



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 PM UTC

PDB ID : 6TDE / pdb_00006tde
Title : Tubulin-inhibitor complex
Authors : Varela, P.F.; Gigant, B.
Deposited on : 2019-11-08
Resolution : 2.29 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

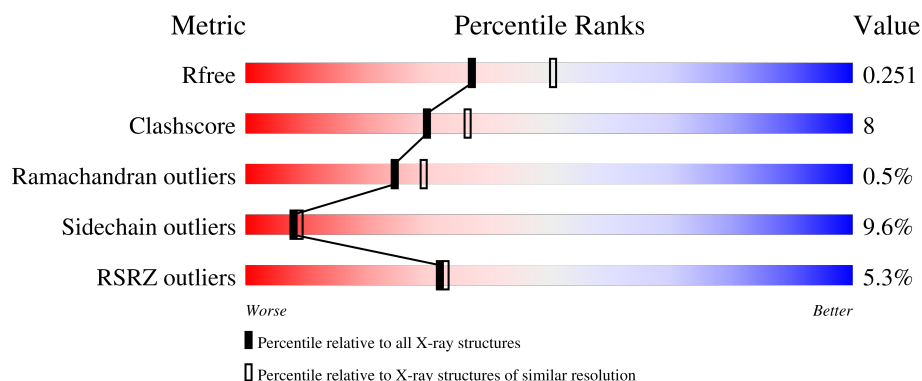
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	5% 73% 19% • •
1	C	451	4% 76% 18% • •
2	B	445	5% 71% 20% • • •
2	D	445	4% 75% 18% • •
3	E	143	12% 73% 17% • 8%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15022 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	434	Total	C	N	O	S	0	0	0
			3390	2145	577	646	22			
1	C	434	Total	C	N	O	S	0	0	0
			3397	2151	577	647	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3375	2116	576	656	27			
2	D	429	Total	C	N	O	S	0	3	0
			3387	2122	578	660	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	131	Total	C	N	O	S	0	0	0
			1075	664	195	212	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	-	expression tag	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	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).

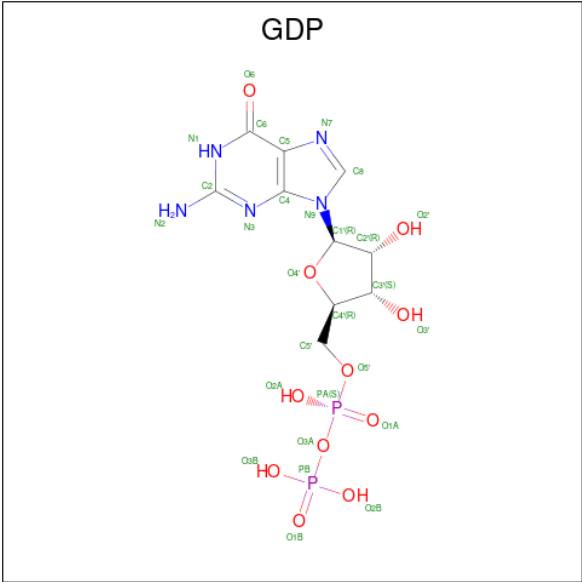


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

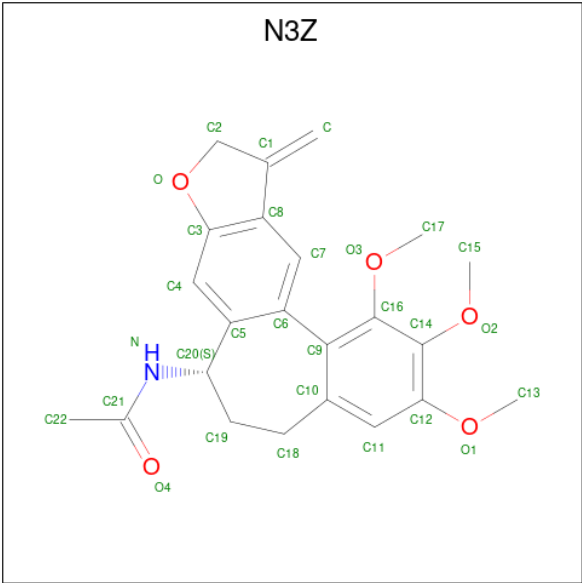
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- 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 {N}-[(10 {S})-3,4,5-trimethoxy-16-methylidene-14-oxatetracyclo[9.7.0.0[^]{2,7}.0[^]{13,17}]octadeca-1(18),2,4,6,11,13(17)-hexaen-10-yl]ethanamide (CCD ID: N3Z) (formula: C₂₃H₂₅NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O		0	0
			29	23	1	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			29	23	1	5		

