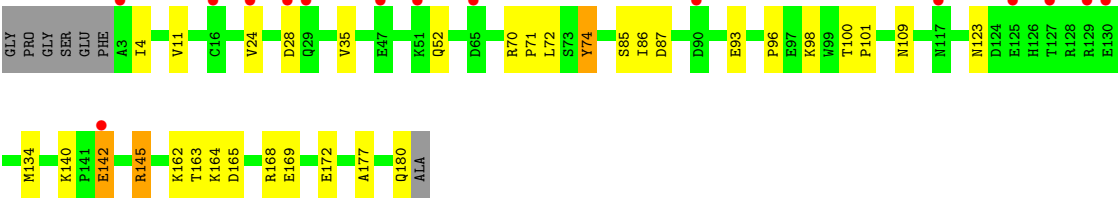
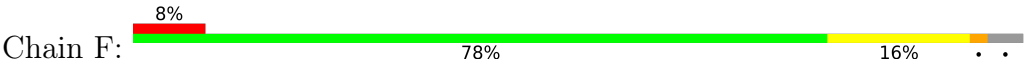
• Molecule 1: Unconventional myosin-IXb



• Molecule 2: Transforming protein RhoA



• Molecule 2: Transforming protein RhoA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.06Å 90.76Å 93.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.40 48.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.70-2.40) 99.7 (48.70-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.211 , 0.246 0.212 , 0.246	Depositor DCC
R_{free} test set	1869 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5968	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7810e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/1527	0.89	5/2067 (0.2%)
1	D	0.52	0/1523	0.86	2/2061 (0.1%)
2	B	0.62	0/1428	0.93	4/1936 (0.2%)
2	F	0.60	0/1397	0.90	4/1898 (0.2%)
All	All	0.57	0/5875	0.89	15/7962 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	70	ARG	CA-C-N	-6.38	113.24	119.87
2	F	70	ARG	C-N-CA	-6.38	113.24	119.87
2	B	70	ARG	CA-C-N	-6.24	113.38	119.87
2	B	70	ARG	C-N-CA	-6.24	113.38	119.87
1	A	196	GLY	CA-C-N	6.15	132.77	121.70
1	A	196	GLY	C-N-CA	6.15	132.77	121.70
2	B	74	TYR	CA-C-N	-5.80	113.98	119.90
2	B	74	TYR	C-N-CA	-5.80	113.98	119.90
2	F	74	TYR	CA-C-N	-5.31	114.29	119.76
2	F	74	TYR	C-N-CA	-5.31	114.29	119.76
1	A	283	MET	N-CA-C	-5.20	103.17	110.50
1	D	253	ASP	CA-C-N	5.15	124.60	119.24
1	D	253	ASP	C-N-CA	5.15	124.60	119.24
1	A	253	ASP	CA-C-N	5.06	125.09	119.32
1	A	253	ASP	C-N-CA	5.06	125.09	119.32

