



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:25 AM UTC

PDB ID : 6TH4 / pdb_00006th4
Title : Tubulin-inhibitor complex
Authors : Varela, P.F.; Gigant, B.
Deposited on : 2019-11-18
Resolution : 2.12 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

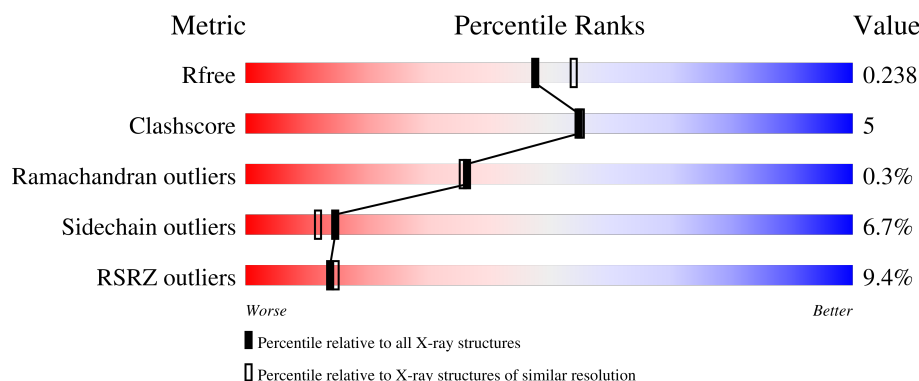
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	12% 83% 10% • 5%
1	C	451	5% 83% 12% • •
2	B	445	9% 76% 17% • •
2	D	445	5% 82% 13% • •
3	E	143	22% 74% 13% • 10%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14923 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	428	Total	C	N	O	S	0	0	0
			3345	2118	566	639	22			
1	C	434	Total	C	N	O	S	0	0	0
			3390	2145	577	646	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	7	0
			3411	2141	584	659	27			
2	D	429	Total	C	N	O	S	0	5	0
			3401	2132	581	661	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	128	Total	C	N	O	S	0	0	0
			1052	651	189	208	4			

There are 4 discrepancies between the modelled and reference sequences:

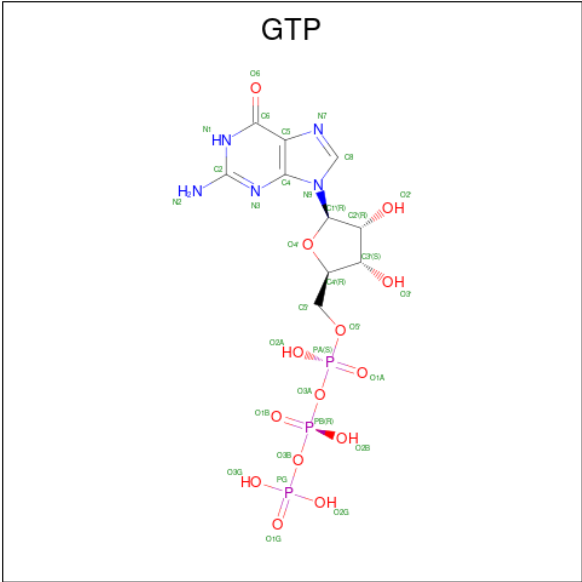
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ACE	-	acetylation	UNP P63043
E	4	ALA	SER	conflict	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

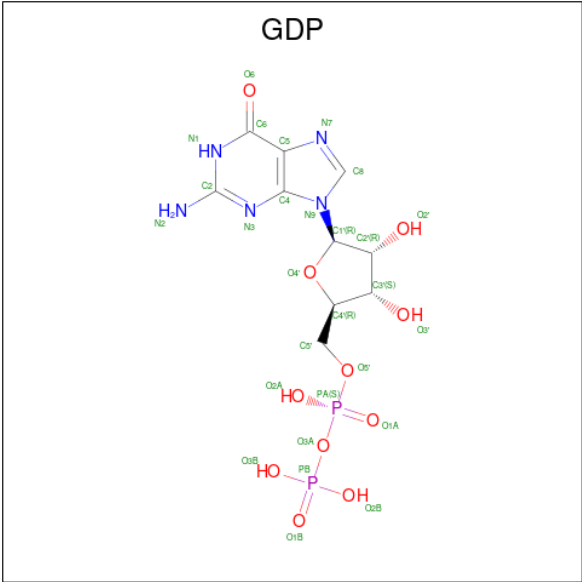


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

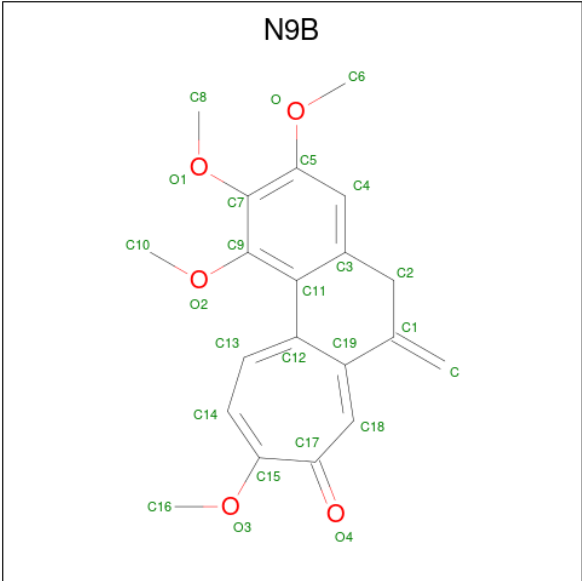
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 8 is 1,2,3,9-tetramethoxy-6-methylidene-5 {H}-cyclohepta[a]naphthalen-8-one (CCD ID: N9B) (formula: C₂₀H₂₀O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	1
			25	20	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			25	20	5		

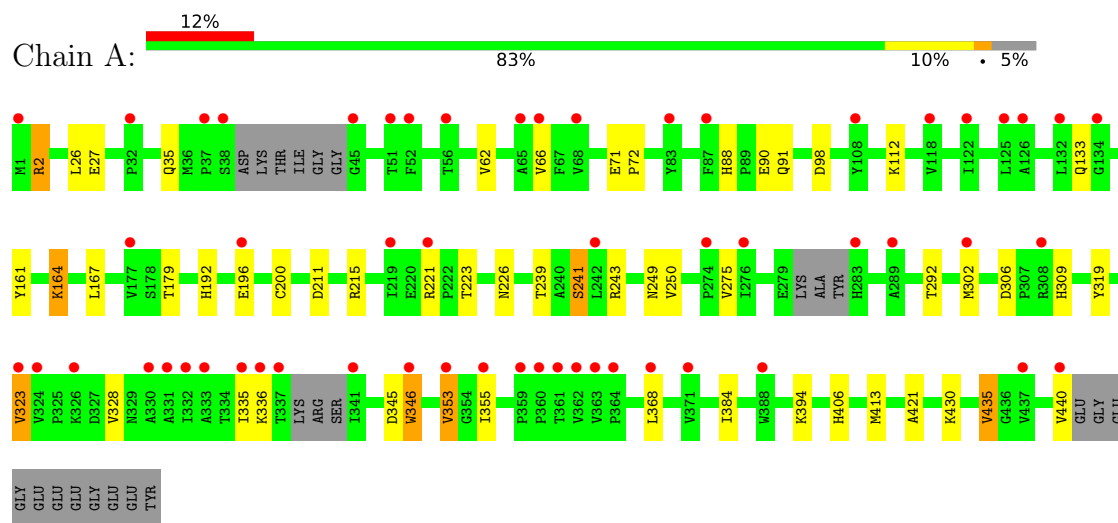
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	17	Total	O	0	0
			17	17		
9	B	19	Total	O	0	0
			19	19		
9	C	49	Total	O	0	0
			49	49		
9	D	29	Total	O	0	0
			29	29		
9	E	3	Total	O	0	0
			3	3		

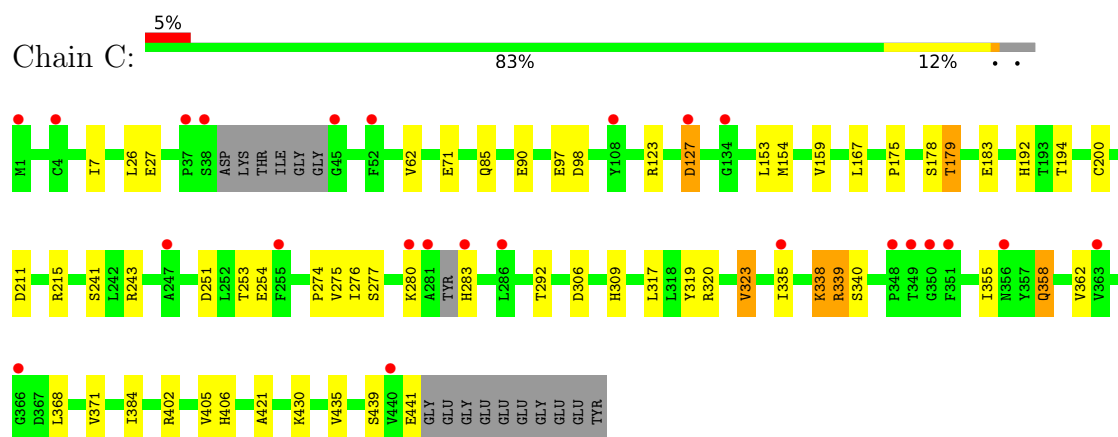
3 Residue-property plots [i](#)

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.