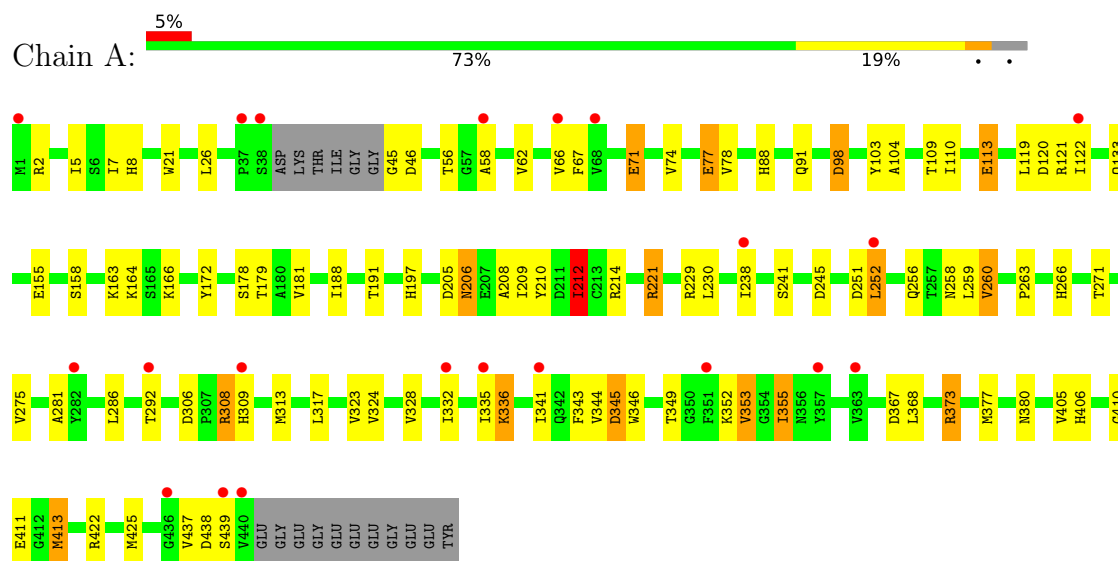
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	39	Total	O	0	0
			39	39		
9	B	31	Total	O	0	0
			31	31		
9	C	54	Total	O	0	0
			54	54		
9	D	34	Total	O	0	0
			34	34		
9	E	15	Total	O	0	0
			15	15		

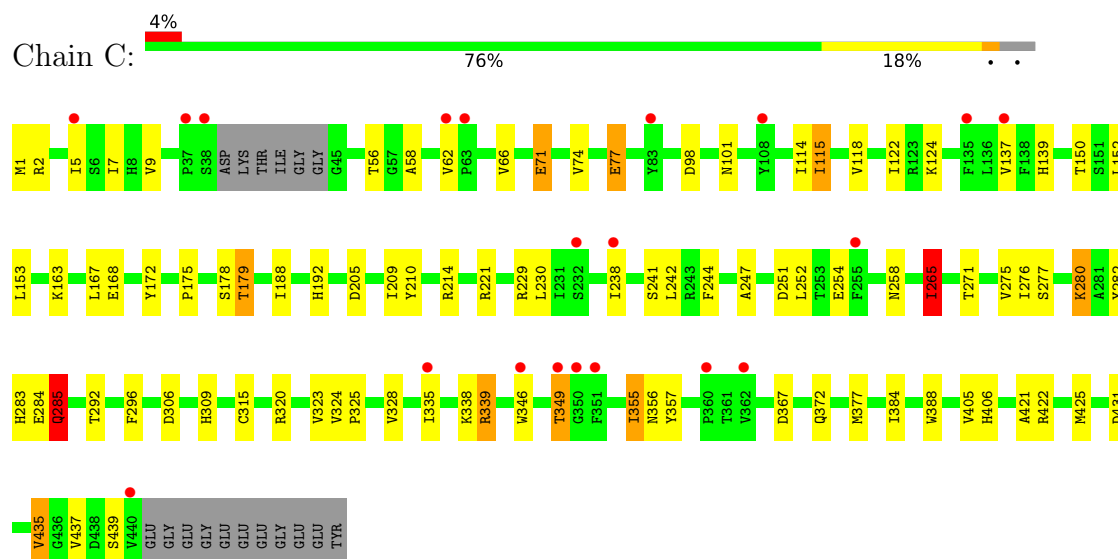
3 Residue-property plots [i](#)

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.