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	1501	0	1526	20	0
1	D	1496	0	1535	21	0
2	B	1398	0	1374	22	0
2	F	1370	0	1325	19	0
3	B	4	0	0	0	0
3	F	4	0	0	0	0
4	B	1	0	0	0	0
4	F	2	0	0	0	0
5	B	28	0	12	0	0
5	F	28	0	12	0	0
6	A	28	0	0	1	0
6	B	45	0	0	0	0
6	D	20	0	0	2	0
6	F	43	0	0	3	0
All	All	5968	0	5784	80	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 (80) 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:351:ALA:HB1	1:A:373:ILE:HG13	1.56	0.87
1:D:351:ALA:HB1	1:D:373:ILE:HG13	1.54	0.86
1:A:293:ARG:HD2	2:F:140:LYS:HZ3	1.41	0.81
2:B:118:LYS:HB3	2:B:121:LEU:HD12	1.76	0.67
1:D:284:THR:N	6:D:501:HOH:O	2.29	0.66
1:D:383:GLU:OE1	1:D:386:ARG:NH1	2.28	0.65
2:F:85:SER:OG	2:F:87:ASP:OD1	2.13	0.63
1:A:362:ASP:HB3	1:A:364:LEU:H	1.66	0.61
2:B:28:ASP:OD1	2:B:164:LYS:NZ	2.31	0.61
1:A:362:ASP:HB3	1:A:364:LEU:N	2.17	0.58
1:A:311:LEU:HD11	1:A:380:LEU:HD21	1.87	0.56
1:A:196:GLY:HA2	1:A:197:HIS:CB	2.37	0.55
2:B:113:ILE:HG12	2:B:173:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:THR:HG22	1:D:318:ASN:HD22	1.72	0.55
2:B:123:ASN:O	2:B:128:ARG:NH1	2.40	0.54
1:D:311:LEU:HD11	1:D:380:LEU:HD21	1.89	0.54
1:D:388:TYR:CZ	1:D:392:MET:HE3	2.42	0.54
2:B:23[B]:ILE:HD12	2:B:31:PRO:HG3	1.91	0.52
1:D:363:PRO:HB2	2:F:72:LEU:HD21	1.91	0.52
2:B:46:ILE:HG22	2:B:53:VAL:HB	1.93	0.51
1:A:284:THR:OG1	1:A:287:GLN:HG2	2.10	0.51
2:F:142:GLU:HA	2:F:145:ARG:NH1	2.26	0.51
2:F:162:LYS:NZ	6:F:306:HOH:O	2.41	0.51
2:F:4:ILE:HD12	2:F:52:GLN:O	2.11	0.50
2:B:86:ILE:HG12	2:B:117:ASN:O	2.11	0.50
2:F:169:GLU:N	2:F:169:GLU:OE1	2.44	0.50
1:D:367:MET:O	1:D:370:VAL:HG12	2.11	0.50
1:D:362:ASP:OD1	1:D:365:THR:OG1	2.30	0.50
2:B:119:LYS:HB2	2:B:159:CYS:O	2.12	0.49
1:A:241:ASN:O	1:A:245:GLU:HG3	2.13	0.48
1:A:363:PRO:O	1:A:366:SER:HB2	2.14	0.48
1:A:288:TYR:HD2	1:A:355:LEU:HD22	1.79	0.47
1:A:386:ARG:HG3	1:A:387:LYS:N	2.29	0.47
1:A:387:LYS:O	1:A:391:LYS:HG2	2.13	0.47
2:B:19:THR:OG1	2:B:59:ASP:OD2	2.32	0.47
1:D:306:ALA:O	1:D:310:VAL:HG23	2.15	0.47
2:F:163:THR:OG1	2:F:165:ASP:HB2	2.15	0.47
1:D:370:VAL:HG13	1:D:371:LEU:HG	1.96	0.47
2:F:164:LYS:N	2:F:164:LYS:HD2	2.30	0.47
2:B:19:THR:O	2:B:23[A]:ILE:HG12	2.15	0.46
2:B:86:ILE:HD12	2:B:122:ARG:NH2	2.31	0.46
1:D:220:LEU:HD22	1:D:328:HIS:CD2	2.51	0.46
