Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 08:44 AM EDT

PDB ID	:	3RYF
Title	:	GTP-Tubulin: RB3 Stathmin-like domain complex
Authors	:	Nawrotek, A.; Knossow, M.; Gigant, B.
Deposited on	:	2011-05-11
Resolution	:	2.52 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 (i) 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 (i)) were used in the production of this report:

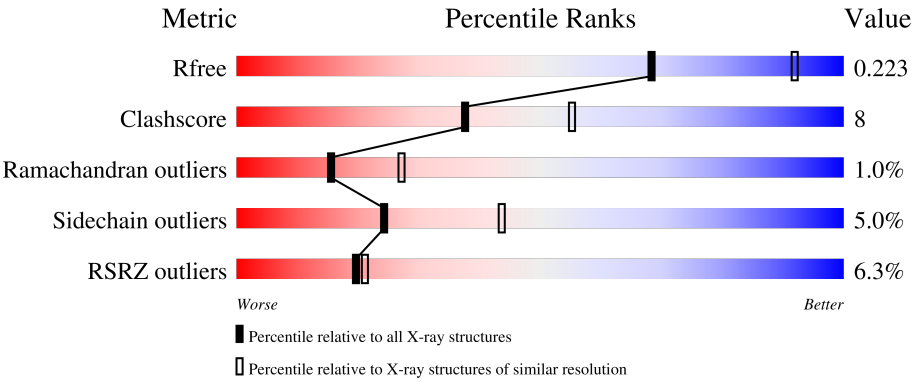
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	451	3% 78% 17%
1	C	451	8% 80% 13%
2	B	445	7% 77% 19%
2	D	445	4% 80% 15%
3	E	143	14% 78% 15% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15301 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	1	0
			3416	2162	580	651	23			
1	C	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	7	0
			3443	2163	585	668	27			
2	D	431	Total	C	N	O	S	0	8	0
			3442	2159	588	668	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

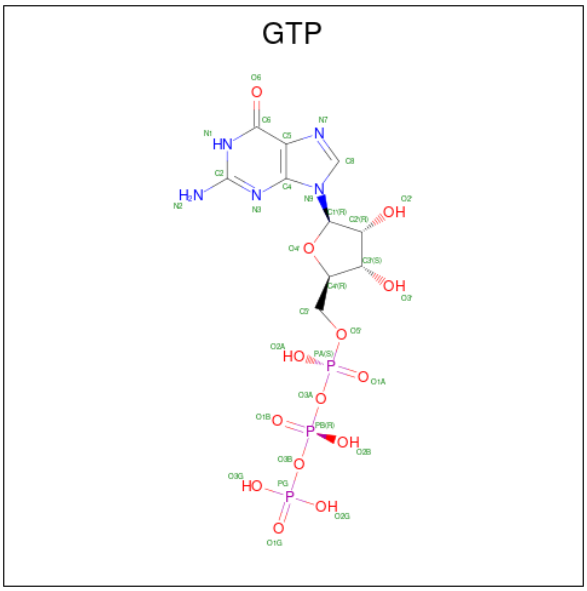
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	136	Total	C	N	O	S	0	0	0
			1070	663	195	208	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ACE	-	SEE REMARK 999	UNP P63043
E	4	ALA	-	SEE REMARK 999	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

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

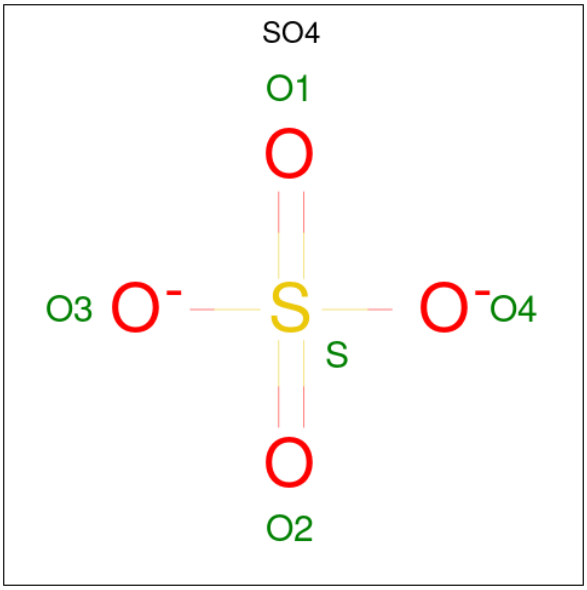


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	1
			60	20	10	25	5		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

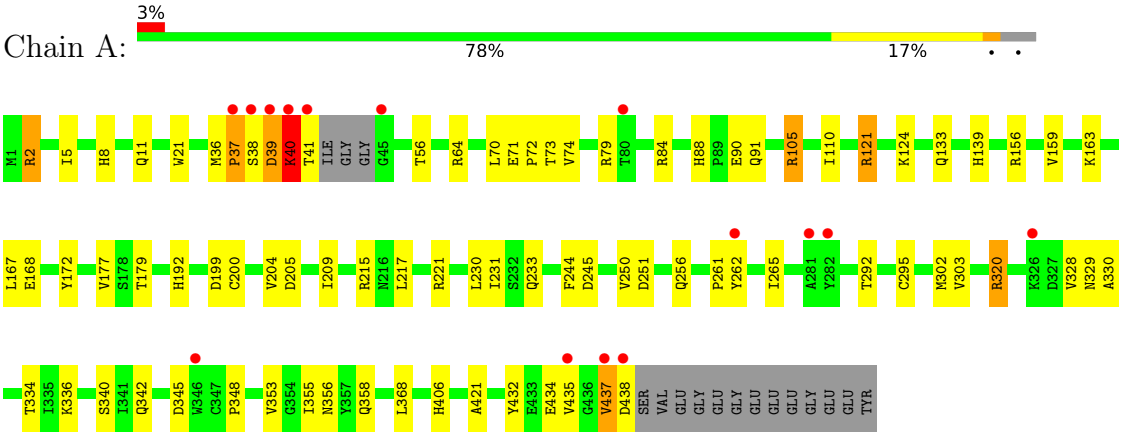
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	118	Total O 118 118	0	0
7	B	70	Total O 73 73	0	3
7	C	76	Total O 76 76	0	0
7	D	88	Total O 88 88	0	1
7	E	8	Total O 8 8	0	0

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.

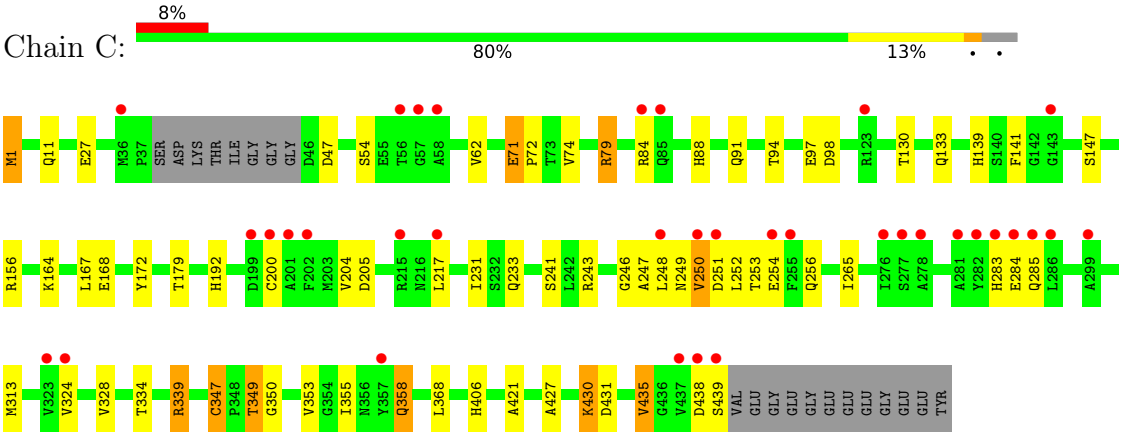
• Molecule 1: Tubulin alpha chain

Chain A:



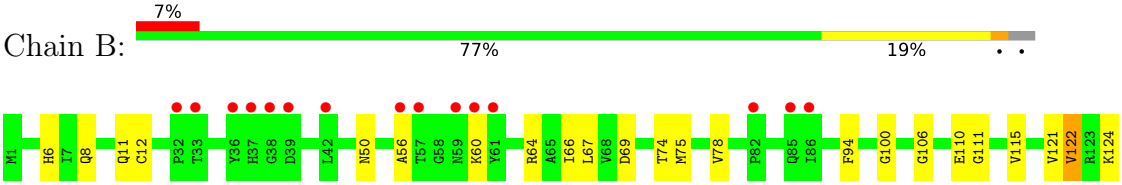
• Molecule 1: Tubulin alpha chain

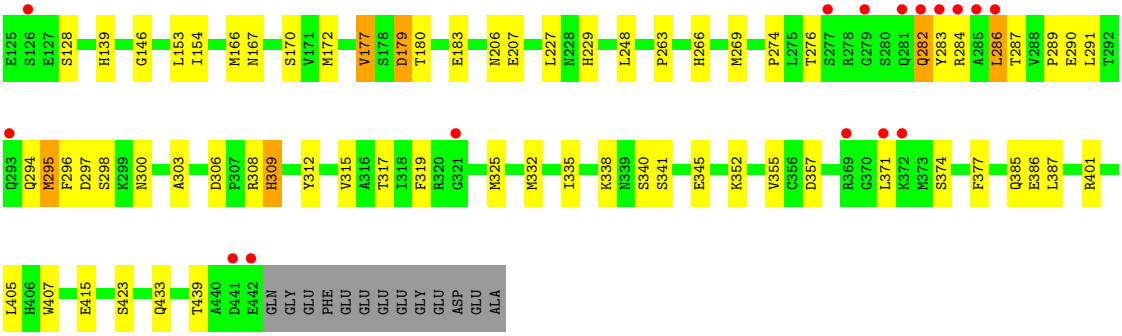
Chain C:



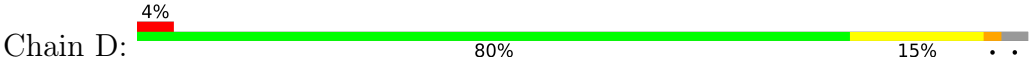
• Molecule 2: Tubulin beta chain

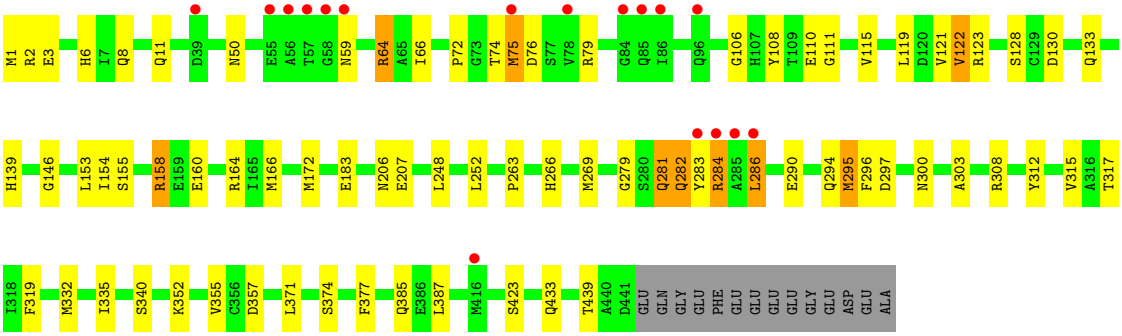
Chain B:



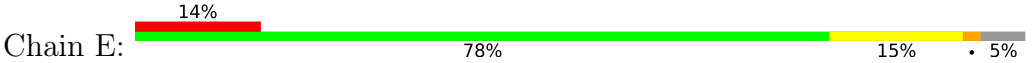


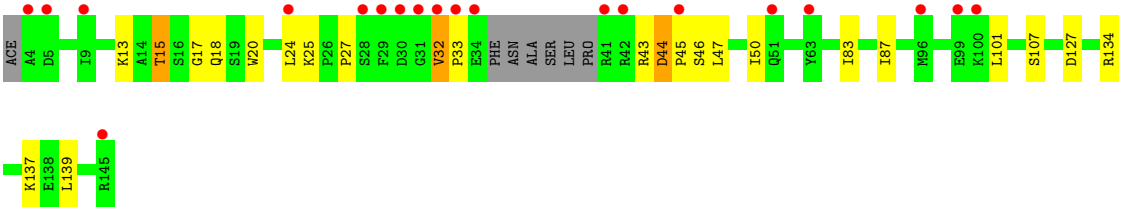
• Molecule 2: Tubulin beta chain





• Molecule 3: Stathmin-4





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.64Å 127.44Å 250.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.90 – 2.52 42.67 – 2.52	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.90-2.52) 99.3 (42.67-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.168 , 0.208 0.179 , 0.223	Depositor DCC
R_{free} test set	3570 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15301	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, SO4

