



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:55 AM EDT

PDB ID : 2GJ9 / pdb_00002gj9
Title : Structure of the MnmE G-domain in complex with GDP*AlF₄⁻, Mg²⁺ and Rb⁺
Authors : Scrima, A.; Wittinghofer, A.
Deposited on : 2006-03-30
Resolution : 2.00 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

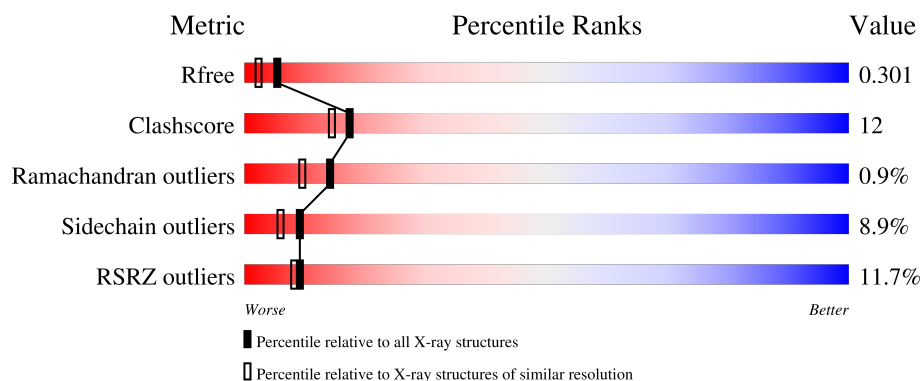
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	172	8% 78% 13% 6%
1	B	172	8% 70% 20% 7%
1	C	172	6% 63% 24% 6% 6%
1	D	172	22% 62% 25% 5% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5042 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.

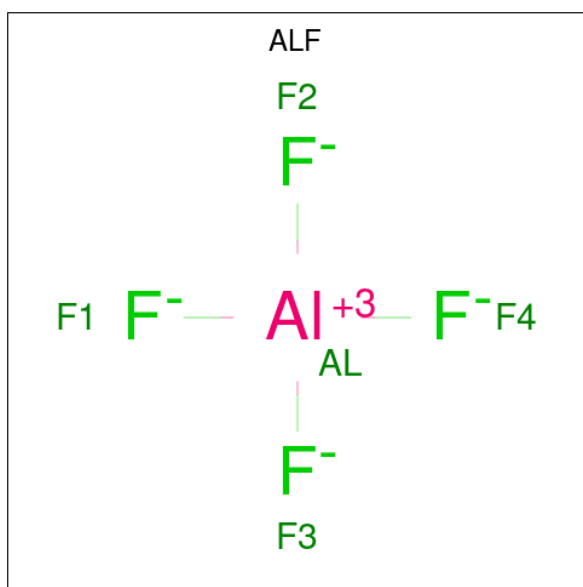
- Molecule 1 is a protein called tRNA modification GTPase trmE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1224	760	225	234	5			
1	B	160	Total	C	N	O	S	0	0	0
			1220	758	224	233	5			
1	C	161	Total	C	N	O	S	0	0	0
			1224	760	225	234	5			
1	D	160	Total	C	N	O	S	0	0	0
			1220	758	224	233	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLY	-	cloning artifact	UNP P25522
A	214	SER	-	cloning artifact	UNP P25522
A	215	HIS	-	cloning artifact	UNP P25522
B	213	GLY	-	cloning artifact	UNP P25522
B	214	SER	-	cloning artifact	UNP P25522
B	215	HIS	-	cloning artifact	UNP P25522
C	213	GLY	-	cloning artifact	UNP P25522
C	214	SER	-	cloning artifact	UNP P25522
C	215	HIS	-	cloning artifact	UNP P25522
D	213	GLY	-	cloning artifact	UNP P25522
D	214	SER	-	cloning artifact	UNP P25522
D	215	HIS	-	cloning artifact	UNP P25522

- Molecule 2 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			5	1	4		
2	B	1	Total	Al	F	0	0
			5	1	4		
2	C	1	Total	Al	F	0	0
			5	1	4		
2	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

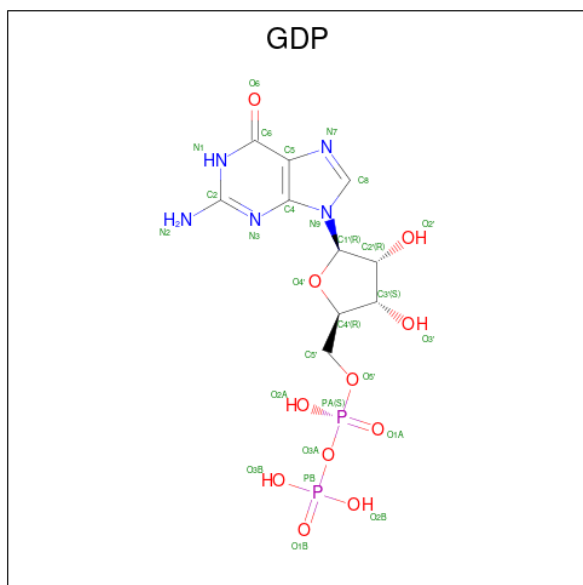
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Rb	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Rb	0	0
			1	1		
4	C	1	Total	Rb	0	0
			1	1		
4	D	1	Total	Rb	0	0
			1	1		

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	2	Total	O	0	0
			2	2		

Continued on next page...

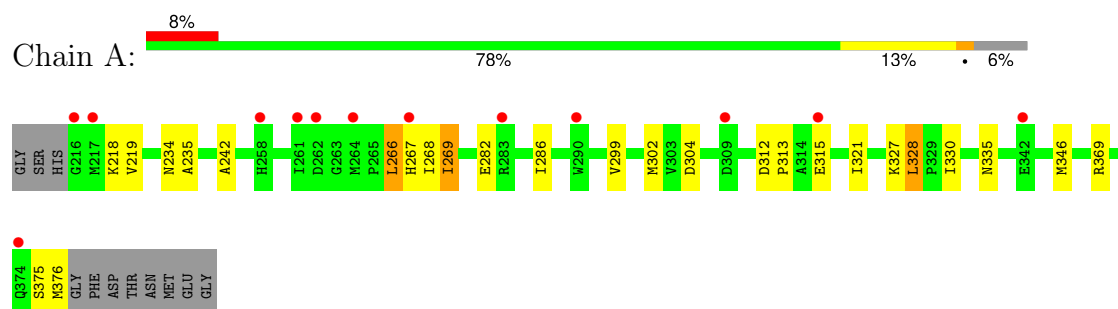
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	O	0	0
			4	4		
6	D	3	Total	O	0	0
			3	3		

