



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:42 PM UTC

PDB ID : 3RYC / pdb_00003ryc
Title : Tubulin: RB3 stathmin-like domain complex
Authors : Nawrotek, A.; Knossow, M.; Gigant, B.
Deposited on : 2011-05-11
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

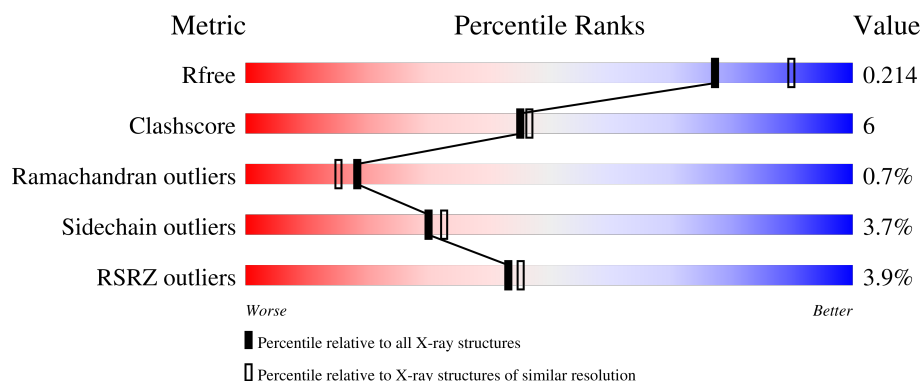
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	451	3% 80% 15% ..
1	C	451	5% 79% 15% ..
2	B	445	3% 79% 16% ..
2	D	445	2% 83% 12% ..
3	E	143	10% 78% 14% .. 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15686 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	431	Total	C	N	O	S	0	2	0
			3394	2150	576	645	23			
1	C	431	Total	C	N	O	S	0	4	0
			3366	2133	570	638	25			

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	10	0
			3445	2161	588	670	26			

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

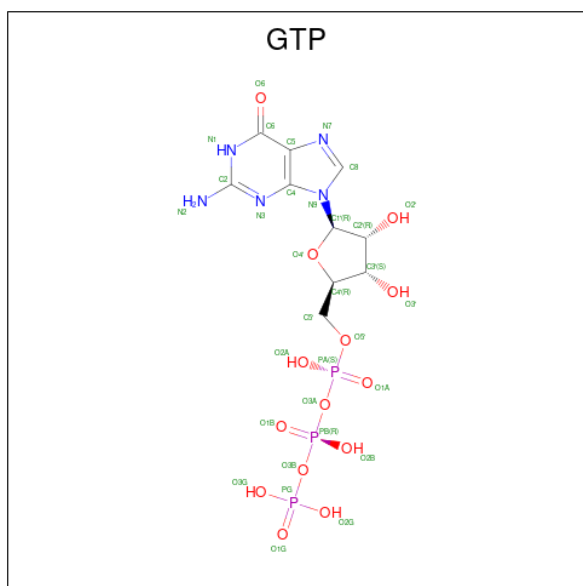
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	136	Total	C	N	O	S	0	0	0
			1096	677	200	215	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 (CCD ID: 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	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	1
			60	20	10	25	5		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	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	D	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	E	1	Total O S 5 4 1	0	0

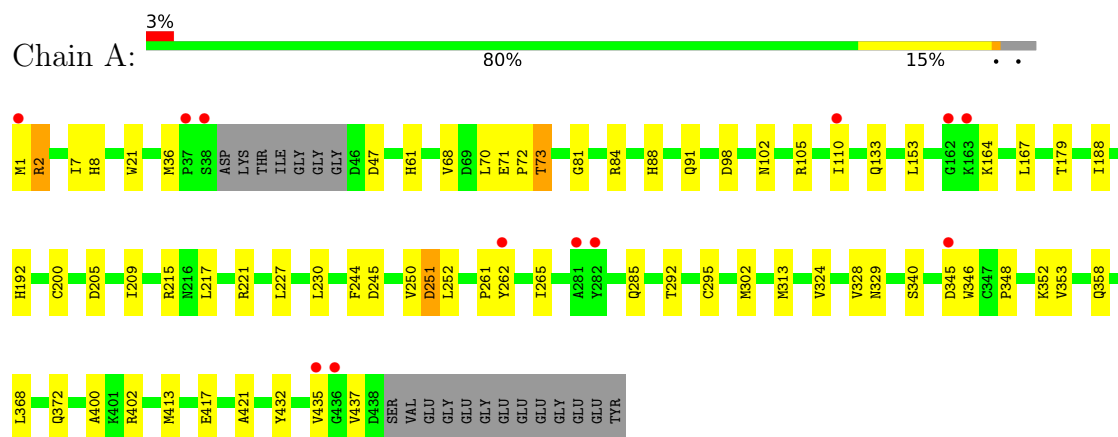
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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including an amino group at the 2-position and a carbonyl group at the 6-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group being the terminal one. The structure is labeled with various atoms and bonds, including the guanine base (N1, N2, N3, N7, C2, C4, C5, C6, C8), the ribose sugar (C1', C2', C3', C4', C5'), and the phosphate groups (P1, P2, O1A, O1B, O2A, O2B, O3A, O3B, O4A, O4B, O5A, O5B). The overall structure is shown in a 3D perspective view.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	221	Total O 221 221	0	0
8	B	146	Total O 147 147	0	1
8	C	146	Total O 146 146	0	0
8	D	182	Total O 186 186	0	4
8	E	32	Total O 32 32	0	0

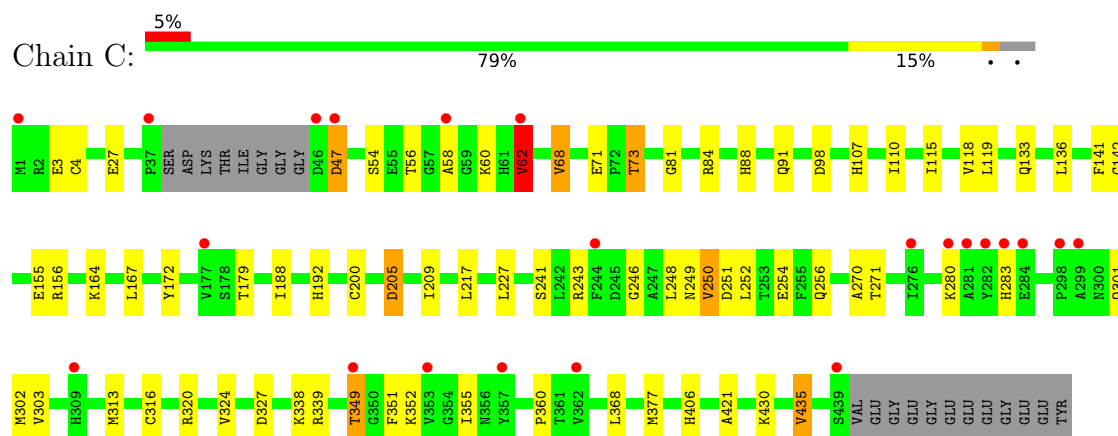
3 Residue-property plots [i](#)

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.