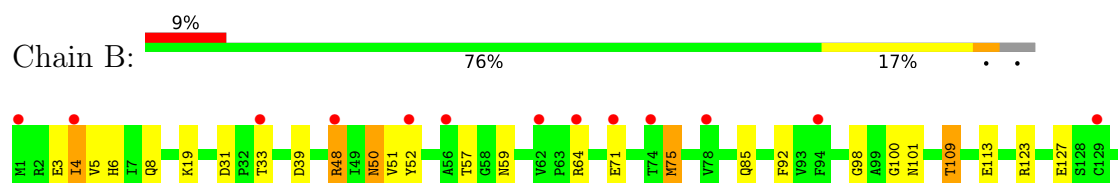
• Molecule 1: Tubulin alpha chain

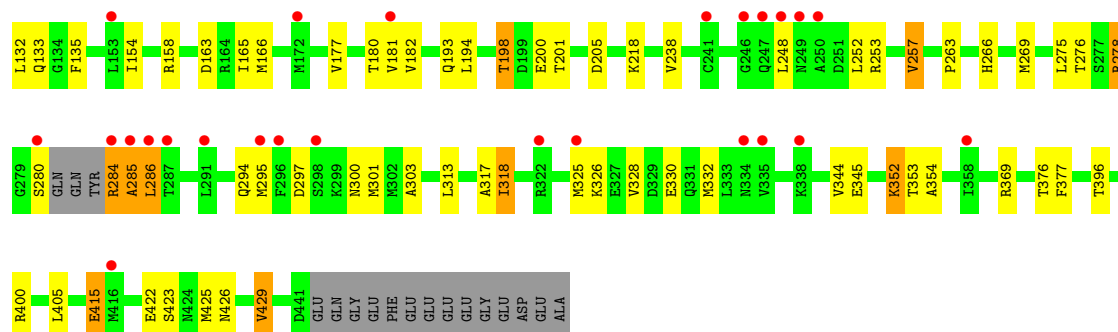


• Molecule 1: Tubulin alpha chain

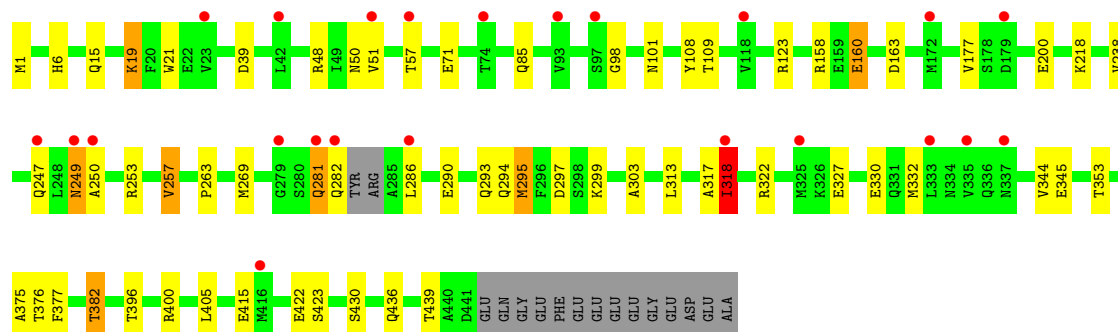
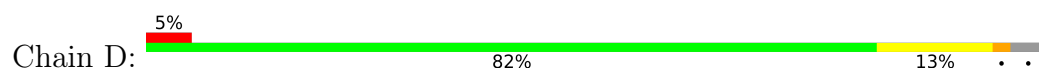


• Molecule 2: Tubulin beta chain

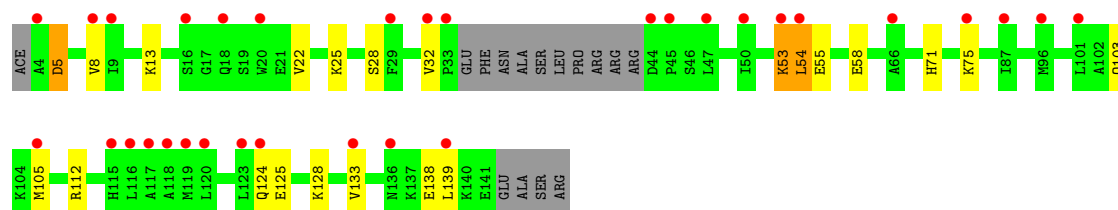
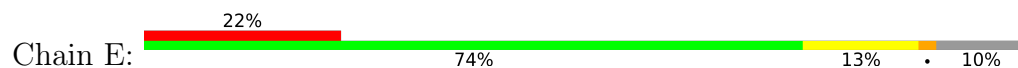




• Molecule 2: Tubulin beta chain



• 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	65.12Å 128.30Å 252.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	126.00 – 2.12 126.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	52.0 (126.00-2.12) 52.0 (126.00-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.192 , 0.226 0.204 , 0.238	Depositor DCC
R_{free} test set	3166 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14923	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: MG, N9B, GDP, SO4, GTP

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	0.68	1/3419 (0.0%)	1.02	2/4641 (0.0%)
1	C	0.72	0/3465	1.04	6/4702 (0.1%)
2	B	0.71	1/3486 (0.0%)	1.02	5/4721 (0.1%)
2	D	0.73	2/3478 (0.1%)	1.03	4/4711 (0.1%)
3	E	0.66	0/1063	1.09	2/1415 (0.1%)
All	All	0.71	4/14911 (0.0%)	1.03	19/20190 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	MET	SD-CE	-6.09	1.64	1.79
2	D	109	THR	CA-C	5.94	1.55	1.52
2	D	281	GLN	CA-C	5.81	1.59	1.52
2	B	109	THR	CA-C	5.22	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	249	ASN	CA-CB-CG	8.14	120.74	112.60
1	C	251	ASP	CA-CB-CG	7.28	119.88	112.60
2	B	71	GLU	CB-CG-CD	6.88	124.30	112.60
1	C	127	ASP	CA-CB-CG	6.37	118.97	112.60
2	D	297	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	98	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	98	ASP	CA-CB-CG	5.86	118.46	112.60
2	B	415	GLU	CA-C-N	5.44	127.57	120.28
2	B	415	GLU	C-N-CA	5.44	127.57	120.28
1	C	338	LYS	CA-C-N	5.31	127.65	120.38
1	C	338	LYS	C-N-CA	5.31	127.65	120.38
1	C	62	VAL	N-CA-C	5.20	113.56	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	VAL	N-CA-C	5.15	113.51	107.89
2	D	318	ILE	CB-CA-C	5.09	116.78	110.73
2	B	297	ASP	CA-CB-CG	5.08	117.68	112.60
2	B	313	LEU	N-CA-C	-5.07	105.21	111.40
2	D	313	LEU	N-CA-C	-5.04	105.25	111.40
3	E	138	GLU	CA-C-N	5.04	127.03	120.28
3	E	138	GLU	C-N-CA	5.04	127.03	120.28

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	3345	0	3247	26	0
1	C	3390	0	3299	25	0
2	B	3411	0	3288	60	0
2	D	3401	0	3274	28	0
3	E	1052	0	1060	10	0
4	A	5	0	0	1	0
4	B	10	0	0	1	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	28	0	12	0	0
7	D	28	0	12	0	0
8	B	25	0	0	0	0
8	D	25	0	0	1	0
9	A	17	0	0	0	0
9	B	19	0	0	0	0
9	C	49	0	0	0	0
9	D	29	0	0	1	0
9	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14923	0	14216	138	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 5.