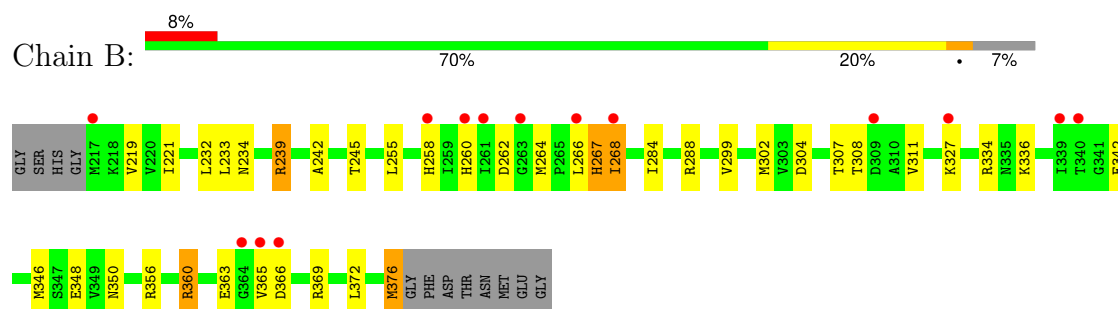
3 Residue-property plots

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.

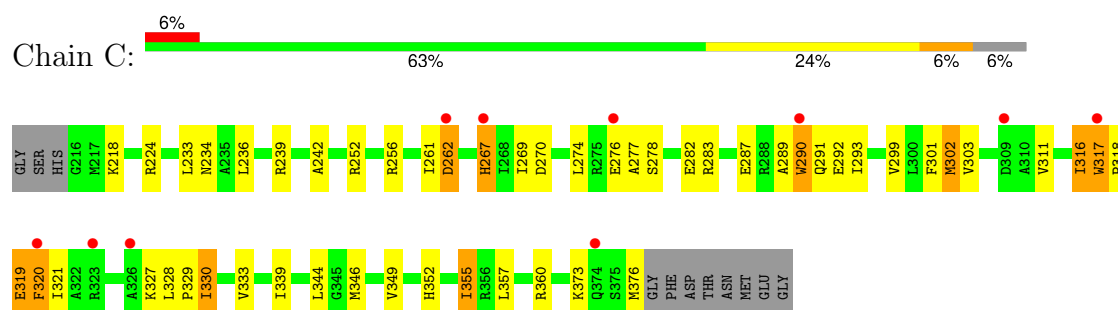
• Molecule 1: tRNA modification GTPase trmE



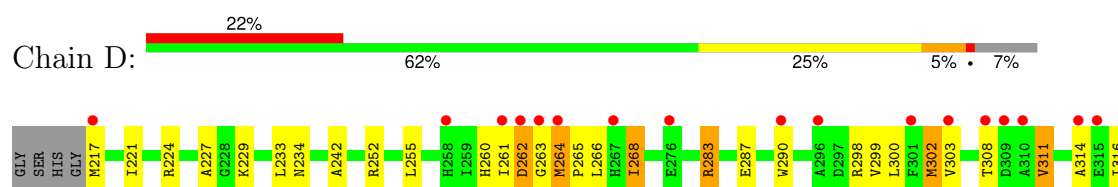
• Molecule 1: tRNA modification GTPase trmE

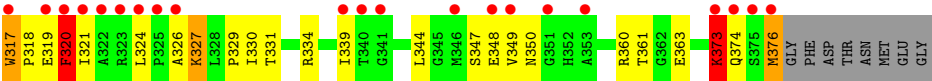


• Molecule 1: tRNA modification GTPase trmE



• Molecule 1: tRNA modification GTPase trmE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.24Å 70.10Å 90.21Å 90.00° 95.76° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.00) 99.3 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.250 , 0.299 0.252 , 0.301	Depositor DCC
R_{free} test set	2446 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5042	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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, RB, ALF, 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	1.21	1/1240 (0.1%)	1.14	2/1680 (0.1%)
1	B	1.12	2/1236 (0.2%)	1.10	0/1675
1	C	1.24	2/1240 (0.2%)	1.21	3/1680 (0.2%)
1	D	0.96	0/1236	1.12	8/1675 (0.5%)
All	All	1.14	5/4952 (0.1%)	1.14	13/6710 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	VAL	CA-CB	7.56	1.64	1.54
1	C	299	VAL	CA-CB	6.18	1.61	1.54
1	B	327	LYS	CA-C	5.61	1.60	1.53
1	A	269	ILE	CA-CB	5.40	1.61	1.54
1	C	339	ILE	CA-CB	5.32	1.61	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ILE	N-CA-C	7.27	117.40	110.42
1	C	290	TRP	CA-CB-CG	-6.38	101.48	113.60
1	D	317	TRP	CA-C-N	6.08	125.80	119.05
1	D	317	TRP	C-N-CA	6.08	125.80	119.05
1	D	224	ARG	CA-C-N	-5.42	114.19	119.78
1	D	224	ARG	C-N-CA	-5.42	114.19	119.78
1	C	317	TRP	N-CA-C	5.34	119.60	108.39
1	A	328	LEU	CA-C-N	-5.21	115.20	120.31
1	A	328	LEU	C-N-CA	-5.21	115.20	120.31
1	D	264	MET	CA-C-N	-5.19	114.61	119.85
1	D	264	MET	C-N-CA	-5.19	114.61	119.85
1	D	252	ARG	NE-CZ-NH1	-5.11	116.39	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	PHE	CB-CA-C	5.09	117.97	109.56

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	1224	0	1242	20	0
1	B	1220	0	1239	24	0
1	C	1224	0	1242	42	0
1	D	1220	0	1239	39	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	12	0	0
5	B	28	0	12	0	0
5	C	28	0	12	1	0
5	D	28	0	12	3	0
6	A	5	0	0	0	0
6	B	2	0	0	0	0
6	C	4	0	0	0	0
6	D	3	0	0	0	0
All	All	5042	0	5010	125	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 12.