2:B:168:ARG:O	2:B:172:GLU:OE1	2.34	0.46
2:B:173:MET:HE3	2:B:173:MET:HB2	1.83	0.46
2:F:168:ARG:O	2:F:172:GLU:HG3	2.16	0.45
1:D:370:VAL:O	1:D:373:ILE:HG12	2.16	0.45
2:F:177:ALA:O	2:F:180:GLN:HG2	2.16	0.45
2:B:168:ARG:HE	2:B:168:ARG:HB3	1.46	0.45
1:D:385:MET:HE1	6:D:513:HOH:O	2.17	0.45
2:B:24:VAL:HG12	2:B:167:VAL:HG11	1.99	0.45
1:D:248:GLN:O	1:D:252:THR:HG23	2.17	0.45
1:A:392:MET:HA	1:A:392:MET:HE2	1.98	0.44
1:A:289:GLY:O	1:A:293:ARG:HG3	2.17	0.44
1:A:391:LYS:O	1:A:395:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:MET:O	1:A:370:VAL:HG12	2.17	0.44
2:F:123:ASN:HA	6:F:318:HOH:O	2.17	0.43
2:F:71:PRO:HA	2:F:74:TYR:CD2	2.52	0.43
2:F:24:VAL:O	2:F:28:ASP:HA	2.18	0.43
2:F:93:GLU:O	2:F:96:PRO:HD2	2.19	0.43
2:F:98:LYS:C	2:F:101:PRO:HD2	2.44	0.43
1:D:284:THR:HG22	1:D:318:ASN:ND2	2.31	0.43
1:A:298:PRO:HG2	1:A:302:GLU:OE2	2.19	0.42
2:B:85:SER:OG	2:B:118:LYS:HD2	2.20	0.42
1:D:345:ALA:O	1:D:349:ILE:HG12	2.19	0.42
2:B:24:VAL:O	2:B:28:ASP:HA	2.20	0.42
2:B:169:GLU:H	2:B:169:GLU:CD	2.28	0.42
2:B:8:LEU:HD11	2:B:81:LEU:HG	2.02	0.42
1:D:383:GLU:CD	1:D:386:ARG:HH12	2.27	0.41
2:F:100:THR:HB	2:F:101:PRO:HD3	2.02	0.41
2:B:142:GLU:H	2:B:142:GLU:HG3	1.35	0.41
2:F:134:MET:HE3	2:F:134:MET:HB2	1.94	0.41
1:A:386:ARG:O	1:A:390:VAL:HG13	2.21	0.41
1:D:250:LEU:HD23	1:D:257:VAL:HG11	2.03	0.41
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.56	0.41
2:F:163:THR:C	2:F:165:ASP:H	2.29	0.41
2:B:166:GLY:O	2:B:169:GLU:HG2	2.21	0.40
1:D:241:ASN:O	1:D:245:GLU:HG3	2.21	0.40
1:D:262:PHE:HA	1:D:263:PRO:HD3	1.97	0.40
1:A:298:PRO:HG3	6:F:318:HOH:O	2.21	0.40
1:A:247:ARG:HD2	6:A:504:HOH:O	2.20	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	186/232 (80%)	179 (96%)	6 (3%)	1 (0%)	24	37
1	D	184/232 (79%)	179 (97%)	4 (2%)	1 (0%)	24	37
2	B	177/185 (96%)	173 (98%)	4 (2%)	0	100	100
2	F	176/185 (95%)	172 (98%)	4 (2%)	0	100	100
All	All	723/834 (87%)	703 (97%)	18 (2%)	2 (0%)	36	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	D	298	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	159/200 (80%)	150 (94%)	9 (6%)	18	33
1	D	162/200 (81%)	154 (95%)	8 (5%)	22	39
2	B	153/160 (96%)	150 (98%)	3 (2%)	48	70
2	F	147/160 (92%)	141 (96%)	6 (4%)	27	46
All	All	621/720 (86%)	595 (96%)	26 (4%)	26	45