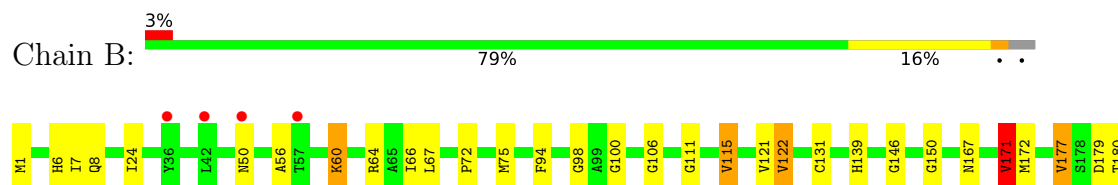
• Molecule 1: Tubulin alpha chain

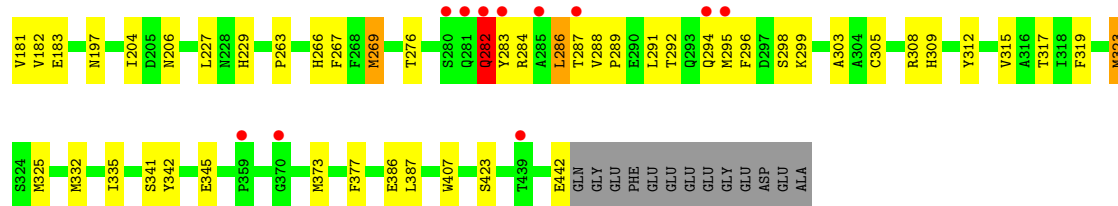


• Molecule 1: Tubulin alpha chain

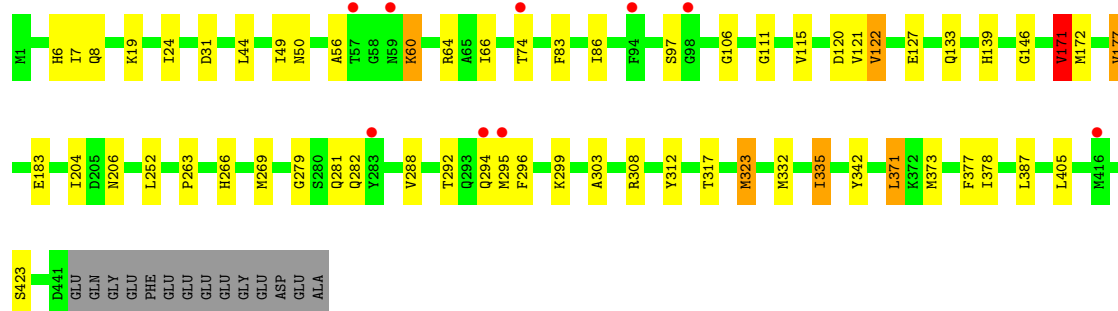
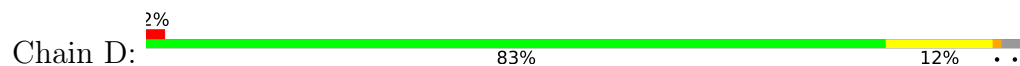


• Molecule 2: Tubulin beta chain

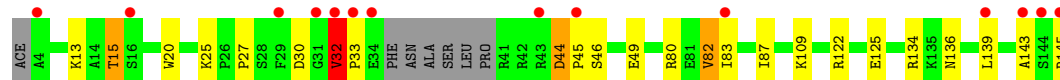
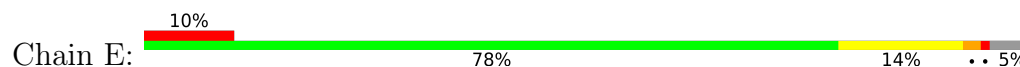




• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.45Å 127.24Å 250.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.14 – 2.10 43.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.14-2.10) 95.0 (43.14-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.171 , 0.201 0.183 , 0.214	Depositor DCC
R_{free} test set	5924 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15686	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, SO4, MG, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.83	1/3474 (0.0%)	1.24	7/4715 (0.1%)
1	C	0.85	0/3453	1.30	17/4689 (0.4%)
2	B	0.84	1/3531 (0.0%)	1.27	14/4782 (0.3%)
2	D	0.84	0/3543	1.29	18/4797 (0.4%)
3	E	0.84	0/1107	1.45	6/1475 (0.4%)
All	All	0.84	2/15108 (0.0%)	1.29	62/20458 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	269	MET	SD-CE	-6.84	1.62	1.79
1	A	340	SER	CB-OG	5.79	1.53	1.42

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	281	GLN	CA-C-N	8.56	137.12	121.70
2	D	281	GLN	C-N-CA	8.56	137.12	121.70
2	B	171	VAL	N-CA-CB	7.07	119.06	111.00
2	D	171	VAL	N-CA-CB	6.99	118.97	111.00
3	E	82	VAL	N-CA-CB	6.88	120.91	110.58
2	B	282	GLN	CA-C-N	6.67	133.71	121.70
2	B	282	GLN	C-N-CA	6.67	133.71	121.70
2	D	122	VAL	N-CA-CB	6.63	120.53	110.58
1	C	205	ASP	CA-CB-CG	6.55	119.15	112.60
2	B	179	ASP	CA-CB-CG	6.38	118.98	112.60
2	D	97	SER	N-CA-C	6.32	119.11	111.40
1	C	338	LYS	CA-C-N	6.21	128.89	120.38
1	C	338	LYS	C-N-CA	6.21	128.89	120.38
2	D	371	LEU	CD1-CG-CD2	6.11	124.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	120	ASP	CA-CB-CG	6.04	118.64	112.60
2	D	177	VAL	CB-CA-C	5.99	116.33	111.06
1	C	351	PHE	N-CA-C	5.98	118.99	109.24
1	C	250	VAL	CB-CA-C	5.88	117.11	110.41
1	C	142	GLY	N-CA-C	5.88	122.68	113.86
2	B	60	LYS	N-CA-C	5.87	119.48	110.20
1	C	110	ILE	CA-C-N	5.86	126.49	119.98
1	C	110	ILE	C-N-CA	5.86	126.49	119.98
2	D	60	LYS	N-CA-C	5.80	119.36	110.20
2	D	171	VAL	CB-CA-C	5.59	117.73	110.96
1	A	81	GLY	CA-C-N	5.59	128.04	120.38
1	A	81	GLY	C-N-CA	5.59	128.04	120.38
1	A	73	THR	N-CA-C	5.58	117.80	111.11
1	A	102	ASN	CA-CB-CG	5.54	118.14	112.60
2	D	74	THR	CA-C-N	5.52	127.61	120.44
2	D	74	THR	C-N-CA	5.52	127.61	120.44
1	C	81	GLY	CA-C-N	5.45	127.85	120.38
1	C	81	GLY	C-N-CA	5.45	127.85	120.38
2	B	171	VAL	CB-CA-C	5.42	117.51	110.96
2	D	378	ILE	CA-C-N	-5.42	118.38	122.33
2	D	378	ILE	C-N-CA	-5.42	118.38	122.33
1	A	251	ASP	CA-CB-CG	5.41	118.01	112.60
1	C	73	THR	N-CA-C	5.41	117.60	111.11
1	A	352	LYS	N-CA-C	-5.39	99.95	108.73
2	D	127	GLU	CB-CG-CD	5.36	121.71	112.60
1	C	115	ILE	N-CA-C	5.32	115.95	110.36
3	E	30	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	122	VAL	N-CA-CB	5.26	120.30	110.77
1	C	141	PHE	CA-C-N	5.26	126.97	120.34
1	C	141	PHE	C-N-CA	5.26	126.97	120.34
2	B	267	PHE	CA-CB-CG	-5.25	108.55	113.80
1	C	47	ASP	CA-CB-CG	5.23	117.83	112.60
2	D	7	ILE	CA-C-N	5.16	130.61	123.07
2	D	7	ILE	C-N-CA	5.16	130.61	123.07
2	B	7	ILE	CA-C-N	5.16	130.60	123.07
2	B	7	ILE	C-N-CA	5.16	130.60	123.07
2	B	115	VAL	N-CA-C	5.15	116.49	110.62
1	C	327	ASP	CA-CB-CG	5.14	117.75	112.60
1	C	62	VAL	N-CA-C	5.13	113.58	107.73
2	D	31	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	197	ASN	N-CA-C	5.09	120.33	113.72
2	B	72	PRO	CA-C-N	5.07	125.70	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	PRO	C-N-CA	5.07	125.70	120.03
1	A	205	ASP	CA-CB-CG	5.06	117.66	112.60
3	E	109	LYS	CA-C-N	5.05	127.00	120.44
3	E	109	LYS	C-N-CA	5.05	127.00	120.44
3	E	143	ALA	CA-C-N	5.03	131.15	121.54
3	E	143	ALA	C-N-CA	5.03	131.15	121.54