All (125) 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:B:308:THR:O	1:B:334:ARG:NH2	1.89	1.06
1:B:221:ILE:HD11	1:B:268:ILE:HD11	1.04	1.01
1:C:317:TRP:NE1	1:C:319:GLU:HB2	1.79	0.96
1:B:221:ILE:HD11	1:B:268:ILE:CD1	1.95	0.95
1:A:312:ASP:HB3	1:A:315:GLU:HG2	1.47	0.94
1:C:355:ILE:HD11	1:C:357:LEU:HD23	1.49	0.94
1:D:308:THR:O	1:D:334:ARG:NH2	2.00	0.93
1:B:221:ILE:CD1	1:B:268:ILE:HD11	1.98	0.92
1:D:233:LEU:HD12	1:D:268:ILE:HD13	1.53	0.90
1:C:234:ASN:HD21	1:C:242:ALA:H	1.18	0.90
1:B:258:HIS:CE1	1:B:267:HIS:HD2	1.91	0.89
1:B:234:ASN:HD21	1:B:242:ALA:H	1.15	0.88
1:D:317:TRP:CE3	1:D:320:PHE:HB3	2.09	0.87
1:D:221:ILE:HD11	1:D:268:ILE:HD11	1.57	0.86
1:C:330:ILE:HG23	1:C:352:HIS:CD2	2.10	0.86
1:A:218:LYS:HE3	1:A:269:ILE:HD13	1.62	0.81
1:C:218:LYS:HE3	1:C:269:ILE:CD1	2.11	0.80
1:A:234:ASN:HD21	1:A:242:ALA:H	1.26	0.79
1:C:218:LYS:HE3	1:C:269:ILE:HD13	1.64	0.79
1:D:233:LEU:HD12	1:D:268:ILE:CD1	2.14	0.77
1:D:321:ILE:HA	1:D:324:LEU:HD12	1.66	0.77
1:C:320:PHE:CD1	1:C:321:ILE:HD13	2.21	0.75
1:D:233:LEU:CD1	1:D:268:ILE:HD13	2.17	0.74
1:C:330:ILE:HG23	1:C:352:HIS:HD2	1.51	0.74
1:B:258:HIS:CE1	1:B:267:HIS:CD2	2.76	0.73
1:A:299:VAL:HG23	1:A:328:LEU:HD21	1.71	0.71
1:C:224:ARG:NH2	1:C:317:TRP:CD1	2.58	0.70
1:A:313:PRO:HB2	1:A:321:ILE:HG13	1.74	0.70
1:B:372:LEU:O	1:B:376:MET:HG2	1.90	0.69
1:A:266:LEU:HD21	1:A:376:MET:HE1	1.74	0.69
1:D:262:ASP:HB2	1:D:373:LYS:HD2	1.74	0.69
1:B:264:MET:HE3	1:B:266:LEU:HD23	1.80	0.64
1:D:283:ARG:CZ	1:D:283:ARG:HB3	2.29	0.62
1:D:326:ALA:O	1:D:327:LYS:HB2	1.98	0.62
1:A:302:MET:HE3	1:A:335:ASN:HB2	1.80	0.62
1:C:274:LEU:HD12	1:C:317:TRP:HZ3	1.66	0.61
1:D:234:ASN:HD21	1:D:242:ALA:H	1.50	0.59
1:B:304:ASP:OD2	1:B:336:LYS:HD2	2.04	0.58
1:D:283:ARG:NH1	1:D:287:GLU:OE1	2.34	0.58
1:A:266:LEU:HD21	1:A:376:MET:CE	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:HD12	1:B:268:ILE:HD13	1.85	0.57
1:B:360:ARG:HH11	1:B:360:ARG:HG2	1.68	0.57
1:D:303:VAL:HG21	1:D:316:ILE:HD13	1.86	0.57
1:D:317:TRP:NE1	1:D:319:GLU:HB2	2.19	0.57
1:B:232:LEU:HD22	1:B:302:MET:HE1	1.87	0.56
1:A:299:VAL:CG2	1:A:328:LEU:HD21	2.35	0.56
1:C:303:VAL:HG21	1:C:316:ILE:HG21	1.87	0.56
1:C:252:ARG:HG2	1:C:282:GLU:HA	1.87	0.56
1:C:320:PHE:CE1	1:C:321:ILE:HD13	2.41	0.56
1:C:311:VAL:HG23	1:C:349:VAL:HG21	1.88	0.56
1:C:302:MET:HG3	1:C:333:VAL:HB	1.88	0.55
1:C:317:TRP:CD1	1:C:319:GLU:HB2	2.40	0.55
1:D:317:TRP:O	1:D:321:ILE:HG12	2.07	0.55
1:C:317:TRP:CE3	1:C:320:PHE:HB2	2.42	0.55
1:D:299:VAL:CG1	1:D:330:ILE:HG12	2.37	0.55
1:C:224:ARG:HH22	1:C:317:TRP:CD1	2.25	0.54
1:C:224:ARG:NH2	1:C:317:TRP:CG	2.76	0.54
1:D:298:ARG:NH1	1:D:329:PRO:HB3	2.22	0.54
1:C:278:SER:O	1:C:283:ARG:NH1	2.41	0.53
1:C:233:LEU:HD22	1:C:270:ASP:HB2	1.90	0.53
1:C:256:ARG:HB3	1:C:267:HIS:CD2	2.44	0.53
1:A:218:LYS:HE3	1:A:269:ILE:CD1	2.37	0.53
1:C:283:ARG:O	1:C:287:GLU:HG3	2.09	0.52
1:A:375:SER:OG	1:A:376:MET:HG3	2.09	0.52
1:A:302:MET:HE3	1:A:335:ASN:CB	2.39	0.52
1:C:360:ARG:HB2	5:C:600:GDP:C5	2.44	0.52
1:C:320:PHE:HD1	1:C:321:ILE:N	2.09	0.51
1:D:262:ASP:CB	1:D:373:LYS:HD2	2.40	0.51
1:C:261:ILE:HG22	1:C:373:LYS:HB2	1.93	0.50
1:C:234:ASN:ND2	1:C:242:ALA:H	1.99	0.50
1:A:266:LEU:HD13	1:A:268:ILE:CD1	2.42	0.50
1:A:282:GLU:O	1:A:286:ILE:HG13	2.11	0.50
1:D:290:TRP:HH2	1:D:320:PHE:HB2	1.74	0.50
1:B:360:ARG:HG2	1:B:360:ARG:NH1	2.25	0.50
1:D:317:TRP:CE3	1:D:320:PHE:CB	2.91	0.50
1:C:320:PHE:CD1	1:C:320:PHE:C	2.90	0.49
1:D:261:ILE:HD12	1:D:266:LEU:HD21	1.94	0.49
1:B:284:ILE:O	1:B:288:ARG:HG3	2.12	0.49
1:C:320:PHE:HD1	1:C:321:ILE:HD13	1.74	0.49
1:D:217:MET:HB2	1:D:376:MET:CE	2.44	0.48
1:B:308:THR:HG23	1:B:334:ARG:HH21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:TRP:CE2	1:C:319:GLU:HB2	2.48	0.48
1:D:326:ALA:O	1:D:327:LYS:CB	2.62	0.48
1:C:261:ILE:CG2	1:C:373:LYS:HB2	2.44	0.47
1:C:256:ARG:NH2	1:C:292:GLU:OE2	2.44	0.47
1:A:302:MET:HE3	1:A:335:ASN:CG	2.40	0.47
1:D:260:HIS:CE1	1:D:265:PRO:HB3	2.50	0.47
1:D:314:ALA:HA	1:D:321:ILE:HG13	1.97	0.46
1:B:372:LEU:O	1:B:376:MET:CG	2.61	0.46
1:B:233:LEU:CD1	1:B:268:ILE:HD13	2.46	0.46
1:D:221:ILE:CG2	1:D:302:MET:CE	2.94	0.46
1:D:300:LEU:HD23	1:D:331:THR:HB	1.98	0.46
1:B:365:VAL:O	1:B:369:ARG:HG3	2.17	0.45
1:C:218:LYS:HE2	1:C:218:LYS:HB3	1.66	0.45
1:C:218:LYS:CE	1:C:269:ILE:CD1	2.90	0.45
1:D:264:MET:HG3	1:D:265:PRO:O	2.17	0.45
1:C:317:TRP:HE1	1:C:319:GLU:HB2	1.73	0.44
1:D:217:MET:HB2	1:D:376:MET:HE1	1.99	0.44
1:C:344:LEU:HD12	1:C:344:LEU:N	2.33	0.44
1:D:360:ARG:HB2	5:D:700:GDP:C5	2.52	0.44
1:A:234:ASN:ND2	1:A:242:ALA:H	2.05	0.44
1:C:289:ALA:O	1:C:293:ILE:HD12	2.17	0.44
1:D:234:ASN:HD21	1:D:242:ALA:N	2.16	0.43
1:B:342:GLU:OE2	1:B:356:ARG:NH2	2.51	0.43
1:D:339:ILE:HD11	5:D:700:GDP:N2	2.34	0.43
1:C:236:LEU:HD23	1:C:236:LEU:HA	1.91	0.42
1:D:311:VAL:HB	1:D:349:VAL:HG21	2.01	0.42
1:D:227:ALA:HB1	1:D:302:MET:HG2	2.01	0.42
1:A:235:ALA:O	1:A:369:ARG:NH2	2.53	0.42
1:C:277:ALA:O	1:C:283:ARG:CG	2.67	0.42
1:D:361:THR:OG1	1:D:363:GLU:HG3	2.19	0.42
1:A:266:LEU:HD13	1:A:268:ILE:HD13	2.01	0.42
1:D:317:TRP:HA	1:D:318:PRO:HD2	1.71	0.42
1:C:317:TRP:HA	1:C:318:PRO:HD2	1.79	0.42
1:D:302:MET:HE2	1:D:302:MET:HB2	1.40	0.41
1:B:304:ASP:O	1:B:307:THR:OG1	2.36	0.41
1:B:233:LEU:HD23	1:B:242:ALA:HB2	2.02	0.41
1:A:304:ASP:OD2	1:A:304:ASP:C	2.64	0.41
1:D:360:ARG:HD3	5:D:700:GDP:C2	2.54	0.41
1:B:311:VAL:HG12	1:B:334:ARG:HD2	2.02	0.41
1:C:328:LEU:HA	1:C:329:PRO:HD3	1.86	0.41
1:A:219:VAL:CG2	1:A:376:MET:HE1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ASN:HD22	1:B:350:ASN:HA	1.73	0.41
1:D:229:LYS:HA	1:D:302:MET:HE3	2.02	0.40
1:C:301:PHE:CZ	1:C:317:TRP:HB2	2.57	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	159/172 (92%)	155 (98%)	4 (2%)	0	100	100
1	B	158/172 (92%)	148 (94%)	8 (5%)	2 (1%)	9	5
1	C	159/172 (92%)	153 (96%)	5 (3%)	1 (1%)	21	17
1	D	158/172 (92%)	147 (93%)	8 (5%)	3 (2%)	6	3
All	All	634/688 (92%)	603 (95%)	25 (4%)	6 (1%)	14	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	LYS
1	B	363	GLU
1	D	373	LYS
1	B	239	ARG
1	C	262	ASP
1	D	263	GLY

