Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:53 PM BST

PDB ID	:	6S6A
Title	:	Crystal structure of RagA-Q66L/RagC-T90N GTPase heterodimer complex
Authors	:	Anandapadamanaban, M.; Masson, G.R.; Perisic, O.; Kaufman, J.; Williams, R.L.
Deposited on	:	2019-07-02
Resolution	:	2.63 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 following versions of software and data (see references ⓘ) were used in the production of this report:

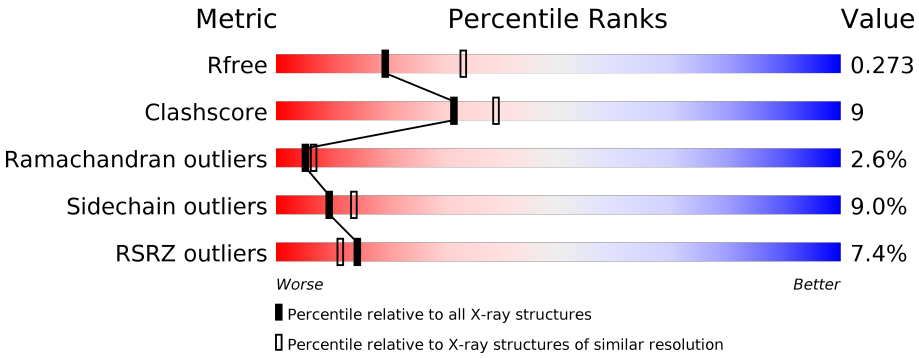
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 on 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	313	71% 21% • 5%
1	B	313	4% 68% 22% • 5%
2	C	399	% 52% 14% • 32%
2	D	399	17% 47% 18% • • 31%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9540 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 Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2444	1553	424	450	17			
1	B	298	Total	C	N	O	S	0	0	0
			2448	1555	427	449	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	LEU	GLN	engineered mutation	UNP Q7L523
B	66	LEU	GLN	engineered mutation	UNP Q7L523

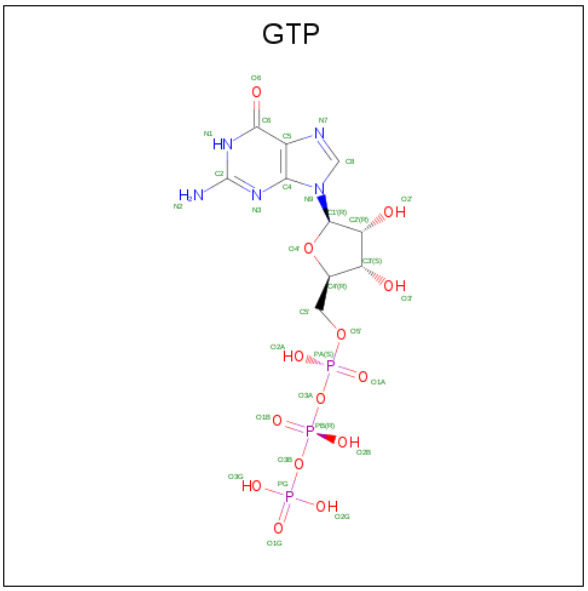
- Molecule 2 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	273	Total	C	N	O	S	0	1	0
			2210	1421	364	413	12			
2	D	275	Total	C	N	O	S	0	0	0
			2222	1431	362	417	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	ASN	THR	engineered mutation	UNP Q9HB90
D	90	ASN	THR	engineered mutation	UNP Q9HB90

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by author).

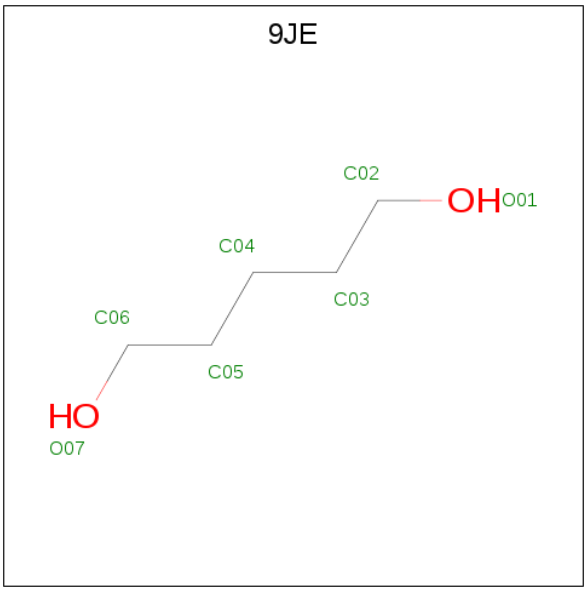


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

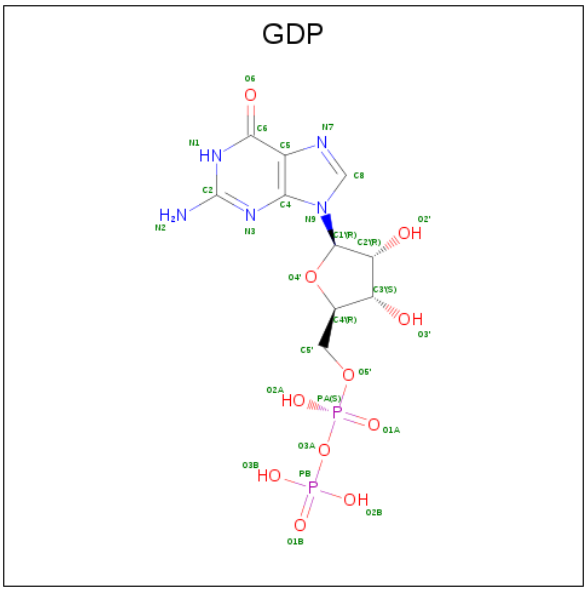
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is pentane-1,5-diol (three-letter code: 9JE) (formula: $C_5H_{12}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 5 2	0	0
5	B	1	Total C O 7 5 2	0	0
5	B	1	Total C O 7 5 2	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by author).



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

- Molecule 7 is water.

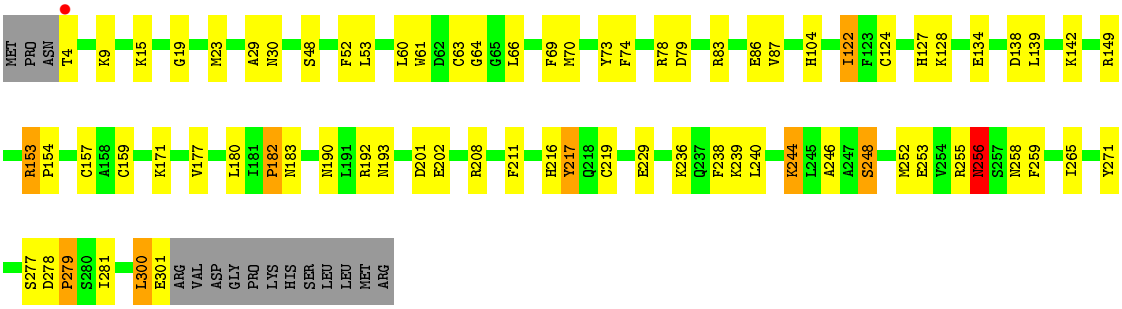
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	29	Total	O	0	0
			29	29		
7	B	26	Total	O	0	0
			26	26		
7	C	17	Total	O	0	0
			17	17		
7	D	1	Total	O	0	0
			1	1		

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.