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	VAL
1	A	251	GLN
1	A	299	GLU
1	A	362	ASP
1	A	364	LEU
1	A	370	VAL
1	A	373	ILE
1	A	387	LYS
1	A	395	ILE

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Mol	Chain	Res	Type
2	B	142	GLU
2	B	145	ARG
2	B	169	GLU
1	D	212	VAL
1	D	215	VAL
1	D	260	GLU
1	D	283	MET
1	D	323	GLU
1	D	364	LEU
1	D	395	ILE
1	D	398	LEU
2	F	11	VAL
2	F	35	VAL
2	F	86	ILE
2	F	109	ASN
2	F	142	GLU
2	F	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	261	ASN
1	A	384	GLN
2	F	126	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 7 ligands modelled in this entry, 3 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	MGF	B	201	6,5	0,3,3	-	-	-		
5	GDP	F	202	4,3	29,30,30	1.18	2 (6%)	45,47,47	1.78	6 (13%)
3	MGF	F	201	6,5	0,3,3	-	-	-		
5	GDP	B	203	4,3	29,30,30	1.29	3 (10%)	45,47,47	1.69	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	F	202	4,3	-	1/16/32/32	0/3/3/3
5	GDP	B	203	4,3	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	203	GDP	C5-C4	3.41	1.48	1.38
5	F	202	GDP	C5-C4	3.35	1.48	1.38
5	B	203	GDP	C6-N1	-2.76	1.33	1.38
5	F	202	GDP	C6-N1	-2.24	1.34	1.38
5	B	203	GDP	PB-O2B	-2.02	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	202	GDP	C5-C4-N3	-6.29	118.38	128.39
5	B	203	GDP	C5-C4-N3	-5.62	119.44	128.39
5	F	202	GDP	C2-N3-C4	5.07	121.04	112.30
5	F	202	GDP	N9-C4-N3	4.33	134.61	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	203	GDP	N9-C4-N3	4.29	134.53	125.95
5	B	203	GDP	C2-N3-C4	4.26	119.64	112.30
5	B	203	GDP	C6-C5-N7	3.29	136.28	130.29
5	F	202	GDP	C6-C5-N7	3.26	136.22	130.29
5	B	203	GDP	O3B-PB-O3A	3.12	115.10	104.64
5	F	202	GDP	C4-C5-N7	-2.69	106.41	110.67
5	B	203	GDP	C4-C5-N7	-2.50	106.72	110.67
5	F	202	GDP	C3'-C2'-C1'	2.05	105.35	101.46

There are no chirality outliers.

