



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 03:24 pm GMT

PDB ID : 2BKU
Title : Kap95p:RanGTP complex
Authors : Lee, S.J.; Matsuura, Y.; Liu, S.M.; Stewart, M.
Deposited on : 2005-02-21
Resolution : 2.70 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

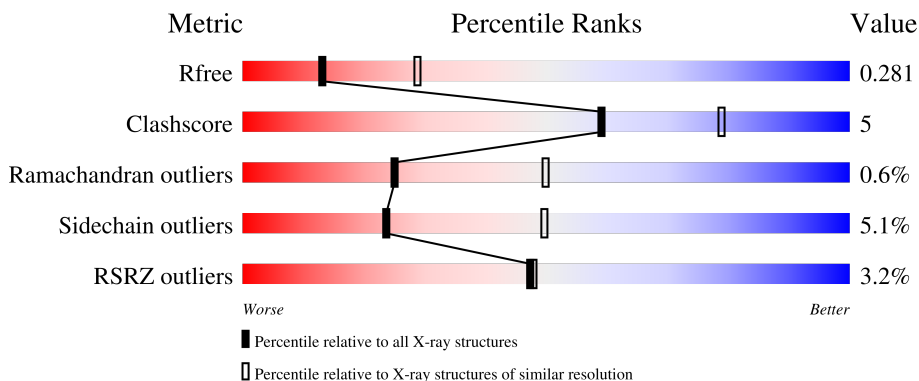
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


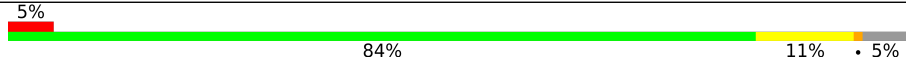
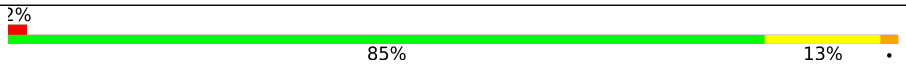

The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	177	 85% 8% • 5%
1	C	177	 5% 84% 11% • 5%
2	B	861	 2% 85% 13% •
2	D	861	 5% 84% 14% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16104 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 GTP-BINDING NUCLEAR PROTEIN RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1377	895	242	236	4	0	0	0
1	C	169	1377	895	242	236	4	0	0	0

- Molecule 2 is a protein called IMPORTIN BETA-1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	857	6624	4188	1095	1305	36	0	0	0
2	D	854	6598	4172	1092	1298	36	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	254	LYS	LEU	conflict	UNP Q06142
D	254	LYS	LEU	conflict	UNP Q06142

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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


- Molecule 5 is water.

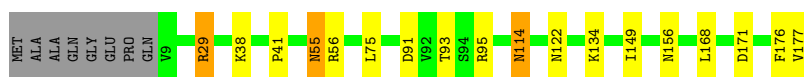
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	29	Total	O	0	0
			29	29		
5	C	7	Total	O	0	0
			7	7		
5	D	22	Total	O	0	0
			22	22		

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: GTP-BINDING NUCLEAR PROTEIN RAN

Chain A: 




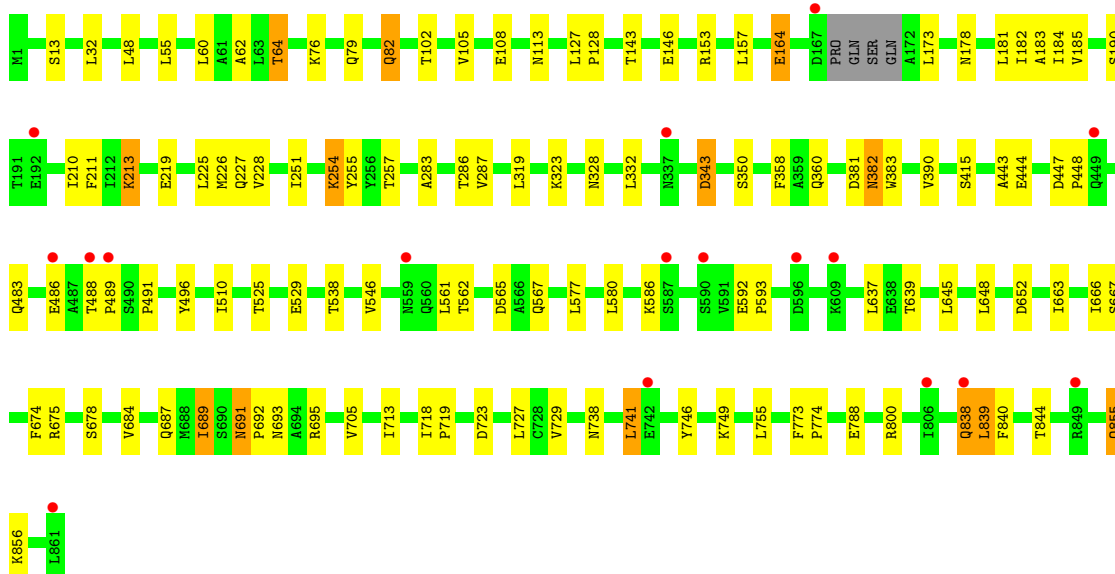
- Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN