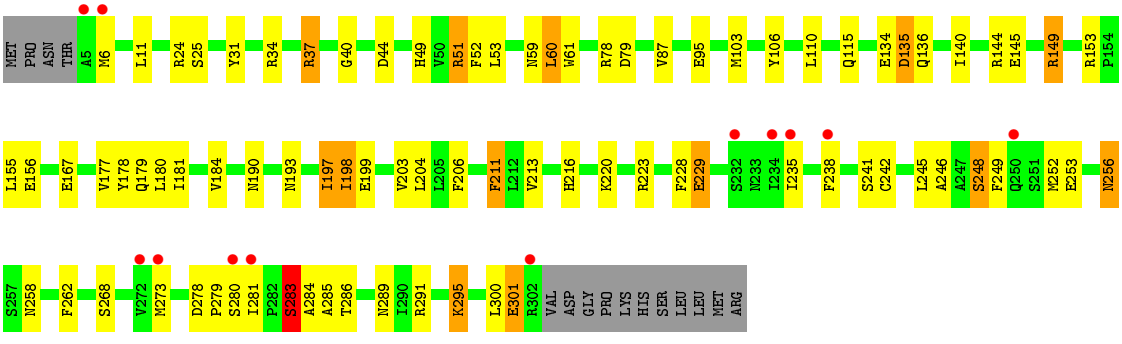
- Molecule 1: Ras-related GTP-binding protein A

Chain A:



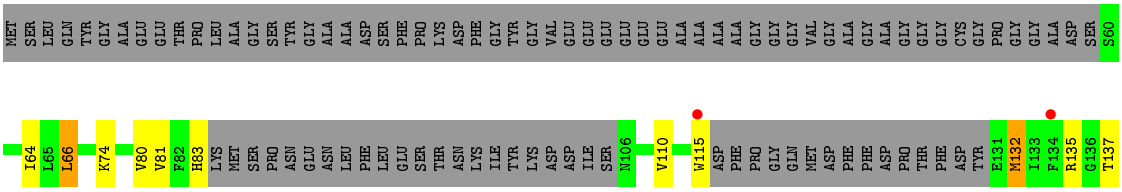
- Molecule 1: Ras-related GTP-binding protein A

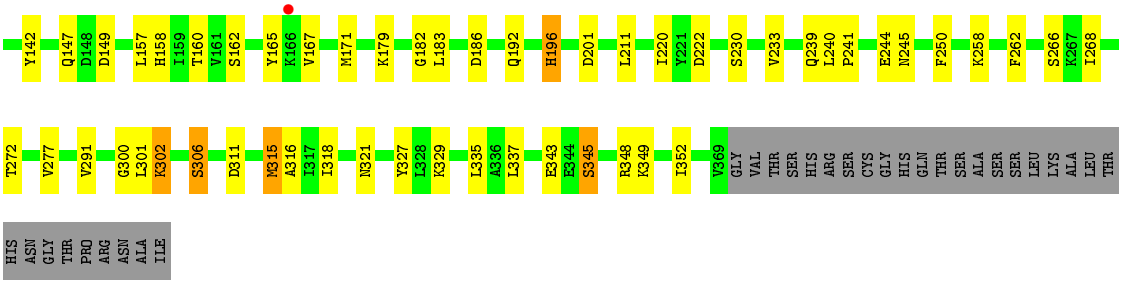
Chain B:



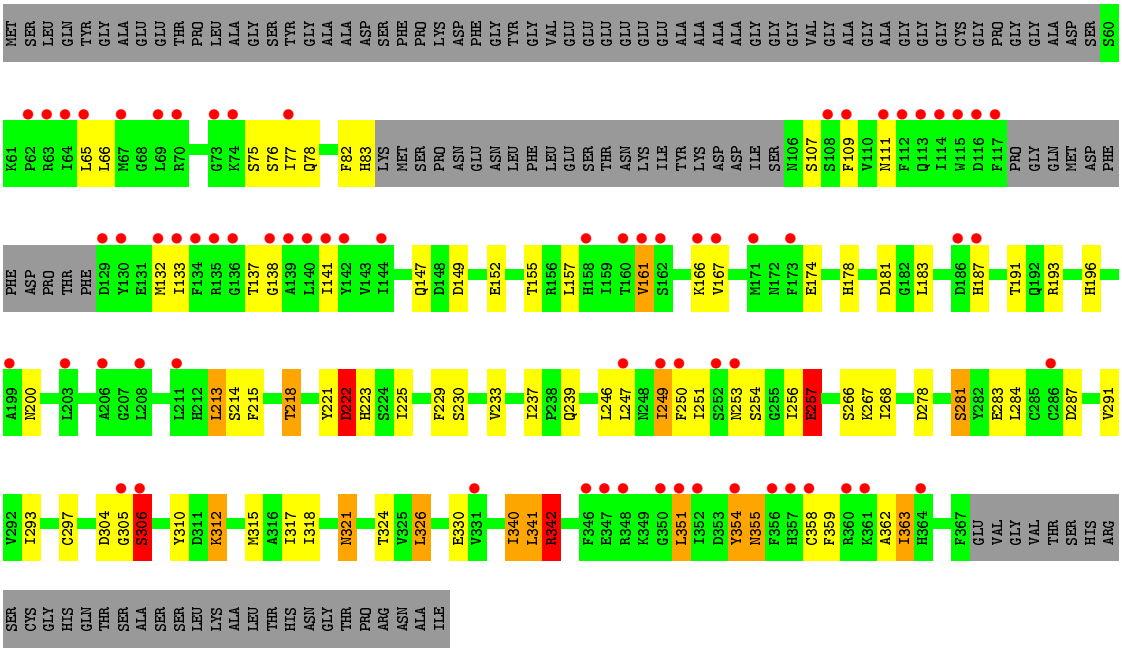
- Molecule 2: Ras-related GTP-binding protein C

Chain C:





• Molecule 2: Ras-related GTP-binding protein C



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.10Å 81.86Å 244.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 2.63 46.58 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.62-2.63) 98.0 (46.58-2.63)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.195 , 0.275 0.201 , 0.273	Depositor DCC
R_{free} test set	2105 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	81.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9540	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: GDP, GTP, MG, 9JE

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	0.82	0/2489	1.03	2/3352 (0.1%)
1	B	0.79	1/2493 (0.0%)	1.01	2/3356 (0.1%)
2	C	0.81	2/2251 (0.1%)	0.97	1/3034 (0.0%)
2	D	1.48	3/2265 (0.1%)	1.00	5/3054 (0.2%)
All	All	1.01	6/9498 (0.1%)	1.00	10/12796 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	257	GLU	CD-OE2	58.18	1.89	1.25
2	D	342	ARG	CZ-NH2	-14.73	1.13	1.33
2	D	342	ARG	CD-NE	5.96	1.56	1.46
2	C	244	GLU	CD-OE1	5.80	1.32	1.25
1	B	156	GLU	CD-OE2	5.30	1.31	1.25
2	C	343	GLU	CD-OE1	5.02	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	342	ARG	NE-CZ-NH1	16.60	128.60	120.30
2	D	342	ARG	NE-CZ-NH2	-12.67	113.97	120.30
2	D	257	GLU	CG-CD-OE2	-12.06	94.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	257	GLU	CG-CD-OE1	-12.04	94.21	118.30
1	B	153	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	D	257	GLU	OE1-CD-OE2	-7.72	114.03	123.30
1	B	153	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	C	306	SER	C-N-CA	5.42	133.68	122.30
1	A	271	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	256	ASN	CB-CA-C	5.01	120.43	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	257	GLU	Sidechain
2	D	342	ARG	Sidechain

5.2 Too-close contacts (i)

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	2444	0	2440	47	0
1	B	2448	0	2446	50	0
2	C	2210	0	2210	39	0
2	D	2222	0	2209	50	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	7	0	0	0	0
5	B	14	0	0	1	0
6	C	28	0	12	2	0
6	D	28	0	12	1	0
7	A	29	0	0	2	0
7	B	26	0	0	0	0
7	C	17	0	0	0	0
7	D	1	0	0	0	0
All	All	9540	0	9353	169	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 9.

