Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:22 pm BST

PDB ID	:	3W3Z
Title	:	Crystal structure of Kap121p bound to RanGTP
Authors	:	Kobayashi, J.; Matsuura, Y.
Deposited on	:	2012-12-28
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 following versions of software and data (see references ⓘ) were used in the production of this report:

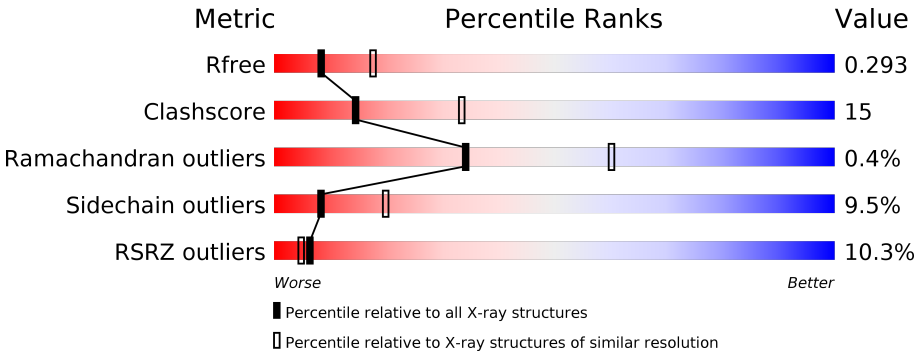
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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 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	1089	10% 70% 20% • 7%
2	B	176	4% 71% 24% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9146 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 Importin subunit beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1013	7713	4956	1250	1471	14	22	0	0	0

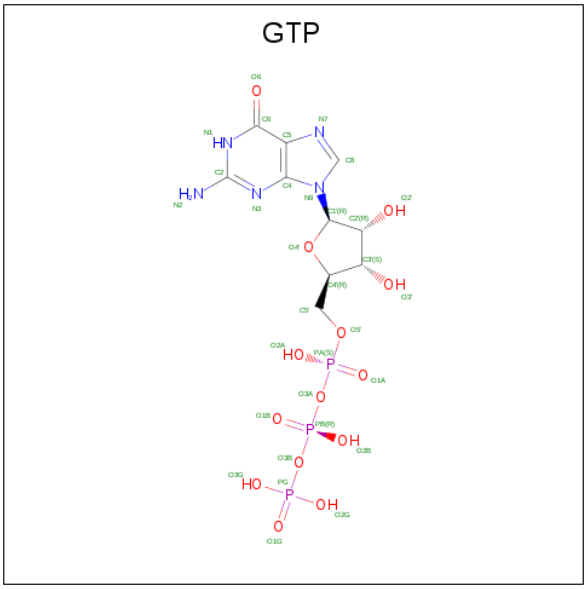
- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	171	1396	905	245	242	4	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is water.

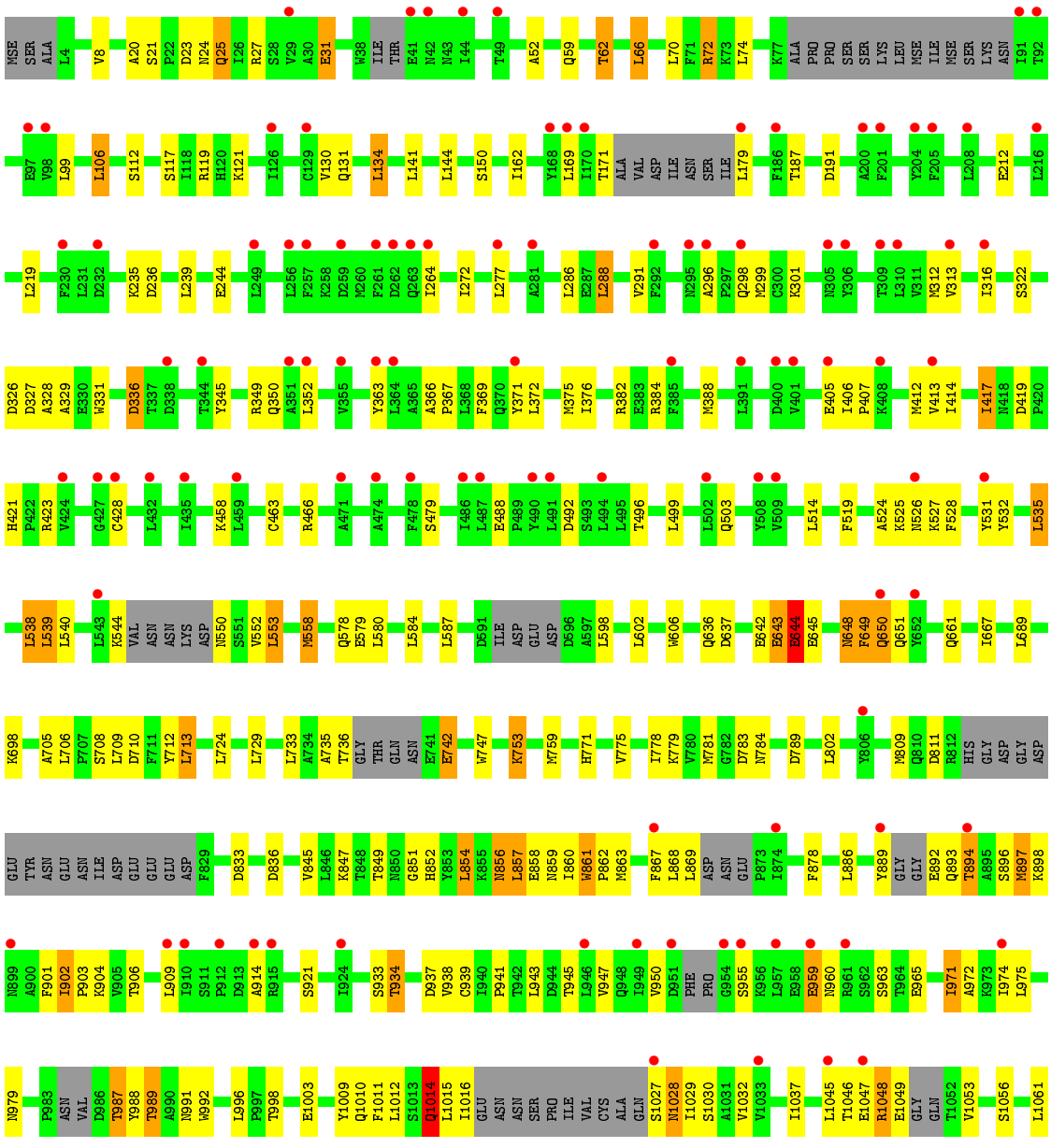
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	O	0	0
			4	4		