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	129/137 (94%)	124 (96%)	5 (4%)	28	28
1	B	129/137 (94%)	116 (90%)	13 (10%)	7	4
1	C	129/137 (94%)	115 (89%)	14 (11%)	6	3
1	D	129/137 (94%)	115 (89%)	14 (11%)	6	3
All	All	516/548 (94%)	470 (91%)	46 (9%)	9	6

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	LEU
1	A	267	HIS
1	A	327	LYS
1	A	330	ILE
1	A	346	MET
1	B	219	VAL
1	B	239	ARG
1	B	245	THR
1	B	255	LEU
1	B	260	HIS
1	B	262	ASP
1	B	267	HIS
1	B	268	ILE
1	B	346	MET
1	B	348	GLU
1	B	360	ARG
1	B	366	ASP
1	B	376	MET
1	C	239	ARG
1	C	262	ASP
1	C	267	HIS
1	C	276	GLU
1	C	290	TRP
1	C	291	GLN
1	C	302	MET
1	C	319	GLU
1	C	320	PHE
1	C	327	LYS
1	C	330	ILE
1	C	346	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	355	ILE
1	C	376	MET
1	D	255	LEU
1	D	262	ASP
1	D	268	ILE
1	D	283	ARG
1	D	302	MET
1	D	311	VAL
1	D	320	PHE
1	D	344	LEU
1	D	347	SER
1	D	348	GLU
1	D	350	ASN
1	D	373	LYS
1	D	374	GLN
1	D	376	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	267	HIS
1	A	352	HIS
1	A	370	ASN
1	B	234	ASN
1	B	258	HIS
1	B	260	HIS
1	B	267	HIS
1	B	350	ASN
1	C	234	ASN
1	C	260	HIS
1	C	352	HIS
1	C	370	ASN
1	D	234	ASN
1	D	258	HIS
1	D	350	ASN
1	D	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
5	GDP	B	500	2,4,3	29,30,30	1.30	3 (10%)	45,47,47	1.89	13 (28%)
2	ALF	C	601	6,5	4,4,4	1.28	0	-		
5	GDP	A	400	2,4,3	29,30,30	1.27	5 (17%)	45,47,47	1.88	8 (17%)
5	GDP	C	600	2,4,3	29,30,30	1.19	4 (13%)	45,47,47	2.05	14 (31%)
2	ALF	A	401	6,5	4,4,4	1.16	0	-		
2	ALF	B	501	6,5	4,4,4	1.13	0	-		
5	GDP	D	700	2,4,3	29,30,30	1.20	1 (3%)	45,47,47	1.83	7 (15%)
2	ALF	D	701	6,5	4,4,4	1.16	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	D	700	2,4,3	-	2/16/32/32	0/3/3/3
5	GDP	A	400	2,4,3	-	2/16/32/32	0/3/3/3
5	GDP	C	600	2,4,3	-	2/16/32/32	0/3/3/3
5	GDP	B	500	2,4,3	-	2/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	700	GDP	C5-C4	3.83	1.49	1.38
5	B	500	GDP	PA-O3A	2.93	1.62	1.59
5	A	400	GDP	C5-C4	2.90	1.46	1.38
5	B	500	GDP	C6-N1	-2.79	1.33	1.38
5	B	500	GDP	C5-C4	2.78	1.46	1.38
5	A	400	GDP	O6-C6	2.75	1.28	1.23
5	C	600	GDP	C6-N1	-2.69	1.33	1.38
5	A	400	GDP	C6-N1	-2.51	1.34	1.38
5	C	600	GDP	C5-C4	2.50	1.45	1.38
5	C	600	GDP	C4-N9	-2.44	1.31	1.38
5	A	400	GDP	PA-O3A	2.34	1.62	1.59
5	C	600	GDP	C5-N7	-2.22	1.34	1.39
5	A	400	GDP	C8-N9	-2.16	1.32	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	400	GDP	C5-C4-N3	-6.08	118.71	128.39
5	D	700	GDP	C5-C4-N3	-5.71	119.31	128.39
5	C	600	GDP	C5-C4-N3	-5.69	119.34	128.39
5	C	600	GDP	C2-N3-C4	5.48	121.75	112.30
5	B	500	GDP	C5-C4-N3	-5.18	120.15	128.39
5	B	500	GDP	C2-N3-C4	5.11	121.10	112.30
5	D	700	GDP	C2-N3-C4	5.09	121.06	112.30
5	A	400	GDP	C2-N3-C4	5.02	120.94	112.30
5	C	600	GDP	C6-C5-N7	4.29	138.10	130.29
5	A	400	GDP	N9-C4-N3	4.16	134.28	125.95
5	A	400	GDP	C4-C5-N7	-4.08	104.21	110.67
5	D	700	GDP	C6-C5-N7	4.05	137.66	130.29
5	B	500	GDP	C6-C5-N7	3.82	137.24	130.29
5	C	600	GDP	N9-C4-N3	3.71	133.38	125.95
5	B	500	GDP	N9-C4-N3	3.65	133.25	125.95
5	D	700	GDP	N9-C4-N3	3.54	133.03	125.95
5	C	600	GDP	O3B-PB-O3A	3.48	116.29	104.64
5	A	400	GDP	C6-C5-N7	3.44	136.56	130.29
5	D	700	GDP	C4-C5-N7	-3.15	105.68	110.67
5	C	600	GDP	C4-C5-N7	-2.88	106.10	110.67
5	B	500	GDP	O3B-PB-O2B	2.87	118.56	107.80
5	A	400	GDP	C8-N7-C5	2.77	109.20	104.26
5	C	600	GDP	O6-C6-C5	-2.56	119.77	126.53
5	B	500	GDP	O6-C6-C5	-2.49	119.96	126.53
5	C	600	GDP	C5-C6-N1	2.39	119.34	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	700	GDP	O2A-PA-O3A	2.39	113.72	107.27
5	B	500	GDP	O3B-PB-O1B	-2.37	101.59	110.83
5	C	600	GDP	C8-N7-C5	2.32	108.40	104.26
5	C	600	GDP	N9-C8-N7	-2.31	109.11	113.40
5	C	600	GDP	O3'-C3'-C4'	-2.31	104.45	111.08
5	C	600	GDP	C2-N1-C6	-2.28	120.97	125.11
5	B	500	GDP	O4'-C1'-N9	2.27	113.51	108.36
5	B	500	GDP	C6-C5-C4	-2.24	115.46	118.83
5	B	500	GDP	C1'-N9-C4	-2.21	119.96	126.49
5	C	600	GDP	N2-C2-N1	2.18	121.36	116.76
5	B	500	GDP	C4-C5-N7	-2.14	107.28	110.67
5	A	400	GDP	O3B-PB-O2B	2.13	115.77	107.80
5	B	500	GDP	C5-C6-N1	2.05	118.46	113.25
5	A	400	GDP	O3'-C3'-C2'	-2.02	105.33	111.82
5	C	600	GDP	C6-C5-C4	-2.01	115.80	118.83
5	D	700	GDP	O2'-C2'-C1'	2.01	117.02	110.10
5	B	500	GDP	N2-C2-N1	2.01	120.99	116.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	400	GDP	PA-O3A-PB-O3B
5	B	500	GDP	PA-O3A-PB-O3B
5	D	700	GDP	PA-O3A-PB-O3B
5	A	400	GDP	PA-O3A-PB-O1B
5	C	600	GDP	PA-O3A-PB-O1B
5	C	600	GDP	PA-O3A-PB-O3B
5	D	700	GDP	PA-O3A-PB-O1B
5	B	500	GDP	PA-O3A-PB-O1B