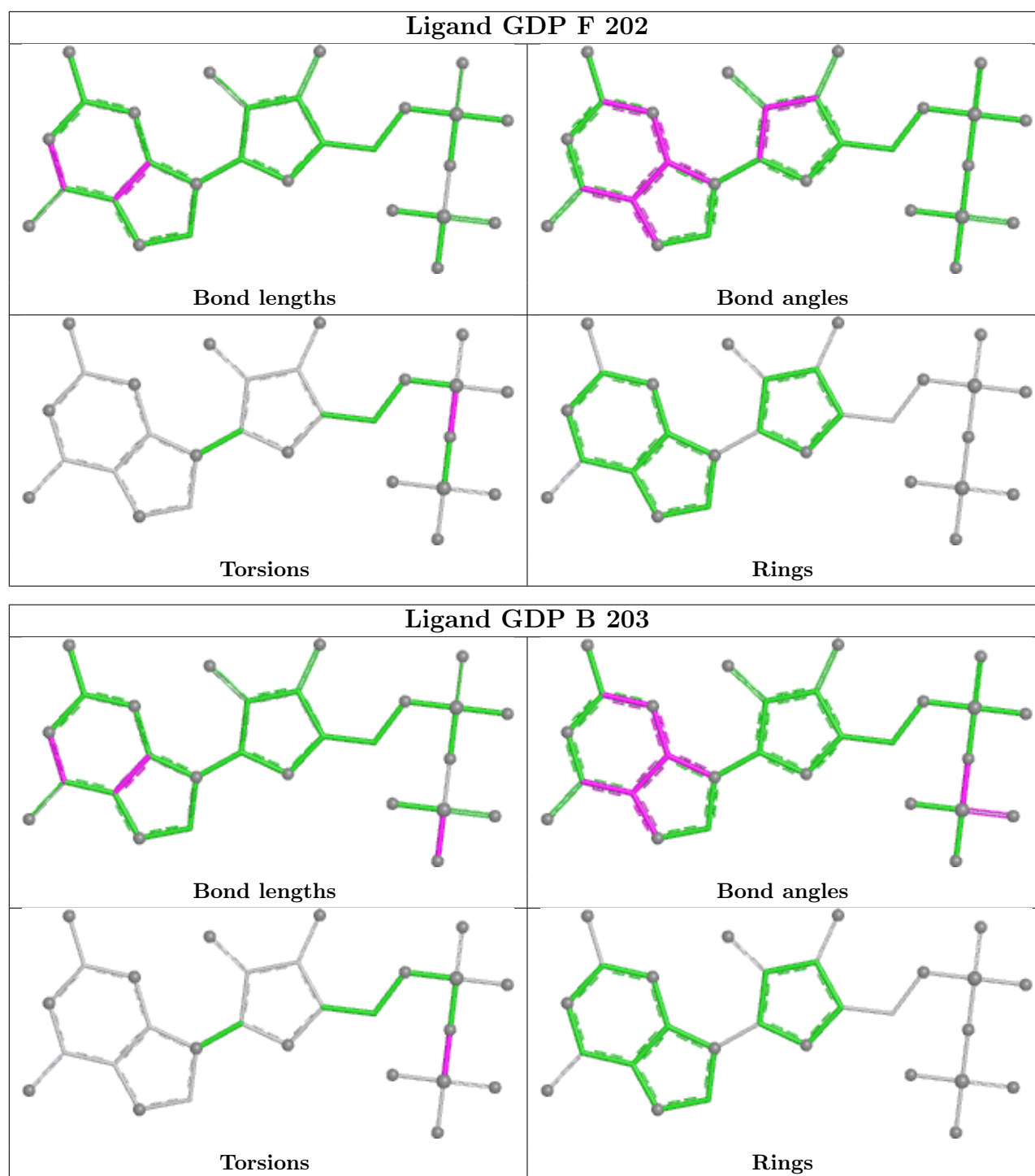
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	203	GDP	PA-O3A-PB-O3B
5	B	203	GDP	PA-O3A-PB-O1B
5	F	202	GDP	PB-O3A-PA-O2A

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.