All (138) 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:269:MET:HE3	2:B:301:MET:HE2	1.51	0.93
3:E:124:GLN:HB3	3:E:128:LYS:HZ2	1.34	0.93
2:B:248[B]:LEU:HD13	2:B:352:LYS:HG2	1.55	0.86
2:B:248[B]:LEU:CD1	2:B:352:LYS:HG2	2.05	0.84
2:D:382:THR:HG21	2:D:436:GLN:HB2	1.60	0.84
2:B:332:MET:HG3	2:B:353:THR:HG21	1.61	0.82
2:D:332:MET:HG3	2:D:353:THR:HG21	1.61	0.81
2:B:5:VAL:HG23	2:B:135:PHE:CD2	2.20	0.76
2:D:48:ARG:O	2:D:51:VAL:HG12	1.87	0.74
3:E:124:GLN:HB3	3:E:128:LYS:NZ	2.02	0.74
1:C:27:GLU:OE1	1:C:243:ARG:NH2	2.20	0.73
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.74	0.69
2:B:284:ARG:HG3	2:B:285:ALA:H	1.58	0.68
2:B:123:ARG:O	2:B:127:GLU:HG2	1.93	0.68
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.75	0.66
2:D:327:GLU:HA	2:D:330:GLU:HG2	1.79	0.65
1:A:306:ASP:OD2	1:A:309:HIS:ND1	2.29	0.65
2:B:133:GLN:HE22	2:B:252:LEU:H	1.43	0.65
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.79	0.65
1:C:306:ASP:OD2	1:C:309:HIS:ND1	2.29	0.64
2:D:286:LEU:HD12	2:D:290:GLU:OE1	1.96	0.64
2:D:250:ALA:HB1	8:D:505:N9B:C6	2.27	0.64
1:C:97:GLU:HG3	2:D:1:MET:HG2	1.80	0.64
2:D:123:ARG:NH1	2:D:160:GLU:OE1	2.30	0.64
2:D:382:THR:HG21	2:D:436:GLN:CB	2.26	0.64
3:E:8:VAL:HG12	3:E:22:VAL:HG22	1.78	0.64
2:D:286:LEU:HD21	2:D:294:GLN:OE1	1.98	0.63
2:D:396:THR:HG22	2:D:422:GLU:OE1	1.98	0.63
2:B:396:THR:HG22	2:B:422:GLU:OE1	1.99	0.62
2:B:425:MET:O	2:B:429:VAL:HG13	1.99	0.62
1:A:328:VAL:HG11	1:A:353:VAL:HG21	1.81	0.62
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.83	0.62
2:B:278:ARG:NH2	4:B:502:SO4:O3	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:MET:HA	2:B:328:VAL:HG12	1.81	0.61
3:E:53:LYS:HE3	3:E:54:LEU:HD13	1.83	0.61
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.84	0.60
1:C:211:ASP:O	1:C:215:ARG:HG3	2.01	0.60
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.84	0.60
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.35	0.59
2:B:31:ASP:OD1	2:B:33:THR:HG22	2.01	0.59
2:D:295:MET:HE2	2:D:375:ALA:HB1	1.85	0.59
2:B:198:THR:HG21	2:B:201:THR:OG1	2.03	0.58
1:A:319:TYR:HB3	1:A:323:VAL:HG11	1.85	0.58
2:B:194:LEU:O	2:B:198:THR:HG22	2.03	0.58
2:B:352:LYS:HA	2:B:352:LYS:HE3	1.84	0.58
1:A:346:TRP:HH2	1:A:435:VAL:HG22	1.67	0.58
1:C:154:MET:HG2	1:C:194:THR:HG23	1.85	0.58
2:B:269:MET:CE	2:B:301:MET:HE2	2.31	0.57
2:B:133:GLN:NE2	2:B:252:LEU:H	2.03	0.57
1:A:221:ARG:HH11	2:B:325:MET:HE3	1.70	0.56
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.88	0.55
2:D:295:MET:CG	2:D:377:PHE:HB2	2.37	0.55
1:C:319:TYR:HB3	1:C:323:VAL:HG11	1.87	0.55
1:A:223:THR:HG22	1:A:226:ASN:OD1	2.09	0.53
1:A:161:TYR:HB3	1:A:164:LYS:HD2	1.91	0.53
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.44	0.52
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.90	0.52
2:D:382:THR:CG2	2:D:436:GLN:OE1	2.58	0.52
2:B:253:ARG:O	2:B:257:VAL:HG13	2.10	0.52
2:D:253:ARG:O	2:D:257:VAL:HG13	2.09	0.52
2:D:382:THR:CG2	2:D:436:GLN:HB2	2.37	0.52
2:B:325:MET:HA	2:B:328:VAL:CG1	2.39	0.52
2:B:5:VAL:HG21	2:B:135:PHE:CE2	2.45	0.52
2:B:51:VAL:HG23	2:B:52:TYR:CD2	2.45	0.52
2:B:75:MET:HE3	2:B:75:MET:HA	1.91	0.51
1:A:211:ASP:O	1:A:215:ARG:HG3	2.10	0.51
1:C:277:SER:HB3	1:C:280:LYS:HG3	1.93	0.51
1:C:179:THR:HG22	1:C:183:GLU:OE2	2.11	0.51
1:A:241:SER:HB2	1:A:249:ASN:O	2.10	0.51
2:B:198:THR:CG2	2:B:266:HIS:NE2	2.74	0.51
2:D:108:TYR:CD1	3:E:133:VAL:HG21	2.46	0.50
1:A:346:TRP:CH2	1:A:435:VAL:HG22	2.45	0.50
2:B:198:THR:HG23	2:B:266:HIS:CD2	2.47	0.50
1:A:2:ARG:HH12	1:A:250:VAL:HG13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:VAL:HG13	1:C:355:ILE:HG23	1.94	0.50
1:C:402:ARG:O	1:C:405:VAL:HG22	2.12	0.50
2:B:50:ASN:O	2:B:64:ARG:NH1	2.44	0.49
2:B:101:ASN:HB3	2:B:180:THR:HG21	1.95	0.49
2:B:4:ILE:HG22	2:B:133:GLN:HG3	1.94	0.49
2:B:400:ARG:HD2	1:C:439:SER:HB3	1.95	0.49
1:A:2:ARG:HB2	1:A:133:GLN:CG	2.42	0.49
2:B:3:GLU:HG2	2:B:64:ARG:NH2	2.27	0.49
2:D:163:ASP:HB2	9:D:626:HOH:O	2.13	0.49
2:B:5:VAL:HG22	2:B:132:LEU:HD11	1.94	0.49
2:B:198:THR:HG22	2:B:266:HIS:NE2	2.27	0.49
1:A:88:HIS:O	1:A:91:GLN:HG2	2.13	0.48
2:B:318:ILE:HG23	2:B:376:THR:HB	1.96	0.47
2:B:248[B]:LEU:HD23	2:B:354:ALA:HB2	1.95	0.47
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.97	0.47
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.48	0.46
1:C:339:ARG:NH2	1:C:340:SER:OG	2.48	0.46
2:B:276:THR:HB	2:B:280:SER:OG	2.14	0.46
2:B:205:ASP:HB2	2:B:303:ALA:HA	1.97	0.46
2:B:48:ARG:O	2:B:51:VAL:HG22	2.15	0.46
2:D:177[A]:VAL:HG22	2:D:177[A]:VAL:O	2.16	0.45
2:D:108:TYR:CG	3:E:133:VAL:HG21	2.51	0.45
2:B:284:ARG:HG3	2:B:285:ALA:N	2.30	0.45
1:C:276:ILE:HG21	1:C:283:HIS:NE2	2.32	0.45
2:B:100:GLY:HA2	1:C:254:GLU:HG3	1.98	0.45
2:B:181:VAL:HG23	2:B:182:VAL:HG13	1.98	0.45
2:B:193:GLN:HE22	3:E:75:LYS:HE3	1.81	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.99	0.45
1:C:320:ARG:HD3	1:C:358:GLN:O	2.17	0.45
1:A:336:LYS:NZ	3:E:5:ASP:HB3	2.32	0.44
1:C:276:ILE:HG23	1:C:280:LYS:HD2	1.98	0.44
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.00	0.44
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.99	0.44
2:B:75:MET:HG3	2:B:92:PHE:HD2	1.82	0.44
1:A:345:ASP:HB2	3:E:28:SER:HB2	2.00	0.44
1:A:223:THR:HG23	1:A:226:ASN:H	1.83	0.43
2:B:133:GLN:NE2	2:B:252:LEU:HG	2.33	0.43
2:B:405:LEU:HD21	2:B:415:GLU:HG3	1.99	0.43
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.43
1:A:394:LYS:NZ	4:A:501:SO4:O4	2.47	0.42
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:VAL:CG2	2:B:135:PHE:CE2	3.02	0.42
2:B:154:ILE:HG12	2:B:166:MET:HE2	2.01	0.42
2:D:318:ILE:HG23	2:D:376:THR:HB	2.02	0.42
1:C:317:LEU:HB3	1:C:319:TYR:CE1	2.54	0.42
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.55	0.42
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.01	0.42
2:B:163:ASP:O	2:B:253:ARG:NH2	2.53	0.42
2:B:109:THR:O	2:B:113:GLU:HG3	2.20	0.42
2:B:6:HIS:HE1	2:B:8:GLN:HB3	1.85	0.42
2:B:369:ARG:HD2	2:B:369:ARG:HA	1.89	0.42
2:B:426:ASN:O	2:B:429:VAL:HG22	2.20	0.41
1:C:175:PRO:HA	1:C:179:THR:OG1	2.19	0.41
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.03	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.41
1:A:292:THR:HG22	1:A:335:ILE:HD11	2.03	0.41
3:E:125:GLU:HA	3:E:128:LYS:HD2	2.01	0.41
2:B:326:LYS:HE2	2:B:330:GLU:OE2	2.21	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
2:D:405:LEU:HD21	2:D:415:GLU:HG3	2.03	0.40
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.02	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.04	0.40
1:A:323:VAL:HG13	1:A:355:ILE:HG23	2.03	0.40
2:D:19:LYS:HD2	2:D:19:LYS:HA	1.84	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	420/451 (93%)	409 (97%)	11 (3%)	0	100	100
1	C	428/451 (95%)	418 (98%)	9 (2%)	1 (0%)	43	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	431/445 (97%)	422 (98%)	6 (1%)	3 (1%)	18	15
2	D	430/445 (97%)	422 (98%)	7 (2%)	1 (0%)	43	44
3	E	124/143 (87%)	122 (98%)	2 (2%)	0	100	100
All	All	1833/1935 (95%)	1793 (98%)	35 (2%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	286	LEU
2	B	98	GLY
2	B	285	ALA
1	C	178	SER
2	D	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	362/379 (96%)	344 (95%)	18 (5%)	22	21
1	C	366/379 (97%)	347 (95%)	19 (5%)	21	19
2	B	374/383 (98%)	348 (93%)	26 (7%)	14	11
2	D	375/383 (98%)	345 (92%)	30 (8%)	11	8
3	E	113/125 (90%)	100 (88%)	13 (12%)	5	3
All	All	1590/1649 (96%)	1484 (93%)	106 (7%)	15	12

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	26	LEU
1	A	35	GLN
1	A	66	VAL
1	A	90	GLU