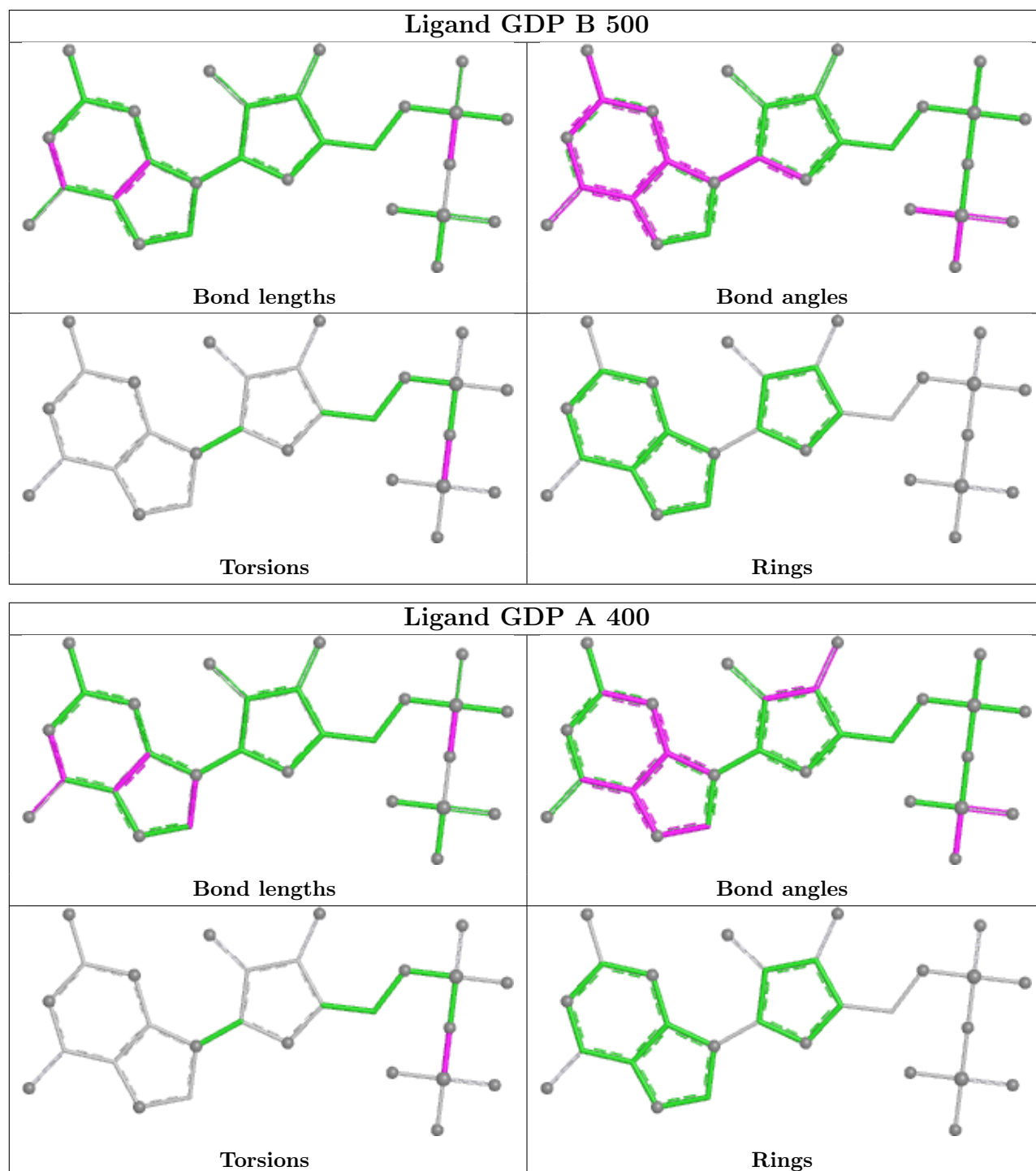
There are no ring outliers.

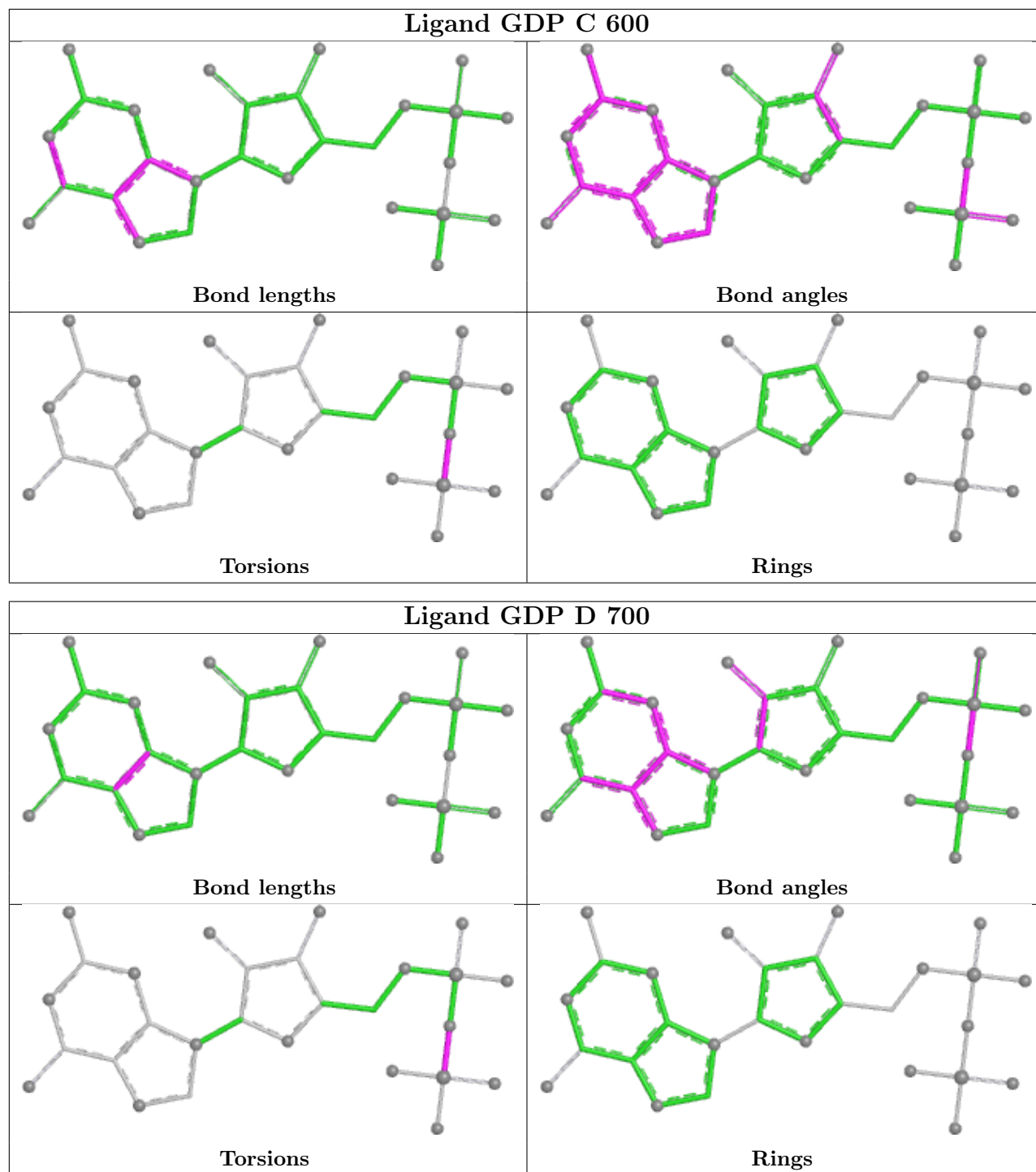
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	600	GDP	1	0
5	D	700	GDP	3	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	161/172 (93%)	0.30	13 (8%) 18 17	10, 19, 37, 47	0
1	B	160/172 (93%)	0.64	14 (8%) 15 14	11, 24, 39, 45	0
1	C	161/172 (93%)	0.32	10 (6%) 26 25	11, 18, 31, 33	0
1	D	160/172 (93%)	1.29	38 (23%) 2 2	13, 33, 54, 57	0
All	All	642/688 (93%)	0.64	75 (11%) 9 8	10, 22, 46, 57	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	263	GLY	8.5
1	D	320	PHE	7.7
1	D	317	TRP	6.1
1	C	317	TRP	5.5
1	D	326	ALA	5.5
1	C	320	PHE	4.6
1	D	376	MET	4.4
1	D	290	TRP	4.4
1	D	262	ASP	4.4
1	B	258	HIS	4.2
1	C	309	ASP	4.0
1	D	324	LEU	3.9
1	D	375	SER	3.7
1	D	308	THR	3.7
1	D	325	PRO	3.6
1	D	309	ASP	3.6
1	C	262	ASP	3.6
1	D	341	GLY	3.6
1	D	322	ALA	3.5
1	D	217	MET	3.5
1	A	262	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	321	ILE	3.3
1	A	290	TRP	3.3
1	C	290	TRP	3.2
1	B	366	ASP	3.2
1	A	283	ARG	3.1
1	D	319	GLU	3.1
1	D	353	ALA	3.0
1	D	301	PHE	3.0
1	B	263	GLY	3.0
1	D	346	MET	3.0
1	C	276	GLU	2.9
1	B	260	HIS	2.9
1	D	374	GLN	2.9
1	B	327	LYS	2.9
1	A	315	GLU	2.8