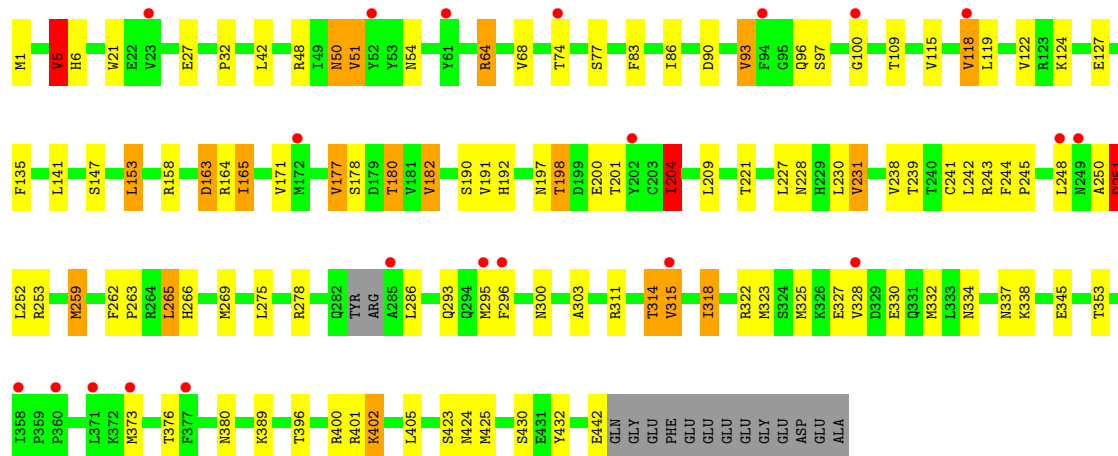
• Molecule 1: Tubulin alpha chain



• Molecule 1: Tubulin alpha chain



• Molecule 2: Tubulin beta chain



Residue	Score	Conservation	Annotations
S430	0.00	0.00	
D441	0.00	0.00	
GLU	0.00	0.00	
GLN	0.00	0.00	
GLY	0.00	0.00	
GLU	0.00	0.00	
PHE	0.00	0.00	
GLU	0.00	0.00	
GLU	0.00	0.00	
GLU	0.00	0.00	
GLU	0.00	0.00	
GLY	0.00	0.00	
GLU	0.00	0.00	
ASP	0.00	0.00	
GLU	0.00	0.00	
ALA	0.00	0.00	
M289	0.00	0.00	
L275	0.00	0.00	
T276	0.00	0.00	
S277	0.00	0.00	
R278	0.00	0.00	
Q281	0.00	0.00	
Q282	0.00	0.00	
TYR	0.00	0.00	
ARG	0.00	0.00	
A285	0.00	0.00	
L286	0.00	0.00	
Q293	0.00	0.00	
Q294	0.00	0.00	
M295	0.00	0.00	
F296	0.00	0.00	
M301	0.00	0.00	
M302	0.00	0.00	
A303	0.00	0.00	
T314	0.00	0.00	
V315	0.00	0.00	
R322	0.00	0.00	
M323	0.00	0.00	
S324	0.00	0.00	
M325	0.00	0.00	
K326	0.00	0.00	
E327	0.00	0.00	
E330	0.00	0.00	
M334	0.00	0.00	
N337	0.00	0.00	
K338	0.00	0.00	
N349	0.00	0.00	
R369	0.00	0.00	
M373	0.00	0.00	
N380	0.00	0.00	
L387	0.00	0.00	
F388	0.00	0.00	
M398	0.00	0.00	
F399	0.00	0.00	
K402	0.00	0.00	
S423	0.00	0.00	
N424	0.00	0.00	
M425	0.00	0.00	
T145	0.00	0.00	
G146	0.00	0.00	
S147	0.00	0.00	
G148	0.00	0.00	
M149	0.00	0.00	
G150	0.00	0.00	
T151	0.00	0.00	
L152	0.00	0.00	
L153	0.00	0.00	
I154	0.00	0.00	
R158	0.00	0.00	
D163	0.00	0.00	
M172	0.00	0.00	
D179	0.00	0.00	
T180	0.00	0.00	
V181	0.00	0.00	
V182	0.00	0.00	
E183	0.00	0.00	
S190	0.00	0.00	
V191	0.00	0.00	
H192	0.00	0.00	
T198	0.00	0.00	
D199	0.00	0.00	
E200	0.00	0.00	
T201	0.00	0.00	
D226	0.00	0.00	
H229	0.00	0.00	
L230	0.00	0.00	
V238	0.00	0.00	
C241	0.00	0.00	
P245	0.00	0.00	
L248	0.00	0.00	
N249	0.00	0.00	
A250	0.00	0.00	
D251	0.00	0.00	
L252	0.00	0.00	
R253	0.00	0.00	
K254	0.00	0.00	
V257	0.00	0.00	
N258	0.00	0.00	
M259	0.00	0.00	
P263	0.00	0.00	
N264	0.00	0.00	
M425	0.00	0.00	
H266	0.00	0.00	
V5	0.00	0.00	
H6	0.00	0.00	
I7	0.00	0.00	
Q8	0.00	0.00	
N14	0.00	0.00	
W21	0.00	0.00	
I30	0.00	0.00	
H37	0.00	0.00	
L42	0.00	0.00	
R48	0.00	0.00	
I49	0.00	0.00	
N50	0.00	0.00	
Y53	0.00	0.00	
T57	0.		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.48Å 128.14Å 251.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.29 45.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	51.9 (45.00-2.29) 51.8 (45.00-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (23-SEP-2019)	Depositor
R, R_{free}	0.198 , 0.232 (Not available) , 0.251	Depositor DCC
R_{free} test set	2431 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.7	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	15022	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, N3Z, 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	0.72	2/3466 (0.1%)	1.06	4/4705 (0.1%)
1	C	0.70	0/3474	1.06	7/4716 (0.1%)
2	B	0.75	2/3448 (0.1%)	1.07	6/4669 (0.1%)
2	D	0.77	5/3460 (0.1%)	1.07	6/4686 (0.1%)
3	E	0.67	0/1086	1.10	1/1444 (0.1%)
All	All	0.73	9/14934 (0.1%)	1.07	24/20220 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	425	MET	SD-CE	-8.77	1.57	1.79
2	D	109	THR	CA-C	7.97	1.57	1.52
1	A	212	ILE	CG1-CD1	-7.79	1.21	1.51
2	B	109	THR	CA-C	6.81	1.56	1.52
2	D	301	MET	SD-CE	-5.83	1.65	1.79
2	D	250	ALA	C-N	5.76	1.41	1.33
2	B	204	ILE	CG1-CD1	-5.25	1.31	1.51
1	A	413	MET	SD-CE	-5.19	1.66	1.79
2	D	250	ALA	CA-C	5.03	1.59	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ASP	CA-CB-CG	7.00	119.60	112.60
2	B	5	VAL	N-CA-CB	6.92	119.31	111.21
2	B	251	ASP	CA-CB-CG	6.91	119.51	112.60
2	D	5	VAL	N-CA-CB	6.53	118.85	111.21
2	D	163	ASP	CA-CB-CG	6.16	118.76	112.60
2	D	337	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	98	ASP	CA-CB-CG	5.97	118.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	VAL	N-CA-CB	-5.87	101.54	111.23
1	C	251	ASP	CA-CB-CG	5.82	118.42	112.60
2	D	251	ASP	CA-CB-CG	5.76	118.36	112.60
2	D	249	ASN	CA-C-N	5.74	132.51	121.54
2	D	249	ASN	C-N-CA	5.74	132.51	121.54
2	B	163	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	281	ALA	CA-C-N	5.48	132.01	121.54
1	A	281	ALA	C-N-CA	5.48	132.01	121.54
1	C	285	GLN	CA-C-N	5.36	128.45	120.95
1	C	285	GLN	C-N-CA	5.36	128.45	120.95
2	B	337	ASN	CA-CB-CG	5.30	117.90	112.60
1	C	265	ILE	CB-CA-C	5.14	119.73	111.29
2	B	296	PHE	CA-CB-CG	-5.11	108.69	113.80
3	E	108	ASN	CA-CB-CG	-5.07	107.53	112.60
1	C	284	GLU	CA-C-N	5.07	131.22	121.54
1	C	284	GLU	C-N-CA	5.07	131.22	121.54
1	C	114	ILE	N-CA-CB	-5.01	106.37	112.33