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Mol	Chain	Res	Type
1	A	112	LYS
1	A	164	LYS
1	A	179	THR
1	A	196	GLU
1	A	241	SER
1	A	302	MET
1	A	323	VAL
1	A	346	TRP
1	A	353	VAL
1	A	384	ILE
1	A	430	LYS
1	A	435	VAL
1	A	440	VAL
2	B	4	ILE
2	B	19	LYS
2	B	39	ASP
2	B	48	ARG
2	B	50	ASN
2	B	57	THR
2	B	59	ASN
2	B	75	MET
2	B	85	GLN
2	B	158	ARG
2	B	177	VAL
2	B	198	THR
2	B	200	GLU
2	B	218	LYS
2	B	238	VAL
2	B	257	VAL
2	B	278	ARG
2	B	284	ARG
2	B	286	LEU
2	B	294	GLN
2	B	318	ILE
2	B	344	VAL
2	B	345	GLU
2	B	352	LYS
2	B	423	SER
2	B	429	VAL
1	C	26	LEU
1	C	71	GLU
1	C	85	GLN

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Mol	Chain	Res	Type
1	C	90	GLU
1	C	123	ARG
1	C	127	ASP
1	C	159	VAL
1	C	179	THR
1	C	241	SER
1	C	253	THR
1	C	323	VAL
1	C	338	LYS
1	C	339	ARG
1	C	358	GLN
1	C	362	VAL
1	C	384	ILE
1	C	430	LYS
1	C	435	VAL
1	C	441	GLU
2	D	15	GLN
2	D	19	LYS
2	D	39	ASP
2	D	50	ASN
2	D	57	THR
2	D	71	GLU
2	D	85	GLN
2	D	101	ASN
2	D	158	ARG
2	D	160	GLU
2	D	200	GLU
2	D	218	LYS
2	D	238	VAL
2	D	247	GLN
2	D	249	ASN
2	D	257	VAL
2	D	281	GLN
2	D	282	GLN
2	D	293	GLN
2	D	295	MET
2	D	299	LYS
2	D	318	ILE
2	D	322	ARG
2	D	344	VAL
2	D	345	GLU
2	D	382	THR

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Mol	Chain	Res	Type
2	D	400	ARG
2	D	423	SER
2	D	430	SER
2	D	439	THR
3	E	5	ASP
3	E	13	LYS
3	E	25	LYS
3	E	32	VAL
3	E	53	LYS
3	E	54	LEU
3	E	55	GLU
3	E	58	GLU
3	E	71	HIS
3	E	103	GLN
3	E	105	MET
3	E	112	ARG
3	E	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	293	ASN
1	A	356	ASN
1	A	372	GLN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	85	GLN
2	B	133	GLN
2	B	193	GLN
2	B	258	ASN
2	B	331	GLN
2	B	406	HIS
1	C	101	ASN
1	C	300	ASN
1	C	393	HIS
2	D	14	ASN
2	D	15	GLN
2	D	50	ASN
2	D	85	GLN

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Mol	Chain	Res	Type
2	D	193	GLN
2	D	281	GLN
2	D	331	GLN
2	D	339	ASN
2	D	433	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	SO4	B	502	-	4,4,4	0.30	0	6,6,6	0.27	0
8	N9B	B	504[A]	-	27,27,27	0.51	0	30,39,39	0.53	0
4	SO4	D	503	-	4,4,4	0.32	0	6,6,6	0.22	0
4	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.07	0
7	GDP	D	504	-	29,30,30	0.65	1 (3%)	45,47,47	0.66	0
4	SO4	D	502	-	4,4,4	0.38	0	6,6,6	0.18	0
4	SO4	C	502	-	4,4,4	0.29	0	6,6,6	0.08	0
8	N9B	D	505	-	27,27,27	0.55	0	30,39,39	0.70	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	501	-	4,4,4	0.26	0	6,6,6	0.13	0
7	GDP	B	503	-	29,30,30	0.59	0	45,47,47	0.65	1 (2%)
5	GTP	A	502	6	33,34,34	0.51	0	50,54,54	0.56	1 (2%)
4	SO4	A	501	-	4,4,4	0.37	0	6,6,6	0.09	0
5	GTP	C	503	6	33,34,34	0.42	0	50,54,54	0.57	1 (2%)

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
8	N9B	B	504[A]	-	-	1/8/20/20	0/3/3/3
7	GDP	D	504	-	-	3/16/32/32	0/3/3/3
8	N9B	D	505	-	-	1/8/20/20	0/3/3/3
7	GDP	B	503	-	-	6/16/32/32	0/3/3/3
5	GTP	A	502	6	-	7/22/38/38	0/3/3/3
5	GTP	C	503	6	-	6/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	504	GDP	PB-O2B	-2.43	1.45	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	505	N9B	C3-C2-C1	2.42	117.13	111.56
7	B	503	GDP	O2A-PA-O5'	2.13	117.23	107.57
5	C	503	GTP	O2B-PB-O3A	2.05	112.82	107.27
5	A	502	GTP	O5'-PA-O1A	2.03	116.99	108.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	GTP	C5'-O5'-PA-O3A
5	A	502	GTP	C5'-O5'-PA-O1A
5	A	502	GTP	C5'-O5'-PA-O2A
5	C	503	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
5	C	503	GTP	C5'-O5'-PA-O3A
5	C	503	GTP	C5'-O5'-PA-O1A
5	C	503	GTP	C5'-O5'-PA-O2A
7	B	503	GDP	C5'-O5'-PA-O3A
7	B	503	GDP	C5'-O5'-PA-O1A
7	B	503	GDP	C5'-O5'-PA-O2A
7	D	504	GDP	C5'-O5'-PA-O3A
7	D	504	GDP	C5'-O5'-PA-O1A
7	D	504	GDP	C5'-O5'-PA-O2A
8	B	504[A]	N9B	C7-C5-O-C6
5	A	502	GTP	PB-O3B-PG-O1G
7	B	503	GDP	C4'-C5'-O5'-PA
7	B	503	GDP	PB-O3A-PA-O1A
8	D	505	N9B	C7-C5-O-C6
5	A	502	GTP	PB-O3B-PG-O2G
5	A	502	GTP	PB-O3B-PG-O3G
5	C	503	GTP	PB-O3B-PG-O3G
5	A	502	GTP	C4'-C5'-O5'-PA
5	C	503	GTP	PB-O3B-PG-O1G
7	B	503	GDP	PB-O3A-PA-O2A

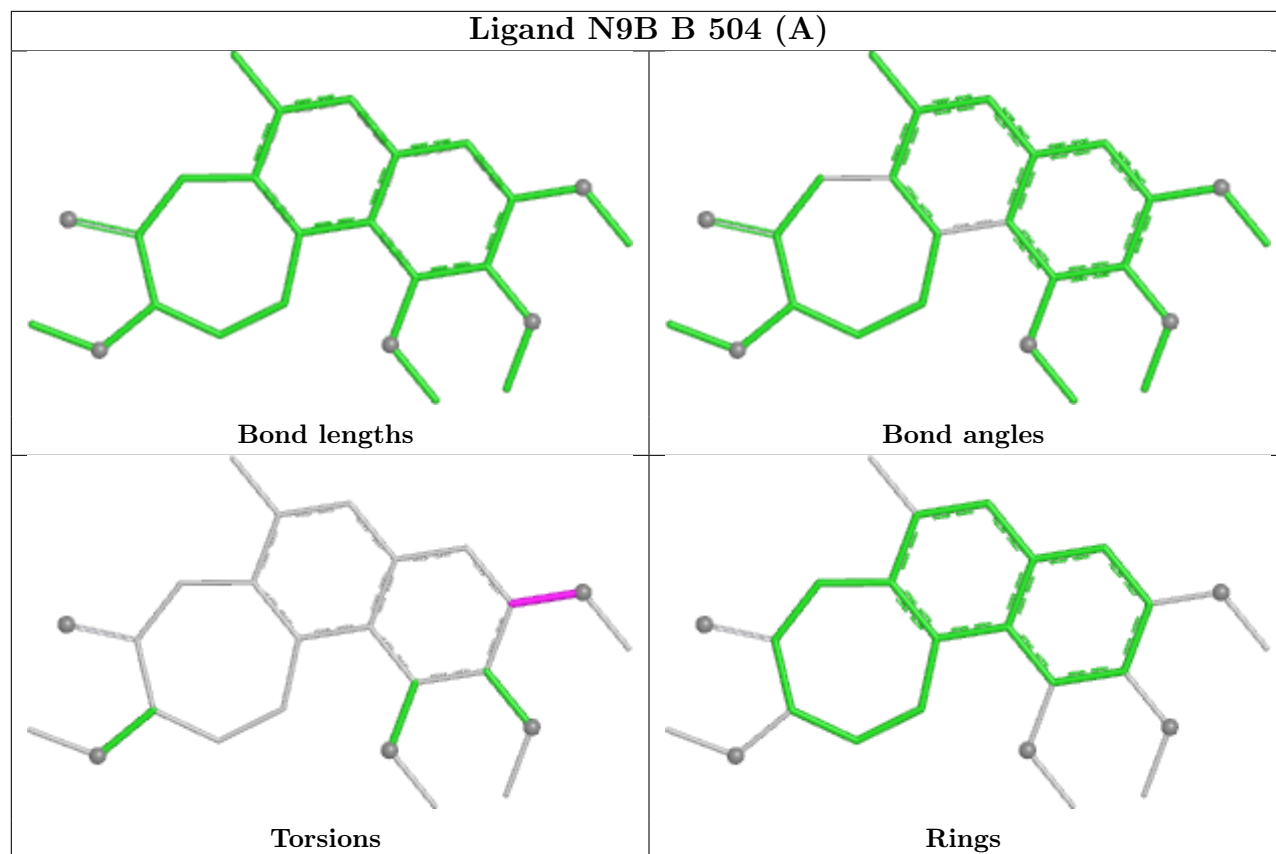
There are no ring outliers.