Chain C: 




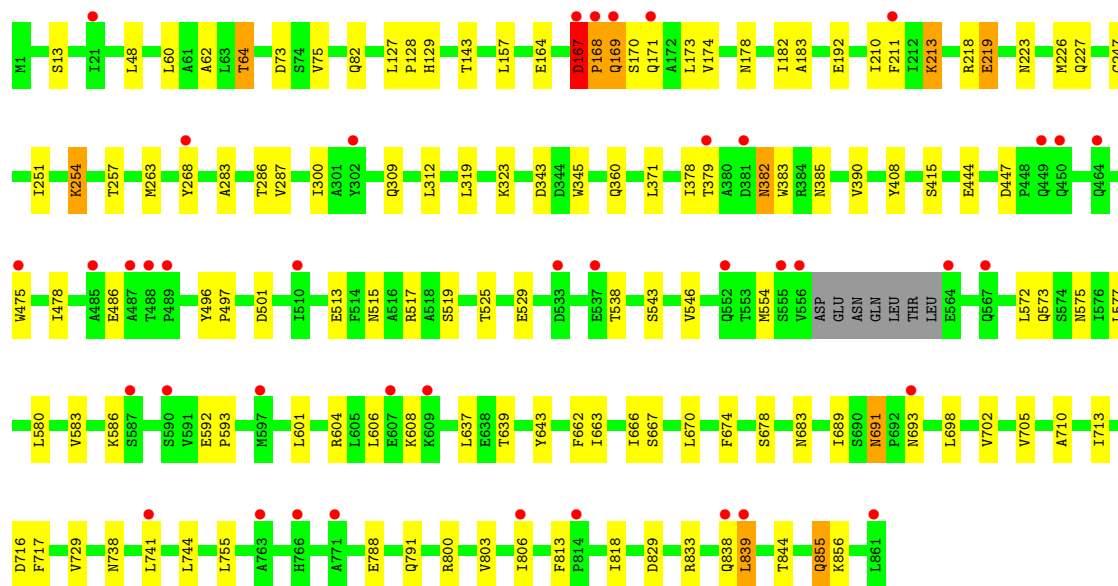
- Molecule 2: IMPORTIN BETA-1 SUBUNIT

Chain B: 



- Molecule 2: IMPORTIN BETA-1 SUBUNIT

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.02Å 127.88Å 161.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.70) 99.6 (19.28-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.223 , 0.279 0.224 , 0.281	Depositor DCC
R_{free} test set	3098 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16104	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1411	0.62	1/1905 (0.1%)
1	C	0.43	0/1411	0.61	1/1905 (0.1%)
2	B	0.43	0/6736	0.55	0/9153
2	D	0.47	2/6711 (0.0%)	0.55	0/9119
All	All	0.44	2/16269 (0.0%)	0.56	2/22082 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	219	GLU	CB-CG	7.54	1.66	1.52
2	D	219	GLU	CG-CD	6.45	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	PRO	N-CA-CB	6.29	110.85	103.30
1	A	41	PRO	N-CA-CB	5.85	110.32	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	167	ASP	Peptide
2	D	168	PRO	Peptide

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	1377	0	1396	16	0
1	C	1377	0	1396	15	0
2	B	6624	0	6580	57	1
2	D	6598	0	6555	71	1
3	A	32	0	12	0	0
3	C	32	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	0	0
5	B	29	0	0	2	0
5	C	7	0	0	2	0
5	D	22	0	0	3	0
All	All	16104	0	15951	149	1

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 5.