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	3390	0	3300	63	0
1	C	3397	0	3307	56	0
2	B	3375	0	3249	74	0
2	D	3387	0	3258	58	0
3	E	1075	0	1086	15	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	1	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
7	B	28	0	12	0	0
7	D	28	0	12	2	0
8	B	29	0	0	0	0
8	D	29	0	0	0	0
9	A	39	0	0	2	0
9	B	31	0	0	1	0
9	C	54	0	0	0	0
9	D	34	0	0	0	0
9	E	15	0	0	1	0
All	All	15022	0	14248	246	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 (246) 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:48:ARG:O	2:B:51:VAL:HG22	1.61	1.00
2:D:192:HIS:HD2	2:D:424:ASN:HD22	1.09	1.00
1:A:133:GLN:HB3	1:A:252:LEU:HD22	1.49	0.94
1:A:336:LYS:HZ1	3:E:4:ALA:N	1.66	0.93
1:C:338:LYS:NZ	1:C:339:ARG:HH12	1.67	0.92
2:B:165:ILE:HG12	2:B:252:LEU:HB3	1.54	0.89
2:B:171:VAL:HG22	2:B:204:ILE:HG12	1.54	0.89
2:D:198:THR:HG22	2:D:266:HIS:NE2	1.89	0.87
2:B:198:THR:HG22	2:B:266:HIS:NE2	1.90	0.87
1:A:206:ASN:HD21	5:A:502:GTP:HN22	1.24	0.83
1:A:328:VAL:HG11	1:A:353:VAL:HG21	1.59	0.82
2:D:388:PHE:HD1	2:D:425:MET:HE3	1.44	0.82
2:B:192:HIS:HD2	2:B:424:ASN:HD22	1.30	0.80
2:D:48:ARG:HH22	2:D:250:ALA:HB3	1.49	0.78
2:D:259:MET:HE3	2:D:314:THR:HG23	1.66	0.77
2:B:259:MET:HE3	2:B:314:THR:HG23	1.66	0.77
1:A:336:LYS:HB2	3:E:24:LEU:HD13	1.66	0.76
1:C:338:LYS:HZ1	1:C:339:ARG:HH12	1.31	0.76
1:A:323:VAL:HB	1:A:355:ILE:HD13	1.70	0.74
2:B:241:CYS:O	2:B:250:ALA:HB2	1.88	0.74
2:D:151:THR:HA	2:D:154:ILE:HG12	1.71	0.73
2:B:171:VAL:HG22	2:B:204:ILE:CG1	2.18	0.72
1:C:9:VAL:CG1	1:C:139:HIS:HB3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.71	0.72
1:A:109:THR:HG21	1:A:411:GLU:OE2	1.89	0.72
2:D:7:ILE:HG12	2:D:66:ILE:HG12	1.72	0.72
2:D:8:GLN:HE21	2:D:14:ASN:HD22	1.36	0.72
2:D:226:ASP:HA	2:D:278:ARG:HG3	1.70	0.71
1:C:431:ASP:O	1:C:435:VAL:HG23	1.90	0.71
2:B:100:GLY:HA2	1:C:254:GLU:HG3	1.71	0.71
1:C:325:PRO:O	1:C:328:VAL:HG22	1.91	0.71
2:D:68:VAL:HG12	2:D:149:MET:HE1	1.72	0.70
2:B:401:ARG:NH2	1:C:437:VAL:O	2.24	0.70
1:A:56:THR:HG22	1:A:58:ALA:H	1.57	0.70
2:D:66:ILE:HD11	2:D:118:VAL:HG13	1.73	0.70
2:B:50:ASN:O	2:B:64:ARG:NH2	2.25	0.69
1:C:346:TRP:HZ2	1:C:435:VAL:HG12	1.58	0.69
2:D:278:ARG:NH2	4:D:503:SO4:O4	2.25	0.69
2:D:388:PHE:CD1	2:D:425:MET:HE3	2.28	0.69
1:C:9:VAL:HG13	1:C:139:HIS:HB3	1.75	0.68
1:C:163:LYS:HE3	3:E:90:ASN:HA	1.73	0.68
2:B:198:THR:HG21	2:B:201:THR:OG1	1.94	0.68
1:A:74:VAL:O	1:A:77:GLU:HG3	1.94	0.67
2:B:191:VAL:HG21	2:B:425:MET:HE3	1.75	0.67
2:B:259:MET:HA	2:B:314:THR:HG21	1.77	0.67
1:C:74:VAL:O	1:C:77:GLU:HG3	1.95	0.67
2:D:241:CYS:O	2:D:250:ALA:HB2	1.94	0.66
2:D:198:THR:HG21	2:D:201:THR:OG1	1.96	0.66
2:B:54:ASN:OD1	2:B:64:ARG:NH1	2.29	0.66
2:B:48:ARG:HH22	2:B:250:ALA:HB3	1.61	0.65
2:B:228:ASN:HA	2:B:231:VAL:HG13	1.78	0.65
1:A:336:LYS:NZ	3:E:4:ALA:N	2.42	0.65
1:C:338:LYS:HZ2	1:C:339:ARG:HH12	1.42	0.65
1:A:308:ARG:HE	1:A:309:HIS:CD2	2.14	0.65
1:C:56:THR:HG22	1:C:58:ALA:H	1.61	0.65
2:B:300:ASN:HB3	9:B:604:HOH:O	1.96	0.64
2:B:262:PHE:HB2	2:B:265:LEU:HD23	1.80	0.64
1:C:276:ILE:HG12	1:C:280:LYS:HE3	1.79	0.64
1:C:9:VAL:HG11	1:C:150:THR:OG1	1.98	0.64
1:A:208:ALA:O	1:A:212:ILE:HG22	1.98	0.63
2:D:259:MET:HA	2:D:314:THR:HG21	1.78	0.63
2:D:8:GLN:HE21	2:D:14:ASN:ND2	1.96	0.62
2:D:192:HIS:HD2	2:D:424:ASN:ND2	1.88	0.61
2:D:192:HIS:CD2	2:D:424:ASN:HD22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:HE22	1:A:251:ASP:HB2	1.67	0.60
2:B:180:THR:HA	1:C:258:ASN:HD21	1.65	0.60
2:D:82:PRO:O	2:D:83:PHE:HB2	2.01	0.59
2:B:83:PHE:O	2:B:86:ILE:HG12	2.02	0.59
2:B:332:MET:HG3	2:B:353:THR:HG21	1.85	0.59
1:C:338:LYS:HZ2	1:C:339:ARG:HH22	1.48	0.59
2:B:318:ILE:HG23	2:B:376:THR:HB	1.85	0.58
1:A:103:TYR:HD1	1:A:413:MET:HE1	1.69	0.57
2:B:119:LEU:O	2:B:122:VAL:HG22	2.04	0.57
1:C:338:LYS:HZ2	1:C:339:ARG:NH1	2.00	0.57
2:B:27:GLU:OE1	2:B:243:ARG:NH2	2.37	0.57
2:D:388:PHE:HD1	2:D:425:MET:CE	2.14	0.57
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.87	0.56
1:C:346:TRP:CZ2	1:C:435:VAL:HG12	2.40	0.56
1:A:163:LYS:HG3	1:A:164:LYS:HD2	1.88	0.56
1:C:306:ASP:OD2	1:C:309:HIS:ND1	2.38	0.56
2:B:68:VAL:HG22	2:B:93:VAL:HG13	1.88	0.56