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	3394	0	3306	41	0
1	C	3366	0	3279	38	0
2	B	3443	0	3293	52	0
2	D	3445	0	3305	43	0
3	E	1096	0	1091	10	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	D	60	0	24	5	0
5	A	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	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
7	B	28	0	12	2	0
8	A	221	0	0	2	0
8	B	147	0	0	1	0
8	C	146	0	0	0	0
8	D	186	0	0	1	0
8	E	32	0	0	0	0
All	All	15686	0	14334	173	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 6.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:HD21	4:D:600[B]:GTP:HN22	1.06	0.99
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.47	0.95
2:D:292:THR:HG22	2:D:335:ILE:HD12	1.49	0.91
2:B:206:ASN:HD21	7:B:600:GDP:HN22	1.18	0.88
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.21	0.80
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.63	0.80
1:A:71:GLU:OE2	1:A:73:THR:HB	1.84	0.75
2:D:317:THR:HG21	2:D:332:MET:HE2	1.68	0.73
2:D:263:PRO:O	2:D:266:HIS:HD2	1.72	0.72
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.37	0.72
2:B:1:MET:N	2:B:131:CYS:SG	2.62	0.72
1:C:71:GLU:OE2	1:C:73:THR:HB	1.91	0.71
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.30	0.71
2:B:317:THR:HG21	2:B:332:MET:HE2	1.71	0.71
2:D:206:ASN:HD21	4:D:600[B]:GTP:N2	1.87	0.69
2:B:263:PRO:O	2:B:266:HIS:HD2	1.76	0.68
1:A:245:ASP:HB3	3:E:15:THR:HG22	1.76	0.68
3:E:44:ASP:H	3:E:45:PRO:HA	1.57	0.68
3:E:32:VAL:HB	3:E:33:PRO:CD	2.24	0.67
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.29	0.67
2:D:50:ASN:O	2:D:64:ARG:NH2	2.29	0.66
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.80	0.65
2:D:206:ASN:ND2	4:D:600[B]:GTP:HN22	1.89	0.64
1:A:133[B]:GLN:HG3	1:A:252:LEU:HB2	1.79	0.63
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.63	0.63
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.47	0.62
1:A:221:ARG:HG2	2:B:325:MET:HB3	1.82	0.62
2:B:312:TYR:CE2	2:B:377[A]:PHE:HZ	2.18	0.61
2:D:312:TYR:CE2	2:D:377[A]:PHE:HZ	2.19	0.61
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.84	0.61
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.83	0.61
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.47	0.61
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.37	0.60
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.65	0.60
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.84	0.60
1:C:339:ARG:H	1:C:339:ARG:HD3	1.67	0.59
2:D:288:VAL:HG22	2:D:323:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:GLN:NE2	2:D:252:LEU:H	2.00	0.59
2:D:295[A]:MET:CG	2:D:377[A]:PHE:HB2	2.33	0.59
2:B:295[A]:MET:CG	2:B:377[A]:PHE:HB2	2.34	0.58
2:D:139:HIS:HD2	2:D:146:GLY:O	1.87	0.58
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.85	0.57
2:B:282:GLN:CB	2:B:283:TYR:HA	2.35	0.56
1:C:313:MET:SD	1:C:435:VAL:CG1	2.93	0.56
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.39	0.56
1:C:54:SER:OG	1:C:62:VAL:HG13	2.06	0.56
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.24	0.56
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.41	0.55
1:A:71:GLU:OE2	1:A:73:THR:CB	2.53	0.55
1:C:246:GLY:H	1:C:249:ASN:HD21	1.52	0.55
2:D:295[B]:MET:HE1	2:D:332:MET:HE1	1.87	0.55
1:A:262:TYR:CE1	1:A:346:TRP:CH2	2.94	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.89	0.55
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.54
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.25	0.54
2:B:295[B]:MET:HE1	2:B:332:MET:HE1	1.90	0.54
2:B:286:LEU:HD12	2:B:291:LEU:HD23	1.88	0.54
2:D:206:ASN:HD21	4:D:600[A]:GTP:HN22	1.53	0.54
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.54
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.90	0.54
2:B:50:ASN:O	2:B:64:ARG:NH2	2.32	0.53
1:A:285:GLN:NE2	1:A:372:GLN:H	2.05	0.53
2:B:106:GLY:O	2:B:111:GLY:HA3	2.10	0.52
2:D:292:THR:HG22	2:D:335:ILE:CD1	2.31	0.52
2:B:100:GLY:HA2	1:C:254:GLU:HG3	1.91	0.52
2:B:269:MET:CE	2:B:305:CYS:HB2	2.40	0.52
1:A:261:PRO:HD2	8:A:692:HOH:O	2.10	0.52
2:B:206:ASN:HD21	7:B:600:GDP:N2	1.99	0.52
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.92	0.51
2:B:66:ILE:HG12	2:B:121:VAL:HG12	1.90	0.51
1:C:313:MET:SD	1:C:435:VAL:HG11	2.51	0.51
2:B:139:HIS:HD2	2:B:146:GLY:O	1.94	0.51
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.94	0.50
1:A:346:TRP:CD1	1:A:346:TRP:H	2.30	0.50
3:E:80:ARG:O	3:E:83:ILE:HG22	2.10	0.50
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.47	0.50
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.49
1:A:133[A]:GLN:OE1	1:A:251:ASP:HB2	2.12	0.49
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.93	0.49
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.47	0.49
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.94	0.48
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.93	0.48
1:A:2:ARG:HB2	1:A:133[A]:GLN:CD	2.39	0.48
2:B:317:THR:HG21	2:B:332:MET:CE	2.42	0.48
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.36	0.48
2:B:295[A]:MET:HG3	2:B:377[A]:PHE:HB2	1.96	0.48
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.94	0.48
2:D:106:GLY:O	2:D:111:GLY:HA3	2.13	0.48
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.48
2:B:292:THR:HG22	2:B:319:PHE:CZ	2.49	0.47
2:D:296[B]:PHE:HB3	2:D:308:ARG:HE	1.79	0.47
2:B:296[B]:PHE:CE1	2:B:342:TYR:HB2	2.50	0.47
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.97	0.47
1:A:105:ARG:HG2	1:A:110:ILE:HD13	1.96	0.47
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.32	0.47
1:A:329:ASN:HD21	3:E:20:TRP:NE1	2.10	0.47
2:B:229:HIS:HE1	2:B:276:THR:HG23	1.79	0.47
2:B:296[B]:PHE:HB3	2:B:308:ARG:HE	1.78	0.47
1:C:56:THR:HG23	1:C:58:ALA:H	1.79	0.47
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:HB2	1.96	0.47
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.61	0.47
1:C:217:LEU:HD21	1:C:368:LEU:HD23	1.96	0.47
2:B:67:LEU:O	2:B:75:MET:HE1	2.14	0.47
2:B:269:MET:HE3	2:B:305:CYS:HB2	1.96	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.55	0.47
2:D:56:ALA:HB3	2:D:60:LYS:HG3	1.97	0.46
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.98	0.46
1:C:71:GLU:OE2	1:C:73:THR:CB	2.61	0.46
1:C:192:HIS:CG	1:C:421:ALA:HA	2.51	0.46
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.46
1:A:88:HIS:H	1:A:91:GLN:NE2	2.14	0.46
2:D:133:GLN:HE22	2:D:252:LEU:H	1.64	0.45
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.98	0.45
3:E:83:ILE:O	3:E:87:ILE:HG12	2.16	0.45
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.81	0.45
2:D:317:THR:HG21	2:D:332:MET:CE	2.40	0.45
2:D:312:TYR:CE2	2:D:377[A]:PHE:CZ	3.02	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:VAL:HG11	2:B:227:LEU:HD21	1.98	0.45
2:B:312:TYR:CE2	2:B:377[A]:PHE:CZ	3.02	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.45
2:D:183:GLU:OE2	4:D:600[B]:GTP:H3'	2.16	0.45
1:A:88:HIS:H	1:A:91:GLN:HE21	1.65	0.44
1:A:402:ARG:NH2	8:A:723:HOH:O	2.51	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.44
2:D:139:HIS:CD2	2:D:146:GLY:O	2.69	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.82	0.44
2:B:180:THR:HG23	2:B:183:GLU:HG3	1.99	0.44
2:B:181:VAL:HG13	2:B:182:VAL:HG13	1.99	0.43
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.67	0.43
2:D:19:LYS:HE3	8:D:723:HOH:O	2.18	0.43
1:A:244:PHE:CG	1:A:358:GLN:HG3	2.52	0.43
1:C:68:VAL:HG11	1:C:118:VAL:HG21	2.01	0.43
1:C:133:GLN:NE2	1:C:252:LEU:H	2.16	0.43
2:D:296[B]:PHE:CE1	2:D:342:TYR:HB2	2.54	0.43
1:C:56:THR:HG22	1:C:60:LYS:H	1.84	0.43
1:C:271:THR:HG22	1:C:301:GLN:HA	2.00	0.43
2:B:75:MET:HE2	2:B:94:PHE:HB3	2.00	0.43
1:C:316:CYS:HA	1:C:352:LYS:O	2.19	0.43
2:D:292:THR:CG2	2:D:335:ILE:HD12	2.34	0.43
1:A:400:ALA:HB2	2:B:442:GLU:HG2	2.01	0.43
2:B:309:HIS:CD2	2:B:386:GLU:OE1	2.67	0.43
3:E:136:ASN:HA	3:E:139:LEU:HD12	2.01	0.43
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.82	0.42
1:C:271:THR:OG1	1:C:377:MET:HB3	2.19	0.42
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.37	0.42
1:A:261:PRO:HG3	1:A:313:MET:HG3	2.00	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.20	0.42
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.00	0.42
2:B:167:ASN:ND2	8:B:689:HOH:O	2.52	0.42
1:A:413:MET:HE3	1:A:417:GLU:HB3	2.01	0.42
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.02	0.42
2:D:44:LEU:HA	2:D:49:ILE:HB	2.02	0.42
1:A:262:TYR:HE1	1:A:346:TRP:CZ2	2.37	0.42
2:B:323:MET:HE3	2:B:373:MET:HE3	2.02	0.42
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.02	0.41
1:A:292:THR:O	1:A:295:CYS:HB2	2.20	0.41
2:B:345:GLU:H	2:B:345:GLU:HG2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295[A]:MET:HE2	2:D:295[A]:MET:HB3	1.95	0.41
1:A:36:MET:HG2	1:A:61:HIS:CD2	2.56	0.41
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.41
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.02	0.41
2:B:146:GLY:O	2:B:150:GLY:HA3	2.21	0.41
2:D:49:ILE:HD12	2:D:49:ILE:HA	1.92	0.41
2:D:323:MET:HE3	2:D:373:MET:HE3	2.02	0.41
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.86	0.40
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:CB	2.51	0.40
2:B:181:VAL:HG23	1:C:349:THR:O	2.21	0.40
2:B:295[B]:MET:HE2	2:B:315:VAL:HG11	2.03	0.40
2:D:296[B]:PHE:CE1	2:D:342:TYR:CB	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	429/451 (95%)	417 (97%)	11 (3%)	1 (0%)	43	44
1	C	430/451 (95%)	414 (96%)	13 (3%)	3 (1%)	18	15
2	B	437/445 (98%)	418 (96%)	14 (3%)	5 (1%)	11	8
2	D	439/445 (99%)	425 (97%)	12 (3%)	2 (0%)	24	22
3	E	132/143 (92%)	125 (95%)	5 (4%)	2 (2%)	8	4
All	All	1867/1935 (96%)	1799 (96%)	55 (3%)	13 (1%)	18	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	VAL
1	C	47	ASP