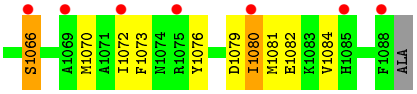
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Importin subunit beta-3

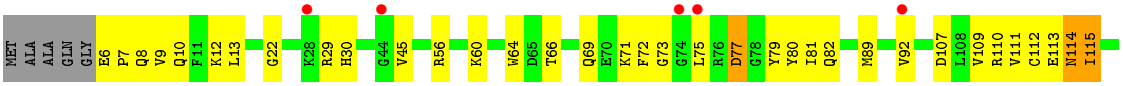
Chain A:

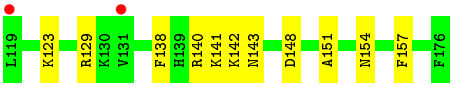




- Molecule 2: GTP-binding nuclear protein Ran

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.75Å 97.75Å 289.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.36 – 2.70 46.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.36-2.70) 99.7 (46.31-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.261 , 0.298 0.261 , 0.293	Depositor DCC
R_{free} test set	2223 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9146	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 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	0.60	0/7823	0.78	4/10619 (0.0%)
2	B	0.74	0/1431	0.86	3/1931 (0.2%)
All	All	0.62	0/9254	0.79	7/12550 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	MSE	CA-CB-CG	-7.76	100.11	113.30
2	B	56	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	809	MSE	CB-CG-SE	-5.71	95.58	112.70
2	B	148	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	A	1014	GLN	CB-CA-C	-5.31	99.78	110.40
2	B	77	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	558	MSE	CB-CA-C	-5.05	100.31	110.40

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	7713	0	7644	235	1
2	B	1396	0	1412	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	B	32	0	12	1	0
5	B	4	0	0	1	0
All	All	9146	0	9068	280	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 15.