All (169) 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:D:257:GLU:OE2	2:D:257:GLU:CD	1.89	1.11
2:D:257:GLU:OE2	2:D:342:ARG:HG2	1.62	0.98
1:B:211:PHE:CZ	1:B:235:ILE:HG21	2.08	0.88
1:A:171:LYS:HB2	1:A:229:GLU:HG2	1.57	0.86
2:D:253:ASN:HB3	2:D:355:ASN:HD22	1.52	0.73
1:B:190:ASN:HD22	1:B:300:LEU:HD11	1.57	0.69
2:D:250:PHE:HB2	2:D:359:PHE:HD2	1.60	0.66
1:B:198:ILE:HG13	1:B:289:ASN:HD22	1.60	0.65
2:D:82:PHE:O	2:D:83:HIS:CD2	2.50	0.65
2:D:266:SER:O	2:D:267:LYS:HB2	1.97	0.65
1:B:216:HIS:HD2	5:B:403:9JE:O01	1.79	0.64
2:D:196:HIS:O	2:D:200:ASN:ND2	2.30	0.63
1:A:248:SER:CB	2:C:321:ASN:HD22	2.12	0.63
1:A:190:ASN:ND2	1:A:300:LEU:HD11	2.13	0.62
1:A:248:SER:HB2	2:C:321:ASN:HD22	1.64	0.62
2:D:287:ASP:O	2:D:291:VAL:HG23	1.99	0.62
2:D:304:ASP:O	2:D:306:SER:N	2.32	0.61
1:A:53:LEU:O	1:A:301:GLU:HG2	2.00	0.61
2:C:262:PHE:O	2:C:335:LEU:HA	1.99	0.61
2:D:257:GLU:OE2	2:D:342:ARG:CG	2.45	0.61
1:B:135:ASP:OD1	1:B:136:GLN:HG2	2.00	0.61
1:B:245:LEU:O	1:B:245:LEU:HD12	2.00	0.61
1:A:153:ARG:HB2	1:A:154:PRO:HD2	1.83	0.61
1:B:262:PHE:O	1:B:273:MET:HA	2.01	0.60
1:A:52:PHE:CZ	1:A:177:VAL:HG11	2.38	0.59
2:D:321:ASN:ND2	2:D:321:ASN:O	2.36	0.58
1:A:190:ASN:HD22	1:A:300:LEU:HD11	1.68	0.58
2:D:351:LEU:O	2:D:354:TYR:HB2	2.02	0.58
1:B:283:SER:O	1:B:285:ALA:N	2.33	0.58
2:C:258:LYS:HE3	2:C:277:VAL:HG22	1.85	0.58
2:D:257:GLU:OE2	2:D:257:GLU:CG	2.51	0.58
1:A:277:SER:O	1:A:279:PRO:HD3	2.03	0.58
1:B:211:PHE:CZ	1:B:235:ILE:CG2	2.86	0.58
2:C:179:LYS:HD3	6:C:401:GDP:C4	2.39	0.57
2:D:293:ILE:O	2:D:297:CYS:SG	2.56	0.57
1:B:24:ARG:HD3	1:B:60:LEU:HD22	1.87	0.56
2:C:74:LYS:NZ	6:C:401:GDP:O3B	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:SER:HB2	1:B:31:TYR:CD1	2.41	0.56
2:D:250:PHE:HB2	2:D:359:PHE:CD2	2.41	0.56
1:A:153:ARG:CB	1:A:154:PRO:CD	2.84	0.55
1:A:201:ASP:OD2	1:A:277:SER:HB3	2.06	0.55
1:B:197:ILE:O	1:B:199:GLU:N	2.39	0.55
1:B:256:ASN:C	1:B:256:ASN:HD22	2.08	0.55
2:D:229:PHE:O	2:D:233:VAL:HG23	2.06	0.55
2:D:310:TYR:OH	2:D:330:GLU:HG2	2.06	0.55
2:D:213:LEU:HB3	2:D:215:PHE:CZ	2.42	0.55
2:D:77:ILE:HG23	2:D:225:ILE:HD11	1.88	0.55
1:A:153:ARG:CB	1:A:154:PRO:HD2	2.37	0.54
1:B:213:VAL:HG21	1:B:228:PHE:HB3	1.89	0.54
2:C:349:LYS:HA	2:C:352:ILE:HD12	1.89	0.54
1:A:87:VAL:CG2	1:A:180:LEU:HD21	2.38	0.53
2:C:301:LEU:O	2:C:302:LYS:HB2	2.08	0.53
1:A:79:ASP:OD1	1:A:83:ARG:NH1	2.42	0.53
1:A:171:LYS:CB	1:A:229:GLU:HG2	2.33	0.53
1:A:252:MET:HE1	2:C:291:VAL:HG11	1.91	0.53
1:A:281:ILE:O	1:A:281:ILE:HD12	2.08	0.53
1:A:149:ARG:HG2	1:A:157:CYS:SG	2.50	0.52
2:D:359:PHE:CE1	2:D:363:ILE:HD11	2.45	0.52
1:B:245:LEU:HD11	2:D:284:LEU:HD13	1.92	0.52
2:D:249:ILE:O	2:D:253:ASN:HB2	2.09	0.52
1:A:208:ARG:NH1	1:A:265:ILE:HD11	2.24	0.52
1:A:74:PHE:O	1:A:78:ARG:HD2	2.09	0.52
2:D:355:ASN:N	2:D:355:ASN:OD1	2.43	0.52
1:B:211:PHE:CE1	1:B:235:ILE:HG21	2.43	0.52
1:A:259:PHE:CD1	2:C:300:GLY:HA3	2.45	0.52
1:B:49:HIS:CD2	1:B:59:ASN:OD1	2.63	0.51
2:C:327:TYR:CZ	2:C:329:LYS:HD2	2.45	0.51
2:D:253:ASN:HB3	2:D:355:ASN:ND2	2.24	0.51
2:D:157:LEU:O	2:D:161:VAL:HB	2.11	0.51
2:D:247:LEU:HA	2:D:359:PHE:HE2	1.77	0.50
2:C:137:THR:HB	2:C:171:MET:CE	2.42	0.50
1:A:104:HIS:HB3	7:A:527:HOH:O	2.10	0.49
1:A:217:TYR:CD1	1:A:217:TYR:C	2.85	0.49
1:A:253:GLU:O	2:C:316:ALA:HA	2.12	0.49
2:D:65:LEU:HD12	2:D:137:THR:HG21	1.94	0.49
1:A:240:LEU:O	1:A:244:LYS:HD2	2.12	0.49
1:B:242:CYS:HB3	1:B:248:SER:O	2.11	0.49
2:D:326:LEU:HD23	2:D:340:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASN:ND2	1:A:258:ASN:H	2.11	0.49
2:D:66:LEU:HD12	2:D:141:ILE:HB	1.95	0.48
1:A:9:LYS:HE3	1:A:61:TRP:CZ2	2.49	0.47
1:B:256:ASN:C	1:B:256:ASN:ND2	2.67	0.47
2:D:141:ILE:HA	2:D:174:GLU:O	2.15	0.47
1:A:124:CYS:O	1:A:159:CYS:HA	2.14	0.47
1:A:122:ILE:CD1	1:A:122:ILE:N	2.78	0.46
2:C:311:ASP:C	2:C:311:ASP:OD1	2.53	0.46
1:B:145:GLU:OE2	1:B:149:ARG:NH2	2.49	0.46
1:B:178:TYR:HA	1:B:181:ILE:HD12	1.98	0.46
2:C:192:GLN:O	2:C:196:HIS:HB2	2.15	0.46
1:B:248:SER:HB2	2:D:321:ASN:HB2	1.98	0.46
1:B:252:MET:HE1	2:D:291:VAL:HG11	1.97	0.46
2:C:132:MET:HA	2:C:135:ARG:HD3	1.98	0.46
1:B:167:GLU:HB2	1:B:229:GLU:CB	2.46	0.46
2:D:237:ILE:HG23	2:D:239:GLN:HE21	1.81	0.46
1:A:70:MET:HA	1:A:73:TYR:CD2	2.51	0.45
1:B:258:ASN:OD1	1:B:258:ASN:N	2.49	0.45
2:D:183:LEU:HB3	2:D:187:HIS:HB3	1.98	0.45
1:A:52:PHE:O	1:A:53:LEU:HB2	2.17	0.45
1:A:79:ASP:O	1:A:83:ARG:HG2	2.16	0.45
1:B:52:PHE:CZ	1:B:177:VAL:HG11	2.51	0.45
2:D:178:HIS:HA	2:D:218:THR:O	2.17	0.45
2:C:64:ILE:HD12	2:C:110:VAL:HG11	1.98	0.45
1:A:248:SER:HB3	2:C:321:ASN:HD22	1.81	0.45
2:C:250:PHE:CE2	2:C:337:LEU:HD21	2.52	0.45
2:C:80:VAL:HG21	2:C:220:ILE:HB	1.98	0.45
2:C:147:GLN:OE1	2:C:182:GLY:HA3	2.17	0.44
1:B:179:GLN:HG2	2:C:348[A]:ARG:HD2	2.00	0.44
2:D:246:LEU:HD21	2:D:362:ALA:HB1	1.99	0.44
2:D:75:SER:OG	6:D:401:GDP:O1B	2.18	0.44
1:B:78:ARG:HE	1:B:115:GLN:NE2	2.16	0.44
1:B:95:GLU:O	1:B:95:GLU:HG2	2.17	0.44
2:C:157:LEU:O	2:C:157:LEU:HD12	2.18	0.44
1:B:167:GLU:HB2	1:B:229:GLU:HB2	1.99	0.44
1:B:206:PHE:CE2	1:B:213:VAL:HG22	2.52	0.43
2:C:158:HIS:O	2:C:162:SER:OG	2.25	0.43
2:C:345:SER:HA	2:C:348[A]:ARG:NH2	2.34	0.43
1:B:203:VAL:O	1:B:216:HIS:HA	2.18	0.43
1:A:63:CYS:O	1:A:64:GLY:C	2.57	0.43
1:B:253:GLU:OE1	2:D:317:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HH12	1:A:265:ILE:HD11	1.83	0.43
1:B:106:TYR:CZ	1:B:110:LEU:HD11	2.54	0.43
1:B:241:SER:OG	2:D:287:ASP:OD2	2.22	0.43
1:B:204:LEU:HD23	1:B:216:HIS:HB2	2.01	0.43
1:A:252:MET:CE	2:C:291:VAL:HG11	2.49	0.43
2:D:109:PHE:O	2:D:109:PHE:CG	2.72	0.43
1:A:87:VAL:HG23	1:A:180:LEU:HD21	2.01	0.43
1:B:149:ARG:CZ	1:B:149:ARG:HB2	2.49	0.43
2:D:351:LEU:O	2:D:354:TYR:CB	2.66	0.43
1:A:138:ASP:O	1:A:142:LYS:HG2	2.18	0.42
1:B:78:ARG:HE	1:B:115:GLN:HE22	1.67	0.42
2:C:301:LEU:O	2:C:302:LYS:CB	2.67	0.42
1:B:53:LEU:O	1:B:301:GLU:HG3	2.19	0.42
1:A:29:ALA:O	1:A:30:ASN:HB2	2.20	0.42
1:B:197:ILE:C	1:B:199:GLU:N	2.73	0.42
2:C:165:TYR:CG	2:C:211:LEU:HD12	2.55	0.42
1:B:193:ASN:O	1:B:197:ILE:HD12	2.19	0.42
1:B:78:ARG:HH11	1:B:115:GLN:NE2	2.17	0.42
1:B:198:ILE:HG13	1:B:289:ASN:ND2	2.32	0.42
2:D:147:GLN:NE2	2:D:181:ASP:O	2.52	0.42
2:C:272:THR:HG21	2:C:277:VAL:HG21	2.01	0.42
1:A:66:LEU:HB2	1:A:69:PHE:CD2	2.55	0.42
1:B:238:PHE:CE2	2:D:318:ILE:HD13	2.55	0.42
1:A:238:PHE:CZ	2:C:318:ILE:HD13	2.55	0.42
1:B:295:LYS:HE2	1:B:295:LYS:N	2.35	0.42
1:A:255:ARG:HB2	2:C:315:MET:HG3	2.02	0.42
1:B:11:LEU:HD23	1:B:61:TRP:HB2	2.01	0.42
1:B:136:GLN:O	1:B:140:ILE:HG12	2.20	0.41
2:D:82:PHE:O	2:D:83:HIS:HD2	1.98	0.41
2:C:258:LYS:HD3	2:C:258:LYS:HA	1.86	0.41
2:C:64:ILE:HD11	2:C:233:VAL:HG22	2.01	0.41
2:C:66:LEU:HD23	2:C:74:LYS:HG2	2.02	0.41
2:D:183:LEU:HD22	2:D:187:HIS:CE1	2.56	0.41
1:A:19:GLY:O	1:A:23:MET:HG3	2.20	0.41
1:A:202:GLU:HA	1:A:217:TYR:O	2.20	0.41
2:D:256:ILE:HA	2:D:341:LEU:HB3	2.01	0.41
2:D:221:TYR:C	2:D:222:ASP:O	2.59	0.41
1:A:127:HIS:O	1:A:128:LYS:HB2	2.21	0.41
2:C:81:VAL:O	2:C:266:SER:HA	2.20	0.41
2:D:278:ASP:HB3	2:D:281:SER:HB2	2.02	0.41
1:B:87:VAL:CG2	1:B:180:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:HE2	2:C:348[B]:ARG:HB3	1.86	0.41
1:A:122:ILE:HD12	1:A:122:ILE:N	2.36	0.41
1:A:236:LYS:HE2	7:A:516:HOH:O	2.21	0.41
2:C:240:LEU:HB3	2:C:241:PRO:HD3	2.03	0.41
2:C:142:TYR:CD1	2:C:142:TYR:C	2.94	0.40
2:D:230:SER:HA	2:D:268:ILE:HG23	2.02	0.40
2:D:312:LYS:HG3	2:D:312:LYS:H	1.64	0.40
2:C:230:SER:HA	2:C:268:ILE:HG23	2.04	0.40
1:B:51:ARG:HB2	1:B:51:ARG:HE	1.76	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	296/313 (95%)	268 (90%)	21 (7%)	7 (2%)	6 7
1	B	296/313 (95%)	253 (86%)	31 (10%)	12 (4%)	3 3
2	C	268/399 (67%)	248 (92%)	18 (7%)	2 (1%)	22 32
2	D	269/399 (67%)	219 (81%)	42 (16%)	8 (3%)	4 5
All	All	1129/1424 (79%)	988 (88%)	112 (10%)	29 (3%)	5 7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	182	PRO
1	B	6	MET
1	B	246	ALA
1	B	278	ASP
1	B	283	SER