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Mol	Chain	Res	Type
2	D	282	GLN
3	E	32	VAL
2	B	282	GLN
2	B	284	ARG
2	B	286	LEU
1	C	280	LYS
1	C	283	HIS
2	D	279	GLY
3	E	44	ASP
2	B	177	VAL
2	B	98	GLY

5.3.2 Protein sidechains ⓘ

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	367/379 (97%)	354 (96%)	13 (4%)	32	35
1	C	363/379 (96%)	351 (97%)	12 (3%)	33	37
2	B	378/385 (98%)	366 (97%)	12 (3%)	34	38
2	D	381/385 (99%)	368 (97%)	13 (3%)	32	35
3	E	114/125 (91%)	103 (90%)	11 (10%)	8	5
All	All	1603/1653 (97%)	1542 (96%)	61 (4%)	30	32

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	47	ASP
1	A	68	VAL
1	A	84	ARG
1	A	164	LYS
1	A	179	THR
1	A	188	ILE

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Mol	Chain	Res	Type
1	A	215	ARG
1	A	250	VAL
1	A	324	VAL
1	A	345	ASP
1	A	435	VAL
2	B	24	ILE
2	B	115	VAL
2	B	122	VAL
2	B	171	VAL
2	B	294[A]	GLN
2	B	294[B]	GLN
2	B	298	SER
2	B	299	LYS
2	B	323	MET
2	B	335	ILE
2	B	341	SER
2	B	423	SER
1	C	62	VAL
1	C	68	VAL
1	C	84	ARG
1	C	164	LYS
1	C	179	THR
1	C	188	ILE
1	C	241	SER
1	C	250	VAL
1	C	324	VAL
1	C	349	THR
1	C	430	LYS
1	C	435	VAL
2	D	24	ILE
2	D	115	VAL
2	D	122	VAL
2	D	171	VAL
2	D	177	VAL
2	D	294[A]	GLN
2	D	294[B]	GLN
2	D	299	LYS
2	D	323	MET
2	D	335	ILE
2	D	371	LEU
2	D	405	LEU
2	D	423	SER

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Mol	Chain	Res	Type
3	E	13	LYS
3	E	15	THR
3	E	25	LYS
3	E	32	VAL
3	E	46	SER
3	E	49	GLU
3	E	82	VAL
3	E	122	ARG
3	E	125	GLU
3	E	134	ARG
3	E	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	91	GLN
1	A	139	HIS
1	A	249	ASN
1	A	256	GLN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	393	HIS
2	B	6	HIS
2	B	14	ASN
2	B	37	HIS
2	B	50	ASN
2	B	101	ASN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	300	ASN
2	B	309	HIS
2	B	334	ASN
2	B	433	GLN
2	B	436	GLN
1	C	8	HIS
1	C	11	GLN
1	C	50	ASN

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Mol	Chain	Res	Type
1	C	91	GLN
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	216	ASN
1	C	249	ASN
1	C	258	ASN
1	C	301	GLN
1	C	329	ASN
1	C	342	GLN
1	C	393	HIS
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	50	ASN
2	D	133	GLN
2	D	139	HIS
2	D	197	ASN
2	D	206	ASN
2	D	247	GLN
2	D	266	HIS
2	D	300	ASN
2	D	385	GLN
2	D	433	GLN
3	E	111	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 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	D	456	-	4,4,4	0.31	0	6,6,6	0.19	0
4	GTP	D	600[A]	5	33,34,34	1.21	4 (12%)	50,54,54	1.84	14 (28%)
6	SO4	D	457	-	4,4,4	0.34	0	6,6,6	0.17	0
7	GDP	B	600	-	29,30,30	1.63	1 (3%)	45,47,47	1.73	9 (20%)
4	GTP	D	600[B]	5	29,30,34	1.10	1 (3%)	45,47,54	1.49	5 (11%)
4	GTP	C	600	5	33,34,34	1.44	4 (12%)	50,54,54	1.72	9 (18%)
4	GTP	A	600	5	33,34,34	1.29	3 (9%)	50,54,54	1.62	9 (18%)
6	SO4	A	452	-	4,4,4	0.61	0	6,6,6	0.17	0
6	SO4	A	454	-	4,4,4	0.42	0	6,6,6	0.19	0
6	SO4	A	455	-	4,4,4	0.30	0	6,6,6	0.15	0
6	SO4	C	453	-	4,4,4	0.30	0	6,6,6	0.12	0
6	SO4	E	146	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	453	-	4,4,4	0.33	0	6,6,6	0.12	0
6	SO4	B	457	-	4,4,4	0.28	0	6,6,6	0.07	0
6	SO4	B	456	-	4,4,4	0.37	0	6,6,6	0.19	0
6	SO4	C	452	-	4,4,4	0.28	0	6,6,6	0.11	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	D	600[A]	5	-	6/22/38/38	0/3/3/3
4	GTP	D	600[B]	5	-	2/16/32/38	0/3/3/3
4	GTP	C	600	5	-	6/22/38/38	0/3/3/3
4	GTP	A	600	5	-	6/22/38/38	0/3/3/3
7	GDP	B	600	-	-	5/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	GDP	PA-O3A	7.43	1.67	1.59
4	C	600	GTP	PA-O3A	6.04	1.66	1.59
4	A	600	GTP	PA-O3A	4.20	1.64	1.59
4	A	600	GTP	PB-O3A	3.01	1.62	1.59
4	D	600[B]	GTP	PA-O3A	2.80	1.62	1.59
4	D	600[A]	GTP	O6-C6	-2.58	1.18	1.23
4	C	600	GTP	O4'-C4'	2.58	1.50	1.45
4	D	600[A]	GTP	PA-O3A	2.47	1.62	1.59
4	D	600[A]	GTP	C2-N2	2.34	1.39	1.34
4	C	600	GTP	C5-C4	2.22	1.44	1.38
4	D	600[A]	GTP	PB-O3A	2.21	1.61	1.59
4	A	600	GTP	O4'-C4'	2.19	1.49	1.45
4	C	600	GTP	PB-O3B	2.08	1.61	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	GTP	C2-N3-C4	4.98	120.87	112.30
4	D	600[A]	GTP	C2-N3-C4	4.87	120.69	112.30
4	A	600	GTP	C2-N3-C4	4.60	120.22	112.30
4	D	600[A]	GTP	C5-C4-N3	-4.51	121.22	128.39
4	D	600[B]	GTP	C5-C4-N3	-4.46	121.29	128.39
4	C	600	GTP	C5-C4-N3	-4.40	121.39	128.39
4	A	600	GTP	C5-C4-N3	-4.19	121.72	128.39
7	B	600	GDP	C2-N3-C4	4.17	119.48	112.30
7	B	600	GDP	C5-C4-N3	-4.13	121.81	128.39
4	D	600[B]	GTP	C2-N3-C4	4.04	119.26	112.30
4	D	600[A]	GTP	C6-C5-N7	3.93	137.44	130.29
4	D	600[B]	GTP	N9-C4-N3	3.65	133.25	125.95
7	B	600	GDP	N9-C4-N3	3.49	132.94	125.95
4	D	600[A]	GTP	N9-C4-N3	3.45	132.86	125.95
7	B	600	GDP	C8-N7-C5	3.41	110.34	104.26
4	C	600	GTP	C6-C5-N7	3.32	136.34	130.29
4	A	600	GTP	C6-C5-N7	3.20	136.11	130.29
7	B	600	GDP	C6-C5-N7	3.17	136.06	130.29
7	B	600	GDP	O2B-PB-O3A	3.08	114.98	104.64
4	C	600	GTP	N9-C4-N3	3.08	132.12	125.95
4	D	600[A]	GTP	C8-N7-C5	2.93	109.48	104.26
4	A	600	GTP	N9-C4-N3	2.88	131.72	125.95
4	A	600	GTP	C8-N7-C5	2.85	109.34	104.26
4	A	600	GTP	O2B-PB-O3A	2.83	114.92	107.27
4	C	600	GTP	C8-N7-C5	2.82	109.28	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600[A]	GTP	O6-C6-N1	-2.71	115.02	120.11
4	C	600	GTP	C4-C5-N7	-2.65	106.46	110.67
7	B	600	GDP	N9-C8-N7	-2.62	108.55	113.40
4	D	600[A]	GTP	C5-C6-N1	2.58	119.83	113.25
4	C	600	GTP	O2B-PB-O3A	2.58	114.25	107.27
4	D	600[A]	GTP	O2B-PB-O3A	2.46	113.92	107.27
4	A	600	GTP	C4-C5-N7	-2.44	106.80	110.67
7	B	600	GDP	C4-C5-N7	-2.44	106.81	110.67
4	C	600	GTP	O5'-C5'-C4'	-2.43	100.72	108.99
4	D	600[A]	GTP	O5'-C5'-C4'	-2.38	100.88	108.99
4	D	600[A]	GTP	C6-C5-C4	-2.34	115.31	118.83
4	D	600[A]	GTP	O3A-PB-O1B	2.34	117.73	110.70
4	C	600	GTP	O3A-PA-O1A	-2.32	103.73	110.70
4	D	600[A]	GTP	N9-C8-N7	-2.31	109.12	113.40
4	D	600[B]	GTP	O2B-PB-O3A	2.27	112.25	104.64
4	D	600[A]	GTP	N2-C2-N3	2.24	124.05	119.67
4	A	600	GTP	O3A-PA-O1A	-2.22	104.03	110.70
4	D	600[A]	GTP	C4-C5-N7	-2.16	107.24	110.67
4	D	600[B]	GTP	C6-C5-N7	2.12	134.15	130.29
7	B	600	GDP	O5'-C5'-C4'	-2.09	101.89	108.99
4	A	600	GTP	C2-N1-C6	-2.03	121.44	125.11