All (149) 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)
5:B:2006:HOH:O	2:D:257:THR:HG22	1.72	0.90
2:B:60:LEU:O	2:B:64:THR:HG23	1.76	0.85
2:D:60:LEU:O	2:D:64:THR:HG23	1.82	0.78
2:D:226:MET:HE1	2:D:251:ILE:HD13	1.66	0.78
2:B:226:MET:HE1	2:B:251:ILE:HD13	1.68	0.76
2:D:167:ASP:HB3	2:D:168:PRO:HD3	1.70	0.73
1:A:134:LYS:NZ	2:B:360:GLN:HE22	1.87	0.73
2:D:167:ASP:HB3	2:D:168:PRO:CD	2.25	0.67
2:B:689:ILE:HD12	2:B:727:LEU:HD22	1.77	0.66
2:D:167:ASP:CB	2:D:168:PRO:CD	2.74	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:838:GLN:O	2:B:840:PHE:N	2.29	0.64
2:D:382:ASN:HB3	2:D:385:ASN:HD22	1.63	0.64
2:D:263:MET:O	2:D:268:TYR:HB2	1.99	0.62
2:B:838:GLN:O	2:B:839:LEU:C	2.38	0.61
2:D:226:MET:CE	2:D:251:ILE:HD13	2.31	0.61
2:D:855:GLN:HE21	2:D:855:GLN:C	2.03	0.61
2:B:113:ASN:HD21	2:B:153:ARG:HH12	1.48	0.60
1:A:134:LYS:HZ1	2:B:360:GLN:HE22	1.48	0.60
2:B:746:TYR:HA	2:B:749:LYS:HE3	1.83	0.60
1:A:114:ASN:C	1:A:114:ASN:HD22	2.07	0.58
2:B:226:MET:CE	2:B:251:ILE:HD13	2.34	0.58
2:D:838:GLN:O	2:D:839:LEU:C	2.42	0.58
2:B:856:LYS:HE2	2:B:856:LYS:HA	1.86	0.57
2:D:219:GLU:HG2	2:D:223:ASN:HD21	1.71	0.54
2:D:143:THR:HG21	2:D:183:ALA:HB1	1.88	0.54
2:D:525:THR:O	2:D:529:GLU:HG2	2.06	0.54
2:D:378:ILE:HG23	2:D:379:THR:HG23	1.89	0.54
2:B:546:VAL:HG23	2:B:580:LEU:HD13	1.90	0.53
2:D:856:LYS:HA	2:D:856:LYS:HE2	1.90	0.53
2:D:663:ILE:HA	2:D:666:ILE:HD11	1.91	0.53
2:B:689:ILE:C	2:B:689:ILE:HD13	2.29	0.53
2:D:210:ILE:O	2:D:213:LYS:HG3	2.08	0.53
1:C:134:LYS:NZ	2:D:360:GLN:HE22	2.07	0.52
1:C:114:ASN:HD22	1:C:114:ASN:C	2.12	0.52
2:B:648:LEU:HD11	2:B:663:ILE:HD11	1.92	0.52
2:B:645:LEU:HD22	2:B:684:VAL:HG21	1.92	0.52
1:C:149:ILE:HD12	1:C:156:ASN:HB2	1.91	0.51
1:A:176:PHE:O	1:A:177:VAL:C	2.48	0.51
2:D:744:LEU:HD23	2:D:791:GLN:HE22	1.74	0.51
2:D:497:PRO:O	2:D:501:ASP:HB2	2.09	0.51
2:D:382:ASN:HD22	2:D:383:TRP:N	2.09	0.51
2:D:800:ARG:HD3	2:D:844:THR:HA	1.93	0.50
2:D:738:ASN:N	2:D:738:ASN:OD1	2.44	0.50
1:C:75:LEU:HD11	2:D:13:SER:HB3	1.93	0.50
2:B:164:GLU:HA	2:B:211:PHE:CE2	2.46	0.50
2:B:800:ARG:HD3	2:B:844:THR:HA	1.93	0.50
2:D:515:ASN:O	2:D:519:SER:OG	2.22	0.49
1:A:149:ILE:HD12	1:A:156:ASN:HB2	1.93	0.49
2:B:219:GLU:OE1	2:D:219:GLU:OE2	2.30	0.49
2:B:82:GLN:HE21	2:B:82:GLN:C	2.16	0.49
2:B:443:ALA:HB2	2:B:483:GLN:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:691:ASN:HD22	2:B:691:ASN:C	2.16	0.49
2:D:129:HIS:CE1	5:D:2005:HOH:O	2.66	0.49
2:B:674:PHE:CD2	2:B:713:ILE:HD11	2.48	0.48
2:D:283:ALA:O	2:D:287:VAL:HG23	2.13	0.48
2:B:666:ILE:HD12	2:B:667:SER:N	2.28	0.48
1:A:149:ILE:HD11	1:A:156:ASN:O	2.12	0.48
2:D:254:LYS:HZ1	2:D:254:LYS:HA	1.79	0.48
2:B:592:GLU:HB2	2:B:593:PRO:HD3	1.96	0.48
5:C:2005:HOH:O	2:D:64:THR:HG22	2.12	0.48
2:D:164:GLU:HA	2:D:211:PHE:CE2	2.48	0.48
2:D:813:PHE:CD2	2:D:818:ILE:HD13	2.48	0.48
2:D:604:ARG:HD3	5:D:2015:HOH:O	2.13	0.48
2:B:562:THR:HG23	2:B:565:ASP:H	1.79	0.48
2:D:475:TRP:O	2:D:478:ILE:HB	2.14	0.47
2:B:181:LEU:HD21	2:B:225:LEU:HD12	1.95	0.47
2:B:510:ILE:H	2:B:510:ILE:HD12	1.79	0.47
2:B:738:ASN:N	2:B:738:ASN:OD1	2.47	0.47
2:B:146:GLU:OE2	2:B:146:GLU:N	2.44	0.47
1:C:149:ILE:HD11	1:C:156:ASN:O	2.14	0.47
2:D:517:ARG:NE	2:D:572:LEU:HD13	2.29	0.47
2:B:525:THR:O	2:B:529:GLU:HG2	2.13	0.47
1:A:114:ASN:C	1:A:114:ASN:ND2	2.68	0.46
2:D:543:SER:HB3	2:D:583:VAL:HG11	1.98	0.46