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Mol	Chain	Res	Type
2	C	302	LYS
2	D	111	ASN
2	D	222	ASP
2	D	305	GLY
1	B	198	ILE
1	B	249	PHE
1	B	279	PRO
1	B	284	ALA
2	D	138	GLY
2	D	306	SER
1	A	248	SER
1	A	279	PRO
1	B	197	ILE
1	B	134	GLU
2	D	133	ILE
1	A	246	ALA
1	A	278	ASP
2	D	107	SER
1	A	300	LEU
1	B	37	ARG
2	C	167	VAL
2	D	167	VAL
1	B	40	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	273/287 (95%)	254 (93%)	19 (7%)	15 23
1	B	273/287 (95%)	247 (90%)	26 (10%)	8 11
2	C	249/340 (73%)	233 (94%)	16 (6%)	17 27
2	D	250/340 (74%)	217 (87%)	33 (13%)	4 4
All	All	1045/1254 (83%)	951 (91%)	94 (9%)	9 14

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	15	LYS
1	A	48	SER
1	A	60	LEU
1	A	86	GLU
1	A	122	ILE
1	A	134	GLU
1	A	139	LEU
1	A	182	PRO
1	A	183	ASN
1	A	192	ARG
1	A	193	ASN
1	A	211	PHE
1	A	216	HIS
1	A	217	TYR
1	A	219	CYS
1	A	239	LYS
1	A	244	LYS
1	A	256	ASN
1	B	34	ARG
1	B	37	ARG
1	B	44	ASP
1	B	51	ARG
1	B	60	LEU
1	B	79	ASP
1	B	103	MET
1	B	135	ASP
1	B	144	ARG
1	B	149	ARG
1	B	155	LEU
1	B	184	VAL
1	B	211	PHE
1	B	220	LYS
1	B	223	ARG
1	B	229	GLU
1	B	248	SER
1	B	256	ASN
1	B	268	SER
1	B	280	SER
1	B	281	ILE
1	B	283	SER
1	B	286	THR
1	B	291	ARG