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

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

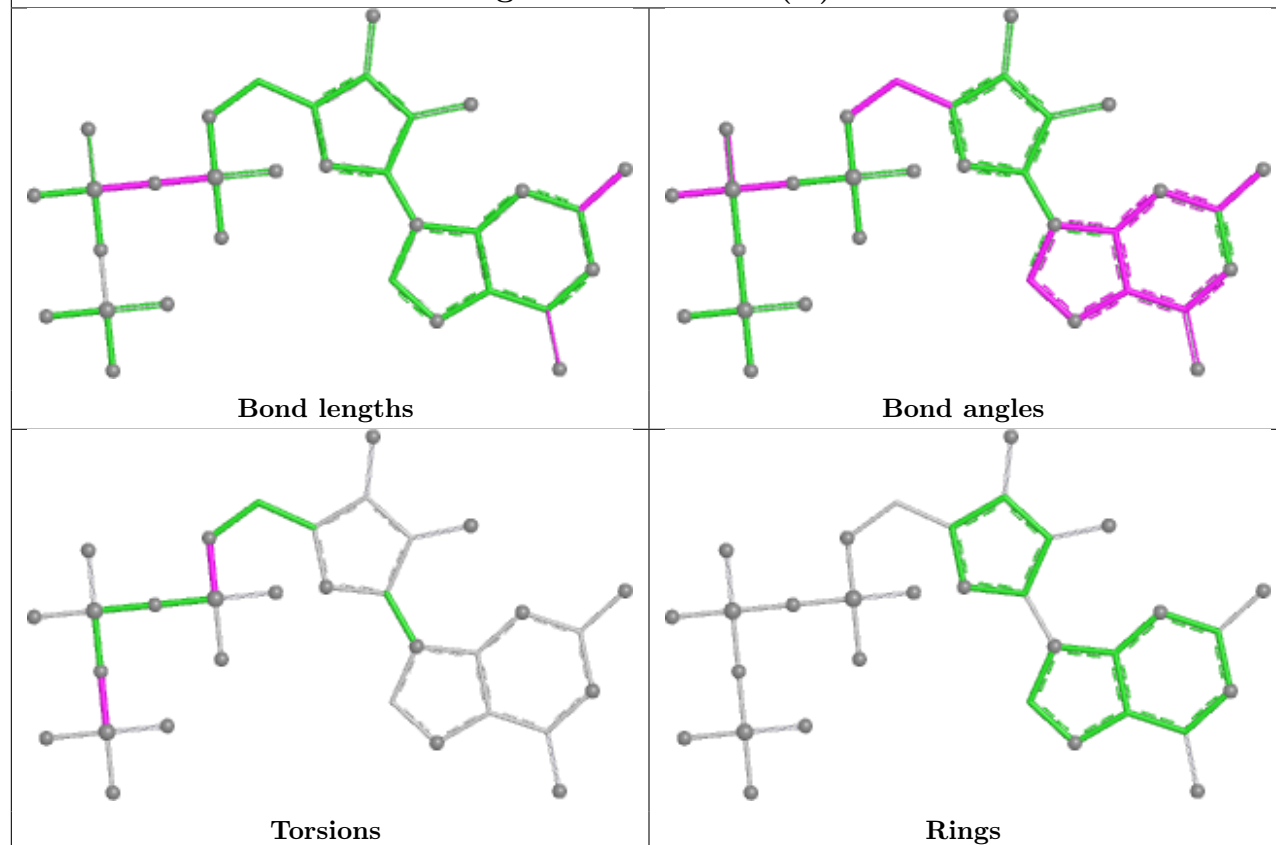
There are no ring outliers.

3 monomers are involved in 7 short contacts:

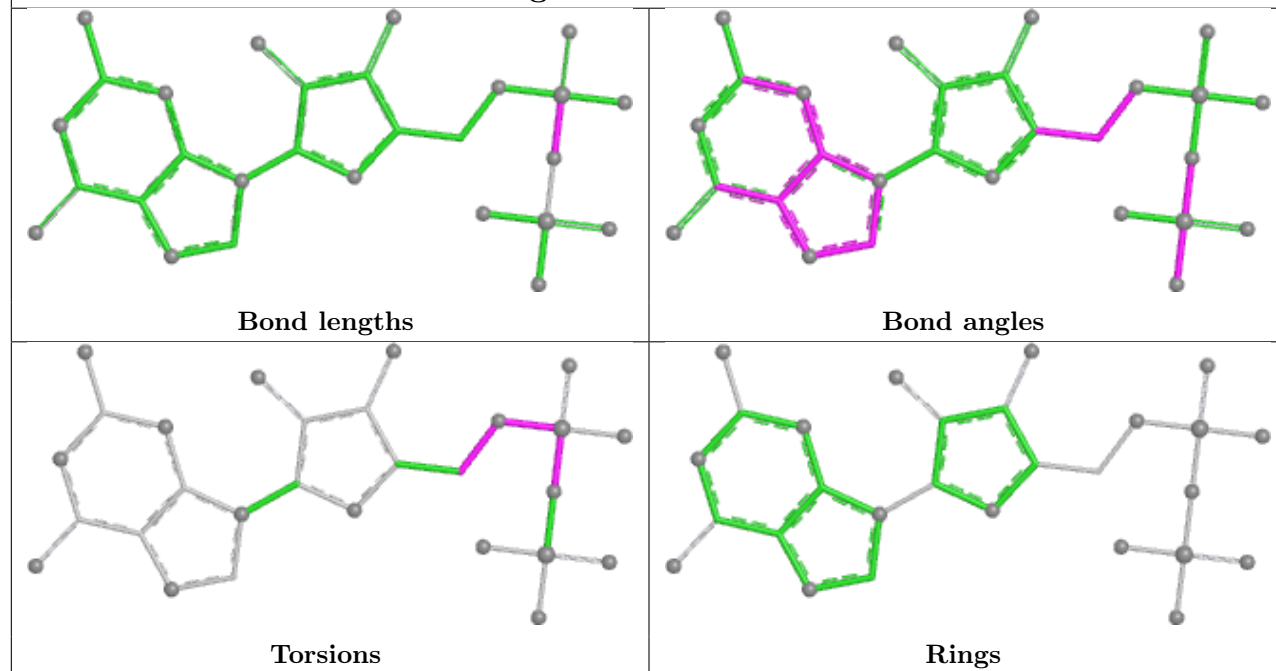
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	600[A]	GTP	1	0
7	B	600	GDP	2	0
4	D	600[B]	GTP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