All (280) 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:B:71:LYS:HE3	2:B:72:PHE:CE2	1.83	1.12
1:A:312:MSE:SE	1:A:371:TYR:CE1	2.55	1.10
2:B:69:GLN:OE1	2:B:71:LYS:HE2	1.51	1.08
1:A:544:LYS:NZ	1:A:579:GLU:OE2	1.88	1.07
1:A:499:LEU:HD21	1:A:535:LEU:HD11	1.36	1.06
1:A:499:LEU:HD22	1:A:535:LEU:HG	1.37	1.06
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.38	1.01
1:A:21:SER:OG	1:A:23:ASP:HB3	1.62	1.00
1:A:24:ASN:OD1	1:A:27:ARG:NH2	1.97	0.96
1:A:499:LEU:HD21	1:A:535:LEU:CD1	1.95	0.96
2:B:114:ASN:HD22	2:B:115:ILE:N	1.64	0.95
1:A:558:MSE:SE	1:A:602:LEU:HD23	2.17	0.94
1:A:496:THR:HG22	1:A:531:TYR:HE1	1.32	0.93
1:A:1046:THR:OG1	1:A:1047:GLU:HA	1.70	0.92
1:A:1028:ASN:O	1:A:1032:VAL:HG23	1.70	0.92
1:A:636:GLN:NE2	1:A:713:LEU:HB2	1.86	0.89
1:A:369:PHE:CD1	1:A:412:MSE:HE1	2.08	0.89
1:A:863:MSE:HE1	1:A:867:PHE:CE2	2.08	0.88
2:B:69:GLN:OE1	2:B:71:LYS:CE	2.20	0.88
2:B:71:LYS:HE3	2:B:72:PHE:CZ	2.09	0.87
1:A:858:GLU:HG3	1:A:897:MSE:HE1	1.57	0.85
1:A:384:ARG:NH2	1:A:421:HIS:HD2	1.75	0.84
1:A:902:ILE:N	1:A:903:PRO:HD2	1.92	0.83
1:A:21:SER:OG	1:A:23:ASP:N	2.11	0.82
1:A:66:LEU:HA	2:B:81:ILE:CD1	2.09	0.82
1:A:698:LYS:HE2	1:A:742:GLU:OE1	1.80	0.82
1:A:336:ASP:OD2	1:A:466:ARG:NE	2.13	0.81
1:A:742:GLU:HA	1:A:742:GLU:OE2	1.82	0.79
1:A:21:SER:OG	1:A:23:ASP:CB	2.31	0.79
2:B:107:ASP:OD1	2:B:110:ARG:NH2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLN:HE22	1:A:713:LEU:N	1.81	0.78
1:A:499:LEU:CD2	1:A:535:LEU:HG	2.14	0.78
1:A:1046:THR:HA	1:A:1048:ARG:H	1.48	0.77
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.12	0.77
1:A:384:ARG:NH2	1:A:421:HIS:CD2	2.52	0.77
1:A:636:GLN:HE22	1:A:713:LEU:H	1.30	0.77
1:A:499:LEU:HD22	1:A:535:LEU:CG	2.14	0.76
1:A:854:LEU:HD12	1:A:854:LEU:O	1.85	0.76
1:A:544:LYS:CE	1:A:579:GLU:OE2	2.32	0.76
2:B:66:THR:O	5:B:302:HOH:O	2.04	0.75
1:A:648:ASN:C	1:A:648:ASN:OD1	2.25	0.75
1:A:802:LEU:HB3	1:A:863:MSE:HE2	1.68	0.75
2:B:29:ARG:HG2	2:B:157:PHE:CE2	2.22	0.74
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.52	0.74
2:B:114:ASN:O	2:B:115:ILE:HG22	1.88	0.74
1:A:892:GLU:CD	1:A:934:THR:HG22	2.08	0.74
1:A:496:THR:HG22	1:A:531:TYR:CE1	2.22	0.73
1:A:771:HIS:O	1:A:775:VAL:HG23	1.87	0.73
1:A:414:ILE:O	1:A:417:ILE:HG22	1.88	0.73
2:B:114:ASN:HD22	2:B:114:ASN:C	1.84	0.73
1:A:384:ARG:HH22	1:A:421:HIS:CD2	2.06	0.73
1:A:312:MSE:SE	1:A:371:TYR:HE1	2.19	0.72
1:A:584:LEU:HB3	1:A:606:TRP:CZ2	2.24	0.72
1:A:898:LYS:HG3	1:A:902:ILE:HD11	1.72	0.71
1:A:384:ARG:NE	1:A:419:ASP:OD1	2.19	0.70
1:A:62:THR:HG23	2:B:82:GLN:HE22	1.57	0.69
1:A:499:LEU:CD2	1:A:535:LEU:CG	2.71	0.68
1:A:72:ARG:HH11	1:A:72:ARG:HG2	1.57	0.68
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.76	0.68
2:B:12:LYS:HE2	2:B:64:TRP:CE2	2.29	0.68
1:A:499:LEU:CD2	1:A:535:LEU:CD1	2.71	0.68
1:A:21:SER:HG	1:A:23:ASP:HB3	1.55	0.68
2:B:112:CYS:CB	2:B:115:ILE:HD13	2.24	0.67
1:A:31:GLU:OE1	2:B:79:TYR:OH	2.12	0.67
2:B:114:ASN:C	2:B:114:ASN:ND2	2.46	0.67
1:A:479:SER:HB3	1:A:519:PHE:HE2	1.60	0.66
1:A:1029:ILE:CG2	1:A:1030:SER:N	2.58	0.66
1:A:636:GLN:NE2	1:A:713:LEU:H	1.94	0.65
1:A:856:ASN:H	1:A:856:ASN:ND2	1.93	0.65
1:A:312:MSE:SE	1:A:371:TYR:CZ	3.00	0.64
1:A:856:ASN:HD22	1:A:856:ASN:H	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHE:CE1	1:A:412:MSE:HE1	2.32	0.64
1:A:479:SER:CB	1:A:519:PHE:HE2	2.11	0.64
1:A:25:GLN:HE21	1:A:25:GLN:HA	1.62	0.64
2:B:112:CYS:HB3	2:B:115:ILE:HD13	1.80	0.64
1:A:1046:THR:HA	1:A:1048:ARG:N	2.13	0.64
1:A:21:SER:OG	1:A:23:ASP:CA	2.46	0.63
1:A:937:ASP:O	1:A:941:PRO:HG2	1.99	0.63
2:B:22:GLY:C	2:B:89:MET:HE1	2.19	0.63
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.80	0.63
1:A:25:GLN:HE21	1:A:25:GLN:CA	2.12	0.63
1:A:20:ALA:O	1:A:21:SER:C	2.33	0.62
1:A:857:LEU:HD23	1:A:886:LEU:HD21	1.81	0.62
1:A:492:ASP:OD2	1:A:527:LYS:HD3	2.00	0.61
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.83	0.61
1:A:66:LEU:HD13	2:B:81:ILE:HD12	1.82	0.61
1:A:1029:ILE:HG23	1:A:1030:SER:N	2.14	0.61
1:A:698:LYS:CE	1:A:742:GLU:OE1	2.49	0.61
2:B:114:ASN:C	2:B:115:ILE:CG2	2.69	0.61
1:A:742:GLU:CA	1:A:742:GLU:OE2	2.49	0.60
1:A:296:ALA:CB	1:A:299:MSE:HE2	2.31	0.60
2:B:114:ASN:O	2:B:115:ILE:CG2	2.48	0.60
2:B:69:GLN:CD	2:B:72:PHE:HE2	2.05	0.60