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	0.52	1/3493 (0.0%)	0.70	0/4740
1	C	0.51	0/3427	0.72	0/4655
2	B	0.50	0/3531	0.72	1/4782 (0.0%)
2	D	0.50	0/3534	0.72	1/4784 (0.0%)
3	E	0.52	0/1081	0.73	0/1444
All	All	0.51	1/15066 (0.0%)	0.72	2/20405 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	SER	CB-OG	8.54	1.53	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	281	GLN	C-N-CA	5.04	134.30	121.70
2	B	179	ASP	CB-CA-C	5.02	120.43	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	3416	0	3325	67	0
1	C	3352	0	3253	42	0
2	B	3443	0	3293	56	0
2	D	3442	0	3302	63	0
3	E	1070	0	1051	16	0
4	A	32	0	12	0	0
4	B	60	0	24	4	0
4	C	32	0	12	0	0
4	D	32	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	0	0	0
6	B	5	0	0	0	0
6	C	15	0	0	0	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
7	A	118	0	0	5	0
7	B	73	0	0	3	0
7	C	76	0	0	1	0
7	D	88	0	0	3	0
7	E	8	0	0	0	0
All	All	15301	0	14284	226	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 8.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HG3	1:A:121:ARG:NH1	1.51	1.24
1:A:90:GLU:HG3	1:A:121:ARG:HH12	0.98	1.12
1:A:90:GLU:CG	1:A:121:ARG:NH1	2.16	1.09
2:D:75:MET:CE	2:D:79:ARG:NH1	2.21	1.02
2:D:75:MET:CG	2:D:79:ARG:NH1	2.23	1.01
2:D:75:MET:SD	2:D:79:ARG:NH1	2.35	1.00
1:A:156:ARG:NH2	7:A:722:HOH:O	1.98	0.97
1:A:90:GLU:HB2	1:A:121:ARG:NH1	1.84	0.93
2:B:206:ASN:HD21	4:B:600[B]:GTP:HN22	1.17	0.92
2:D:75:MET:HE3	2:D:79:ARG:NH1	1.84	0.91
1:A:90:GLU:CG	1:A:121:ARG:HH12	1.78	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:CB	1:A:121:ARG:NH1	2.37	0.86
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.55	0.86
1:A:71:GLU:OE2	1:A:73:THR:HB	1.75	0.85
2:D:206:ASN:HD21	4:D:600:GTP:HN22	1.26	0.81
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.28	0.81
1:A:121:ARG:HH21	1:A:124:LYS:HD2	1.45	0.80
2:B:206:ASN:HD21	4:B:600[A]:GTP:HN22	1.28	0.79
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.65	0.79
2:D:75:MET:CE	2:D:79:ARG:HH11	1.97	0.77
3:E:44:ASP:H	3:E:45:PRO:HA	1.48	0.77
1:A:245:ASP:HB3	3:E:15:THR:HG22	1.68	0.74
2:D:75:MET:HG2	2:D:79:ARG:HH11	1.52	0.74
2:D:75:MET:CE	2:D:76:ASP:OD1	2.37	0.73
1:A:90:GLU:CG	1:A:121:ARG:HH11	1.99	0.73
2:B:66:ILE:HG12	2:B:121:VAL:HG12	1.71	0.72
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.72	0.71
2:D:75:MET:HG2	2:D:79:ARG:NH1	2.06	0.70
1:C:233:GLN:NE2	7:C:676:HOH:O	2.25	0.70
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.76	0.69
2:D:263:PRO:O	2:D:266:HIS:HD2	1.75	0.69
1:A:37:PRO:C	1:A:39:ASP:H	1.96	0.68
2:D:317:THR:HG21	2:D:332:MET:HE1	1.76	0.68
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:HB2	1.77	0.67
1:C:427:ALA:O	1:C:430:LYS:HD2	1.94	0.67
2:B:295[A]:MET:HG3	2:B:377[A]:PHE:HB2	1.78	0.66
2:D:75:MET:CG	2:D:79:ARG:HH11	2.03	0.66
2:D:133:GLN:NE2	2:D:252:LEU:H	1.94	0.65
2:D:283:TYR:O	2:D:284:ARG:HB3	1.98	0.64
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.63	0.64
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.62	0.63
2:D:75:MET:HG3	2:D:79:ARG:NH1	2.13	0.63
2:D:50:ASN:O	2:D:64:ARG:NH2	2.30	0.62
2:B:263:PRO:O	2:B:266:HIS:HD2	1.82	0.62
2:B:317:THR:HG21	2:B:332:MET:HE1	1.81	0.62
2:D:2:ARG:HD2	2:D:130:ASP:HB3	1.81	0.62
1:A:71:GLU:OE2	1:A:73:THR:CB	2.47	0.62
2:D:75:MET:HE2	2:D:76:ASP:OD1	2.00	0.62
2:D:281:GLN:HA	2:D:282:GLN:CB	2.30	0.61
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.66	0.61
3:E:32:VAL:HB	3:E:33:PRO:CD	2.30	0.61
2:B:294[A]:GLN:OE1	7:B:46:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD12	2:B:291:LEU:HD23	1.82	0.60
1:C:1:MET:N	1:C:130:THR:OG1	2.34	0.60
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.36	0.60
2:D:139:HIS:HD2	2:D:146:GLY:O	1.85	0.60
2:B:282:GLN:CB	2:B:283:TYR:HA	2.33	0.59
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.38	0.59
2:B:139:HIS:HD2	2:B:146:GLY:O	1.86	0.59
2:B:295[B]:MET:HE2	2:B:315:VAL:HG11	1.86	0.58
1:C:339:ARG:H	1:C:339:ARG:HD3	1.68	0.58
2:D:1:MET:HA	2:D:1:MET:HE2	1.86	0.57
1:A:261:PRO:HG2	7:A:704:HOH:O	2.04	0.57
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.67	0.57
2:D:295[B]:MET:HE2	2:D:315:VAL:HG11	1.86	0.57
1:C:284:GLU:CB	1:C:285:GLN:HA	2.35	0.57
3:E:45:PRO:HG2	3:E:50:ILE:HD11	1.86	0.57
1:A:121:ARG:NH2	1:A:124:LYS:HD2	2.18	0.57
2:D:2:ARG:HG3	2:D:3:GLU:OE2	2.04	0.57
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.87	0.56
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.41	0.56
2:B:75:MET:HG3	2:B:94:PHE:HB3	1.85	0.56
3:E:83:ILE:O	3:E:87:ILE:HG12	2.06	0.56
1:A:36:MET:O	1:A:38:SER:N	2.39	0.56
1:A:204:VAL:HG11	1:A:231:ILE:HG12	1.86	0.56
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.87	0.56
1:A:265:ILE:HB	7:A:704:HOH:O	2.05	0.56
2:D:312:TYR:CE2	2:D:377[A]:PHE:HZ	2.24	0.55
2:B:296[B]:PHE:HB3	2:B:308:ARG:HE	1.71	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.42	0.55
2:D:296[B]:PHE:HB3	2:D:308:ARG:HE	1.71	0.55
1:A:90:GLU:O	1:A:121:ARG:HD2	2.07	0.55
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.90	0.54
1:C:313:MET:SD	1:C:435:VAL:CG1	2.95	0.54
2:D:75:MET:HE1	2:D:76:ASP:OD1	2.07	0.54
2:B:312:TYR:CE2	2:B:377[A]:PHE:HZ	2.26	0.54
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.54
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.73	0.54
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.90	0.53
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.89	0.53
1:A:159:VAL:HB	7:A:700:HOH:O	2.07	0.53
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.91	0.53
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLU:HG2	1:C:358:GLN:HE22	1.73	0.53
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.53
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.90	0.52
1:A:262:TYR:HB2	1:A:265:ILE:HD12	1.92	0.52
2:B:229:HIS:HE1	2:B:276:THR:HG23	1.75	0.51
2:B:405:LEU:HD21	2:B:415:GLU:HG2	1.91	0.51
2:D:164:ARG:NH1	7:D:692:HOH:O	2.37	0.51
2:D:284:ARG:HH22	2:D:290:GLU:CD	2.13	0.51
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.43	0.51
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.92	0.51
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.91	0.51
1:A:204:VAL:HG22	1:A:302[B]:MET:CE	2.41	0.51
1:A:40:LYS:O	1:A:41:THR:HB	2.11	0.51
2:B:139:HIS:HE1	2:B:170:SER:OG	1.94	0.50
2:D:2:ARG:HH11	2:D:2:ARG:HG2	1.75	0.50
1:C:54:SER:OG	1:C:62:VAL:HG13	2.12	0.50
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.94	0.50
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.94	0.50
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.47	0.50
2:B:100:GLY:HA2	1:C:254:GLU:HG3	1.93	0.50
2:D:317:THR:HG21	2:D:332:MET:CE	2.42	0.50
2:D:75:MET:CG	2:D:79:ARG:HH12	2.06	0.50
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.11	0.49
1:C:79:ARG:NH2	1:C:94:THR:OG1	2.41	0.49
2:D:133:GLN:HE22	2:D:252:LEU:H	1.60	0.49
2:D:183:GLU:OE2	4:D:600:GTP:H3'	2.13	0.49
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.94	0.49
1:C:313:MET:SD	1:C:435:VAL:HG11	2.52	0.49
2:D:11:GLN:HB2	7:D:612:HOH:O	2.12	0.49
2:B:11:GLN:HB2	7:B:612[A]:HOH:O	2.12	0.49
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.94	0.49
2:D:1:MET:HA	2:D:1:MET:CE	2.41	0.49
1:A:38:SER:C	1:A:40:LYS:H	2.16	0.49
2:B:206:ASN:ND2	4:B:600[A]:GTP:HN22	2.05	0.49
2:D:286:LEU:HD11	2:D:294[A]:GLN:NE2	2.27	0.48
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.95	0.48
1:A:88:HIS:H	1:A:91:GLN:NE2	2.11	0.48
3:E:13:LYS:HD3	3:E:18:GLN:HG3	1.96	0.48
2:B:319:PHE:HB2	2:B:355:VAL:HG22	1.96	0.48
2:D:281:GLN:CA	2:D:282:GLN:CB	2.92	0.48
2:D:286:LEU:HD11	2:D:294[A]:GLN:HE22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:HD2	7:A:704:HOH:O	2.14	0.48
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.44	0.48
2:D:139:HIS:CD2	2:D:146:GLY:O	2.64	0.48
1:C:250:VAL:HG23	1:C:254:GLU:HB3	1.96	0.47
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.96	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
1:A:37:PRO:C	1:A:39:ASP:N	2.66	0.47
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.95	0.47
1:A:434:GLU:O	1:A:437:VAL:HG22	2.15	0.47
1:C:204:VAL:HG11	1:C:231:ILE:HG12	1.97	0.47
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.97	0.47
2:B:309:HIS:CD2	2:B:386:GLU:OE1	2.62	0.47
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.50	0.47
2:B:317:THR:HG21	2:B:332:MET:CE	2.43	0.46
1:A:221:ARG:HG2	2:B:325:MET:HB3	1.98	0.46
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.97	0.46
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.63	0.46
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.96	0.46
1:A:329:ASN:ND2	3:E:20:TRP:HE1	2.03	0.46
2:D:119:LEU:O	2:D:123:ARG:HG3	2.16	0.46
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.64	0.46
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.46
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.64	0.46
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.97	0.46
1:A:121:ARG:HH21	1:A:124:LYS:CD	2.21	0.46
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.99	0.46
1:C:217:LEU:HD21	1:C:368:LEU:HD23	1.96	0.46
2:D:284:ARG:NH2	2:D:290:GLU:OE2	2.48	0.46
2:B:167:ASN:ND2	7:B:648:HOH:O	2.48	0.46
2:D:319:PHE:HB2	2:D:355:VAL:HG22	1.97	0.46
2:B:297[A]:ASP:HB3	2:B:300:ASN:HD22	1.81	0.45
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.98	0.45
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.98	0.45
2:D:106:GLY:O	2:D:111:GLY:HA3	2.16	0.45
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.51	0.45
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.99	0.45
2:D:108:TYR:O	3:E:134:ARG:HD3	2.16	0.45
1:A:204:VAL:HG22	1:A:302[B]:MET:HE2	1.99	0.45
2:B:100:GLY:HA3	1:C:253:THR:HG22	1.99	0.45
1:C:265:ILE:HD11	1:C:431:ASP:HB3	1.98	0.45
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.44
2:D:248:LEU:HD11	2:D:352:LYS:HB3	2.00	0.44
2:D:385:GLN:HE22	2:D:433:GLN:HE21	1.65	0.44
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.35	0.44
1:C:133:GLN:NE2	1:C:251:ASP:HB2	2.30	0.44
2:B:75:MET:HG3	2:B:94:PHE:CB	2.47	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
2:B:248:LEU:HD11	2:B:352:LYS:HB3	1.99	0.43
1:A:105:ARG:HG2	1:A:110:ILE:HD13	2.00	0.43
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.43
1:A:40:LYS:HD3	1:A:41:THR:H	1.83	0.43
1:A:292:THR:O	1:A:295:CYS:HB2	2.18	0.43
1:A:355:ILE:O	3:E:17:GLY:HA2	2.19	0.43
1:C:246:GLY:H	1:C:249:ASN:HD21	1.65	0.43
1:A:88:HIS:H	1:A:91:GLN:HE21	1.66	0.43
2:B:177:VAL:HG11	2:B:227:LEU:HD21	2.00	0.43
2:B:306:ASP:O	2:B:309:HIS:HB2	2.19	0.43
2:D:297[A]:ASP:HB3	2:D:300:ASN:HD22	1.83	0.42
1:C:139:HIS:HE1	1:C:168:GLU:OE1	2.01	0.42
2:D:2:ARG:HG3	2:D:3:GLU:H	1.84	0.42
1:A:437:VAL:HG23	1:A:438:ASP:H	1.85	0.42
2:B:50:ASN:O	2:B:64:ARG:NH2	2.39	0.42
1:A:5:ILE:HD13	1:A:64:ARG:HB3	2.02	0.42
1:A:320:ARG:HA	1:A:356:ASN:O	2.19	0.42
1:C:133:GLN:NE2	1:C:252:LEU:H	2.18	0.42
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:CB	2.49	0.42
1:C:347:CYS:C	1:C:349:THR:H	2.23	0.42
1:C:156:ARG:HD3	3:E:101:LEU:HD21	2.02	0.42
2:B:11:GLN:HA	2:B:74:THR:HG21	2.02	0.41
1:A:2:ARG:HB2	1:A:133:GLN:CD	2.40	0.41
2:B:286:LEU:HD13	2:B:290:GLU:HB3	2.02	0.41
1:C:141:PHE:O	1:C:147:SER:HB3	2.20	0.41
2:B:385:GLN:HE22	2:B:433:GLN:HE21	1.66	0.41
2:B:180:THR:HG23	2:B:183:GLU:HG3	2.02	0.41
1:C:97:GLU:OE2	2:D:1:MET:CE	2.68	0.41
2:D:72:PRO:O	2:D:75:MET:HB3	2.20	0.41
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.61	0.41
1:A:244:PHE:CD2	1:A:358:GLN:HG3	2.56	0.41
2:B:67:LEU:CD2	2:B:78:VAL:HG11	2.51	0.41
2:B:274:PRO:HD2	2:B:371:LEU:HD13	2.03	0.41
1:A:330:ALA:O	1:A:334:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:HA	1:C:94:THR:HG21	2.03	0.41
2:D:11:GLN:HA	2:D:74:THR:HG21	2.01	0.41
1:C:79:ARG:H	1:C:79:ARG:HG2	1.73	0.41
1:C:88:HIS:H	1:C:91:GLN:NE2	2.19	0.41
2:B:12:CYS:HB2	4:B:600[A]:GTP:C8	2.56	0.41
2:B:401:ARG:HD3	1:C:439:SER:HB3	2.03	0.41
2:D:158:ARG:NH2	7:D:661:HOH:O	2.54	0.40
3:E:43:ARG:HA	3:E:44:ASP:HA	1.94	0.40
2:B:274:PRO:HB3	2:B:286:LEU:HG	2.03	0.40
1:C:247:ALA:HB3	1:C:355:ILE:HB	2.03	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	432/451 (96%)	414 (96%)	14 (3%)	4 (1%)	17	30
1	C	427/451 (95%)	408 (96%)	15 (4%)	4 (1%)	17	30
2	B	437/445 (98%)	415 (95%)	18 (4%)	4 (1%)	17	30
2	D	437/445 (98%)	421 (96%)	12 (3%)	4 (1%)	17	30
3	E	132/143 (92%)	125 (95%)	5 (4%)	2 (2%)	10	17
All	All	1865/1935 (96%)	1783 (96%)	64 (3%)	18 (1%)	15	27