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Mol	Chain	Res	Type
1	B	295	LYS
1	B	301	GLU
2	C	66	LEU
2	C	83	HIS
2	C	115	TRP
2	C	132	MET
2	C	149	ASP
2	C	160	THR
2	C	183	LEU
2	C	186	ASP
2	C	196	HIS
2	C	201	ASP
2	C	222	ASP
2	C	239	GLN
2	C	245	ASN
2	C	306	SER
2	C	315	MET
2	C	345	SER
2	D	76	SER
2	D	78	GLN
2	D	132	MET
2	D	149	ASP
2	D	152	GLU
2	D	155	THR
2	D	161	VAL
2	D	166	LYS
2	D	191	THR
2	D	193	ARG
2	D	213	LEU
2	D	214	SER
2	D	218	THR
2	D	222	ASP
2	D	223	HIS
2	D	249	ILE
2	D	251	ILE
2	D	254	SER
2	D	281	SER
2	D	283	GLU
2	D	306	SER
2	D	312	LYS
2	D	315	MET
2	D	321	ASN

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Mol	Chain	Res	Type
2	D	324	THR
2	D	326	LEU
2	D	340	ILE
2	D	341	LEU
2	D	351	LEU
2	D	354	TYR
2	D	355	ASN
2	D	358	CYS
2	D	363	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	116	ASN
1	A	190	ASN
1	A	237	GLN
1	A	256	ASN
1	B	115	GLN
1	B	190	ASN
1	B	216	HIS
1	B	256	ASN
1	B	289	ASN
2	C	106	ASN
2	C	253	ASN
2	C	321	ASN
2	D	78	GLN
2	D	83	HIS
2	D	113	GLN
2	D	239	GLN
2	D	248	ASN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	9JE	B	404	-	6,6,6	0.37	0	5,5,5	0.32	0
6	GDP	D	401	-	24,30,30	1.16	2 (8%)	31,47,47	1.92	7 (22%)
3	GTP	A	401	4	26,34,34	1.05	1 (3%)	33,54,54	2.20	5 (15%)
5	9JE	B	403	-	6,6,6	0.30	0	5,5,5	0.55	0
5	9JE	A	403	-	6,6,6	0.37	0	5,5,5	0.22	0
3	GTP	B	401	4	26,34,34	1.03	1 (3%)	33,54,54	2.15	4 (12%)
6	GDP	C	401	-	24,30,30	1.13	2 (8%)	31,47,47	2.15	9 (29%)

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	9JE	B	404	-	-	2/4/4/4	-
6	GDP	D	401	-	-	0/12/32/32	0/3/3/3
3	GTP	A	401	4	-	3/18/38/38	0/3/3/3
5	9JE	B	403	-	-	1/4/4/4	-
5	9JE	A	403	-	-	1/4/4/4	-
3	GTP	B	401	4	-	1/18/38/38	0/3/3/3
6	GDP	C	401	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	401	GDP	C6-C5	3.97	1.48	1.41
3	B	401	GTP	C6-N1	3.69	1.39	1.33
3	A	401	GTP	C6-N1	3.62	1.39	1.33
6	C	401	GDP	C6-C5	3.44	1.47	1.41
6	D	401	GDP	C5-C4	2.49	1.47	1.40
6	C	401	GDP	C5-C4	2.07	1.46	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	GTP	C5-C6-N1	-9.00	111.12	123.43
3	B	401	GTP	C5-C6-N1	-8.80	111.39	123.43
3	A	401	GTP	C6-N1-C2	6.17	125.73	115.93
3	B	401	GTP	C6-N1-C2	5.86	125.24	115.93
6	C	401	GDP	C6-C5-C4	-5.73	115.33	120.80
6	D	401	GDP	C5-C6-N1	-4.39	117.43	123.43
6	C	401	GDP	C6-N1-C2	4.38	122.89	115.93
6	D	401	GDP	C6-C5-C4	-4.12	116.86	120.80
6	D	401	GDP	C6-N1-C2	4.10	122.45	115.93
6	C	401	GDP	C2-N3-C4	4.01	119.94	115.36
6	C	401	GDP	N3-C2-N1	-3.80	122.16	127.22
6	D	401	GDP	C2-N3-C4	3.72	119.61	115.36
6	C	401	GDP	C5-C6-N1	-3.65	118.44	123.43
6	C	401	GDP	PA-O3A-PB	-3.59	120.51	132.83
3	B	401	GTP	C2-N3-C4	-3.26	111.64	115.36
3	A	401	GTP	C2-N3-C4	-3.17	111.74	115.36
6	C	401	GDP	C1'-N9-C4	-3.05	121.28	126.64
6	D	401	GDP	N3-C2-N1	-2.92	123.33	127.22
6	D	401	GDP	C3'-C2'-C1'	2.79	105.19	100.98
3	A	401	GTP	N3-C2-N1	-2.79	123.50	127.22
3	B	401	GTP	N3-C2-N1	-2.52	123.86	127.22
6	D	401	GDP	C4-C5-N7	-2.34	106.96	109.40
3	A	401	GTP	O3'-C3'-C2'	-2.18	104.77	111.82
6	C	401	GDP	C4-C5-N7	-2.11	107.20	109.40
6	C	401	GDP	N2-C2-N1	2.00	120.37	117.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	GDP	PA-O3A-PB-O2B
5	B	404	9JE	C04-C05-C06-O07

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Mol	Chain	Res	Type	Atoms
5	A	403	9JE	O01-C02-C03-C04
3	A	401	GTP	PA-O3A-PB-O1B
5	B	404	9JE	C03-C04-C05-C06
5	B	403	9JE	C03-C04-C05-C06
3	B	401	GTP	PA-O3A-PB-O1B
6	C	401	GDP	PA-O3A-PB-O3B
3	A	401	GTP	PA-O3A-PB-O2B
3	A	401	GTP	O4'-C4'-C5'-O5'
6	C	401	GDP	PA-O3A-PB-O1B

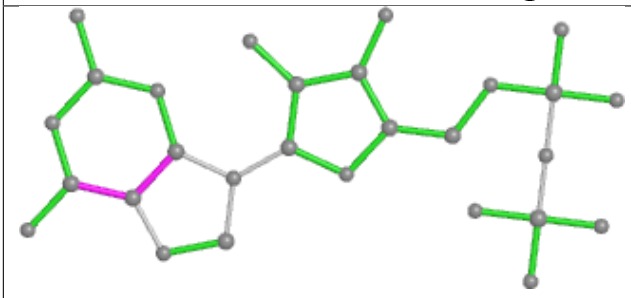
There are no ring outliers.

3 monomers are involved in 4 short contacts:

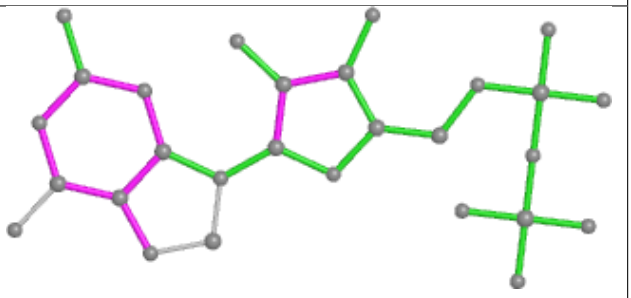
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	GDP	1	0
5	B	403	9JE	1	0
6	C	401	GDP	2	0

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 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.