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	192/232 (82%)	0.95	31 (16%)	4 4	43, 74, 97, 109	0
1	D	190/232 (81%)	1.04	30 (15%)	5 4	44, 76, 100, 122	0
2	B	178/185 (96%)	0.51	11 (6%)	26 23	33, 59, 89, 104	1 (0%)
2	F	178/185 (96%)	0.75	15 (8%)	17 14	39, 62, 100, 111	0
All	All	738/834 (88%)	0.82	87 (11%)	9 6	33, 67, 97, 122	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	364	LEU	5.0
1	D	225	MET	5.0
2	F	125	GLU	4.7
1	D	358	PRO	4.6
1	A	363	PRO	4.4
1	A	364	LEU	4.4
1	A	365	THR	4.1
1	A	197	HIS	3.9
1	A	361	SER	3.8
1	D	200	VAL	3.6
1	A	199	GLY	3.6
1	D	253	ASP	3.4
1	D	215	VAL	3.4
1	A	281	PRO	3.4
2	F	3	ALA	3.4
1	D	252	THR	3.4
1	D	297	LEU	3.4
2	F	47	GLU	3.3
1	A	390	VAL	3.3
1	D	199	GLY	3.2
1	D	390	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	129	ARG	3.1
1	A	253	ASP	3.1
2	B	145	ARG	3.1
2	B	3	ALA	3.0
2	B	170	VAL	3.0
1	A	252	THR	3.0
1	D	374	THR	3.0
1	D	357	CYS	2.9
1	D	198	PHE	2.9
2	B	172	GLU	2.9
1	A	201	CYS	2.9
1	D	398	LEU	2.8
2	F	90	ASP	2.8
1	A	320	ASN	2.8
2	F	29	GLN	2.7
2	B	51	LYS	2.7
2	F	51	LYS	2.7
1	D	293	ARG	2.6
1	D	365	THR	2.6
1	D	211	SER	2.6
1	D	254	PRO	2.6
2	F	117	ASN	2.5
1	D	281	PRO	2.5
1	A	302	GLU	2.5
1	A	301	GLN	2.5
2	B	48	VAL	2.5
2	F	65	ASP	2.4
1	D	282	LEU	2.4
1	A	356	ARG	2.4
1	A	254	PRO	2.4
1	D	316	GLU	2.4
2	F	24	VAL	2.4
1	A	373	ILE	2.4
1	A	366	SER	2.4
1	A	398	LEU	2.4
2	B	133	LYS	2.3
1	A	200	VAL	2.3
2	F	127	THR	2.3
1	A	196	GLY	2.3
1	A	357	CYS	2.3
1	A	297	LEU	2.3
1	D	371	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	377	VAL	2.3
1	D	201	CYS	2.2
1	A	362	ASP	2.2
1	A	255	ALA	2.2
1	A	284	THR	2.2
1	D	362	ASP	2.2
2	F	142	GLU	2.1
2	B	134	MET	2.1
1	A	271	LEU	2.1
1	D	322	LEU	2.1
2	B	140	LYS	2.1
1	D	331	LYS	2.1
2	F	28	ASP	2.1
1	D	367	MET	2.1
1	A	280	GLU	2.1
1	D	323	GLU	2.1
2	F	16	CYS	2.1
2	F	130	GLU	2.0
1	A	285	PHE	2.0
1	A	256	ALA	2.0
1	D	256	ALA	2.0
2	B	125	GLU	2.0
2	B	17	GLY	2.0
1	A	396	SER	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](#)

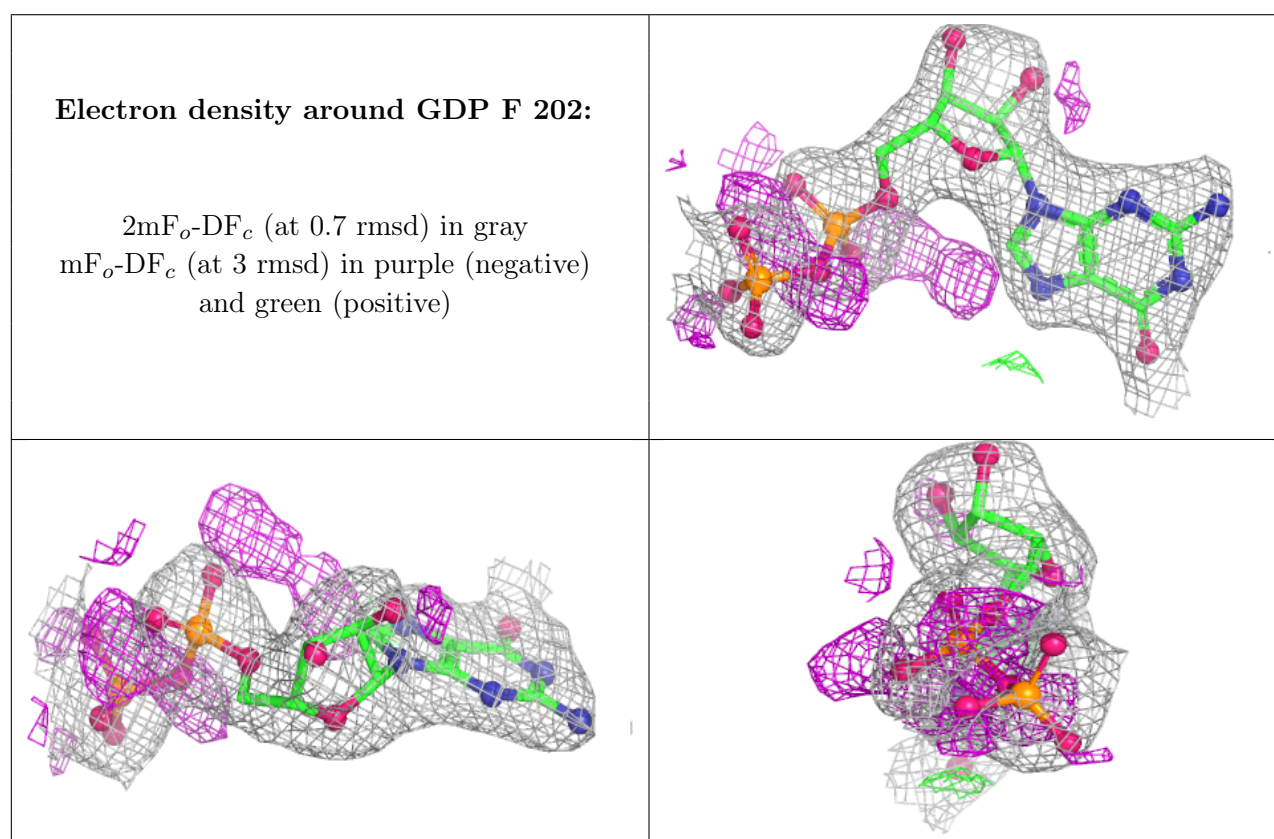
There are no oligosaccharides in this entry.