1:C:55:ASN:ND2	1:C:56:ARG:HG3	2.31	0.46
2:D:219:GLU:HG2	2:D:223:ASN:ND2	2.30	0.46
2:D:666:ILE:HD12	2:D:667:SER:N	2.31	0.46
2:D:554:MET:HE3	2:D:601:LEU:HD22	1.97	0.46
2:D:592:GLU:N	2:D:593:PRO:CD	2.79	0.46
1:C:122:ASN:HA	1:C:149:ILE:HG22	1.96	0.46
2:D:662:PHE:O	2:D:666:ILE:HG13	2.15	0.46
2:B:328:ASN:O	2:B:332:LEU:HG	2.16	0.46
2:D:382:ASN:HB3	2:D:385:ASN:ND2	2.30	0.46
2:B:855:GLN:HE21	2:B:855:GLN:C	2.19	0.45
2:D:691:ASN:HD22	2:D:693:ASN:H	1.64	0.45
2:B:48:LEU:HD13	2:B:62:ALA:HB2	1.99	0.45
1:C:42:THR:HG21	5:C:2004:HOH:O	2.17	0.45
2:D:592:GLU:HB2	2:D:593:PRO:HD3	1.98	0.45
2:B:102:THR:O	2:B:105:VAL:HG22	2.17	0.45
2:B:185:VAL:CG1	2:B:228:VAL:HG21	2.47	0.45
2:D:803:VAL:HA	2:D:806:ILE:HD12	1.98	0.45
1:C:56:ARG:HD2	1:C:171:ASP:OD1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:LYS:HA	2:D:254:LYS:NZ	2.33	0.44
1:A:55:ASN:C	1:A:55:ASN:HD22	2.21	0.44
2:B:178:ASN:O	2:B:182:ILE:HG12	2.18	0.44
1:A:55:ASN:C	1:A:55:ASN:ND2	2.71	0.43
1:C:140:ARG:HG3	2:D:345:TRP:CZ2	2.53	0.43
2:D:572:LEU:HA	2:D:575:ASN:HD22	1.82	0.43
1:C:114:ASN:C	1:C:114:ASN:ND2	2.70	0.43
2:B:652:ASP:O	2:B:695:ARG:HD3	2.18	0.43
2:B:691:ASN:HD22	2:B:693:ASN:H	1.65	0.43
2:D:178:ASN:O	2:D:182:ILE:HG12	2.18	0.43
2:D:674:PHE:HB3	2:D:713:ILE:HD11	1.99	0.43
2:B:448:PRO:HG3	2:B:491:PRO:HG3	2.00	0.43
2:B:691:ASN:HD22	2:B:692:PRO:N	2.16	0.43
2:D:713:ILE:CG2	2:D:716:ASP:HB3	2.49	0.43
1:A:122:ASN:HA	1:A:149:ILE:HG22	1.99	0.43
1:A:134:LYS:HZ1	2:B:360:GLN:NE2	2.16	0.43
2:D:829:ASP:O	2:D:833:ARG:HG3	2.19	0.43
2:B:382:ASN:HD22	2:B:383:TRP:N	2.16	0.43
2:B:674:PHE:HB3	2:B:713:ILE:HD11	2.00	0.43
1:A:55:ASN:ND2	1:A:56:ARG:HG3	2.34	0.43
1:A:91:ASP:OD1	1:A:93:THR:HB	2.19	0.43
2:D:48:LEU:HD13	2:D:62:ALA:HB2	2.01	0.43
2:D:573:GLN:HE22	2:D:608:LYS:NZ	2.17	0.43
2:D:371:LEU:HD13	2:D:408:TYR:CE1	2.54	0.42
2:B:127:LEU:N	2:B:128:PRO:CD	2.82	0.42
2:D:218:ARG:O	2:D:219:GLU:C	2.58	0.42
2:B:76:LYS:HA	2:B:79:GLN:HE21	1.85	0.42
2:B:488:THR:HB	2:B:489:PRO:HD3	2.02	0.42
2:D:710:ALA:HA	2:D:717:PHE:CD1	2.55	0.42
2:B:718:ILE:N	2:B:719:PRO:CD	2.82	0.42
2:D:73:ASP:OD2	2:D:75:VAL:N	2.51	0.42
1:A:56:ARG:HD2	1:A:171:ASP:OD1	2.19	0.42
2:D:211:PHE:CD2	2:D:211:PHE:N	2.87	0.42
2:D:169:GLN:O	2:D:174:VAL:HB	2.20	0.41
2:D:300:ILE:HG12	2:D:312:LEU:HD21	2.01	0.41
1:A:29:ARG:HD2	2:B:567:GLN:NE2	2.35	0.41
2:D:127:LEU:N	2:D:128:PRO:CD	2.83	0.41
2:D:129:HIS:HE1	5:D:2005:HOH:O	2.01	0.41
2:D:698:LEU:O	2:D:702:VAL:HG23	2.20	0.41
2:B:254:LYS:HB2	2:B:255:TYR:CD2	2.55	0.41
2:B:283:ALA:O	2:B:287:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LEU:HD21	2:B:108:GLU:HG2	2.03	0.41
1:C:134:LYS:NZ	2:D:360:GLN:NE2	2.69	0.41
2:B:210:ILE:O	2:B:213:LYS:HG3	2.21	0.41
2:D:667:SER:O	2:D:670:LEU:O	2.38	0.41
1:C:176:PHE:O	1:C:177:VAL:C	2.60	0.41
2:B:343:ASP:OD1	2:B:343:ASP:C	2.59	0.41
2:B:773:PHE:HB3	2:B:774:PRO:HD3	2.03	0.41
2:D:371:LEU:HD13	2:D:408:TYR:CD1	2.56	0.41
2:D:855:GLN:HE21	2:D:856:LYS:N	2.18	0.40
1:A:75:LEU:HD11	2:B:13:SER:HB3	2.03	0.40
2:B:675:ARG:HD2	5:B:2018:HOH:O	2.22	0.40
1:C:55:ASN:ND2	1:C:55:ASN:C	2.75	0.40
2:D:546:VAL:HG23	2:D:580:LEU:HD13	2.02	0.40
2:D:606:LEU:HB3	2:D:643:TYR:CE1	2.56	0.40
2:B:143:THR:HG21	2:B:183:ALA:HB1	2.02	0.40
1:C:124:VAL:HG11	1:C:148:ASP:HB3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:723:ASP:OD2	2:D:219:GLU:OE2[2_454]	2.01	0.19