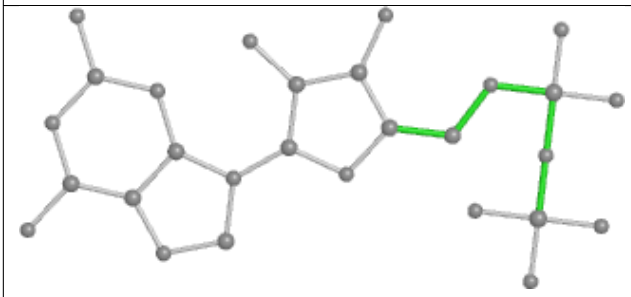
Ligand GDP D 401



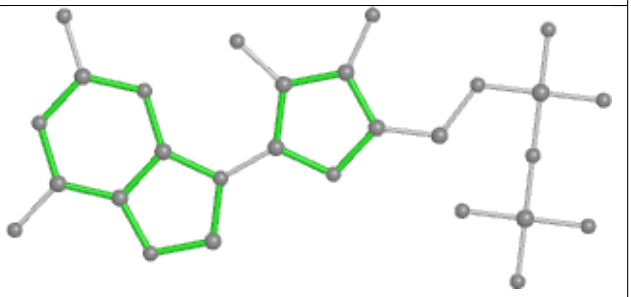
Bond lengths



Bond angles

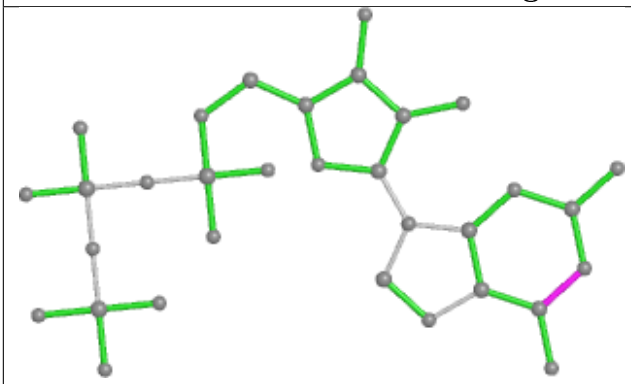


Torsions

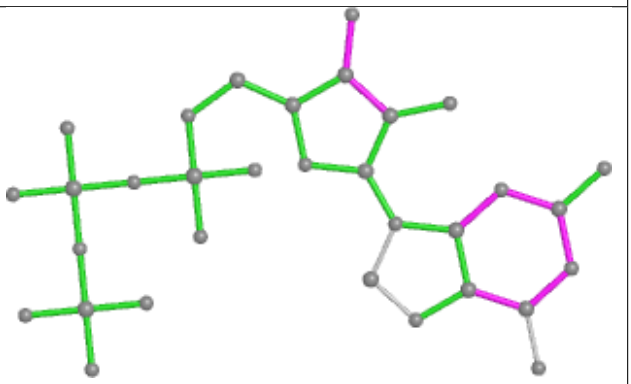


Rings

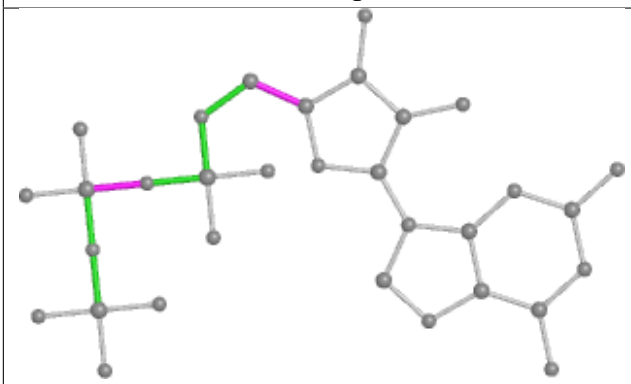
Ligand GTP A 401



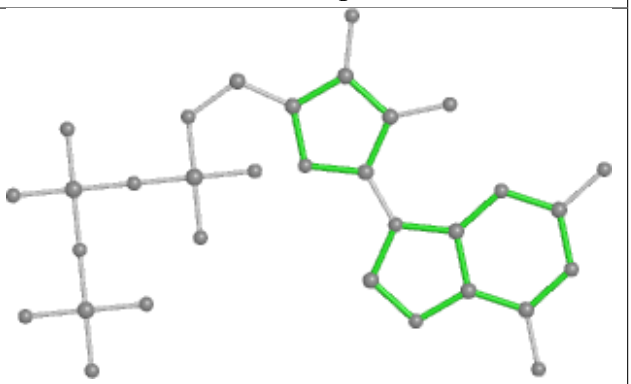
Bond lengths



Bond angles

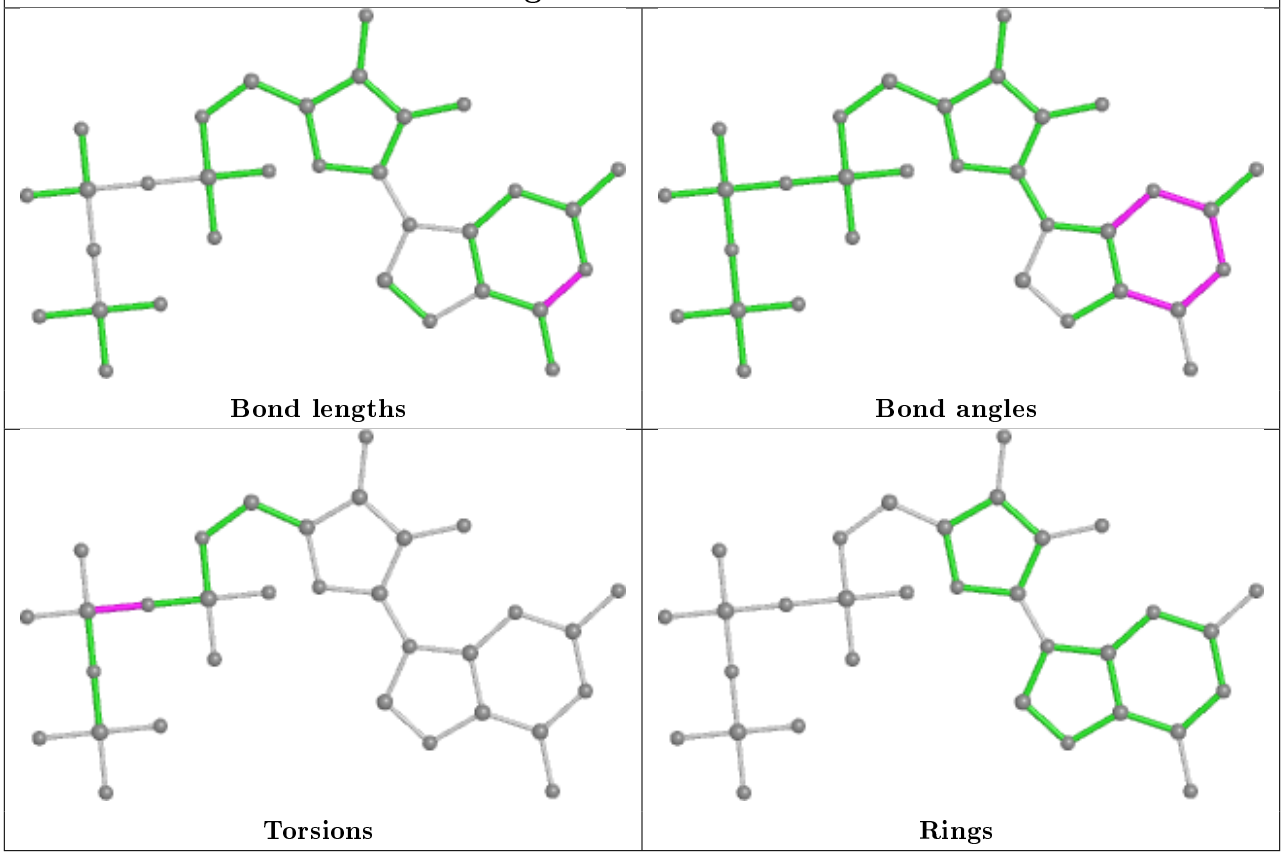


Torsions

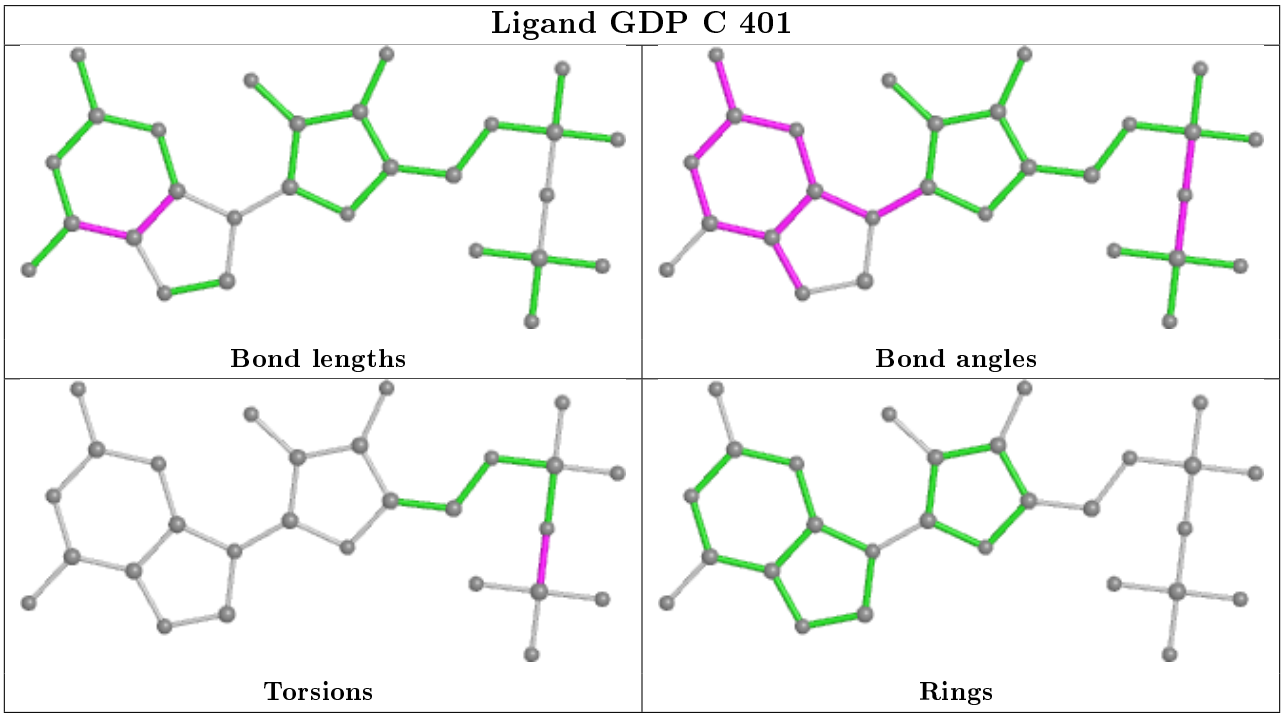


Rings

Ligand GTP B 401



Ligand GDP C 401



5.7 Other polymers

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, 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	298/313 (95%)	0.01	1 (0%) 94 95	55, 76, 118, 142	0
1	B	298/313 (95%)	0.23	12 (4%) 38 35	59, 84, 126, 150	0
2	C	273/399 (68%)	0.04	3 (1%) 80 78	55, 83, 131, 148	0
2	D	275/399 (68%)	1.26	69 (25%) 0 0	81, 139, 171, 200	0
All	All	1144/1424 (80%)	0.37	85 (7%) 14 11	55, 90, 153, 200	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	115	TRP	9.5
2	D	117	PHE	7.4
2	D	354	TYR	6.3
2	D	130	TYR	5.4
2	D	116	ASP	5.0
2	D	69	LEU	4.7
2	D	132	MET	4.6
2	D	134	PHE	4.5
2	D	253	ASN	4.5
2	D	133	ILE	4.3
2	D	63	ARG	4.3
2	D	129	ASP	4.2
2	D	141	ILE	4.0
2	D	67	MET	4.0
1	B	280	SER	4.0
2	D	249	ILE	4.0
1	B	5	ALA	3.9
2	D	65	LEU	3.9
2	D	348	ARG	3.9
2	D	160	THR	3.9
2	D	356	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	208	LEU	3.8
2	D	361	LYS	3.8
2	D	112	PHE	3.8
2	D	199	ALA	3.8
2	D	203	LEU	3.8
2	D	305	GLY	3.6
1	B	281	ILE	3.6
2	D	252	SER	3.5
2	D	111	ASN	3.4
2	D	140	LEU	3.4
2	D	135	ARG	3.4
2	D	167	VAL	3.2