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	437	VAL
1	C	47	ASP
1	C	283	HIS

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Mol	Chain	Res	Type
1	C	349	THR
2	D	282	GLN
3	E	32	VAL
2	B	286	LEU
1	C	350	GLY
2	D	59	ASN
2	B	282	GLN
1	A	39	ASP
2	B	284	ARG
2	D	284	ARG
3	E	44	ASP
2	D	279	GLY
1	A	37	PRO
2	B	177	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	369/379 (97%)	353 (96%)	16 (4%)	29	50
1	C	359/379 (95%)	343 (96%)	16 (4%)	27	48
2	B	378/385 (98%)	357 (94%)	21 (6%)	21	38
2	D	380/385 (99%)	359 (94%)	21 (6%)	21	39
3	E	108/125 (86%)	101 (94%)	7 (6%)	17	31
All	All	1594/1653 (96%)	1513 (95%)	81 (5%)	24	43

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	40	LYS
1	A	56	THR
1	A	79	ARG
1	A	84	ARG

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Mol	Chain	Res	Type
1	A	105	ARG
1	A	121	ARG
1	A	163	LYS
1	A	177	VAL
1	A	179	THR
1	A	215	ARG
1	A	250	VAL
1	A	320	ARG
1	A	342	GLN
1	A	345	ASP
1	A	435	VAL
2	B	110	GLU
2	B	115	VAL
2	B	122	VAL
2	B	124	LYS
2	B	128	SER
2	B	153	LEU
2	B	179	ASP
2	B	207	GLU
2	B	295[A]	MET
2	B	295[B]	MET
2	B	298	SER
2	B	309	HIS
2	B	335	ILE
2	B	338	LYS
2	B	340	SER
2	B	341	SER
2	B	345	GLU
2	B	357	ASP
2	B	374	SER
2	B	423	SER
2	B	439	THR
1	C	1	MET
1	C	71	GLU
1	C	79	ARG
1	C	84	ARG
1	C	164	LYS
1	C	179	THR
1	C	241	SER
1	C	250	VAL
1	C	324	VAL
1	C	334	THR

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Mol	Chain	Res	Type
1	C	339	ARG
1	C	347	CYS
1	C	358	GLN
1	C	430	LYS
1	C	435	VAL
1	C	438	ASP
2	D	64	ARG
2	D	75	MET
2	D	110	GLU
2	D	115	VAL
2	D	122	VAL
2	D	128	SER
2	D	153	LEU
2	D	155	SER
2	D	158	ARG
2	D	160	GLU
2	D	207	GLU
2	D	286	LEU
2	D	295[A]	MET
2	D	295[B]	MET
2	D	335	ILE
2	D	340	SER
2	D	357	ASP
2	D	371	LEU
2	D	374	SER
2	D	423	SER
2	D	439	THR
3	E	15	THR
3	E	25	LYS
3	E	46	SER
3	E	107	SER
3	E	127	ASP
3	E	137	LYS
3	E	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	91	GLN
1	A	139	HIS

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Mol	Chain	Res	Type
1	A	197	HIS
1	A	249	ASN
1	A	258	ASN
1	A	301	GLN
1	A	329	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	101	ASN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	247	GLN
2	B	266	HIS
2	B	309	HIS
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	11	GLN
1	C	50	ASN
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
1	C	329	ASN
1	C	356	ASN
1	C	358	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	206	ASN
2	D	247	GLN
2	D	266	HIS
2	D	300	ASN
2	D	385	GLN

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Mol	Chain	Res	Type
2	D	433	GLN
2	D	436	GLN
3	E	111	ASN
3	E	124	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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
6	SO4	C	453	-	4,4,4	0.29	0	6,6,6	0.16	0
4	GTP	B	600[B]	-	24,30,34	1.24	3 (12%)	30,47,54	1.63	5 (16%)
4	GTP	A	600	5	26,34,34	1.42	4 (15%)	32,54,54	1.26	4 (12%)
6	SO4	C	452	-	4,4,4	0.35	0	6,6,6	0.14	0
6	SO4	D	457	-	4,4,4	0.40	0	6,6,6	0.15	0
4	GTP	B	600[A]	5	26,34,34	1.24	3 (11%)	32,54,54	1.70	5 (15%)
6	SO4	A	454	-	4,4,4	0.33	0	6,6,6	0.09	0
4	GTP	D	600	5	26,34,34	1.17	1 (3%)	32,54,54	1.69	7 (21%)
4	GTP	C	600	5	26,34,34	1.36	4 (15%)	32,54,54	1.27	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	B	456	-	4,4,4	0.33	0	6,6,6	0.38	0
6	SO4	C	454	-	4,4,4	0.16	0	6,6,6	0.27	0
6	SO4	D	456	-	4,4,4	0.40	0	6,6,6	0.18	0
6	SO4	E	146	-	4,4,4	0.31	0	6,6,6	0.17	0
6	SO4	A	455	-	4,4,4	0.08	0	6,6,6	0.15	0
6	SO4	A	452	-	4,4,4	0.42	0	6,6,6	0.22	0
6	SO4	A	453	-	4,4,4	0.33	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	B	600[B]	-	-	7/12/32/38	0/3/3/3
4	GTP	A	600	5	-	8/18/38/38	0/3/3/3
4	GTP	B	600[A]	5	-	5/18/38/38	0/3/3/3
4	GTP	D	600	5	-	7/18/38/38	0/3/3/3
4	GTP	C	600	5	-	5/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	O4'-C1'	3.60	1.46	1.41
4	A	600	GTP	C8-N7	-3.04	1.29	1.35
4	C	600	GTP	C8-N7	-2.99	1.29	1.35
4	B	600[B]	GTP	C6-N1	2.93	1.42	1.37
4	A	600	GTP	O4'-C4'	2.78	1.51	1.45
4	B	600[A]	GTP	C8-N7	-2.75	1.30	1.35
4	B	600[B]	GTP	C5-C6	-2.72	1.41	1.47
4	D	600	GTP	C8-N7	-2.60	1.30	1.35
4	B	600[B]	GTP	C8-N7	-2.53	1.30	1.35
4	B	600[A]	GTP	C5-C6	-2.28	1.42	1.47
4	C	600	GTP	PA-O2A	2.27	1.66	1.55
4	C	600	GTP	O4'-C1'	2.26	1.44	1.41
4	B	600[A]	GTP	O4'-C1'	2.22	1.44	1.41
4	C	600	GTP	C2'-C1'	2.08	1.56	1.53
4	A	600	GTP	PA-O5'	2.07	1.67	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	600	GTP	PA-O3A-PB	-4.88	116.06	132.83
4	B	600[A]	GTP	PB-O3B-PG	-4.77	116.45	132.83
4	B	600[A]	GTP	PA-O3A-PB	-4.44	117.59	132.83
4	B	600[B]	GTP	PA-O3A-PB	-4.35	117.89	132.83
4	D	600	GTP	PB-O3B-PG	-3.83	119.67	132.83
4	B	600[A]	GTP	C8-N7-C5	3.46	109.57	102.99
4	B	600[B]	GTP	C8-N7-C5	3.28	109.24	102.99
4	C	600	GTP	C8-N7-C5	3.14	108.98	102.99
4	B	600[B]	GTP	O2B-PB-O3A	2.95	114.54	104.64
4	C	600	GTP	PB-O3B-PG	-2.93	122.78	132.83
4	A	600	GTP	C8-N7-C5	2.84	108.39	102.99
4	D	600	GTP	C8-N7-C5	2.75	108.23	102.99
4	A	600	GTP	PA-O3A-PB	-2.70	123.55	132.83
4	A	600	GTP	PB-O3B-PG	-2.56	124.04	132.83
4	B	600[A]	GTP	O2G-PG-O3B	2.52	113.08	104.64
4	B	600[B]	GTP	O6-C6-C5	-2.49	119.52	124.37
4	C	600	GTP	PA-O3A-PB	-2.44	124.47	132.83
4	D	600	GTP	O5'-C5'-C4'	-2.37	100.83	108.99
4	B	600[B]	GTP	O5'-C5'-C4'	-2.27	101.17	108.99
4	D	600	GTP	N2-C2-N3	2.26	124.14	119.74
4	A	600	GTP	O6-C6-N1	-2.22	118.03	120.65
4	D	600	GTP	O4'-C4'-C3'	-2.07	101.02	105.11
4	B	600[A]	GTP	O3G-PG-O3B	2.05	111.50	104.64
4	D	600	GTP	O5'-PA-O1A	2.02	116.94	109.07