1:C:66:VAL:HG21	1:C:122:ILE:HD13	1.87	0.56
1:A:221:ARG:HH11	2:B:325:MET:HE2	1.71	0.56
1:C:338:LYS:NZ	1:C:339:ARG:NH1	2.47	0.56
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.87	0.55
2:B:323:MET:HE2	2:B:373:MET:HG2	1.88	0.55
3:E:96:MET:HB3	9:E:214:HOH:O	2.05	0.55
1:A:306:ASP:OD2	1:A:309:HIS:ND1	2.39	0.55
2:B:259:MET:HE3	2:B:314:THR:CG2	2.36	0.55
1:C:9:VAL:HG13	1:C:139:HIS:CB	2.37	0.55
2:D:259:MET:HE3	2:D:314:THR:CG2	2.36	0.55
1:C:296:PHE:CZ	1:C:377:MET:HE1	2.42	0.55
2:D:295:MET:HE2	2:D:315:VAL:HG11	1.88	0.55
1:A:332:ILE:HD13	3:E:22:VAL:HG11	1.89	0.55
2:D:198:THR:HG22	2:D:266:HIS:CD2	2.42	0.55
2:B:192:HIS:CD2	2:B:424:ASN:HD22	2.20	0.55
1:C:115:ILE:HG12	1:C:152:LEU:HD21	1.88	0.55
1:A:158:SER:HB2	1:A:166:LYS:NZ	2.22	0.54
3:E:134:ARG:HH22	3:E:137:LYS:HD3	1.72	0.54
1:A:410:GLY:HA2	3:E:64:GLN:HE22	1.72	0.54
1:A:77:GLU:HG2	9:A:627:HOH:O	2.07	0.54
1:A:191:THR:HG22	1:A:425:MET:HE1	1.90	0.54
1:A:166:LYS:HE3	1:A:197:HIS:O	2.08	0.53
1:A:133:GLN:HB3	1:A:252:LEU:CD2	2.32	0.53
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:LYS:HZ2	1:C:339:ARG:NH2	2.05	0.53
2:B:198:THR:HG22	2:B:266:HIS:CD2	2.43	0.53
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.90	0.53
2:B:197:ASN:HD21	3:E:75:LYS:NZ	2.07	0.53
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.28	0.52
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.91	0.52
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.44	0.52
2:B:295:MET:HE2	2:B:315:VAL:HG11	1.90	0.52
1:A:308:ARG:NE	1:A:309:HIS:CD2	2.77	0.52
2:D:323:MET:HE2	2:D:373:MET:HG2	1.90	0.52
1:A:158:SER:HB2	1:A:166:LYS:HZ1	1.75	0.52
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.92	0.52
1:A:286:LEU:O	1:A:373:ARG:HD3	2.10	0.52
1:C:323:VAL:HB	1:C:355:ILE:HD13	1.90	0.52
2:D:1:MET:CE	2:D:253:ARG:HE	2.23	0.52
2:B:177:VAL:HG21	2:B:227:LEU:HD11	1.91	0.51
2:B:204:ILE:HG13	2:B:204:ILE:O	2.09	0.51
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.36	0.51
1:C:325:PRO:HA	1:C:328:VAL:HG22	1.92	0.51
1:C:247:ALA:HB2	1:C:357:TYR:CZ	2.46	0.51
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.94	0.50
2:B:1:MET:CE	2:B:253:ARG:HE	2.24	0.50
1:C:265:ILE:HG13	1:C:265:ILE:O	2.10	0.50
2:D:399:PHE:O	2:D:402:LYS:HD2	2.12	0.50
1:A:313:MET:HG2	1:A:380:ASN:O	2.12	0.49
2:B:259:MET:CA	2:B:314:THR:HG21	2.42	0.49
2:D:48:ARG:HH12	2:D:250:ALA:HB2	1.77	0.49
2:B:197:ASN:HD21	3:E:75:LYS:HZ2	1.60	0.49
2:B:250:ALA:O	2:B:251:ASP:HB3	2.12	0.49
1:C:137:VAL:HG13	1:C:168:GLU:HG2	1.94	0.49
1:A:346:TRP:CD1	1:A:346:TRP:H	2.31	0.49
2:B:83:PHE:O	2:B:86:ILE:CG1	2.60	0.49
1:C:285:GLN:HG2	1:C:372:GLN:HB2	1.94	0.49
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.61	0.48
2:B:314:THR:HG22	2:B:380:ASN:HB3	1.96	0.48
1:C:137:VAL:CG1	1:C:168:GLU:HG2	2.44	0.48
1:A:103:TYR:CD1	1:A:413:MET:HE1	2.49	0.48
2:B:204:ILE:HD12	2:B:209:LEU:HD11	1.94	0.48
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.96	0.48
2:D:37:HIS:O	2:D:37:HIS:CG	2.67	0.47
2:D:68:VAL:CG1	2:D:149:MET:HE1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:CYS:HB3	1:C:377:MET:HE2	1.96	0.47
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.95	0.47
2:D:30:ILE:HD11	2:D:86:ILE:HD11	1.95	0.47
2:B:198:THR:CG2	2:B:266:HIS:CD2	2.98	0.47
2:D:259:MET:CA	2:D:314:THR:HG21	2.43	0.47
1:A:271:THR:HG23	1:A:377:MET:HB3	1.95	0.47
2:B:119:LEU:HA	2:B:122:VAL:HG22	1.96	0.47
2:D:198:THR:CG2	2:D:266:HIS:CD2	2.97	0.47
3:E:13:LYS:HG3	3:E:18:GLN:HG3	1.96	0.47
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.49	0.47
1:A:323:VAL:HB	1:A:355:ILE:CD1	2.44	0.47
1:A:263:PRO:O	1:A:266:HIS:HD2	1.98	0.47
2:D:42:LEU:HD22	2:D:245:PRO:HG2	1.97	0.46
2:B:165:ILE:HD11	2:B:252:LEU:HD23	1.97	0.46
2:B:163:ASP:O	2:B:253:ARG:NH2	2.49	0.46
1:A:110:ILE:O	1:A:113:GLU:HB2	2.15	0.46
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.50	0.46
1:C:271:THR:HG23	1:C:377:MET:HB3	1.97	0.46
2:D:1:MET:HE1	2:D:253:ARG:HE	1.80	0.46
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.46
2:B:242:LEU:HA	2:B:250:ALA:HB1	1.98	0.46
2:B:42:LEU:HD22	2:B:245:PRO:HG2	1.97	0.45