2	D	211	LEU	3.2
2	D	114	ILE	3.2
2	D	351	LEU	3.2
1	A	4	THR	3.2
2	D	70	ARG	3.2
2	D	357	HIS	3.1
2	D	136	GLY	3.1
2	D	346	PHE	3.1
2	D	171	MET	3.0
2	D	364	HIS	2.9
2	D	161	VAL	2.9
2	D	74	LYS	2.9
2	D	62	PRO	2.8
2	D	360	ARG	2.7
2	D	247	LEU	2.7
2	D	350	GLY	2.7
2	C	134	PHE	2.7
2	D	250	PHE	2.7
2	D	142	TYR	2.7
2	D	162	SER	2.6
2	D	286	CYS	2.6
1	B	234	ILE	2.5
2	D	158	HIS	2.5
2	D	77	ILE	2.5
2	D	138	GLY	2.4
2	C	166	LYS	2.4
2	D	113	GLN	2.4
2	D	108	SER	2.4
2	D	64	ILE	2.4
2	D	352	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	358	CYS	2.3
2	D	109	PHE	2.3
2	D	347	GLU	2.2
2	C	115	TRP	2.2
2	D	139	ALA	2.2
2	D	306	SER	2.2
1	B	302	ARG	2.2
1	B	235	ILE	2.1
2	D	206	ALA	2.1
1	B	238	PHE	2.1
2	D	173	PHE	2.1
1	B	232	SER	2.1
1	B	273	MET	2.1
1	B	272	VAL	2.1
1	B	250	GLN	2.1
2	D	331	VAL	2.1
1	B	6	MET	2.1
2	D	73	GLY	2.1
2	D	186	ASP	2.1
2	D	187	HIS	2.0
2	D	144	ILE	2.0
2	D	166	LYS	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 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
5	9JE	A	403	7/7	0.86	0.22	100,112,123,124	0

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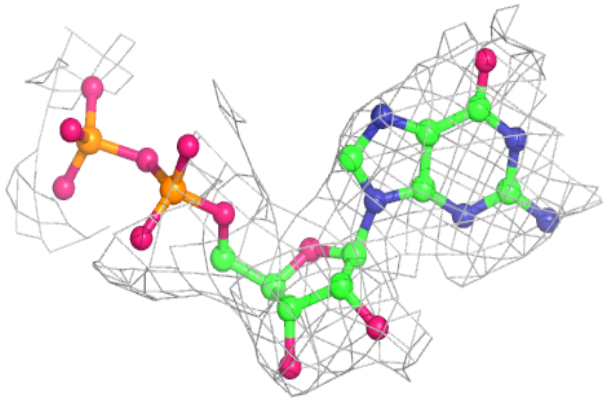
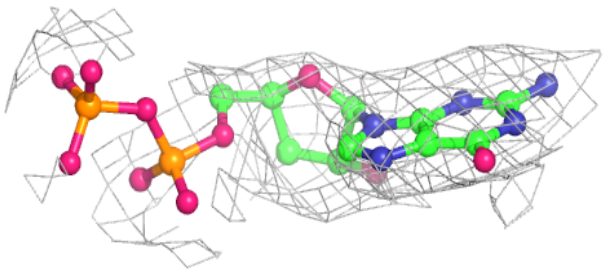
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	9JE	B	404	7/7	0.88	0.29	78,80,90,91	0
6	GDP	D	401	28/28	0.92	0.12	110,123,138,140	0
5	9JE	B	403	7/7	0.95	0.41	73,77,88,107	0
6	GDP	C	401	28/28	0.95	0.14	78,101,112,118	0
4	MG	B	402	1/1	0.96	0.09	114,114,114,114	0
3	GTP	B	401	32/32	0.97	0.13	61,85,101,108	0
4	MG	A	402	1/1	0.98	0.18	70,70,70,70	0
3	GTP	A	401	32/32	0.99	0.18	52,65,68,72	0