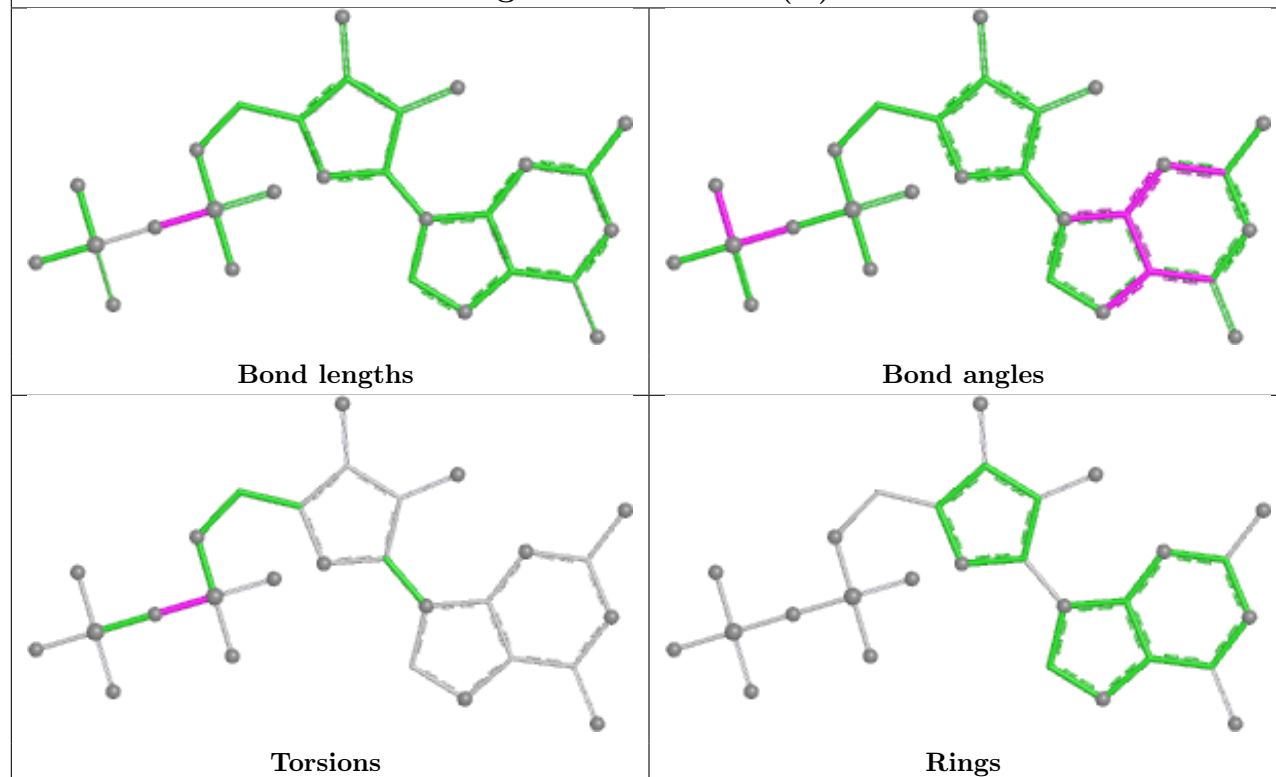
Ligand GTP D 600 (A)