1:A:344:VAL:CG2	1:A:346:TRP:NE1	2.80	0.45
2:D:183:GLU:OE2	7:D:504:GDP:H3'	2.16	0.45
2:B:147:SER:HG	2:B:190:SER:HG	1.63	0.45
2:D:334:ASN:O	2:D:338:LYS:HG2	2.17	0.45
2:B:74:THR:O	2:B:77:SER:OG	2.30	0.45
2:D:241:CYS:O	2:D:250:ALA:CB	2.63	0.45
3:E:50:ILE:HG13	3:E:53:LYS:HE2	1.99	0.45
1:A:258:ASN:ND2	1:A:352:LYS:HZ3	2.15	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.45
1:A:109:THR:HG22	3:E:61:ARG:CZ	2.47	0.45
2:D:30:ILE:HD13	2:D:53:TYR:CE2	2.52	0.45
2:D:198:THR:HG21	2:D:201:THR:HG1	1.80	0.45
2:B:325:MET:HA	2:B:328:VAL:HG22	1.99	0.45
1:A:344:VAL:HG21	1:A:346:TRP:NE1	2.32	0.44
2:B:334:ASN:O	2:B:338:LYS:HG2	2.17	0.44
2:B:243:ARG:HH21	2:B:244:PHE:HE2	1.65	0.44
2:D:254:LYS:HA	2:D:257:VAL:HG22	1.99	0.44
2:D:68:VAL:HG12	2:D:149:MET:CE	2.46	0.44
2:D:147:SER:HB2	2:D:190:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HE1	2:B:253:ARG:HE	1.81	0.44
2:D:314:THR:HG22	2:D:380:ASN:HB3	1.99	0.44
2:B:115:VAL:HG23	2:B:153:LEU:HD22	1.99	0.44
1:A:119:LEU:O	1:A:122:ILE:HG13	2.18	0.43
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.00	0.43
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.43
1:C:338:LYS:HZ2	1:C:339:ARG:CZ	2.32	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.36	0.43
2:B:248:LEU:HG	2:B:250:ALA:H	1.83	0.43
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.43
1:A:212:ILE:HG12	1:A:230:LEU:HD21	2.01	0.43
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.54	0.43
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.01	0.43
2:D:181:VAL:O	2:D:398:MET:SD	2.76	0.43
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.49	0.43
2:B:250:ALA:O	2:B:251:ASP:CB	2.67	0.43
2:B:327:GLU:HA	2:B:330:GLU:HG2	2.01	0.43
1:C:242:LEU:HD11	1:C:252:LEU:HD13	2.00	0.43
2:D:163:ASP:O	2:D:253:ARG:NH2	2.52	0.43
1:A:45:GLY:N	1:A:245:ASP:H	2.17	0.42
1:A:88:HIS:O	1:A:91:GLN:HG2	2.19	0.42
1:C:221:ARG:HD3	2:D:326:LYS:HG3	2.01	0.42
3:E:141:GLU:HG2	3:E:142:GLU:H	1.83	0.42
2:B:32:PRO:O	2:B:86:ILE:HG23	2.19	0.42
1:A:155:GLU:HB3	3:E:50:ILE:HD12	2.01	0.42
1:C:167:LEU:HD22	1:C:252:LEU:HD11	2.01	0.42
1:A:119:LEU:HA	1:A:122:ILE:CG1	2.50	0.42
2:D:326:LYS:H	2:D:326:LYS:HD3	1.84	0.42
2:B:239:THR:OG1	2:B:243:ARG:NH1	2.53	0.42
2:D:327:GLU:HA	2:D:330:GLU:HG2	2.02	0.42
2:B:198:THR:HG21	2:B:201:THR:HG1	1.82	0.42
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.55	0.42
2:D:145:THR:HG23	7:D:504:GDP:PB	2.60	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.42
1:C:118:VAL:O	1:C:122:ILE:HG12	2.20	0.41
2:D:172:MET:HG3	2:D:387:LEU:HD21	2.02	0.41
1:A:258:ASN:ND2	1:A:352:LYS:NZ	2.68	0.41
2:B:165:ILE:CG1	2:B:252:LEU:HD23	2.51	0.41
2:B:402:LYS:HD2	2:B:405:LEU:HB3	2.02	0.41
2:D:5:VAL:HG22	2:D:135:PHE:HD1	1.85	0.41
1:A:292:THR:HG22	1:A:335:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HG21	1:C:152:LEU:HG	2.01	0.41
1:C:175:PRO:HA	1:C:179:THR:OG1	2.20	0.41
2:D:326:LYS:HD3	2:D:326:LYS:N	2.36	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.41
2:B:396:THR:O	2:B:400:ARG:HB2	2.20	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.21	0.41
2:D:229:HIS:HB2	2:D:278:ARG:HG2	2.03	0.41
1:A:8:HIS:ND1	1:A:67:PHE:CZ	2.89	0.41
1:A:119:LEU:HA	1:A:122:ILE:HG13	2.02	0.41
2:B:314:THR:HG22	2:B:380:ASN:CB	2.51	0.41
2:B:178:SER:HB3	1:C:349:THR:HG21	2.01	0.41
1:A:166:LYS:HE2	9:A:602:HOH:O	2.21	0.41
2:B:400:ARG:HH21	1:C:439:SER:HB2	1.87	0.40
1:C:192:HIS:CG	1:C:421:ALA:HA	2.57	0.40
1:C:244:PHE:HB2	1:C:356:ASN:HD22	1.86	0.40
1:A:271:THR:HG21	1:A:377:MET:HE2	2.03	0.40
2:B:5:VAL:HG22	2:B:135:PHE:HD1	1.86	0.40
2:B:265:LEU:HD12	2:B:432:TYR:CZ	2.57	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	430/451 (95%)	419 (97%)	9 (2%)	2 (0%)	24	29
1	C	430/451 (95%)	417 (97%)	9 (2%)	4 (1%)	14	15
2	B	426/445 (96%)	415 (97%)	10 (2%)	1 (0%)	43	53
2	D	428/445 (96%)	415 (97%)	11 (3%)	2 (0%)	24	29
3	E	127/143 (89%)	123 (97%)	4 (3%)	0	100	100
All	All	1841/1935 (95%)	1789 (97%)	43 (2%)	9 (0%)	24	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	ASP
2	D	250	ALA
1	C	283	HIS
1	A	178	SER
1	C	178	SER
1	C	282	TYR
1	C	285	GLN
1	A	46	ASP
2	D	251	ASP