3 monomers are involved in 3 short contacts:

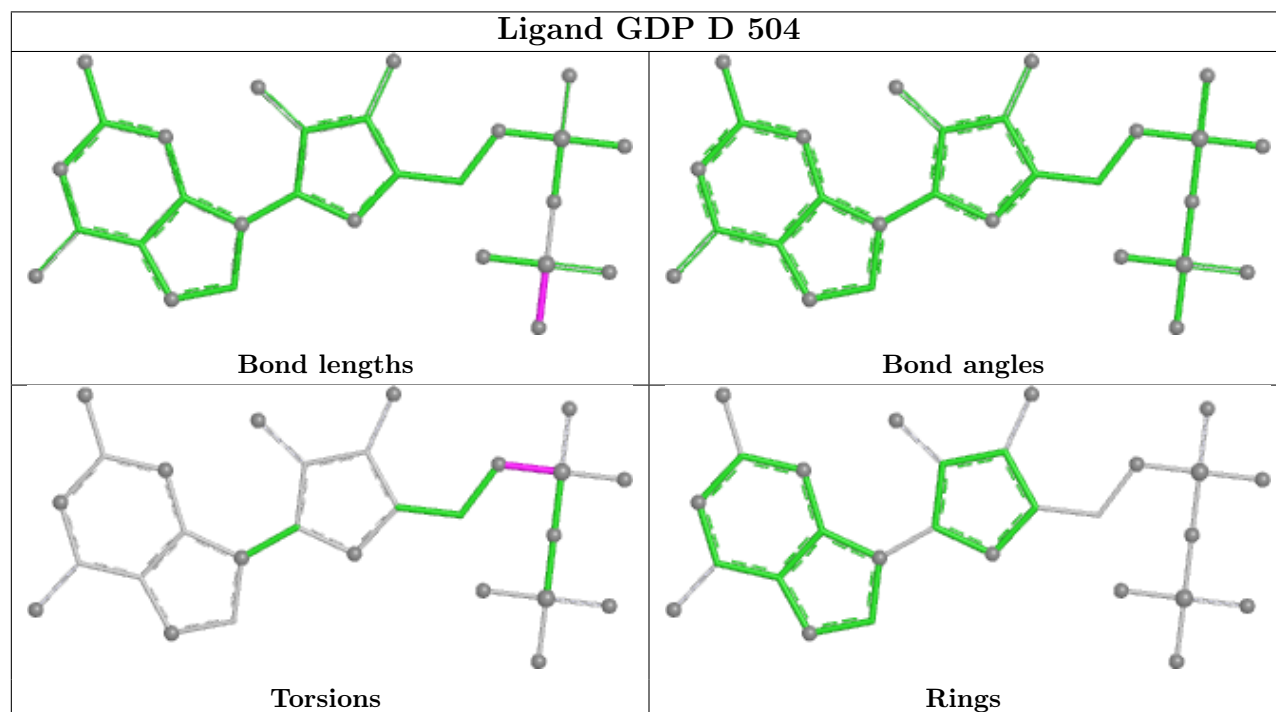
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	SO4	1	0
8	D	505	N9B	1	0
4	A	501	SO4	1	0

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 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.

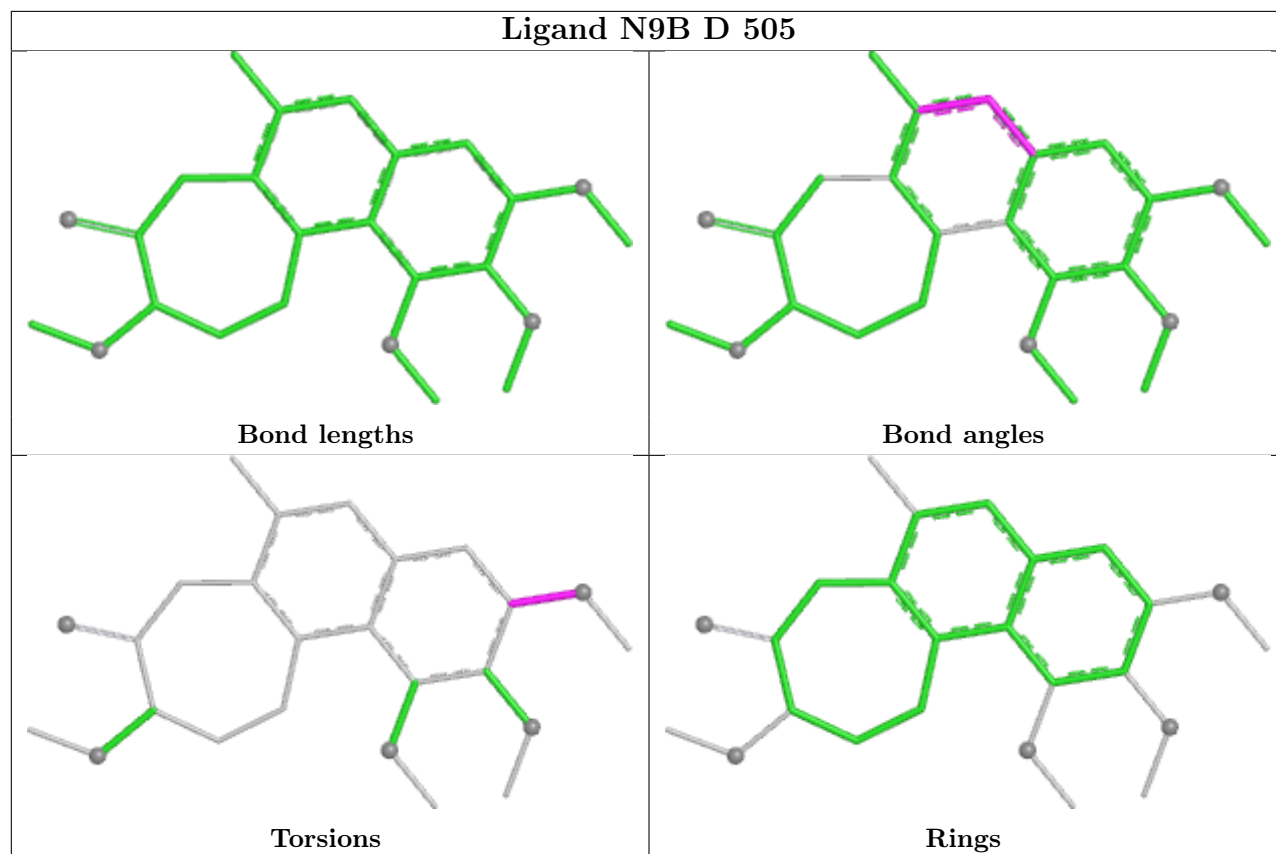
Ligand N9B B 504 (A)