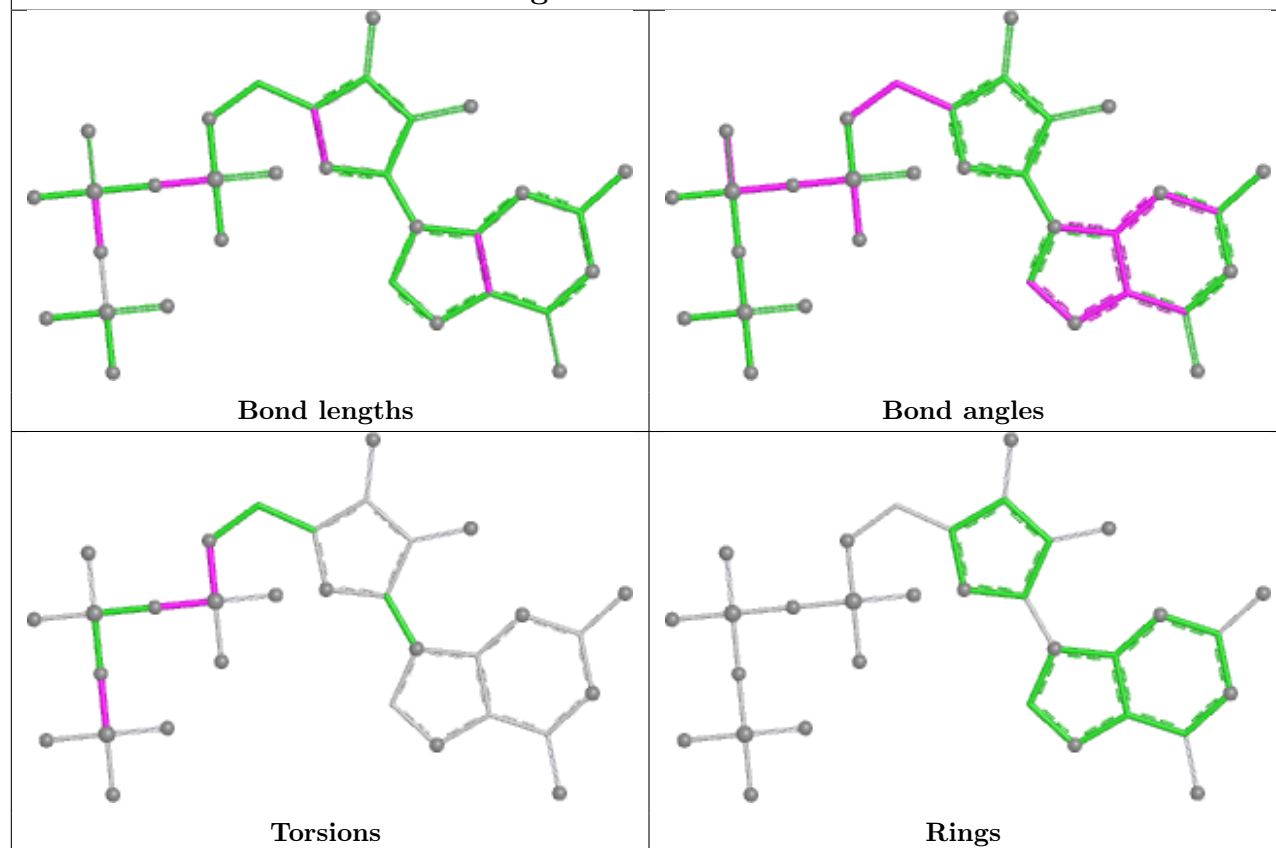
Ligand GDP B 600

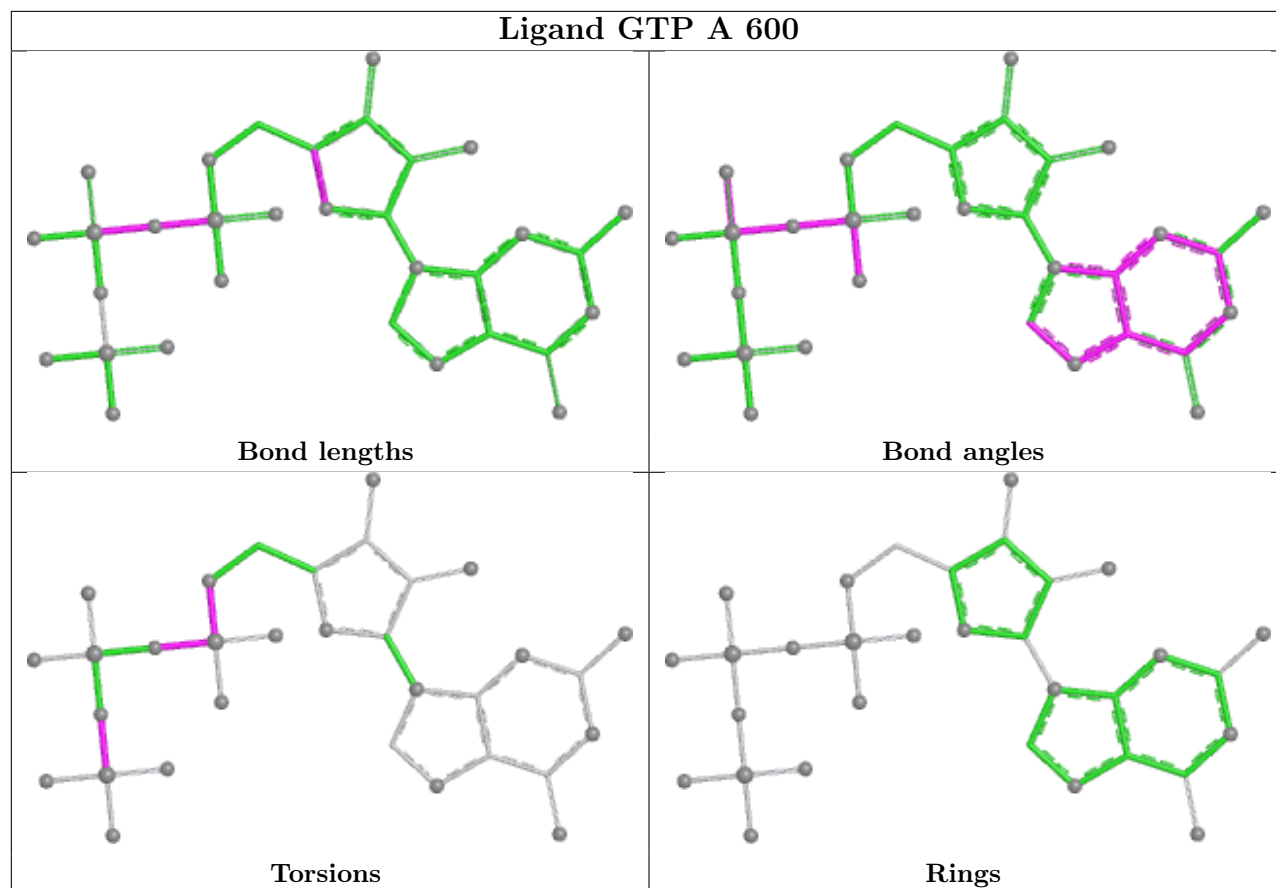


Ligand GTP D 600 (B)



Ligand GTP C 600





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	431/451 (95%)	-0.03	12 (2%)	55	57	18, 45, 72, 130	2 (0%)
1	C	431/451 (95%)	0.34	22 (5%)	33	35	26, 52, 88, 115	4 (0%)
2	B	432/445 (97%)	0.13	15 (3%)	47	49	25, 48, 90, 117	11 (2%)
2	D	431/445 (96%)	-0.00	9 (2%)	63	66	21, 41, 78, 111	14 (3%)
3	E	136/143 (95%)	0.64	14 (10%)	12	12	43, 62, 110, 138	0
All	All	1861/1935 (96%)	0.15	72 (3%)	43	45	18, 48, 86, 138	31 (1%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	283	TYR	5.1
3	E	32	VAL	4.6
2	D	59	ASN	4.5
1	C	282	TYR	3.8
1	C	37	PRO	3.6
1	C	362	VAL	3.6
3	E	143	ALA	3.6
3	E	34	GLU	3.4
3	E	45	PRO	3.4
1	C	439	SER	3.3
1	C	357	TYR	3.2
1	C	177	VAL	3.1
1	C	349	THR	3.1
3	E	139	LEU	3.1
2	D	294[A]	GLN	3.0
2	B	283	TYR	3.0
3	E	31	GLY	2.9
1	C	1[A]	MET	2.9
1	C	58	ALA	2.9
2	D	57	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	295[A]	MET	2.7
1	C	46	ASP	2.7
3	E	145	ARG	2.7
3	E	144	SER	2.7
1	A	282	TYR	2.7
1	C	283	HIS	2.7
2	D	295[A]	MET	2.7
2	B	287	THR	2.6
3	E	16	SER	2.6
2	D	98	GLY	2.5
2	B	294[A]	GLN	2.5
3	E	33	PRO	2.5
1	A	38	SER	2.5
2	B	280	SER	2.5
2	D	74	THR	2.4
3	E	4	ALA	2.4
1	C	281	ALA	2.4
2	D	94	PHE	2.4
1	A	1	MET	2.4
2	D	416	MET	2.4
2	B	439	THR	2.4
1	A	110	ILE	2.4
2	B	57	THR	2.4
2	B	359	PRO	2.4
2	B	285	ALA	2.3
1	C	280	LYS	2.3
1	A	436	GLY	2.3
1	C	284	GLU	2.3
1	A	435	VAL	2.3
1	A	163	LYS	2.3
1	A	281	ALA	2.3
1	C	299	ALA	2.3
3	E	83	ILE	2.2
1	C	298	PRO	2.2
1	C	309	HIS	2.2
2	B	42	LEU	2.2
1	C	62	VAL	2.1
1	C	276	ILE	2.1
3	E	43	ARG	2.1
2	B	281	GLN	2.1
2	B	282	GLN	2.1
2	B	370	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	353	VAL	2.1
1	A	37	PRO	2.1
1	A	262	TYR	2.1
2	B	50	ASN	2.0
1	A	345	ASP	2.0
1	A	162	GLY	2.0
1	C	244	PHE	2.0
3	E	29	PHE	2.0
1	C	47	ASP	2.0
2	B	36	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

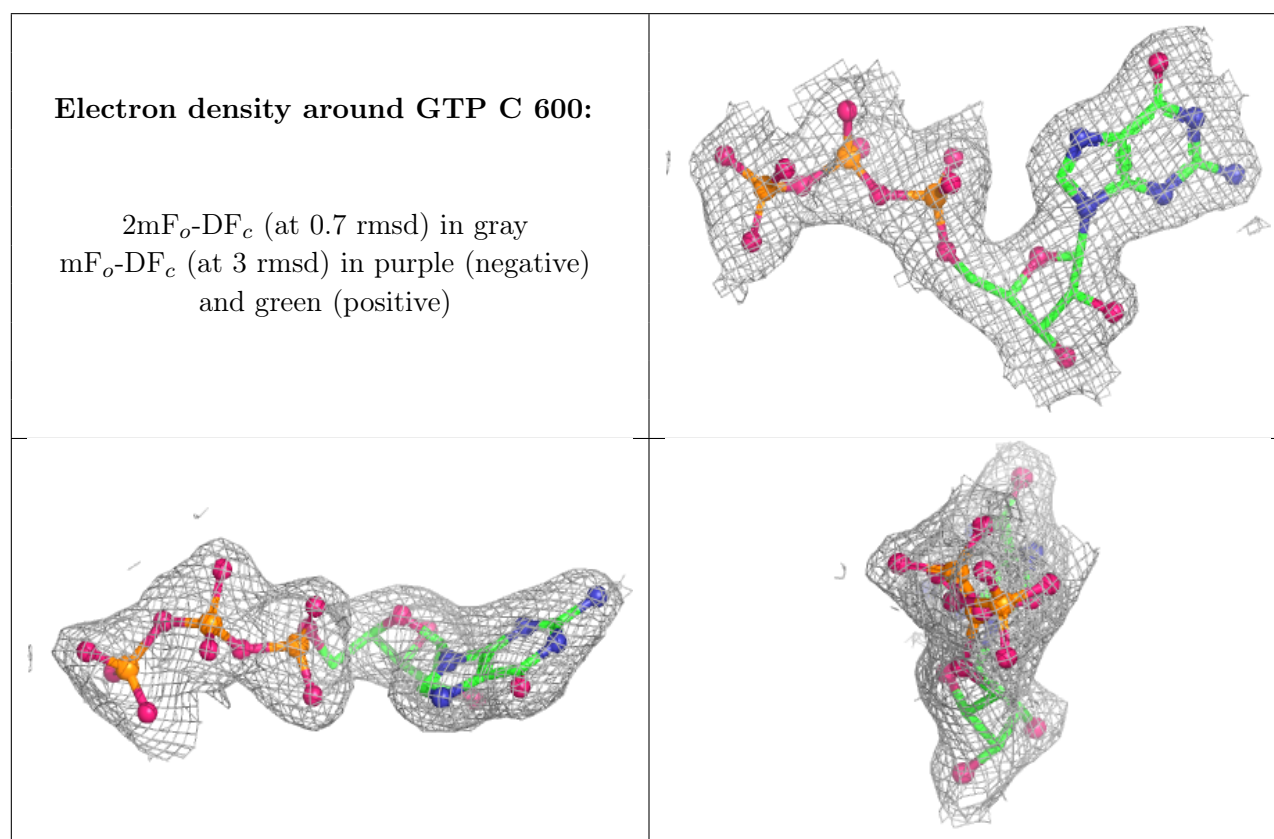
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	455	5/5	0.79	0.16	125,129,130,131	0
6	SO4	B	457	5/5	0.83	0.10	129,133,134,135	0
6	SO4	B	456	5/5	0.84	0.10	94,98,99,100	0
6	SO4	A	453	5/5	0.85	0.16	110,114,116,117	0
6	SO4	E	146	5/5	0.87	0.08	103,107,108,109	0
6	SO4	D	457	5/5	0.88	0.13	112,116,117,117	0
6	SO4	C	452	5/5	0.90	0.07	80,84,85,86	0
6	SO4	C	453	5/5	0.90	0.13	127,132,132,133	0
6	SO4	A	454	5/5	0.90	0.09	84,88,89,89	0
6	SO4	A	452	5/5	0.90	0.09	72,75,76,79	0
5	MG	D	601	1/1	0.96	0.13	38,38,38,38	1
6	SO4	D	456	5/5	0.97	0.06	60,64,64,66	0
4	GTP	C	600	32/32	0.98	0.05	34,40,43,45	0