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	167/177 (94%)	159 (95%)	8 (5%)	0	100	100
1	C	167/177 (94%)	159 (95%)	8 (5%)	0	100	100
2	B	853/861 (99%)	817 (96%)	31 (4%)	5 (1%)	25	50
2	D	850/861 (99%)	809 (95%)	34 (4%)	7 (1%)	19	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2037/2076 (98%)	1944 (95%)	81 (4%)	12 (1%)	25 50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	839	LEU
2	D	167	ASP
2	D	171	GLN
2	D	170	SER
2	D	839	LEU
2	B	190	SER
2	B	586	LYS
2	D	586	LYS
2	B	729	VAL
2	B	741	LEU
2	D	729	VAL
2	D	169	GLN

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	149/155 (96%)	143 (96%)	6 (4%)	31 60
1	C	149/155 (96%)	142 (95%)	7 (5%)	26 54
2	B	722/726 (99%)	682 (94%)	40 (6%)	21 46
2	D	719/726 (99%)	684 (95%)	35 (5%)	25 52
All	All	1739/1762 (99%)	1651 (95%)	88 (5%)	24 50

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	38	LYS
1	A	55	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	ARG
1	A	114	ASN
1	A	168	LEU
2	B	32	LEU
2	B	64	THR
2	B	82	GLN
2	B	157	LEU
2	B	164	GLU
2	B	173	LEU
2	B	184	ILE
2	B	213	LYS
2	B	227	GLN
2	B	254	LYS
2	B	257	THR
2	B	286	THR
2	B	319	LEU
2	B	323	LYS
2	B	343	ASP
2	B	350	SER
2	B	358	PHE
2	B	381	ASP
2	B	382	ASN
2	B	390	VAL
2	B	415	SER
2	B	444	GLU
2	B	447	ASP
2	B	486	GLU
2	B	496	TYR
2	B	538	THR
2	B	561	LEU
2	B	577	LEU
2	B	637	LEU
2	B	639	THR
2	B	678	SER
2	B	687	GLN
2	B	689	ILE
2	B	691	ASN
2	B	705	VAL
2	B	741	LEU
2	B	755	LEU
2	B	788	GLU
2	B	838	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	855	GLN
1	C	29	ARG
1	C	38	LYS
1	C	55	ASN
1	C	93	THR
1	C	95	ARG
1	C	114	ASN
1	C	168	LEU
2	D	64	THR
2	D	82	GLN
2	D	157	LEU
2	D	173	LEU
2	D	192	GLU
2	D	213	LYS
2	D	227	GLN
2	D	247	CYS
2	D	254	LYS
2	D	286	THR
2	D	309	GLN
2	D	319	LEU
2	D	323	LYS
2	D	343	ASP
2	D	382	ASN
2	D	390	VAL
2	D	415	SER
2	D	444	GLU
2	D	447	ASP
2	D	486	GLU
2	D	496	TYR
2	D	513	GLU
2	D	538	THR
2	D	577	LEU
2	D	637	LEU
2	D	639	THR
2	D	678	SER
2	D	683	ASN
2	D	689	ILE
2	D	691	ASN
2	D	705	VAL
2	D	741	LEU
2	D	755	LEU
2	D	788	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	855	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	100	ASN
1	A	114	ASN
2	B	34	ASN
2	B	79	GLN
2	B	82	GLN
2	B	87	GLN
2	B	113	ASN
2	B	215	ASN
2	B	313	GLN
2	B	360	GLN
2	B	382	ASN
2	B	385	ASN
2	B	451	HIS
2	B	552	GLN
2	B	567	GLN
2	B	683	ASN
2	B	691	ASN
2	B	712	ASN
2	B	781	GLN
2	B	785	GLN
2	B	791	GLN
2	B	855	GLN
1	C	100	ASN
1	C	114	ASN
2	D	34	ASN
2	D	79	GLN
2	D	82	GLN
2	D	113	ASN
2	D	117	GLN
2	D	215	ASN
2	D	309	GLN
2	D	313	GLN
2	D	360	GLN
2	D	382	ASN
2	D	385	ASN
2	D	552	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	567	GLN
2	D	573	GLN
2	D	575	ASN
2	D	683	ASN
2	D	691	ASN
2	D	693	ASN
2	D	712	ASN
2	D	733	ASN
2	D	781	GLN
2	D	791	GLN
2	D	855	GLN