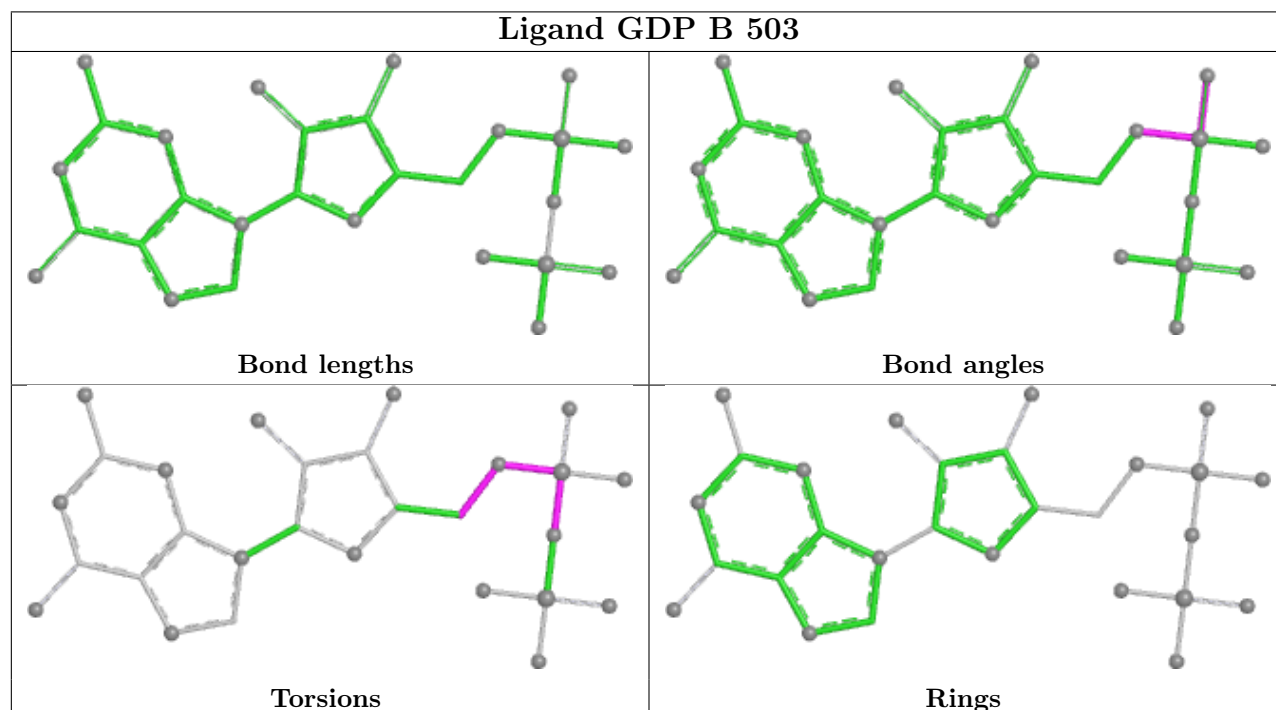
Ligand GDP D 504



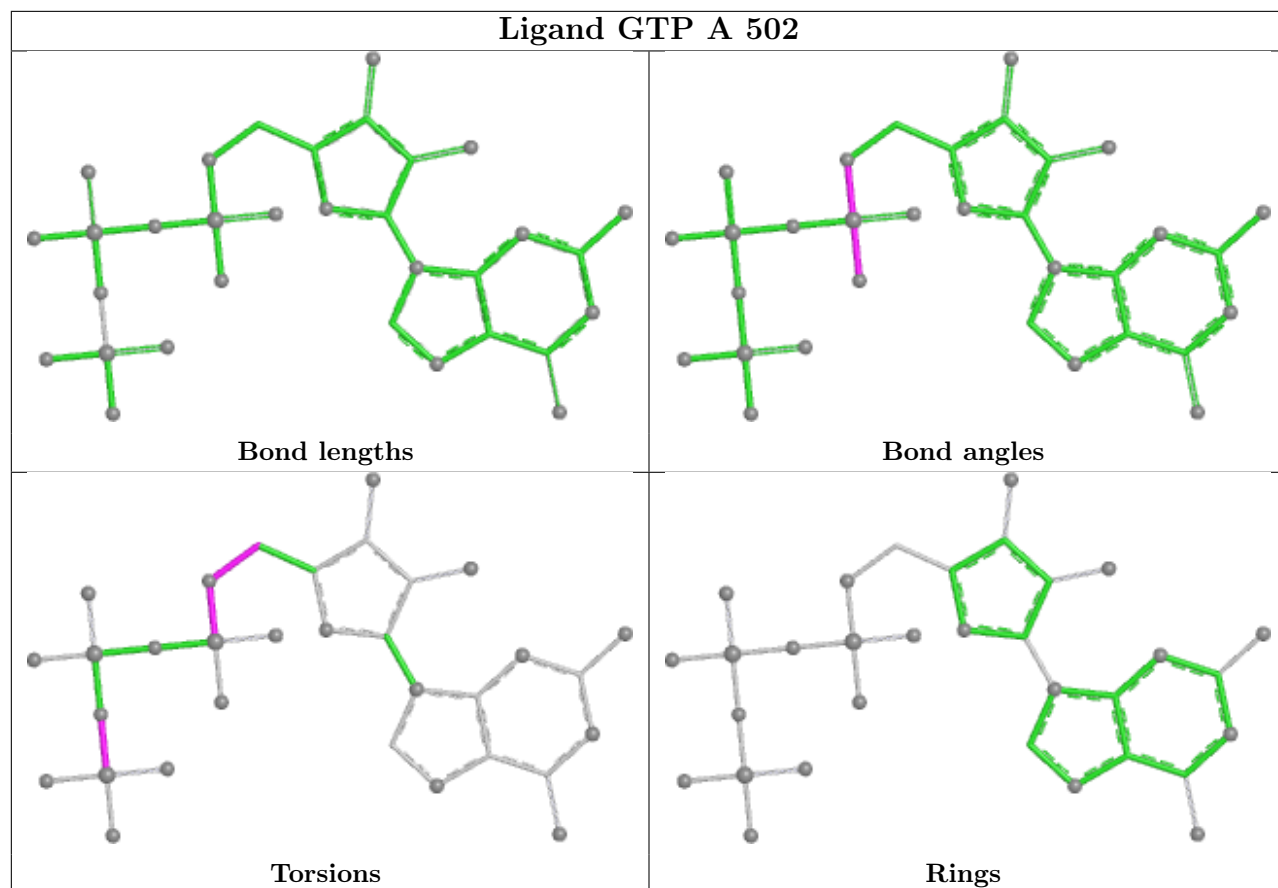
Ligand N9B D 505



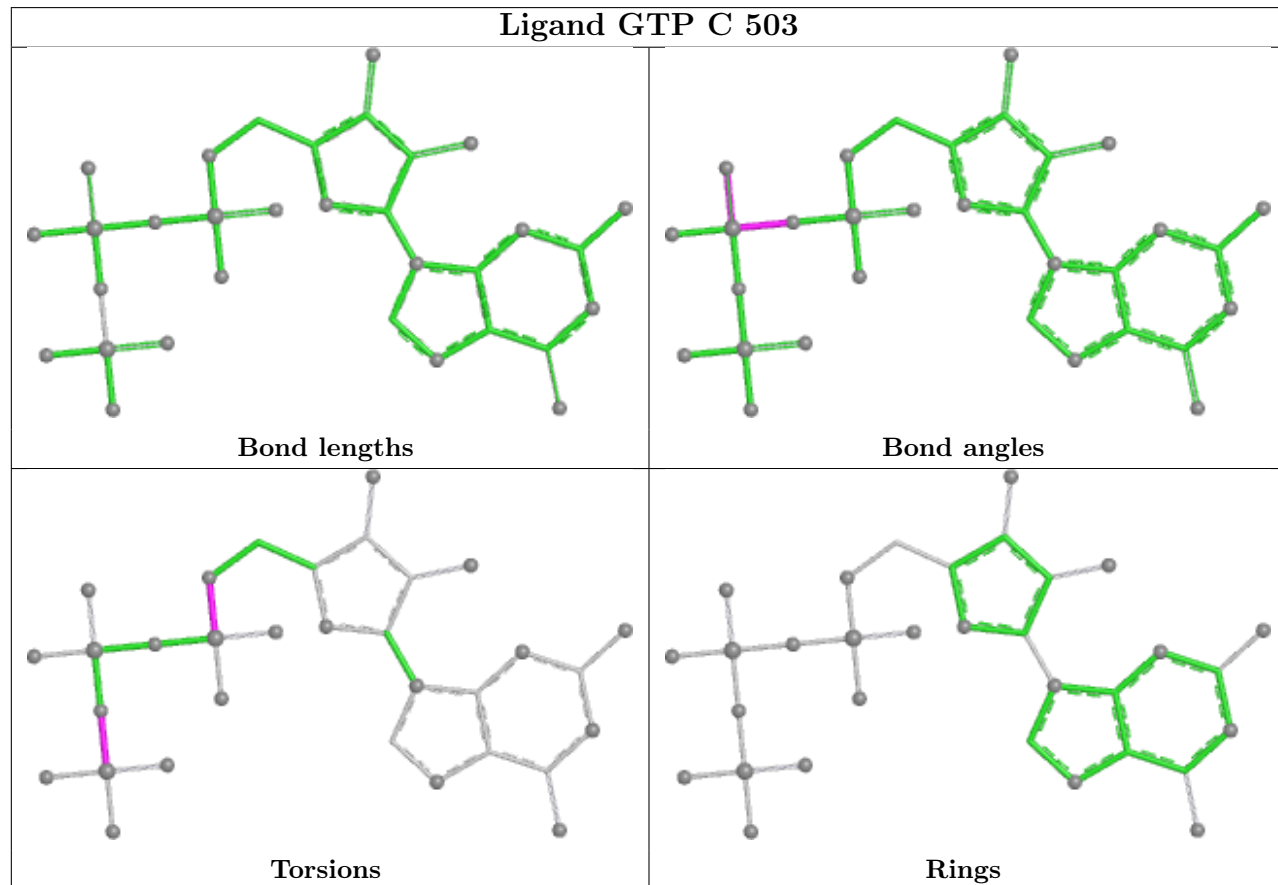
Ligand GDP B 503



Ligand GTP A 502



Ligand GTP C 503



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	428/451 (94%)	0.91	56 (13%) 7 8	41, 73, 106, 135	0
1	C	434/451 (96%)	0.51	24 (5%) 30 33	37, 57, 82, 99	0
2	B	428/445 (96%)	0.76	38 (8%) 15 16	34, 63, 112, 135	7 (1%)
2	D	429/445 (96%)	0.47	23 (5%) 31 34	22, 52, 87, 102	5 (1%)
3	E	128/143 (89%)	1.46	32 (25%) 2 2	63, 88, 126, 132	0
All	All	1847/1935 (95%)	0.72	173 (9%) 14 15	22, 63, 104, 135	12 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	8	VAL	5.0
1	C	349	THR	4.4
1	C	255	PHE	4.4
1	A	337	THR	4.4
2	B	249[A]	ASN	4.3
2	B	286	LEU	4.0
3	E	123	LEU	4.0
2	B	94	PHE	4.0
2	D	97	SER	3.9
1	A	440	VAL	3.8
1	A	65	ALA	3.8
2	D	57	THR	3.8
1	A	1	MET	3.7
2	B	78	VAL	3.7
2	B	285	ALA	3.6
2	B	52	TYR	3.6
2	D	179[A]	ASP	3.6
3	E	117	ALA	3.5
1	A	341	ILE	3.5
1	C	440	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	3.4
2	D	279	GLY	3.4
1	C	281	ALA	3.4
1	A	38	SER	3.3
3	E	33	PRO	3.3
2	B	246[A]	GLY	3.3
2	B	1	MET	3.3
1	C	1	MET	3.3
1	C	38	SER	3.2
1	A	324	VAL	3.2
1	C	108	TYR	3.2
3	E	32	VAL	3.2
1	A	332	ILE	3.2
1	A	335	ILE	3.2
3	E	116	LEU	3.1
1	A	66	VAL	3.1
1	A	362	VAL	3.1
3	E	120	LEU	3.1
3	E	139	LEU	3.1
3	E	47	LEU	3.1
3	E	45	PRO	3.0
2	B	172	MET	3.0
3	E	9	ILE	3.0
1	A	125	LEU	2.9
1	C	335	ILE	2.9
2	B	250[A]	ALA	2.9
3	E	66	ALA	2.9
1	A	353	VAL	2.8
3	E	136	ASN	2.8
1	A	302	MET	2.8
2	B	56	ALA	2.8
3	E	4	ALA	2.8
2	B	248[A]	LEU	2.8
2	D	42	LEU	2.8
2	B	241	CYS	2.8
1	A	276	ILE	2.8
3	E	115	HIS	2.8
3	E	105	MET	2.8
1	A	134	GLY	2.8
1	A	45	GLY	2.7
2	D	333	LEU	2.7
2	B	33	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	247[A]	GLN	2.7
2	D	250	ALA	2.7
2	B	291	LEU	2.7
1	C	356	ASN	2.7
2	D	249	ASN	2.7
3	E	50	ILE	2.7
1	A	346	TRP	2.7
2	B	284	ARG	2.7
1	A	364	PRO	2.7
2	D	281	GLN	2.6
1	A	132	LEU	2.6
1	A	359	PRO	2.6
2	D	282	GLN	2.6
1	A	388	TRP	2.6
2	D	118	VAL	2.6
1	C	247	ALA	2.5
2	B	74	THR	2.5
1	A	242	LEU	2.5
1	A	51	THR	2.5
2	D	247	GLN	2.5
3	E	18	GLN	2.5
2	B	358	ILE	2.5
1	A	361	THR	2.5
2	D	286	LEU	2.5
2	D	337	ASN	2.5
2	B	4	ILE	2.5
2	B	62	VAL	2.4
2	D	172	MET	2.4
3	E	118	ALA	2.4
1	A	283	HIS	2.4
1	C	350	GLY	2.4
1	A	437	VAL	2.4
2	B	338	LYS	2.4
1	C	283	HIS	2.4
3	E	101	LEU	2.4
2	B	48	ARG	2.4
3	E	119	MET	2.4