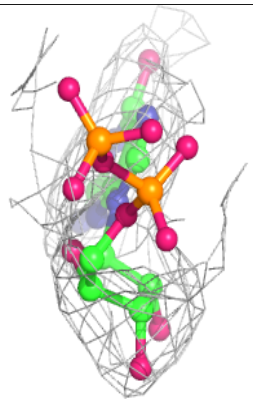
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 401:

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

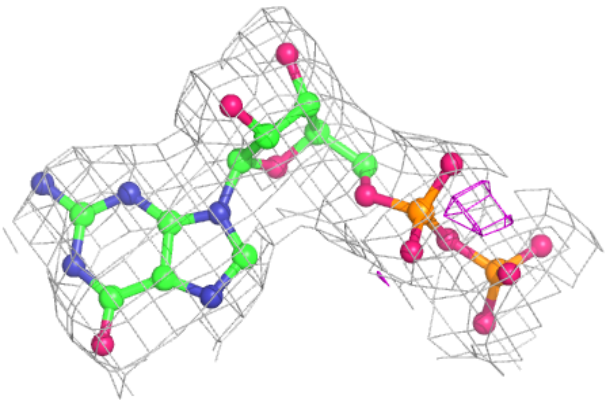


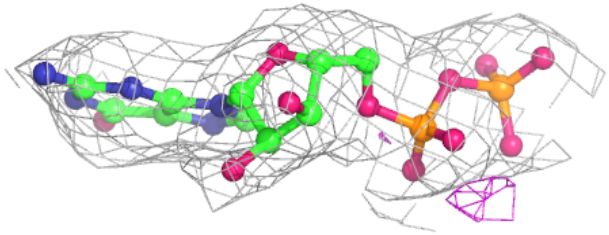


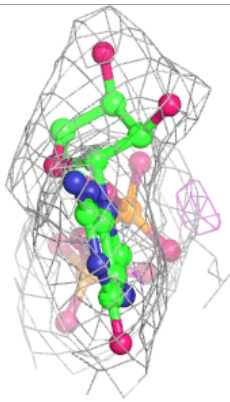


Electron density around GDP C 401:

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

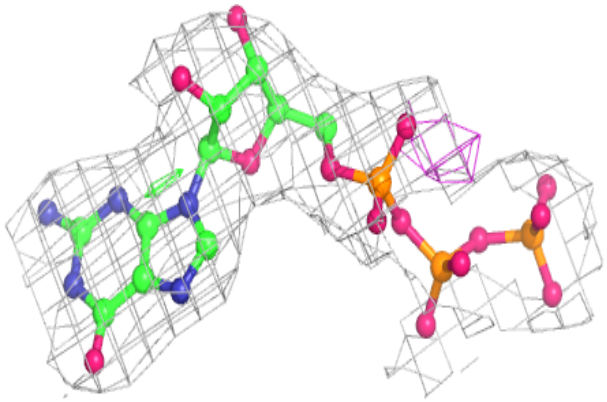


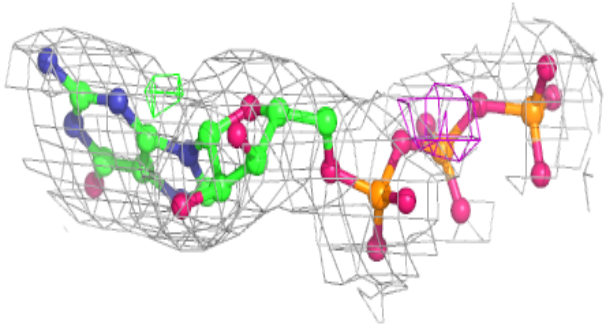


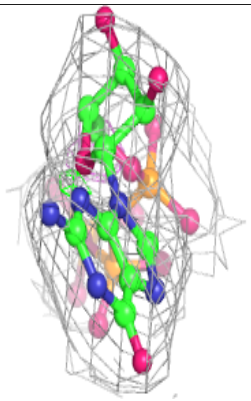


Electron density around GTP B 401:

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

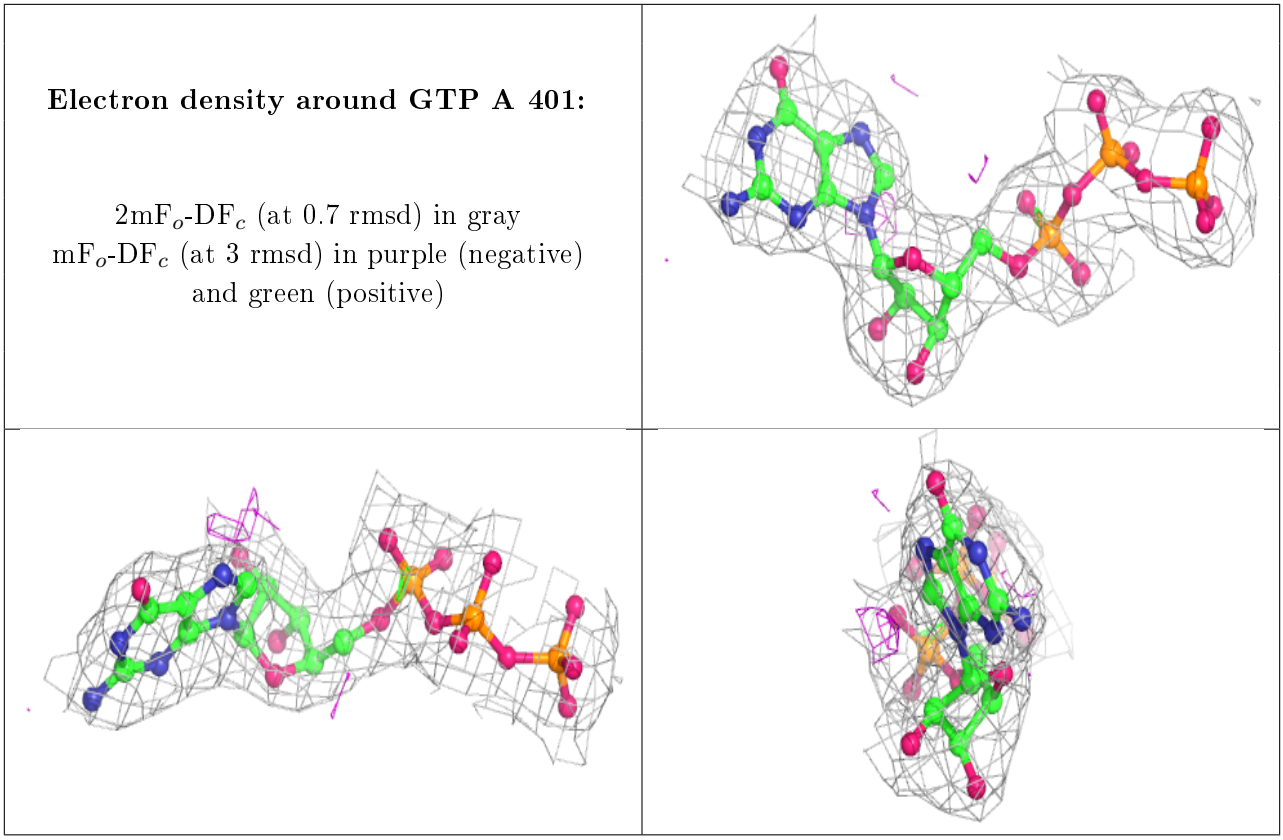






Electron density around GTP A 401:

$2mF_o$-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.