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.

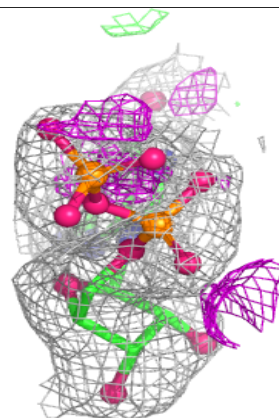
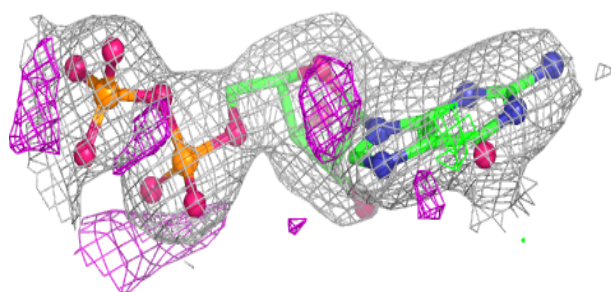
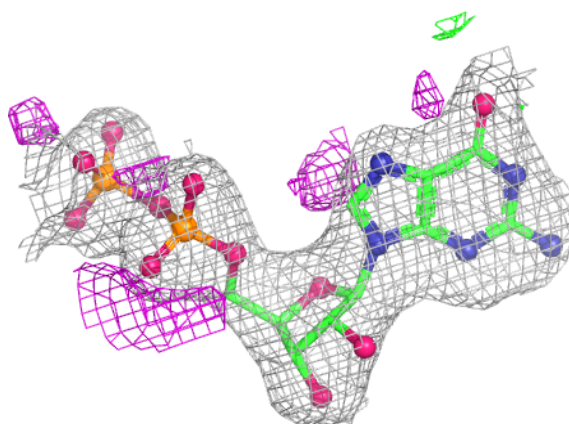
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	F	204	1/1	0.93	0.15	49,49,49,49	0
5	GDP	F	202	28/28	0.94	0.10	39,56,62,68	0
5	GDP	B	203	28/28	0.96	0.08	34,50,58,67	0
3	MGF	F	201	4/4	0.96	0.10	36,40,41,47	0
3	MGF	B	201	4/4	0.98	0.10	37,38,39,40	0
4	MG	F	203	1/1	0.99	0.07	42,42,42,42	0
4	MG	B	202	1/1	0.99	0.03	37,37,37,37	0

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



Electron density around GDP B 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.