2	B	280	SER	2.4
1	A	83	TYR	2.3
1	C	52	PHE	2.3
2	D	325	MET	2.3
1	A	330	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	286	LEU	2.3
2	D	335	VAL	2.3
3	E	124	GLN	2.3
1	A	221	ARG	2.3
1	A	308	ARG	2.3
1	A	368	LEU	2.3
1	A	52	PHE	2.3
2	B	335	VAL	2.3
1	A	289	ALA	2.3
1	A	219	ILE	2.2
1	A	118	VAL	2.2
1	C	45	GLY	2.2
2	B	129	CYS	2.2
2	D	416	MET	2.2
1	C	351	PHE	2.2
3	E	133	VAL	2.2
2	B	295	MET	2.2
1	A	126	ALA	2.2
1	A	196	GLU	2.2
3	E	54	LEU	2.2
2	B	298	SER	2.2
1	C	280	LYS	2.2
1	A	32	PRO	2.2
1	A	360	PRO	2.2
2	D	318	ILE	2.2
3	E	87	ILE	2.2
1	A	363	VAL	2.2
1	A	333	ALA	2.2
3	E	96	MET	2.2
1	C	127	ASP	2.2
1	A	355	ILE	2.1
2	B	296	PHE	2.1
2	B	181	VAL	2.1
1	C	134	GLY	2.1
2	B	334	ASN	2.1
2	B	416	MET	2.1
3	E	44	ASP	2.1
1	A	37	PRO	2.1
3	E	29	PHE	2.1
1	A	177	VAL	2.1
1	A	371	VAL	2.1
2	D	51	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	64	ARG	2.1
2	B	71	GLU	2.1
1	A	108	TYR	2.1
1	A	274	PRO	2.1
3	E	20	TRP	2.1
2	D	93	VAL	2.1
3	E	75	LYS	2.1
2	B	153	LEU	2.1
2	B	325	MET	2.1
1	A	56	THR	2.1
3	E	53	LYS	2.1
1	A	87	PHE	2.1
2	D	23	VAL	2.1
3	E	16	SER	2.1
1	C	366	GLY	2.0
1	A	122	ILE	2.0
1	A	323	VAL	2.0
1	C	363	VAL	2.0
1	A	331	ALA	2.0
2	B	322	ARG	2.0
1	C	4	CYS	2.0
1	A	326	LYS	2.0
1	A	336	LYS	2.0
1	C	37	PRO	2.0
1	C	348	PRO	2.0
2	B	287	THR	2.0
2	D	74	THR	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,

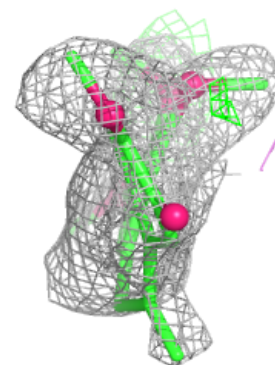
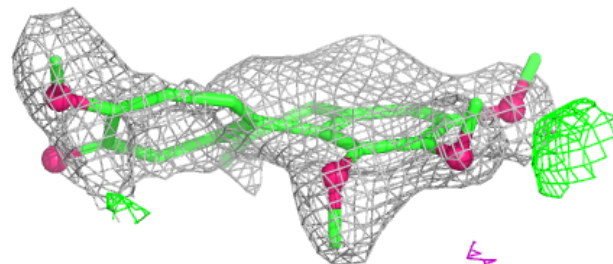
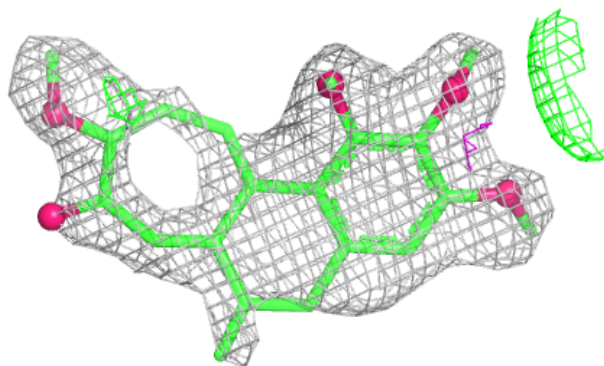
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	502	5/5	0.58	0.15	172,172,172,172	0
4	SO4	C	501	5/5	0.60	0.10	150,151,151,151	0
4	SO4	A	501	5/5	0.63	0.11	124,124,124,124	0
4	SO4	D	503	5/5	0.70	0.18	157,157,157,157	0
4	SO4	B	501	5/5	0.76	0.11	144,145,145,145	0
4	SO4	D	502	5/5	0.82	0.14	118,118,118,118	0
8	N9B	B	504[A]	25/25	0.87	0.13	44,46,47,47	25
4	SO4	B	502	5/5	0.89	0.07	98,98,98,98	0
8	N9B	D	505	25/25	0.94	0.09	50,51,52,53	0
5	GTP	C	503	32/32	0.97	0.06	43,45,45,45	0
7	GDP	B	503	28/28	0.97	0.06	51,52,53,53	0
7	GDP	D	504	28/28	0.98	0.05	40,41,43,43	0
6	MG	D	501	1/1	0.98	0.06	46,46,46,46	0
5	GTP	A	502	32/32	0.98	0.05	47,48,49,49	0
6	MG	A	503	1/1	1.00	0.02	50,50,50,50	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.

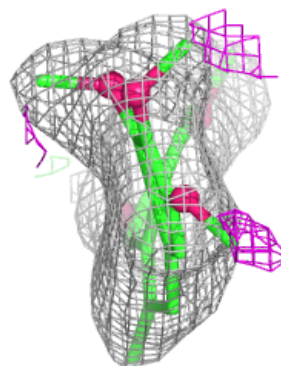
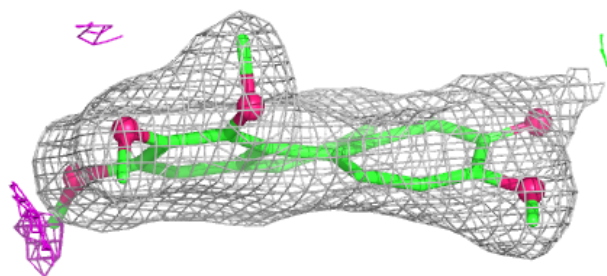
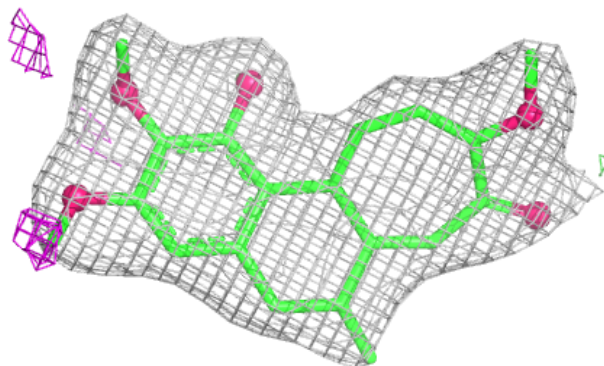
Electron density around N9B B 504 (A):