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O1A
4	A	600	GTP	C5'-O5'-PA-O2A
4	B	600[B]	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
4	B	600[A]	GTP	PB-O3B-PG-O1G
4	D	600	GTP	PB-O3B-PG-O1G
4	B	600[A]	GTP	PB-O3B-PG-O2G
4	B	600[B]	GTP	PA-O3A-PB-O3B
4	B	600[B]	GTP	C5'-O5'-PA-O3A
4	D	600	GTP	C5'-O5'-PA-O3A
4	B	600[A]	GTP	C5'-O5'-PA-O2A
4	B	600[B]	GTP	C5'-O5'-PA-O2A
4	D	600	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	D	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3A-PA-O2A
4	B	600[B]	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
4	A	600	GTP	PB-O3B-PG-O1G
4	B	600[A]	GTP	PB-O3A-PA-O2A
4	B	600[B]	GTP	C4'-C5'-O5'-PA
4	D	600	GTP	PB-O3A-PA-O2A
4	A	600	GTP	PB-O3B-PG-O2G
4	A	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	PB-O3B-PG-O3G
4	D	600	GTP	PB-O3B-PG-O2G
4	D	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	C5'-O5'-PA-O3A
4	B	600[A]	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	PB-O3A-PA-O1A
4	B	600[B]	GTP	PB-O3A-PA-O1A

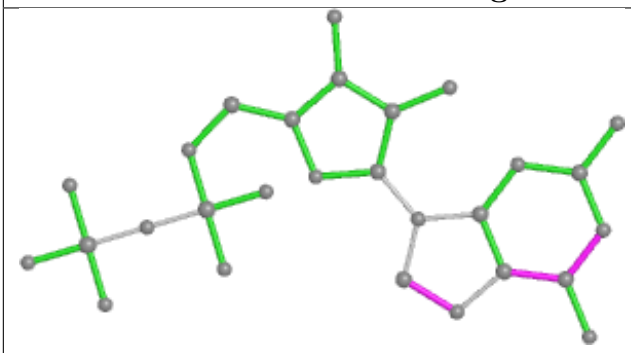
There are no ring outliers.

3 monomers are involved in 6 short contacts:

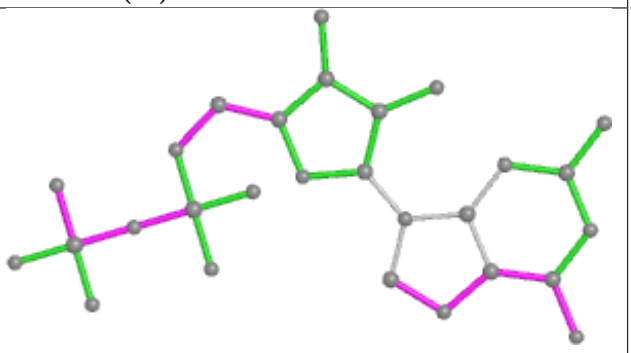
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600[B]	GTP	1	0
4	B	600[A]	GTP	3	0
4	D	600	GTP	2	0

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.

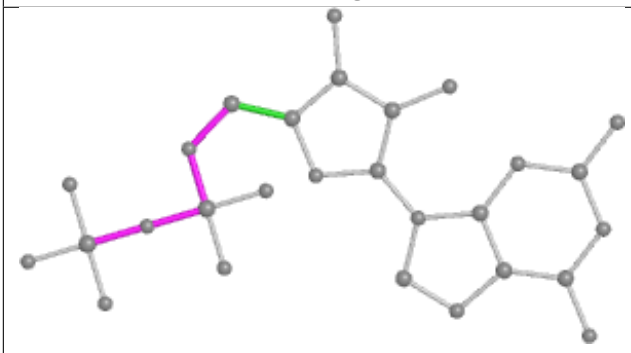
Ligand GTP B 600 (B)