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	366/379 (97%)	330 (90%)	36 (10%)	7	8
1	C	367/379 (97%)	340 (93%)	27 (7%)	13	15
2	B	371/383 (97%)	328 (88%)	43 (12%)	5	5
2	D	373/383 (97%)	336 (90%)	37 (10%)	7	8
3	E	115/125 (92%)	104 (90%)	11 (10%)	8	9
All	All	1592/1649 (96%)	1438 (90%)	154 (10%)	8	8

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	26	LEU
1	A	62	VAL
1	A	71	GLU
1	A	77	GLU
1	A	78	VAL
1	A	113	GLU
1	A	120	ASP
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	179	THR
1	A	181	VAL
1	A	188	ILE
1	A	206	ASN
1	A	212	ILE
1	A	221	ARG
1	A	229	ARG
1	A	238	ILE
1	A	241	SER
1	A	252	LEU
1	A	259	LEU
1	A	260	VAL
1	A	308	ARG
1	A	317	LEU
1	A	324	VAL
1	A	336	LYS
1	A	341	ILE
1	A	345	ASP
1	A	353	VAL
1	A	355	ILE
1	A	367	ASP
1	A	373	ARG
1	A	405	VAL
1	A	422	ARG
1	A	437	VAL
1	A	438	ASP
1	A	439	SER
2	B	5	VAL
2	B	50	ASN
2	B	51	VAL
2	B	64	ARG
2	B	90	ASP
2	B	93	VAL
2	B	96	GLN
2	B	97	SER
2	B	118	VAL
2	B	124	LYS
2	B	127	GLU
2	B	141	LEU
2	B	153	LEU
2	B	158	ARG
2	B	164	ARG