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GTP	A	220	4	26,34,34	1.24	2 (7%)	32,54,54	1.50	7 (21%)
3	GTP	C	220	4	26,34,34	1.14	2 (7%)	32,54,54	1.56	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	220	4	-	6/18/38/38	0/3/3/3
3	GTP	C	220	4	-	7/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	220	GTP	C5-C6	-4.29	1.38	1.47
3	C	220	GTP	C5-C6	-3.83	1.39	1.47
3	A	220	GTP	C2-N3	2.34	1.38	1.33
3	C	220	GTP	C2-N3	2.08	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	220	GTP	PA-O3A-PB	-3.90	119.44	132.83
3	C	220	GTP	PA-O3A-PB	-3.67	120.24	132.83
3	C	220	GTP	C5-C6-N1	3.37	119.91	113.95
3	A	220	GTP	C5-C6-N1	3.31	119.79	113.95
3	C	220	GTP	C2-N1-C6	-3.04	119.51	125.10
3	A	220	GTP	C2-N1-C6	-2.86	119.83	125.10
3	C	220	GTP	C8-N7-C5	2.86	108.43	102.99
3	A	220	GTP	C8-N7-C5	2.81	108.34	102.99
3	A	220	GTP	PB-O3B-PG	-2.56	124.06	132.83
3	C	220	GTP	PB-O3B-PG	-2.29	124.96	132.83
3	C	220	GTP	O6-C6-C5	-2.14	120.19	124.37
3	A	220	GTP	O6-C6-C5	-2.14	120.20	124.37
3	A	220	GTP	O3G-PG-O3B	2.13	111.79	104.64
3	C	220	GTP	O2G-PG-O3B	2.04	111.48	104.64
3	C	220	GTP	O3G-PG-O3B	2.03	111.43	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	220	GTP	C5'-O5'-PA-O3A
3	A	220	GTP	C5'-O5'-PA-O1A
3	A	220	GTP	C5'-O5'-PA-O2A

Continued on next page...