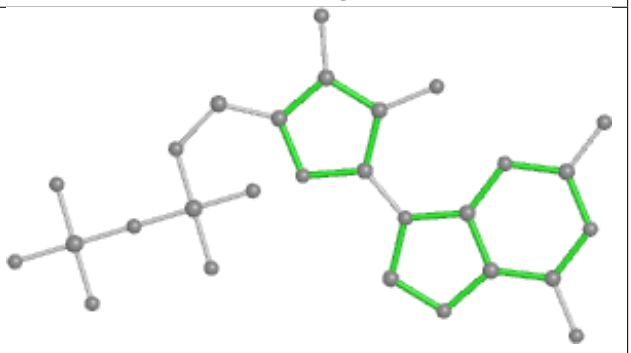
Bond lengths



Bond angles

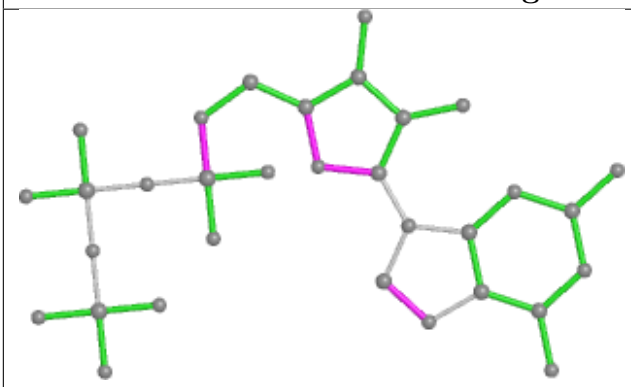


Torsions

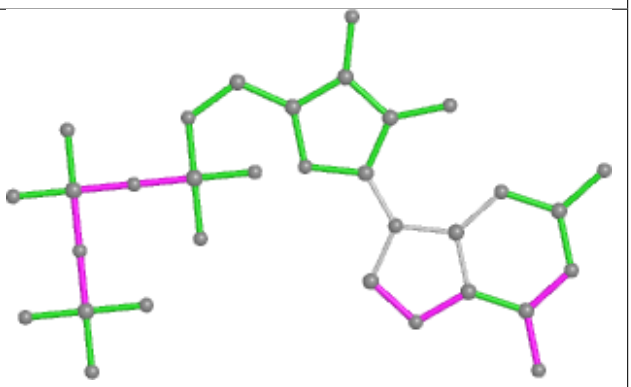


Rings

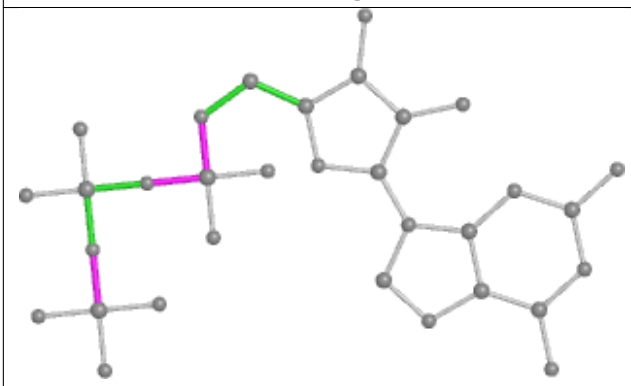
Ligand GTP A 600



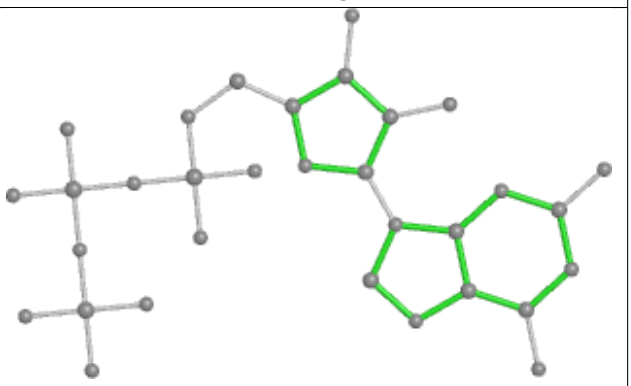
Bond lengths



Bond angles

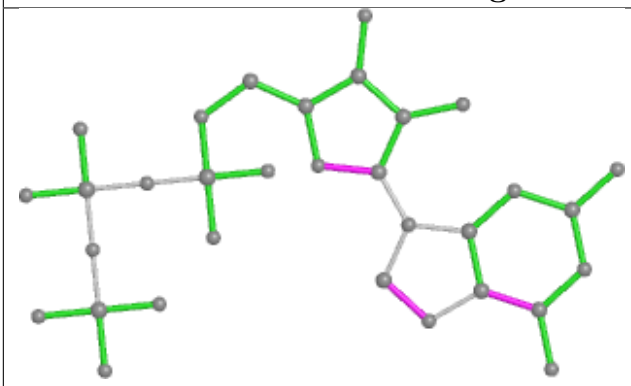


Torsions

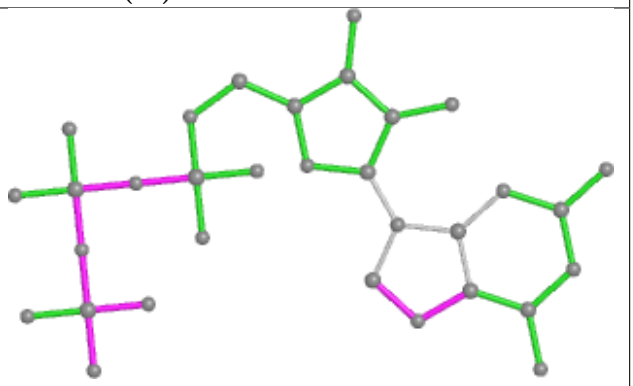


Rings

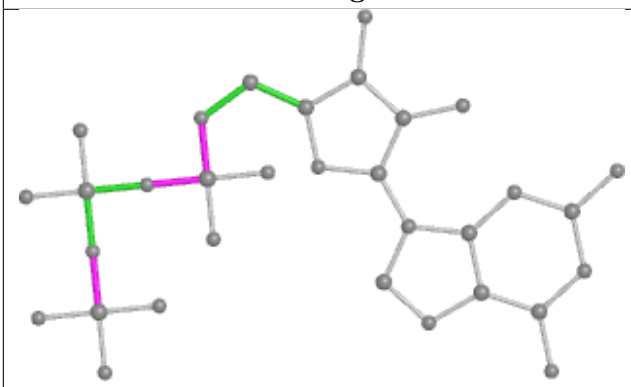
Ligand GTP B 600 (A)