1:A:503:GLN:CG	1:A:538:LEU:HD21	2.32	0.60
1:A:898:LYS:O	1:A:902:ILE:HG12	2.01	0.59
2:B:92:VAL:CG1	2:B:129:ARG:HG2	2.32	0.59
2:B:69:GLN:HB2	2:B:72:PHE:HD2	1.67	0.59
1:A:854:LEU:HD13	1:A:886:LEU:HD22	1.84	0.59
1:A:902:ILE:HG21	1:A:938:VAL:HG11	1.84	0.59
1:A:902:ILE:N	1:A:903:PRO:CD	2.64	0.59
1:A:514:LEU:HD21	1:A:539:LEU:HD11	1.85	0.58
1:A:1066:SER:O	1:A:1070:MSE:HG2	2.03	0.58
1:A:336:ASP:OD2	1:A:466:ARG:NH2	2.36	0.58
1:A:648:ASN:OD1	1:A:649:PHE:N	2.36	0.58
1:A:66:LEU:HA	2:B:81:ILE:HD13	1.86	0.58
1:A:858:GLU:O	1:A:861:TRP:HB2	2.03	0.57
1:A:388:MSE:SE	1:A:413:VAL:HG22	2.54	0.57
1:A:987:THR:HG23	1:A:991:ASN:HD21	1.69	0.57
1:A:996:LEU:HD23	1:A:996:LEU:N	2.19	0.57
1:A:21:SER:HG	1:A:23:ASP:CA	2.18	0.57
1:A:558:MSE:SE	1:A:602:LEU:CD2	3.00	0.57
1:A:898:LYS:O	1:A:902:ILE:CG1	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASP:O	1:A:496:THR:HG23	2.05	0.56
1:A:296:ALA:HB3	1:A:299:MSE:HE2	1.87	0.56
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.21	0.56
1:A:336:ASP:OD2	1:A:466:ARG:CZ	2.54	0.56
1:A:1028:ASN:O	1:A:1032:VAL:CG2	2.51	0.56
1:A:117:SER:O	1:A:121:LYS:NZ	2.37	0.55
1:A:636:GLN:NE2	1:A:713:LEU:CB	2.67	0.55
1:A:854:LEU:HD13	1:A:886:LEU:CD2	2.37	0.55
1:A:1012:LEU:O	1:A:1016:ILE:HG13	2.08	0.54
1:A:1011:PHE:O	1:A:1015:LEU:HG	2.08	0.54
1:A:479:SER:CB	1:A:519:PHE:CE2	2.90	0.54
2:B:73:GLY:O	2:B:75:LEU:N	2.37	0.54
2:B:22:GLY:C	2:B:89:MET:CE	2.75	0.54
1:A:667:ILE:CG2	1:A:713:LEU:HD23	2.38	0.54
1:A:384:ARG:HH21	1:A:421:HIS:HD2	1.52	0.54
1:A:735:ALA:C	1:A:736:THR:HG23	2.28	0.54
2:B:45:VAL:HB	2:B:79:TYR:CE2	2.43	0.53
1:A:21:SER:HG	1:A:23:ASP:CB	2.16	0.53
1:A:25:GLN:NE2	1:A:25:GLN:HA	2.23	0.53
1:A:1073:PHE:HB3	1:A:1081:MSE:SE	2.58	0.53
1:A:479:SER:HB2	1:A:519:PHE:CE2	2.44	0.53
1:A:893:GLN:HG2	1:A:893:GLN:O	2.09	0.53
2:B:71:LYS:CE	2:B:72:PHE:CE2	2.75	0.53
1:A:312:MSE:HE3	1:A:316:ILE:HD11	1.91	0.53
2:B:71:LYS:HE3	2:B:72:PHE:HE2	1.64	0.53
1:A:499:LEU:CD2	1:A:535:LEU:HD11	2.23	0.53
1:A:858:GLU:HG3	1:A:897:MSE:CE	2.36	0.53
1:A:1010:GLN:O	1:A:1014:GLN:HG2	2.09	0.53
1:A:301:LYS:HA	1:A:363:TYR:CE1	2.45	0.52
1:A:558:MSE:HE1	1:A:598:LEU:HD11	1.92	0.52
1:A:898:LYS:HG3	1:A:902:ILE:CD1	2.38	0.52
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.92	0.52
1:A:345:TYR:O	1:A:349:ARG:HG3	2.10	0.52
1:A:802:LEU:HD21	1:A:878:PHE:CZ	2.45	0.51
2:B:112:CYS:HB2	2:B:115:ILE:HD13	1.91	0.51
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.10	0.51
1:A:350:GLN:HG2	2:B:140:ARG:NH2	2.24	0.51
1:A:858:GLU:CG	1:A:897:MSE:HE1	2.35	0.51
1:A:851:GLY:O	1:A:854:LEU:N	2.43	0.51
1:A:544:LYS:HE2	1:A:579:GLU:OE2	2.08	0.51
2:B:6:GLU:O	2:B:7:PRO:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLN:HB3	1:A:134:LEU:HB2	1.92	0.50
1:A:372:LEU:O	1:A:376:ILE:HG12	2.11	0.50
1:A:893:GLN:CG	1:A:893:GLN:O	2.58	0.50
2:B:114:ASN:C	2:B:115:ILE:HG23	2.31	0.50
2:B:29:ARG:HD2	2:B:151:ALA:O	2.11	0.50
1:A:1047:GLU:C	1:A:1049:GLU:N	2.61	0.50
1:A:327:ASP:O	1:A:328:ALA:HB3	2.12	0.50
1:A:747:TRP:CD1	1:A:781:MSE:HG3	2.47	0.50
1:A:458:LYS:HE3	1:A:463:CYS:SG	2.52	0.50
1:A:892:GLU:CG	1:A:934:THR:CG2	2.89	0.50
1:A:858:GLU:O	1:A:861:TRP:N	2.36	0.49
1:A:322:SER:O	1:A:382:ARG:NH2	2.45	0.49
1:A:66:LEU:HA	2:B:81:ILE:HD11	1.90	0.49
2:B:10:GLN:HA	2:B:60:LYS:O	2.12	0.49
1:A:939:CYS:HB3	1:A:974:ILE:HG12	1.94	0.49
2:B:10:GLN:HB3	2:B:60:LYS:HB3	1.95	0.49
1:A:25:GLN:NE2	1:A:25:GLN:CA	2.74	0.48
1:A:987:THR:HG22	1:A:988:TYR:N	2.28	0.48
1:A:861:TRP:HE1	1:A:897:MSE:SE	2.46	0.48
1:A:644:GLU:HG2	1:A:645:GLU:N	2.27	0.48
1:A:854:LEU:C	1:A:854:LEU:HD12	2.30	0.48
1:A:528:PHE:O	1:A:532:TYR:N	2.44	0.48
1:A:859:ASN:OD1	1:A:859:ASN:N	2.46	0.48
1:A:894:THR:O	1:A:897:MSE:HG3	2.13	0.48
2:B:29:ARG:HG2	2:B:157:PHE:CZ	2.48	0.48
2:B:12:LYS:NZ	2:B:79:TYR:O	2.47	0.48
1:A:892:GLU:CG	1:A:934:THR:HG22	2.43	0.47
1:A:52:ALA:HB1	1:A:106:LEU:HD13	1.96	0.47
1:A:499:LEU:HD11	1:A:531:TYR:HB3	1.96	0.47
1:A:712:TYR:HD1	1:A:713:LEU:HD13	1.79	0.47
1:A:861:TRP:NE1	1:A:897:MSE:SE	2.97	0.47
1:A:856:ASN:O	1:A:857:LEU:C	2.52	0.47
1:A:747:TRP:CG	1:A:781:MSE:HG3	2.50	0.47
2:B:13:LEU:C	2:B:13:LEU:HD23	2.34	0.47
1:A:27:ARG:NH1	2:B:45:VAL:CG1	2.77	0.47
1:A:709:LEU:HD12	1:A:753:LYS:HG2	1.96	0.47