1	C	267	HIS	2.8
1	D	303	VAL	2.8
1	D	339	ILE	2.7
1	A	309	ASP	2.6
1	D	258	HIS	2.6
1	D	323	ARG	2.6
1	A	216	GLY	2.5
1	B	266	LEU	2.5
1	A	264	MET	2.4
1	D	310	ALA	2.4
1	A	258	HIS	2.4
1	C	374	GLN	2.4
1	B	309	ASP	2.4
1	D	276	GLU	2.3
1	A	374	GLN	2.3
1	B	365	VAL	2.3
1	A	342	GLU	2.3
1	D	314	ALA	2.3
1	A	267	HIS	2.3
1	B	261	ILE	2.3
1	B	340	THR	2.3
1	D	296	ALA	2.3
1	D	351	GLY	2.3
1	D	315	GLU	2.2
1	D	340	THR	2.2
1	D	267	HIS	2.2
1	B	339	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	349	VAL	2.2
1	B	364	GLY	2.2
1	A	217	MET	2.2
1	D	261	ILE	2.1
1	A	261	ILE	2.1
1	D	348	GLU	2.1
1	C	326	ALA	2.1
1	D	373	LYS	2.1
1	D	264	MET	2.0
1	B	268	ILE	2.0
1	B	217	MET	2.0
1	C	323	ARG	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(Å ²)	Q<0.9
3	MG	B	502	1/1	0.91	0.04	14,14,14,14	0
3	MG	D	702	1/1	0.94	0.05	23,23,23,23	0
5	GDP	D	700	28/28	0.94	0.09	15,25,29,30	0
3	MG	A	402	1/1	0.95	0.07	13,13,13,13	0
5	GDP	B	500	28/28	0.96	0.08	14,26,29,30	0
2	ALF	B	501	5/5	0.96	0.05	12,13,16,16	0
5	GDP	A	400	28/28	0.97	0.06	8,11,14,15	0
3	MG	C	602	1/1	0.97	0.03	15,15,15,15	0
5	GDP	C	600	28/28	0.97	0.06	8,14,16,17	0
2	ALF	D	701	5/5	0.97	0.05	12,16,17,19	0
2	ALF	C	601	5/5	0.98	0.05	12,15,15,20	0