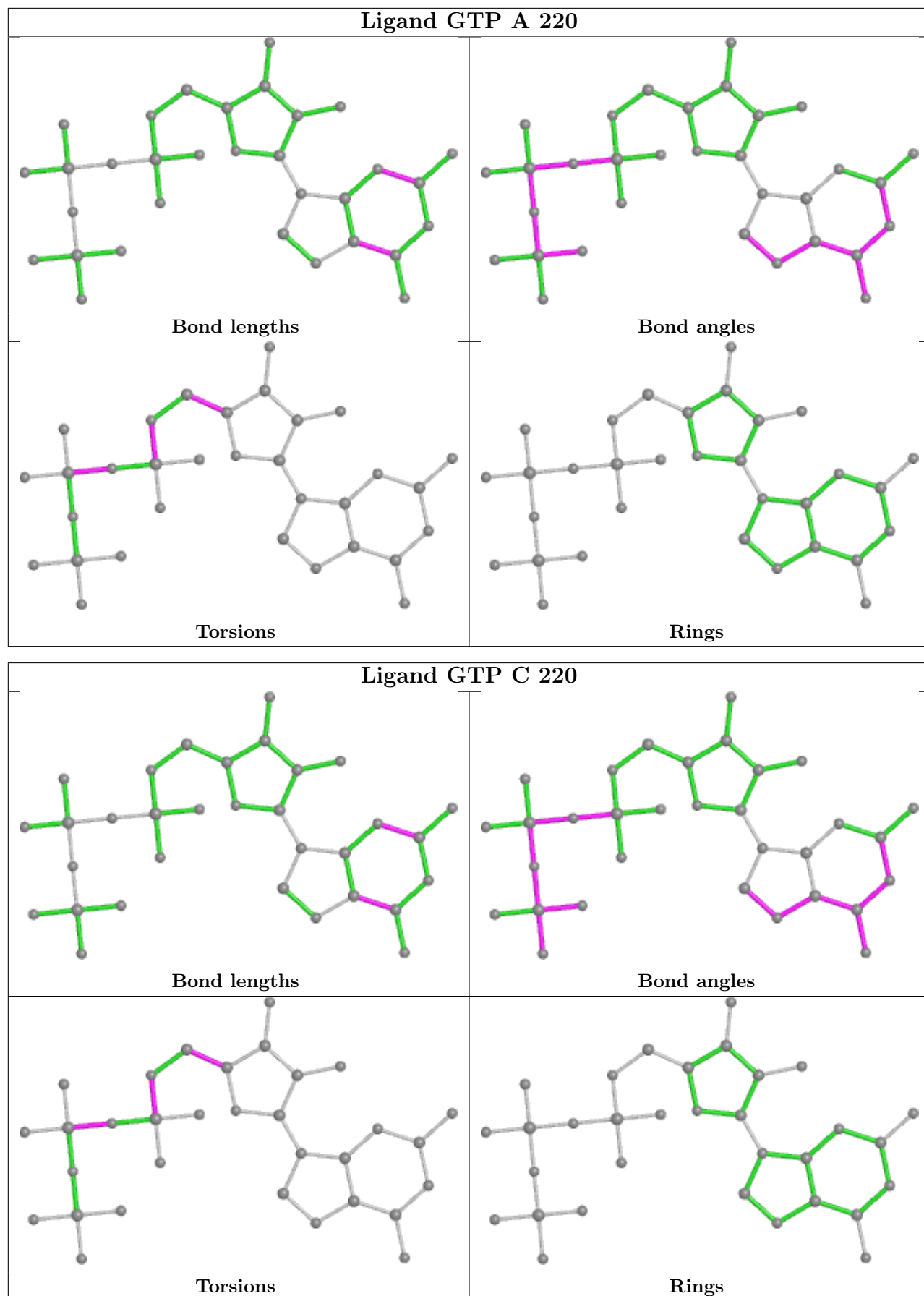
Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	220	GTP	C5'-O5'-PA-O3A
3	C	220	GTP	C5'-O5'-PA-O1A
3	C	220	GTP	C5'-O5'-PA-O2A
3	A	220	GTP	O4'-C4'-C5'-O5'
3	A	220	GTP	C3'-C4'-C5'-O5'
3	C	220	GTP	O4'-C4'-C5'-O5'
3	C	220	GTP	C3'-C4'-C5'-O5'
3	C	220	GTP	PA-O3A-PB-O2B
3	A	220	GTP	PA-O3A-PB-O2B
3	C	220	GTP	PA-O3A-PB-O1B

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	169/177 (95%)	-0.14	0 100 100	35, 49, 72, 88	0
1	C	169/177 (95%)	-0.04	8 (4%) 31 30	42, 53, 74, 90	0
2	B	857/861 (99%)	-0.03	17 (1%) 65 67	34, 55, 84, 108	0
2	D	854/861 (99%)	0.03	41 (4%) 30 28	36, 59, 88, 118	0
All	All	2049/2076 (98%)	-0.02	66 (3%) 47 48	34, 56, 84, 118	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	590	SER	7.2
2	D	556	VAL	7.1
2	B	587	SER	6.4
1	C	177	VAL	5.7
2	D	510	ILE	5.6
2	B	167	ASP	5.3
2	D	488	THR	5.0
2	D	838	GLN	4.1
2	D	171	GLN	4.1
2	D	590	SER	3.8
2	D	741	LEU	3.8
2	D	475	TRP	3.6
2	D	268	TYR	3.5
1	C	170	GLY	3.4
2	D	564	GLU	3.4
2	B	486	GLU	3.4
2	D	839	LEU	3.4
2	D	609	LYS	3.2
2	B	838	GLN	3.2
2	D	555	SER	3.2
2	D	167	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	127	LYS	3.0
2	D	693	ASN	3.0
2	D	763	ALA	3.0
2	B	192	GLU	2.9
2	B	449	GLN	2.9
2	D	771	ALA	2.8
2	D	211	PHE	2.8
2	D	450	GLN	2.8
2	D	766	HIS	2.7
2	D	861	LEU	2.7
2	D	533	ASP	2.7
2	B	742	GLU	2.7
2	B	861	LEU	2.7
2	D	381	ASP	2.7
1	C	175	GLU	2.7
2	D	449	GLN	2.6
2	D	487	ALA	2.6
2	D	607	GLU	2.6
2	B	337	ASN	2.6
2	D	597	MET	2.6
2	D	302	TYR	2.5
2	D	169	GLN	2.5
2	D	537	GLU	2.4
2	B	849	ARG	2.4
2	D	567	GLN	2.4
2	B	596	ASP	2.3
1	C	56	ARG	2.3
2	D	806	ILE	2.3
1	C	55	ASN	2.2
2	D	485	ALA	2.2
2	D	552	GLN	2.2
2	D	814	PRO	2.2
2	D	379	THR	2.2
2	D	168	PRO	2.2
2	D	464	GLN	2.1
2	D	21	ILE	2.1
2	B	488	THR	2.1
2	D	587	SER	2.1
2	D	489	PRO	2.1
2	B	559	ASN	2.1
2	B	489	PRO	2.0
1	C	57	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	609	LYS	2.0
1	C	53	HIS	2.0
2	B	806	ILE	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](#)