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.27	0.47
1:A:550:ASN:O	1:A:553:LEU:N	2.48	0.47
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.29	0.47
1:A:857:LEU:HD23	1:A:886:LEU:CD2	2.44	0.47
1:A:906:THR:HA	1:A:909:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:LEU:O	1:A:947:VAL:HG23	2.15	0.47
1:A:987:THR:CG2	1:A:991:ASN:HD21	2.28	0.46
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.44	0.46
2:B:80:TYR:HB2	2:B:111:VAL:HG21	1.97	0.46
1:A:649:PHE:C	1:A:651:GLN:H	2.18	0.46
1:A:863:MSE:CE	1:A:867:PHE:CE2	2.89	0.46
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.98	0.46
1:A:328:ALA:O	1:A:329:ALA:C	2.53	0.46
1:A:384:ARG:HH21	1:A:419:ASP:CG	2.18	0.46
1:A:987:THR:HG23	1:A:991:ASN:ND2	2.31	0.46
1:A:1011:PHE:HA	1:A:1014:GLN:HG3	1.98	0.46
1:A:833:ASP:O	1:A:836:ASP:HB2	2.16	0.46
1:A:496:THR:CG2	1:A:531:TYR:CE1	2.97	0.45
1:A:130:VAL:HG11	1:A:169:LEU:HD21	1.98	0.45
1:A:369:PHE:CE1	1:A:412:MSE:CE	2.98	0.45
1:A:417:ILE:HG13	1:A:458:LYS:HD3	1.99	0.45
1:A:419:ASP:OD2	1:A:421:HIS:CD2	2.70	0.45
1:A:852:HIS:C	1:A:854:LEU:H	2.20	0.45
1:A:858:GLU:C	1:A:860:ILE:N	2.69	0.45
1:A:417:ILE:CG1	1:A:458:LYS:HD3	2.47	0.45
2:B:69:GLN:OE1	2:B:72:PHE:HE2	2.00	0.45
1:A:21:SER:HG	1:A:23:ASP:C	2.19	0.45
1:A:892:GLU:HG2	1:A:934:THR:CG2	2.47	0.45
1:A:1011:PHE:HA	1:A:1014:GLN:CG	2.48	0.44
1:A:710:ASP:OD2	1:A:753:LYS:NZ	2.46	0.44
1:A:514:LEU:HD21	1:A:539:LEU:CD1	2.48	0.44
2:B:114:ASN:ND2	2:B:115:ILE:N	2.47	0.44
1:A:636:GLN:NE2	1:A:713:LEU:N	2.55	0.44
1:A:854:LEU:CD1	1:A:886:LEU:HD22	2.48	0.44
1:A:112:SER:O	1:A:119:ARG:NH2	2.51	0.44
1:A:66:LEU:CA	2:B:81:ILE:HD13	2.47	0.44
1:A:1003:GLU:CD	1:A:1003:GLU:H	2.22	0.43
1:A:712:TYR:CE1	1:A:713:LEU:HD22	2.53	0.43
1:A:27:ARG:NH1	2:B:45:VAL:HG13	2.33	0.43
1:A:25:GLN:HE21	1:A:25:GLN:N	2.17	0.43
1:A:892:GLU:OE1	1:A:933:SER:OG	2.25	0.43
1:A:1061:LEU:HD21	1:A:1072:ILE:HD12	1.99	0.43
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.99	0.43
1:A:1047:GLU:C	1:A:1049:GLU:H	2.22	0.43
1:A:366:ALA:HB3	1:A:367:PRO:HD3	2.00	0.43
1:A:856:ASN:ND2	1:A:856:ASN:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:ASN:O	1:A:858:GLU:N	2.52	0.43
2:B:154:ASN:O	2:B:157:PHE:HB2	2.19	0.43
1:A:1046:THR:HG1	1:A:1047:GLU:HA	1.79	0.43
1:A:144:LEU:HD21	1:A:162:ILE:HD12	2.01	0.43
1:A:667:ILE:HG23	1:A:713:LEU:HD23	1.99	0.43
2:B:69:GLN:NE2	2:B:72:PHE:HE2	2.17	0.43
1:A:861:TRP:N	1:A:862:PRO:HD2	2.34	0.42
1:A:331:TRP:CZ2	1:A:423:ARG:HG3	2.54	0.42
1:A:934:THR:O	1:A:934:THR:OG1	2.35	0.42
1:A:649:PHE:C	1:A:651:GLN:N	2.72	0.42
1:A:419:ASP:OD2	1:A:421:HIS:HD2	2.02	0.42
1:A:413:VAL:HG13	1:A:428:CYS:SG	2.59	0.42
1:A:1079:ASP:HA	1:A:1082:GLU:CD	2.40	0.42
2:B:12:LYS:HE2	2:B:64:TRP:CZ2	2.53	0.42
1:A:902:ILE:CG2	1:A:938:VAL:HG11	2.49	0.42
2:B:109:VAL:HA	2:B:112:CYS:O	2.20	0.42
1:A:272:ILE:HG21	1:A:313:VAL:HB	2.02	0.42
1:A:648:ASN:C	1:A:650:GLN:N	2.73	0.42
1:A:667:ILE:HD13	1:A:713:LEU:HB3	2.01	0.42
2:B:123:LYS:HG2	4:B:202:GTP:C6	2.54	0.41
1:A:643:GLU:OE2	1:A:643:GLU:N	2.52	0.41
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.54	0.41
1:A:847:LYS:HB2	1:A:889:TYR:OH	2.19	0.41
1:A:959:GLU:N	1:A:959:GLU:OE1	2.53	0.41
2:B:6:GLU:O	2:B:8:GLN:NE2	2.53	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.86	0.41
1:A:1076:TYR:CG	1:A:1080:ILE:HD11	2.55	0.41
1:A:1080:ILE:O	1:A:1080:ILE:HD12	2.21	0.41
1:A:336:ASP:HA	1:A:466:ARG:CZ	2.51	0.41
1:A:345:TYR:CZ	1:A:349:ARG:HD2	2.56	0.41
1:A:636:GLN:HE21	1:A:713:LEU:HB2	1.77	0.41
1:A:735:ALA:C	1:A:736:THR:CG2	2.88	0.41
2:B:138:PHE:CZ	2:B:142:LYS:HG3	2.56	0.41
1:A:540:LEU:HD21	1:A:580:LEU:HD13	2.02	0.41
1:A:901:PHE:C	1:A:903:PRO:HD2	2.40	0.41
1:A:914:ALA:O	1:A:963:SER:OG	2.25	0.41
1:A:849:THR:HB	1:A:852:HIS:HB2	2.03	0.41
1:A:264:ILE:HD11	1:A:288:LEU:CD1	2.51	0.41
1:A:584:LEU:CD2	1:A:602:LEU:HD22	2.51	0.41
1:A:705:ALA:O	1:A:708:SER:HB2	2.21	0.41
1:A:858:GLU:CG	1:A:897:MSE:CE	2.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HG2	2:B:141:LYS:O	2.21	0.40
1:A:503:GLN:CD	1:A:538:LEU:HD21	2.42	0.40
2:B:30:HIS:CE1	2:B:157:PHE:CE2	3.09	0.40
1:A:778:ILE:HD11	1:A:845:VAL:HG22	2.03	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)
1:A:212:GLU:OE1	1:A:212:GLU:OE1[4_555]	1.84	0.36