Continued on next page...

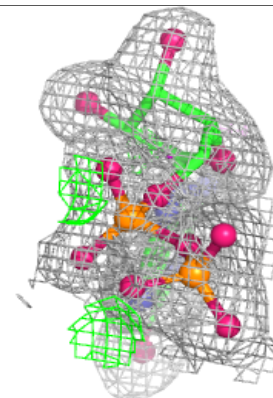
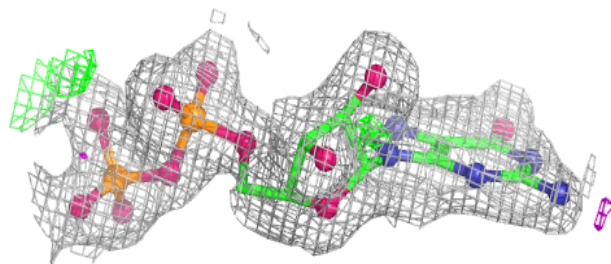
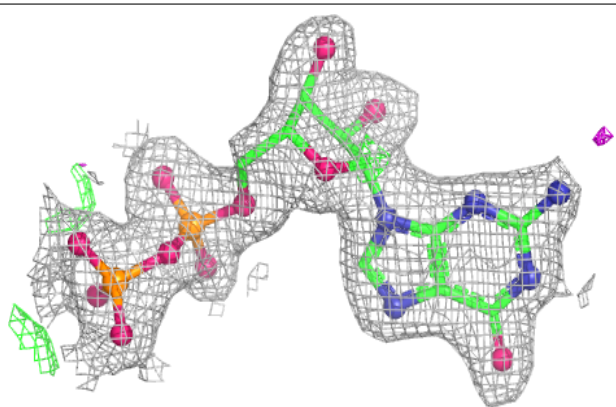
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ALF	A	401	5/5	0.98	0.04	11,13,13,15	0
4	RB	B	503	1/1	0.99	0.07	25,25,25,25	0
4	RB	D	703	1/1	0.99	0.05	25,25,25,25	0
4	RB	C	603	1/1	1.00	0.05	19,19,19,19	0
4	RB	A	403	1/1	1.00	0.03	18,18,18,18	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.