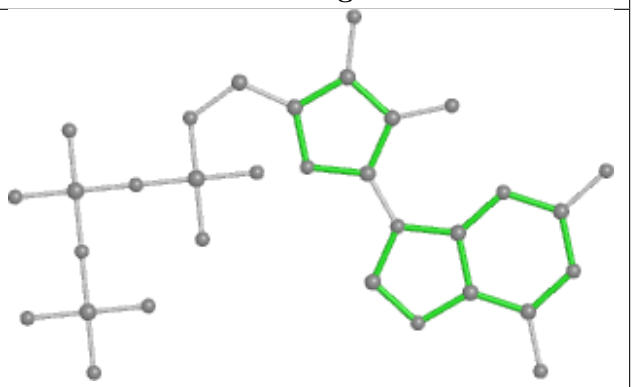
Bond lengths



Bond angles

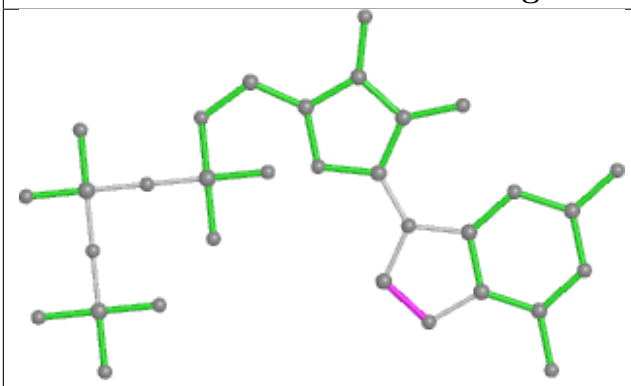


Torsions

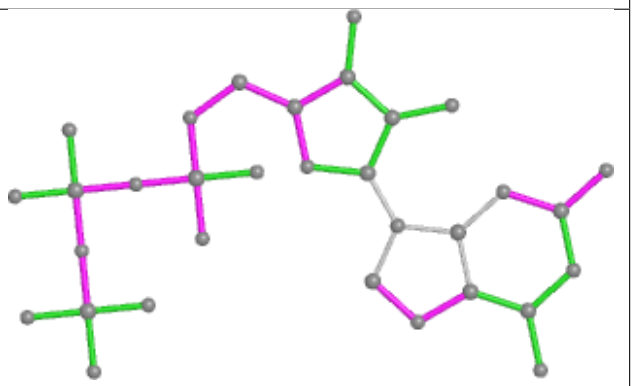


Rings

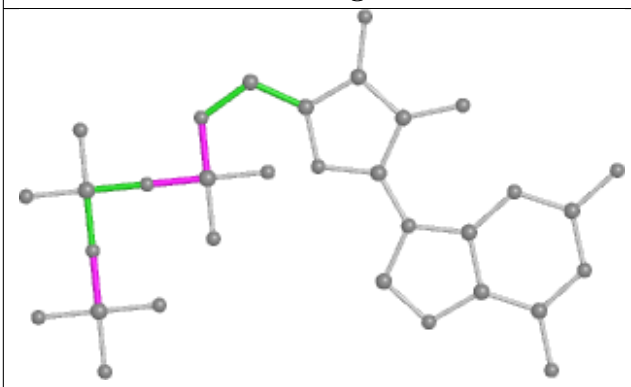
Ligand GTP D 600



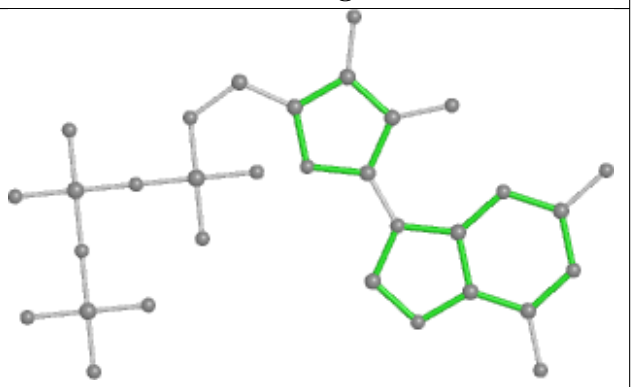
Bond lengths



Bond angles

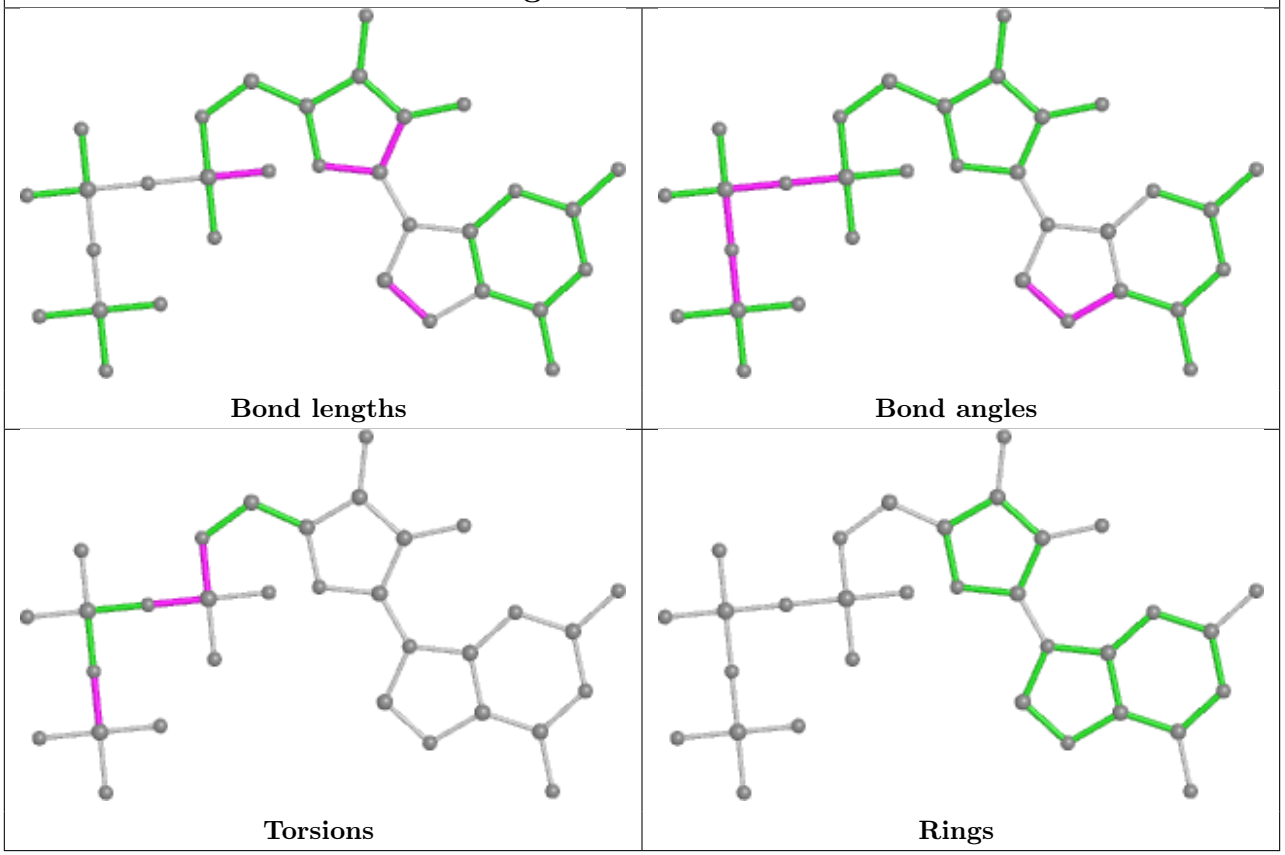


Torsions



Rings

Ligand GTP C 600



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	435/451 (96%)	-0.02	15 (3%)	45	49	44, 65, 95, 143	0
1	C	431/451 (95%)	0.37	35 (8%)	12	12	44, 69, 107, 140	0
2	B	432/445 (97%)	0.29	31 (7%)	15	16	43, 66, 119, 186	4 (0%)
2	D	431/445 (96%)	0.09	17 (3%)	39	43	40, 60, 104, 132	4 (0%)
3	E	136/143 (95%)	0.79	20 (14%)	2	2	62, 84, 129, 154	0
All	All	1865/1935 (96%)	0.23	118 (6%)	20	21	40, 67, 111, 186	8 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	32	VAL	11.3
1	A	38	SER	8.0
1	C	283	HIS	7.4
3	E	33	PRO	7.0
2	D	283	TYR	6.7
1	C	284	GLU	6.6
1	A	346	TRP	6.2
2	B	283	TYR	5.8
3	E	4	ALA	5.6
1	A	282	TYR	5.5
3	E	31	GLY	5.5
2	B	442	GLU	5.0
3	E	41	ARG	4.9
1	A	41	THR	4.7
2	D	59	ASN	4.7
2	D	284	ARG	4.6
2	D	75	MET	4.5
2	D	56	ALA	4.4
1	C	439	SER	4.4
1	C	281	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	36	TYR	4.2
2	B	39	ASP	4.1
2	B	371	LEU	4.1
2	D	39	ASP	4.0
1	C	282	TYR	4.0
1	A	437	VAL	4.0
2	B	279	GLY	4.0
2	B	57	THR	4.0
2	B	37	HIS	4.0
2	B	59	ASN	3.9
1	A	438	ASP	3.9
1	C	276	ILE	3.8
1	A	39	ASP	3.8
1	C	57	GLY	3.7
2	D	96	GLN	3.7
3	E	45	PRO	3.7
2	D	416	MET	3.6
2	D	58	GLY	3.5
2	B	369	ARG	3.5
1	C	217	LEU	3.4
2	B	284	ARG	3.4
2	B	321	GLY	3.3
3	E	5	ASP	3.3
2	B	33	THR	3.2
2	B	42	LEU	3.2
2	B	32	PRO	3.1
3	E	42	ARG	3.1
1	C	56	THR	3.1
2	B	86	ILE	3.0
1	C	357	TYR	3.0
2	B	282	GLN	3.0
1	C	215	ARG	3.0
1	A	281	ALA	3.0
1	C	324	VAL	2.9
2	D	57	THR	2.9
2	D	85	GLN	2.9
2	B	285	ALA	2.9
2	B	286	LEU	2.8
1	C	58	ALA	2.8
3	E	24	LEU	2.8
1	A	262	TYR	2.8
2	B	82	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	200	CYS	2.7
3	E	63	TYR	2.7
2	B	126	SER	2.7
3	E	9	ILE	2.7
1	C	438	ASP	2.7
3	E	29	PHE	2.6
1	C	278	ALA	2.6
1	C	85	GLN	2.6
1	C	250	VAL	2.6
2	D	285	ALA	2.6
1	C	286	LEU	2.6
1	A	435	VAL	2.5
1	A	40	LYS	2.5
3	E	30	ASP	2.5
1	C	255	PHE	2.5
1	C	285	GLN	2.5
3	E	99	GLU	2.5
1	C	84	ARG	2.5
1	C	36	MET	2.5
2	D	78	VAL	2.4
3	E	51	GLN	2.4
2	B	61	TYR	2.4
2	B	293[A]	GLN	2.4
2	B	277	SER	2.4
3	E	100	LYS	2.4
2	D	55	GLU	2.4
2	D	84	GLY	2.3
1	C	199	ASP	2.3
1	C	323	VAL	2.3
1	A	80	THR	2.3
1	C	254	GLU	2.3
1	C	437	VAL	2.3
1	C	277	SER	2.3
2	B	38	GLY	2.3
1	C	143	GLY	2.2
3	E	28	SER	2.2
3	E	96	MET	2.2
1	C	201	ALA	2.2
2	B	372	LYS	2.2
3	E	145	ARG	2.2
2	B	441	ASP	2.2
2	B	56	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	86	ILE	2.1
3	E	34	GLU	2.1
2	B	85	GLN	2.1
2	D	286	LEU	2.1
1	A	45	GLY	2.1
1	C	299	ALA	2.1
2	B	60	LYS	2.1
1	C	248	LEU	2.1
1	A	326	LYS	2.1
1	A	37	PRO	2.0
2	B	281	GLN	2.0
1	C	123	ARG	2.0
1	C	251	ASP	2.0
1	C	202	PHE	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
6	SO4	C	453	5/5	0.75	0.21	154,158,158,159	0
6	SO4	A	455	5/5	0.78	0.28	151,155,156,157	0
6	SO4	B	456	5/5	0.89	0.16	108,112,113,114	0
6	SO4	A	454	5/5	0.89	0.25	134,139,139,140	0
6	SO4	C	454	5/5	0.91	0.26	131,136,136,137	0
6	SO4	E	146	5/5	0.91	0.17	118,122,123,124	0
6	SO4	A	453	5/5	0.93	0.15	105,110,110,111	0
5	MG	B	601[A]	1/1	0.95	0.20	84,84,84,84	1
6	SO4	D	457	5/5	0.96	0.10	107,111,112,112	0

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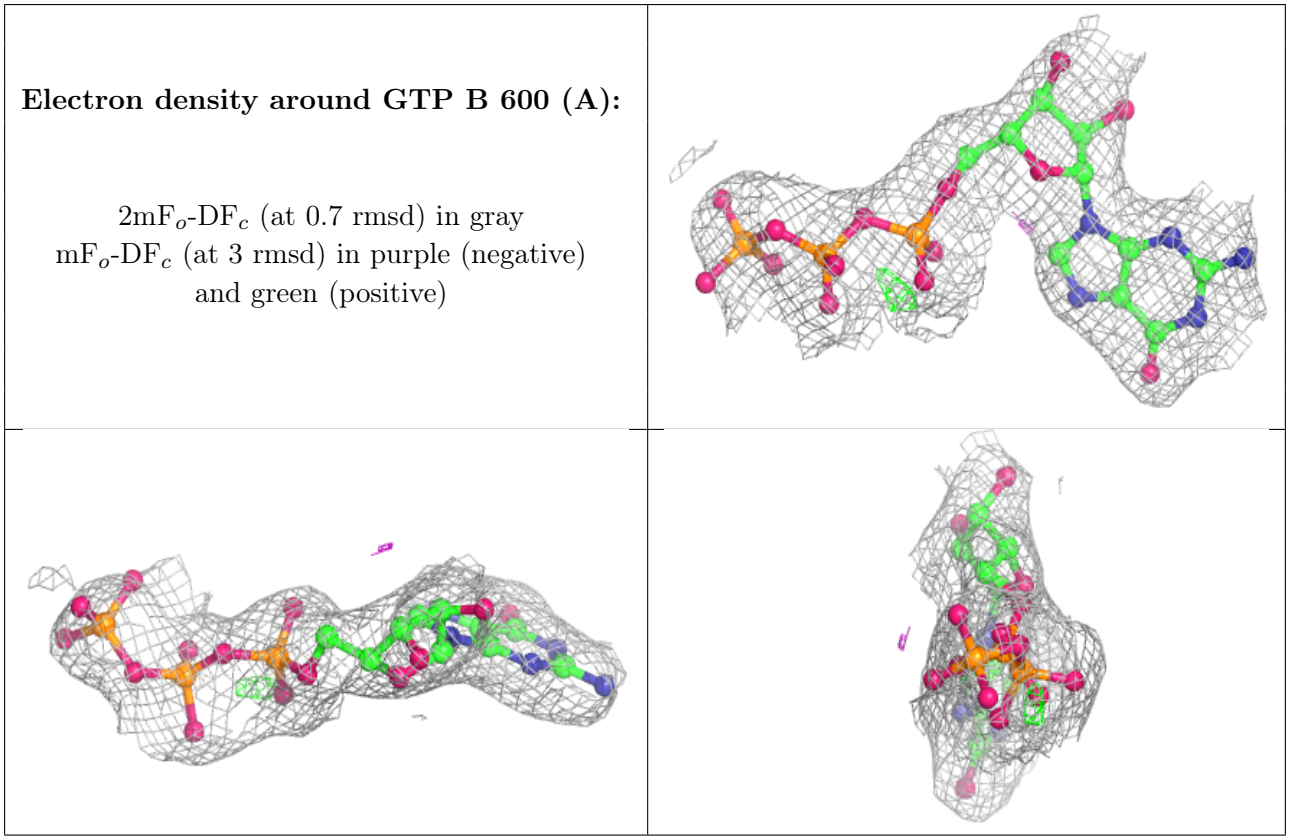
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	452	5/5	0.97	0.09	94,98,99,101	0
6	SO4	D	456	5/5	0.97	0.09	83,88,89,90	0
6	SO4	C	452	5/5	0.97	0.09	97,101,103,103	0
5	MG	A	601	1/1	0.97	0.18	48,48,48,48	0
4	GTP	B	600[A]	32/32	0.98	0.20	75,78,82,85	32
4	GTP	B	600[B]	28/32	0.98	0.20	30,32,36,37	28
5	MG	C	601	1/1	0.98	0.12	47,47,47,47	0
5	MG	D	601	1/1	0.98	0.06	63,63,63,63	0
4	GTP	D	600	32/32	0.98	0.11	46,51,61,62	0
4	GTP	A	600	32/32	0.99	0.20	47,49,53,55	0
4	GTP	C	600	32/32	0.99	0.16	48,55,59,61	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.