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	985/1089 (90%)	945 (96%)	35 (4%)	5 (0%)	29 54
2	B	169/176 (96%)	158 (94%)	11 (6%)	0	100 100
All	All	1154/1265 (91%)	1103 (96%)	46 (4%)	5 (0%)	34 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	525	LYS
1	A	644	GLU
1	A	1048	ARG
1	A	524	ALA
1	A	8	VAL

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	829/923 (90%)	742 (90%)	87 (10%)	7 16
2	B	151/153 (99%)	145 (96%)	6 (4%)	31 60
All	All	980/1076 (91%)	887 (90%)	93 (10%)	8 20

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	31	GLU
1	A	59	GLN
1	A	62	THR
1	A	66	LEU
1	A	72	ARG
1	A	74	LEU
1	A	106	LEU
1	A	134	LEU
1	A	141	LEU
1	A	150	SER
1	A	171	THR
1	A	179	LEU
1	A	187	THR
1	A	219	LEU
1	A	236	ASP
1	A	239	LEU
1	A	277	LEU
1	A	286	LEU
1	A	288	LEU
1	A	291	VAL
1	A	298	GLN
1	A	326	ASP
1	A	336	ASP
1	A	352	LEU
1	A	405	GLU
1	A	417	ILE

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Mol	Chain	Res	Type
1	A	488	GLU
1	A	526	ASN
1	A	535	LEU
1	A	538	LEU
1	A	539	LEU
1	A	552	VAL
1	A	553	LEU
1	A	578	GLN
1	A	587	LEU
1	A	637	ASP
1	A	642	GLU
1	A	643	GLU
1	A	644	GLU
1	A	648	ASN
1	A	649	PHE
1	A	650	GLN
1	A	661	GLN
1	A	689	LEU
1	A	706	LEU
1	A	713	LEU
1	A	724	LEU
1	A	729	LEU
1	A	733	LEU
1	A	742	GLU
1	A	753	LYS
1	A	759	MSE
1	A	779	LYS
1	A	783	ASP
1	A	784	ASN
1	A	789	ASP
1	A	811	ASP
1	A	854	LEU
1	A	856	ASN
1	A	857	LEU
1	A	861	TRP
1	A	868	LEU
1	A	869	LEU
1	A	894	THR
1	A	896	SER
1	A	897	MSE
1	A	902	ILE
1	A	904	LYS

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Mol	Chain	Res	Type
1	A	921	SER
1	A	934	THR
1	A	945	THR
1	A	950	VAL
1	A	955	SER
1	A	959	GLU
1	A	960	ASN
1	A	971	ILE
1	A	979	ASN
1	A	987	THR
1	A	989	THR
1	A	1014	GLN
1	A	1027	SER
1	A	1028	ASN
1	A	1045	LEU
1	A	1056	SER
1	A	1066	SER
1	A	1080	ILE
2	B	9	VAL
2	B	77	ASP
2	B	113	GLU
2	B	114	ASN
2	B	115	ILE
2	B	143	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	25	GLN
1	A	54	GLN
1	A	303	ASN
1	A	308	GLN
1	A	421	HIS
1	A	430	ASN
1	A	541	ASN
1	A	578	GLN
1	A	636	GLN
1	A	650	GLN
1	A	659	GLN
1	A	692	GLN
1	A	856	ASN

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Mol	Chain	Res	Type
1	A	888	GLN
1	A	893	GLN
1	A	991	ASN
1	A	1074	ASN
2	B	30	HIS
2	B	100	ASN
2	B	105	HIS
2	B	114	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	B	202	3	26,34,34	1.17	2 (7%)	33,54,54	2.21	11 (33%)

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
4	GTP	B	202	3	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	GTP	C6-C5	3.68	1.47	1.41
4	B	202	GTP	C5-C4	2.54	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	202	GTP	C2-N3-C4	5.92	122.11	115.36
4	B	202	GTP	C6-C5-C4	-4.54	116.46	120.80
4	B	202	GTP	C6-N1-C2	3.88	122.10	115.93
4	B	202	GTP	N3-C2-N1	-3.77	122.19	127.22
4	B	202	GTP	O5'-PA-O1A	-3.77	94.36	109.07
4	B	202	GTP	C5-C6-N1	-3.22	119.02	123.43
4	B	202	GTP	O3G-PG-O2G	2.91	118.75	107.64
4	B	202	GTP	PA-O3A-PB	-2.67	123.66	132.83
4	B	202	GTP	C3'-C2'-C1'	2.65	104.96	100.98
4	B	202	GTP	O4'-C1'-C2'	-2.64	103.07	106.93
4	B	202	GTP	O2A-PA-O5'	2.21	118.03	107.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	202	GTP	PA-O3A-PB-O2B
4	B	202	GTP	PA-O3A-PB-O1B

There are no ring outliers.