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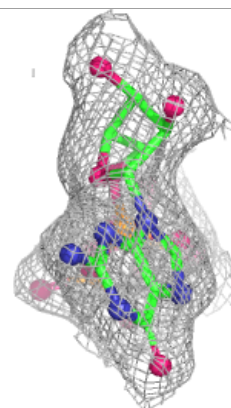
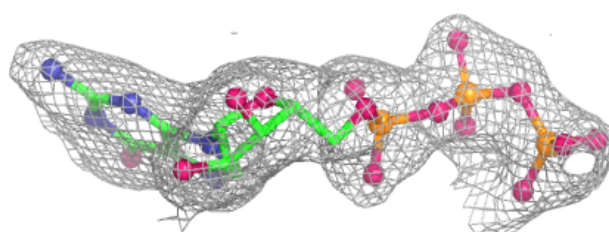
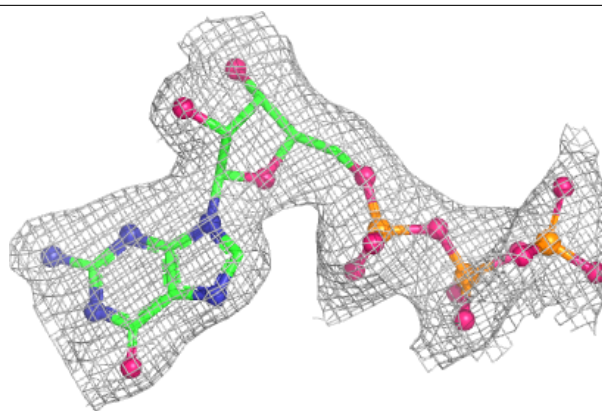
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GTP	D	600[A]	32/32	0.98	0.05	26,29,35,35	32
4	GTP	D	600[B]	28/32	0.98	0.05	30,32,35,35	28
7	GDP	B	600	28/28	0.98	0.05	37,39,41,42	0
5	MG	A	601	1/1	0.99	0.04	42,42,42,42	0
4	GTP	A	600	32/32	0.99	0.04	31,33,36,38	0
5	MG	C	601	1/1	1.00	0.03	36,36,36,36	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.

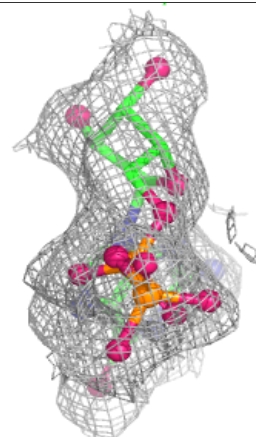
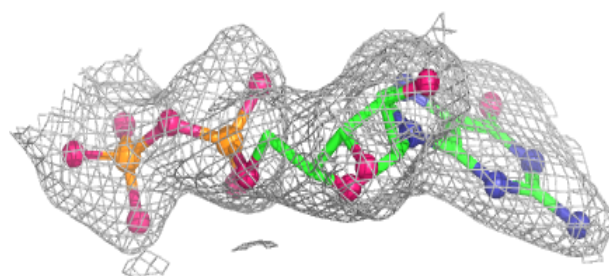
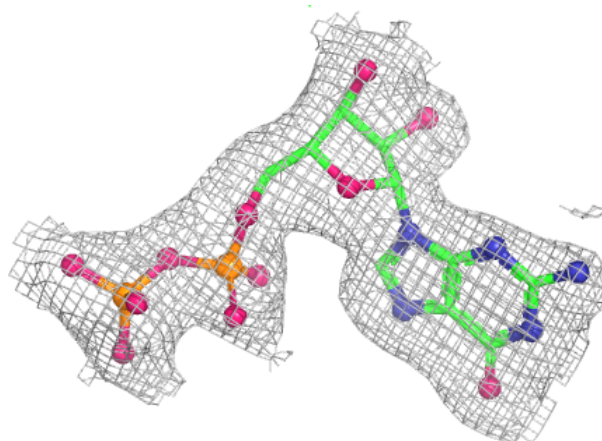


Electron density around GTP D 600 (A):

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

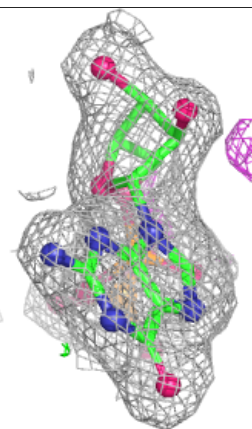
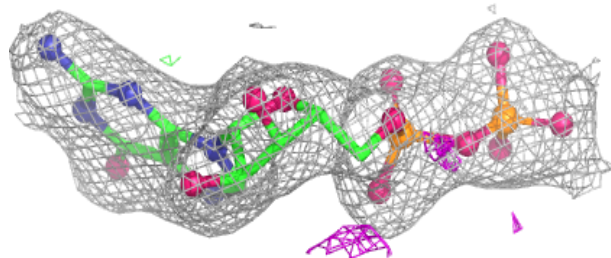
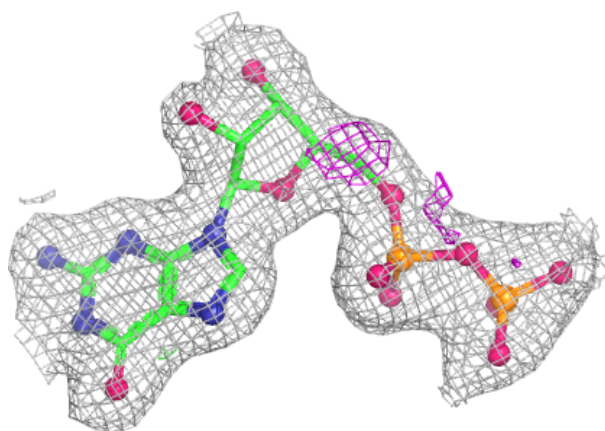
**Electron density around GTP D 600 (B):**

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

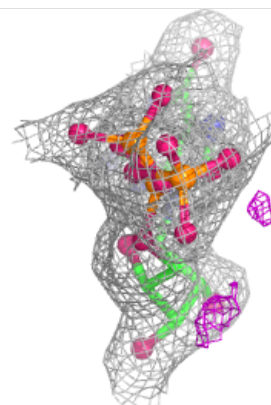
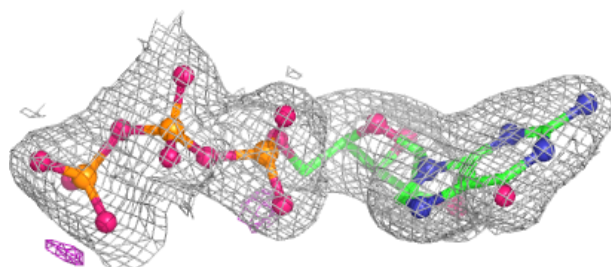
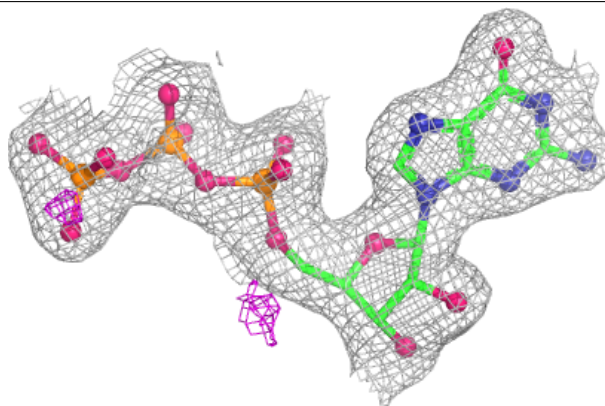


Electron density around GDP B 600:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.