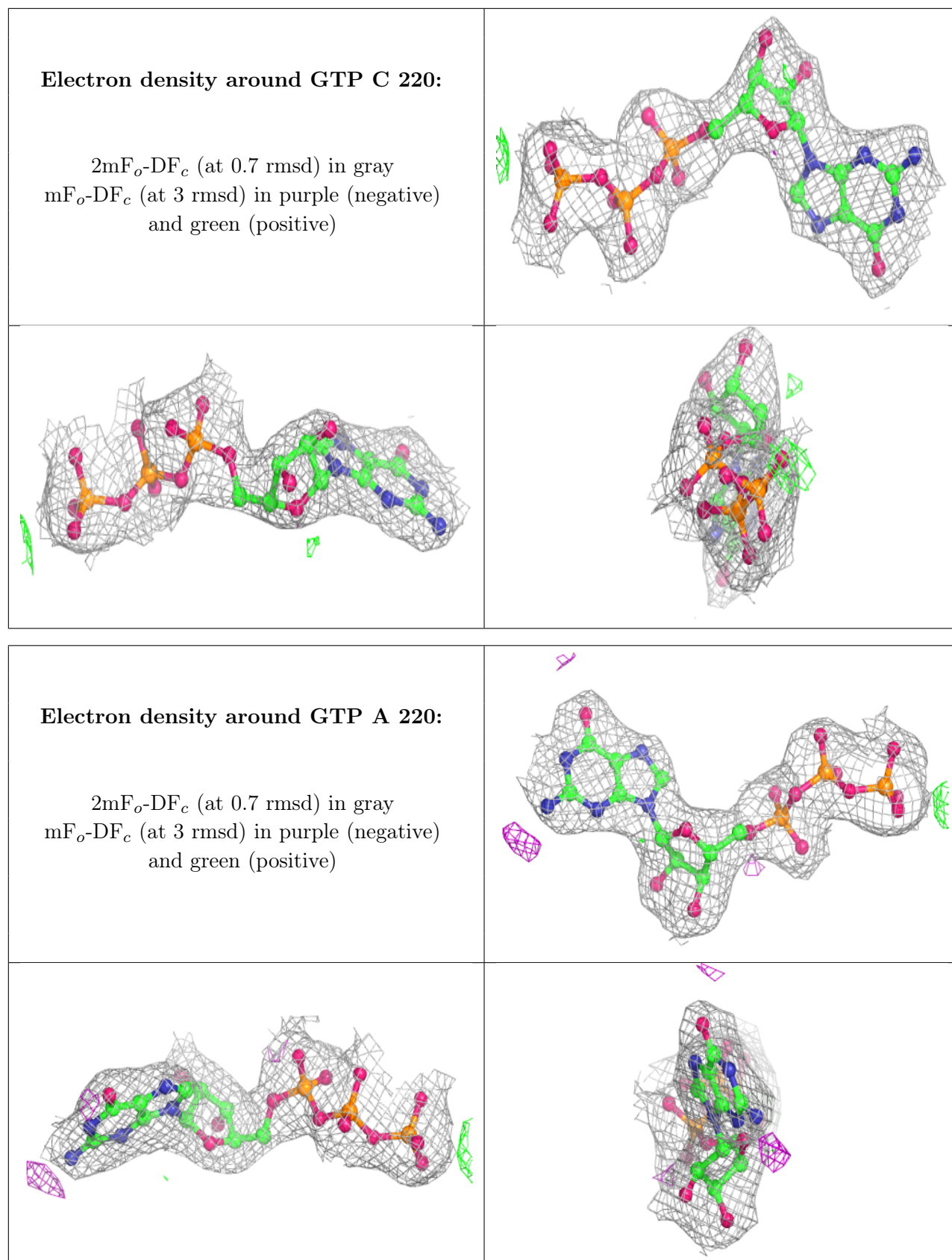
There are no monosaccharides in this entry.

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, 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	GTP	C	220	32/32	0.97	0.10	43,46,51,54	0
4	MG	C	221	1/1	0.98	0.04	47,47,47,47	0
4	MG	A	221	1/1	0.99	0.07	41,41,41,41	0
3	GTP	A	220	32/32	0.99	0.10	32,39,43,45	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.