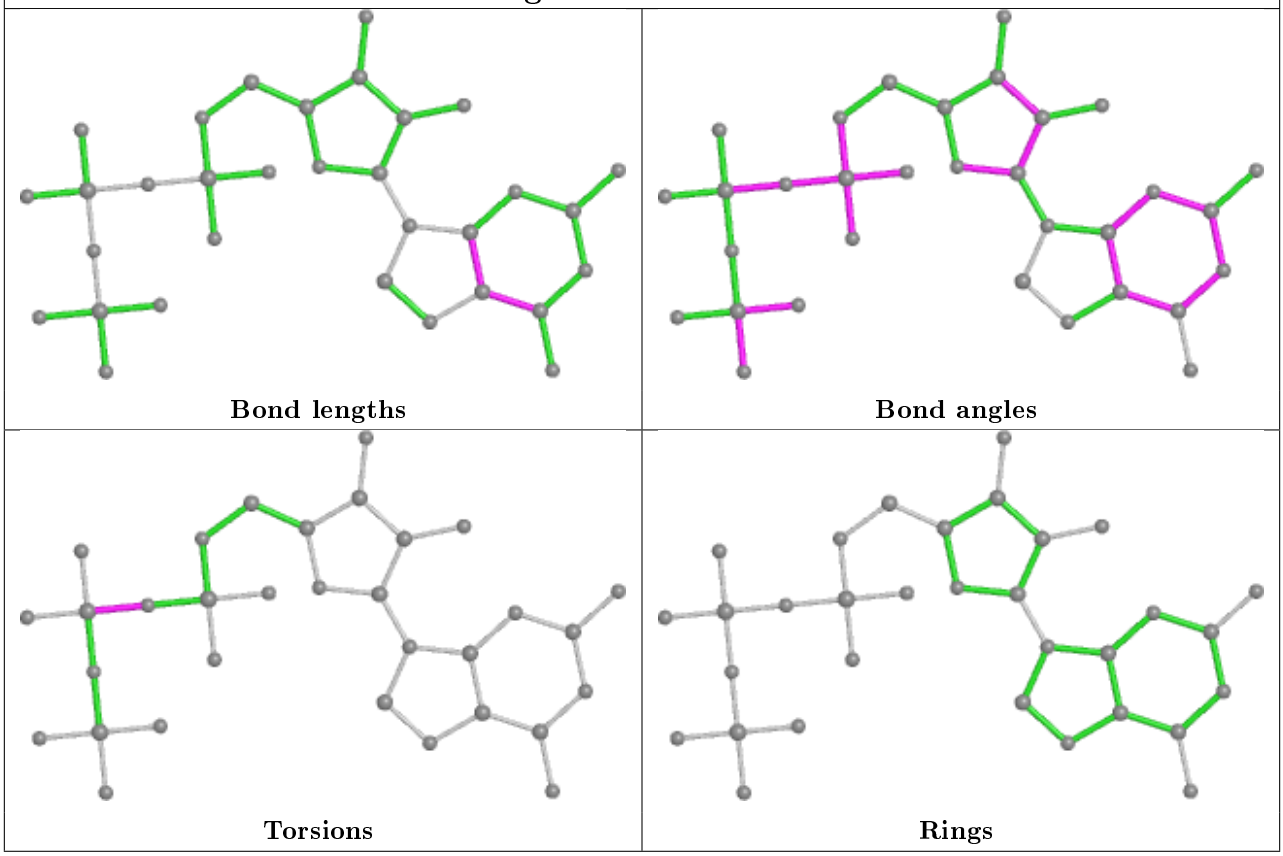
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	GTP	1	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 GTP B 202