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

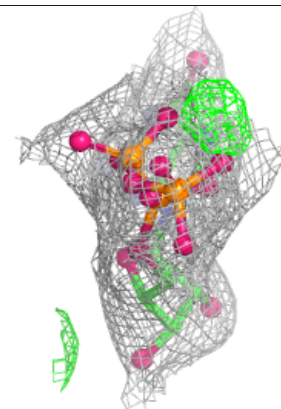
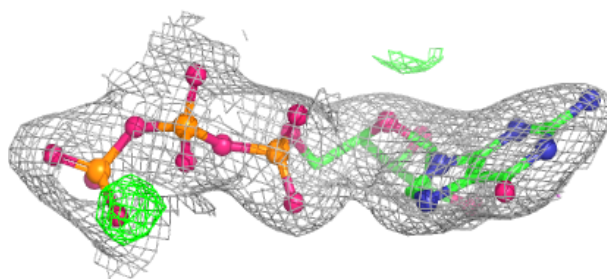
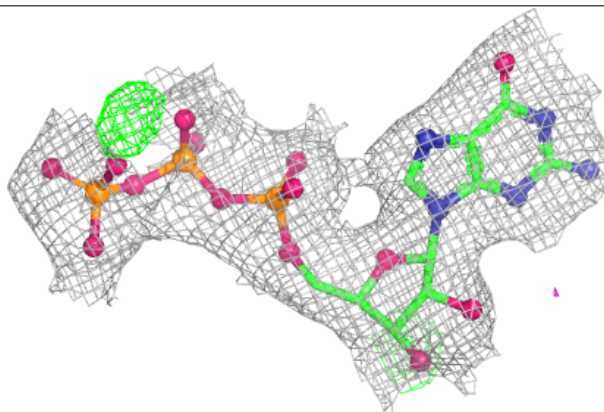


Electron density around N9B D 505:

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

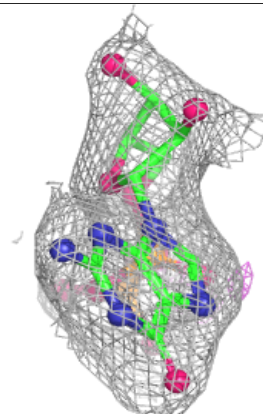
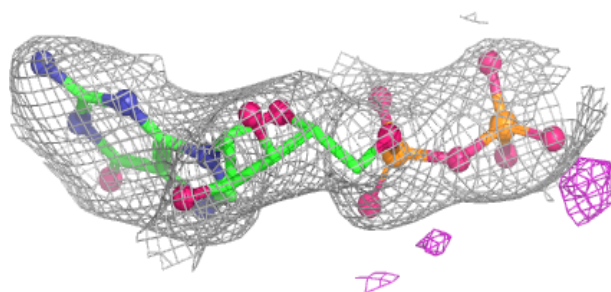
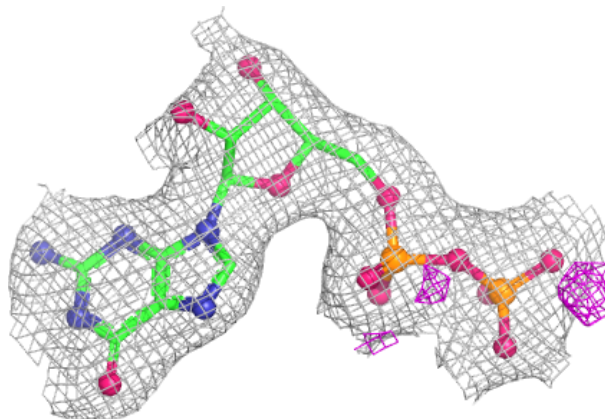
**Electron density around GTP C 503:**

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



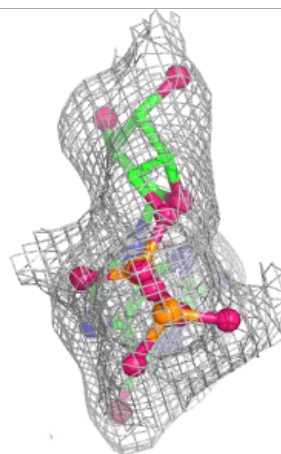
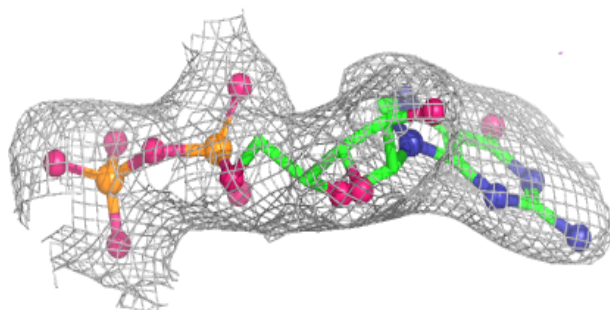
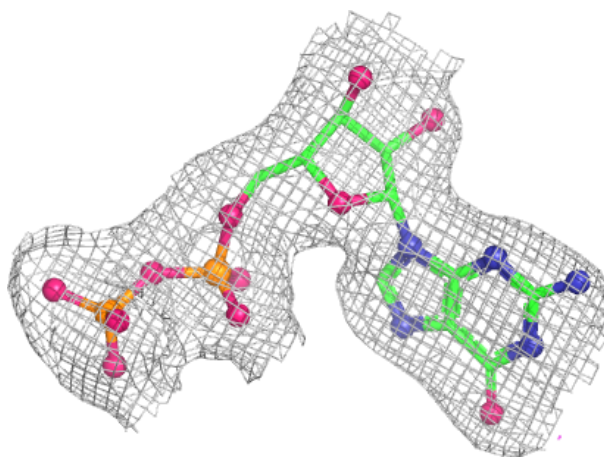
Electron density around GDP B 503:

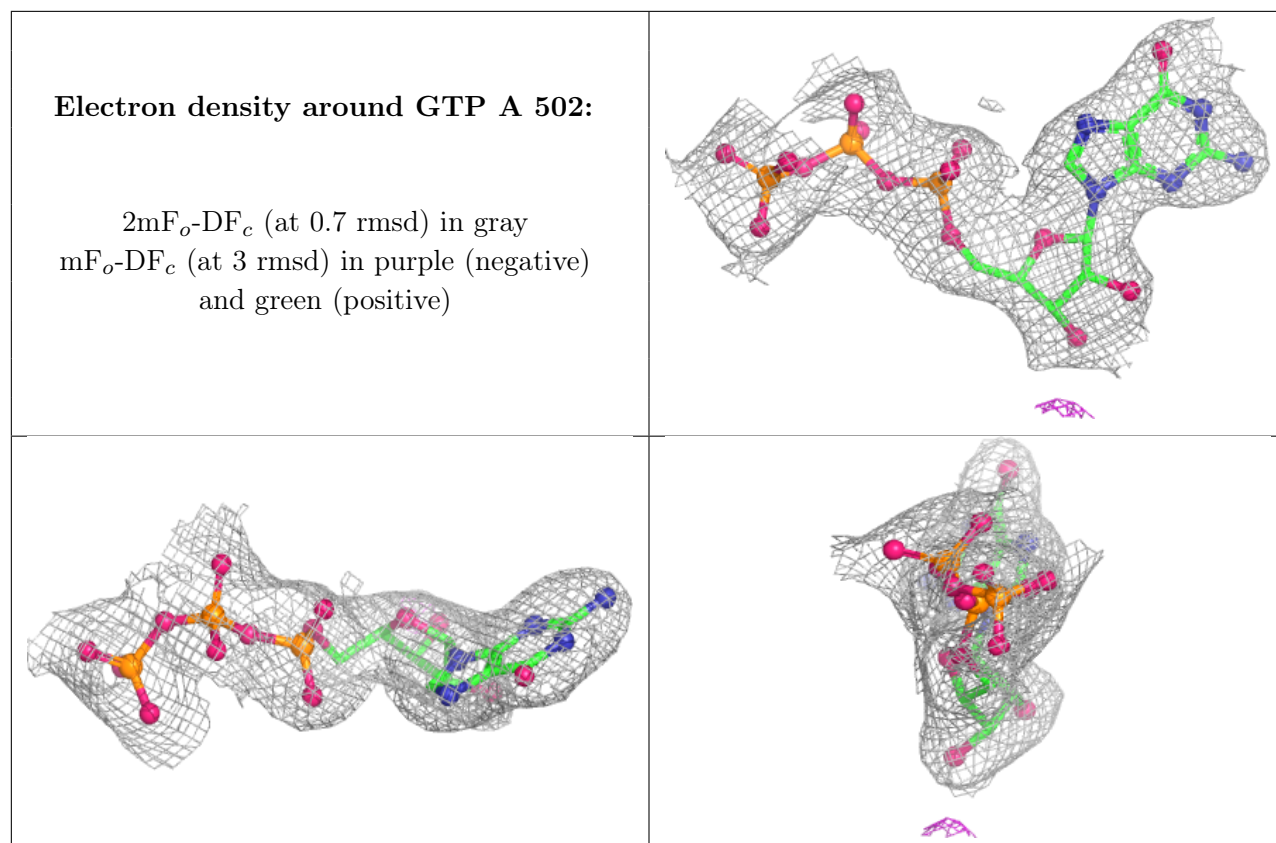
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP D 504:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.