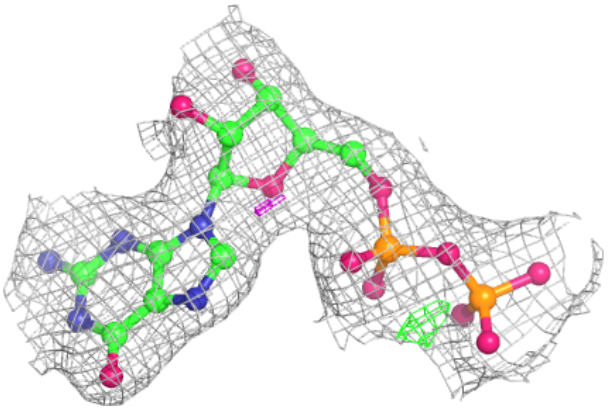
Electron density around GTP B 600 (A):

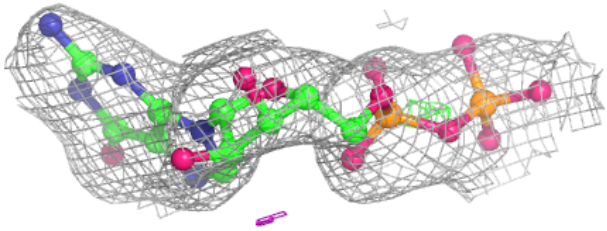
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

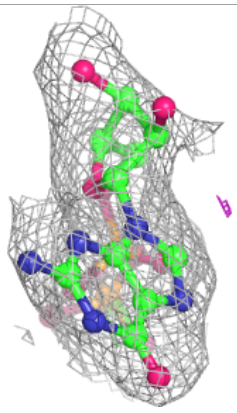


Electron density around GTP B 600 (B):

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

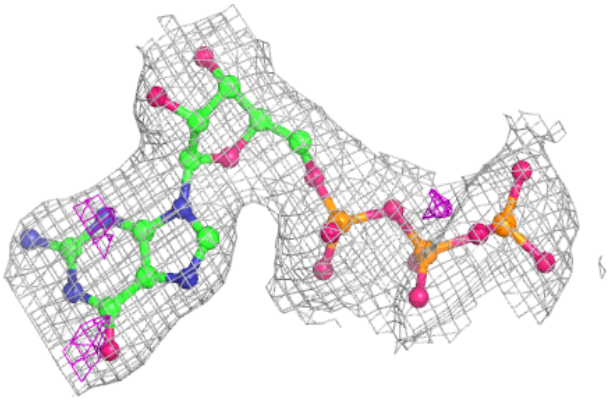


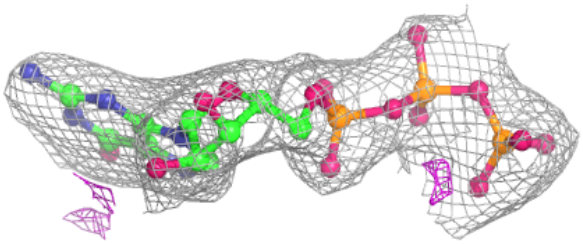


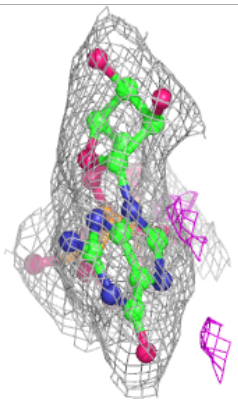


Electron density around GTP D 600:

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

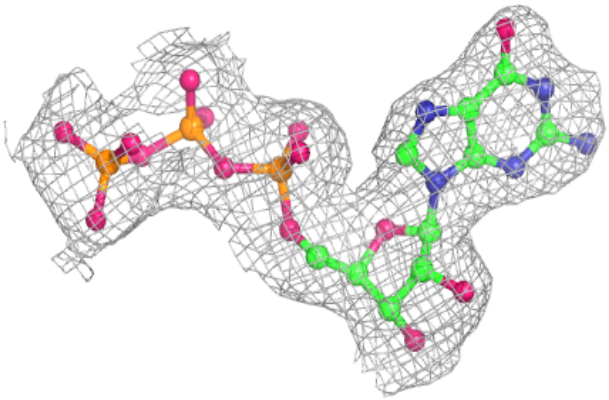


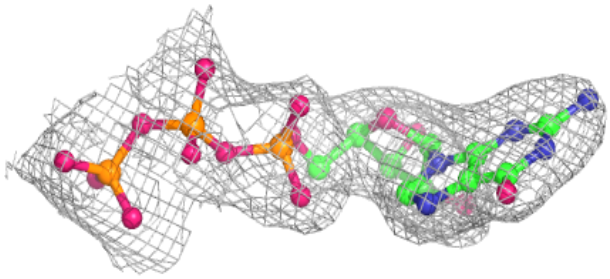


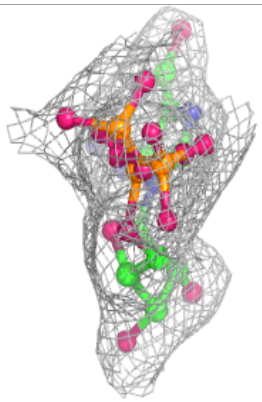


Electron density around GTP A 600:

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

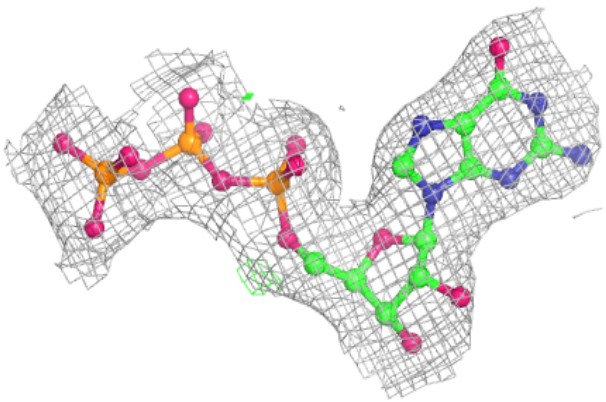


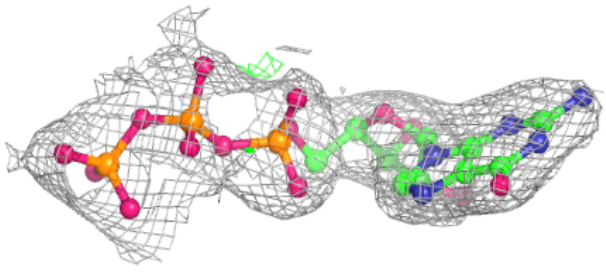


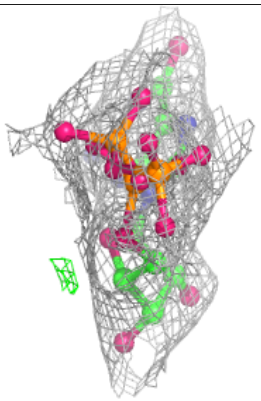


Electron density around GTP C 600:

$2mF_o$-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.