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	991/1089 (91%)	0.63	113 (11%) 5 4	46, 103, 159, 219	0
2	B	171/176 (97%)	0.46	7 (4%) 37 36	50, 78, 122, 147	0
All	All	1162/1265 (91%)	0.60	120 (10%) 6 5	46, 98, 157, 219	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	PHE	5.9
1	A	295	ASN	5.3
1	A	494	LEU	5.2
1	A	168	TYR	5.0
1	A	259	ASP	4.8
1	A	1047	GLU	4.7
1	A	487	LEU	4.4
1	A	92	THR	4.4
1	A	256	LEU	4.3
1	A	91	ILE	4.3
1	A	478	PHE	4.3
1	A	1069	ALA	4.2
1	A	216	LEU	3.9
1	A	298	GLN	3.9
1	A	364	LEU	3.9
1	A	909	LEU	3.8
2	B	131	VAL	3.8
1	A	400	ASP	3.7
1	A	208	LEU	3.7
1	A	874	ILE	3.6
1	A	44	ILE	3.5
1	A	912	PRO	3.5
1	A	924	ILE	3.4
1	A	263	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	292	PHE	3.3
1	A	385	PHE	3.2
1	A	49	THR	3.2
1	A	961	ARG	3.2
1	A	42	ASN	3.1
1	A	650	GLN	3.1
1	A	262	ASP	3.1
1	A	432	LEU	3.1
1	A	486	ILE	3.1
1	A	652	TYR	3.0
1	A	261	PHE	3.0
1	A	313	VAL	3.0
1	A	509	VAL	3.0
1	A	424	VAL	3.0
1	A	1072	ILE	2.9
1	A	309	THR	2.9
1	A	371	TYR	2.9
1	A	205	PHE	2.9
1	A	405	GLU	2.9
1	A	264	ILE	2.8
1	A	169	LEU	2.8
1	A	391	LEU	2.8
1	A	957	LEU	2.8
1	A	806	TYR	2.8
1	A	401	VAL	2.8
1	A	363	TYR	2.8
1	A	867	PHE	2.8
1	A	351	ALA	2.8
1	A	543	LEU	2.8
2	B	119	LEU	2.7
1	A	296	ALA	2.7
1	A	352	LEU	2.7
1	A	316	ILE	2.7
1	A	129	CYS	2.7
1	A	502	LEU	2.7
1	A	179	LEU	2.6
1	A	899	ASN	2.6
1	A	474	ALA	2.5
1	A	959	GLU	2.5
1	A	249	LEU	2.5
1	A	306	TYR	2.5
1	A	490	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	427	GLY	2.5
1	A	955	SER	2.5
1	A	200	ALA	2.4
1	A	531	TYR	2.4
1	A	954	GLY	2.4
2	B	44	GLY	2.4
1	A	310	LEU	2.4
1	A	894	THR	2.4
2	B	75	LEU	2.4
1	A	526	ASN	2.4
1	A	1080	ILE	2.4
1	A	889	TYR	2.4
1	A	277	LEU	2.4
1	A	1027	SER	2.4
1	A	435	ILE	2.3
1	A	471	ALA	2.3
1	A	508	TYR	2.3
1	A	97	GLU	2.3
1	A	949	ILE	2.3
1	A	974	ILE	2.3
1	A	1088	PHE	2.3
1	A	126	ILE	2.3
1	A	951	ASP	2.3
1	A	1066	SER	2.2
1	A	281	ALA	2.2
1	A	29	VAL	2.2
1	A	98	VAL	2.2
1	A	170	ILE	2.2
1	A	338	ASP	2.2
1	A	355	VAL	2.2
1	A	201	PHE	2.2
1	A	413	VAL	2.2
1	A	946	LEU	2.2
1	A	1033	VAL	2.2
2	B	92	VAL	2.2
1	A	491	LEU	2.1
1	A	344	THR	2.1
1	A	914	ALA	2.1
1	A	232	ASP	2.1
1	A	915	ARG	2.1
1	A	428	CYS	2.1
2	B	74	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1075	ARG	2.1
1	A	408	LYS	2.1
1	A	186	PHE	2.1
1	A	204	TYR	2.0
1	A	41	GLU	2.0
1	A	1045	LEU	2.0
1	A	910	ILE	2.0
1	A	305	ASN	2.0
1	A	230	PHE	2.0
1	A	459	LEU	2.0
1	A	1085	HIS	2.0
2	B	28	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 carbohydrates in this entry.

6.4 Ligands (i)

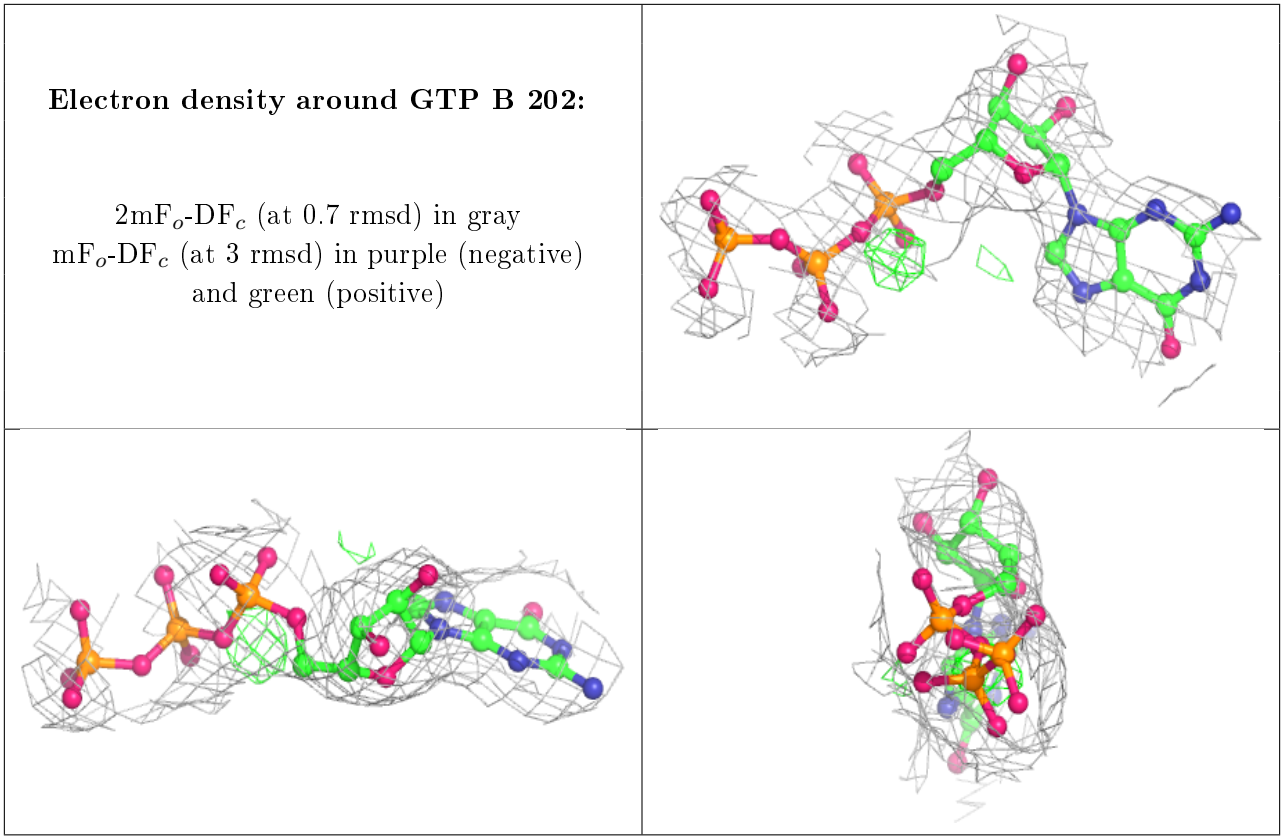
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	B	201	1/1	0.92	0.09	50,50,50,50	0
4	GTP	B	202	32/32	0.96	0.18	58,78,102,120	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 GTP B 202:

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



6.5 Other polymers (i)

There are no such residues in this entry.