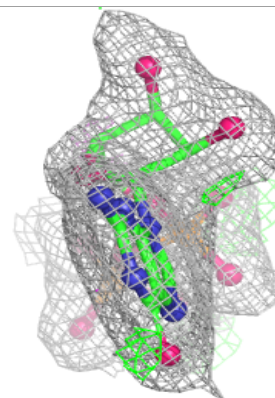
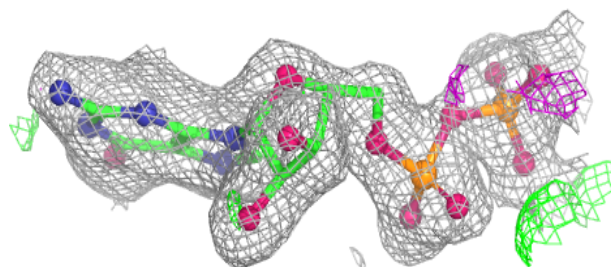
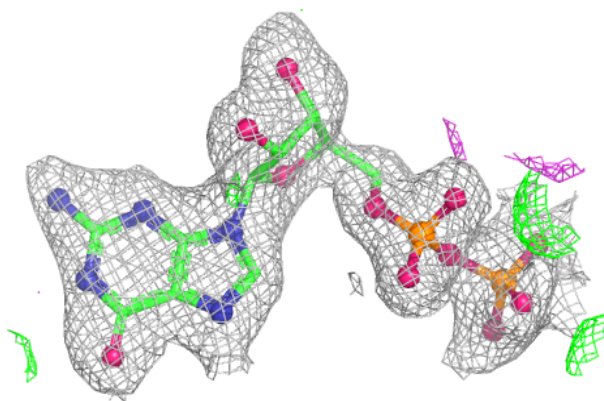
Electron density around GDP D 700:

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

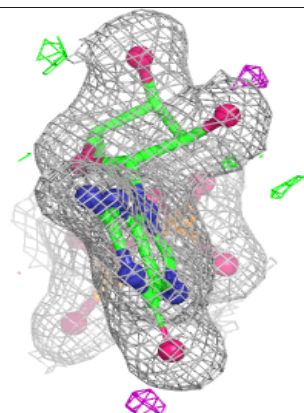
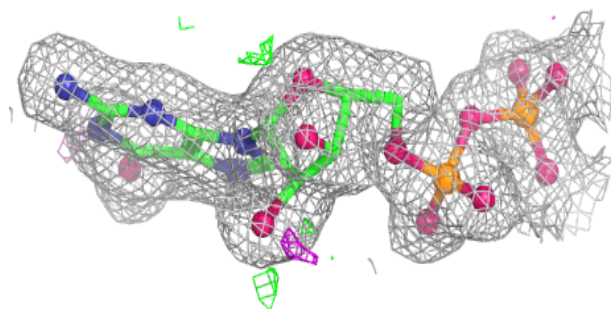
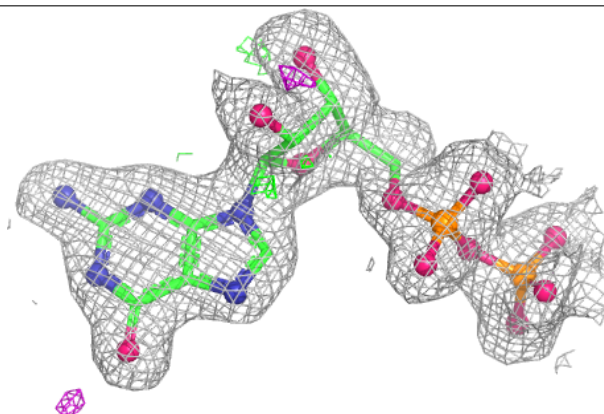


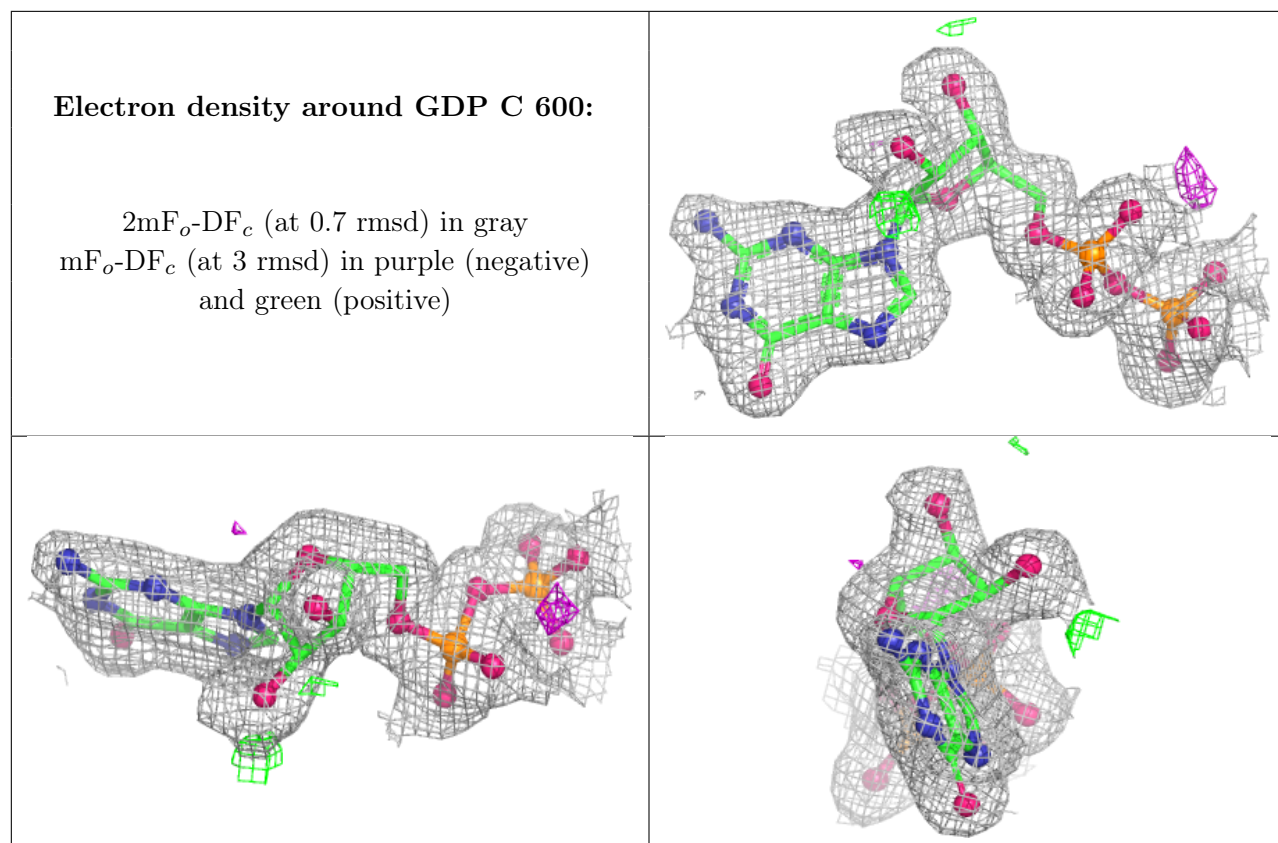
Electron density around GDP B 500:

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

**Electron density around GDP A 400:**

$2mF_o-DF_c$ (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.