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Mol	Chain	Res	Type
2	B	165	ILE
2	B	177	VAL
2	B	180	THR
2	B	182	VAL
2	B	198	THR
2	B	200	GLU
2	B	204	ILE
2	B	221	THR
2	B	230	LEU
2	B	231	VAL
2	B	238	VAL
2	B	259	MET
2	B	265	LEU
2	B	275	LEU
2	B	278	ARG
2	B	286	LEU
2	B	293	GLN
2	B	311	ARG
2	B	314	THR
2	B	315	VAL
2	B	318	ILE
2	B	322	ARG
2	B	345	GLU
2	B	389	LYS
2	B	402	LYS
2	B	423	SER
2	B	430	SER
2	B	442	GLU
1	C	1	MET
1	C	2	ARG
1	C	5	ILE
1	C	62	VAL
1	C	71	GLU
1	C	77	GLU
1	C	115	ILE
1	C	124	LYS
1	C	179	THR
1	C	188	ILE
1	C	229	ARG
1	C	238	ILE
1	C	241	SER
1	C	265	ILE

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Mol	Chain	Res	Type
1	C	275	VAL
1	C	277	SER
1	C	280	LYS
1	C	285	GLN
1	C	324	VAL
1	C	339	ARG
1	C	349	THR
1	C	355	ILE
1	C	367	ASP
1	C	384	ILE
1	C	405	VAL
1	C	422	ARG
1	C	435	VAL
2	D	5	VAL
2	D	30	ILE
2	D	50	ASN
2	D	66	ILE
2	D	71	GLU
2	D	85	GLN
2	D	90	ASP
2	D	96	GLN
2	D	115	VAL
2	D	124	LYS
2	D	127	GLU
2	D	141	LEU
2	D	145	THR
2	D	153	LEU
2	D	158	ARG
2	D	180[A]	THR
2	D	180[B]	THR
2	D	181	VAL
2	D	198	THR
2	D	200	GLU
2	D	230	LEU
2	D	238	VAL
2	D	259	MET
2	D	275	LEU
2	D	277	SER
2	D	278	ARG
2	D	282	GLN
2	D	286	LEU
2	D	293	GLN

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Mol	Chain	Res	Type
2	D	314	THR
2	D	315	VAL
2	D	322	ARG
2	D	325	MET
2	D	349	ASN
2	D	369	ARG
2	D	423	SER
2	D	430	SER
3	E	25	LYS
3	E	29	PHE
3	E	68	LEU
3	E	71	HIS
3	E	83	ILE
3	E	95	LYS
3	E	103	GLN
3	E	108	ASN
3	E	120	LEU
3	E	121	GLU
3	E	142	GLU

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	GLN
1	A	35	GLN
1	A	101	ASN
1	A	107	HIS
1	A	206	ASN
1	A	249	ASN
1	A	256	GLN
1	A	258	ASN
1	A	283	HIS
1	A	285	GLN
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	37	HIS
2	B	136	GLN
2	B	167	ASN
2	B	192	HIS

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Mol	Chain	Res	Type
2	B	197	ASN
2	B	331	GLN
2	B	336	GLN
2	B	349	ASN
2	B	385	GLN
2	B	436	GLN
1	C	15	GLN
1	C	31	GLN
1	C	35	GLN
1	C	101	ASN
1	C	258	ASN
1	C	356	ASN
2	D	8	GLN
2	D	11	GLN
2	D	14	ASN
2	D	85	GLN
2	D	136	GLN
2	D	167	ASN
2	D	192	HIS
2	D	282	GLN
2	D	336	GLN
2	D	339	ASN
2	D	380	ASN
3	E	18	GLN
3	E	51	GLN
3	E	64	GLN
3	E	124	GLN
3	E	129	HIS
3	E	136	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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	D	502	-	4,4,4	0.29	0	6,6,6	0.23	0
4	SO4	A	501	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	D	503	-	4,4,4	0.32	0	6,6,6	0.27	0
4	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.22	0
8	N3Z	B	504	-	31,32,32	0.21	0	42,47,47	0.73	3 (7%)
7	GDP	D	504	-	29,30,30	0.44	0	45,47,47	0.66	0
7	GDP	B	503	-	29,30,30	0.51	0	45,47,47	0.63	0
4	SO4	C	502	-	4,4,4	0.26	0	6,6,6	0.13	0
4	SO4	C	501	-	4,4,4	0.32	0	6,6,6	0.23	0
5	GTP	A	502	6	33,34,34	0.51	0	50,54,54	0.57	0
4	SO4	C	503	-	4,4,4	0.36	0	6,6,6	0.07	0
8	N3Z	D	505	-	31,32,32	0.29	0	42,47,47	0.75	3 (7%)
4	SO4	D	501	-	4,4,4	0.26	0	6,6,6	0.16	0
5	GTP	C	504	6	33,34,34	0.41	0	50,54,54	0.55	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
7	GDP	B	503	-	-	5/16/32/32	0/3/3/3
5	GTP	C	504	6	-	5/22/38/38	0/3/3/3
5	GTP	A	502	6	-	5/22/38/38	0/3/3/3
8	N3Z	D	505	-	-	0/10/32/32	0/4/4/4
7	GDP	D	504	-	-	3/16/32/32	0/3/3/3
8	N3Z	B	504	-	-	0/10/32/32	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	505	N3Z	C4-C3-C8	-2.57	121.76	124.70
8	D	505	N3Z	C2-C1-C	-2.56	125.80	129.96
8	B	504	N3Z	C4-C3-C8	-2.55	121.79	124.70
8	B	504	N3Z	C2-C1-C	-2.47	125.93	129.96
8	D	505	N3Z	O-C3-C4	-2.01	125.19	127.86
8	B	504	N3Z	O-C3-C4	-2.01	125.19	127.86

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	GTP	PB-O3B-PG-O2G
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	504	GTP	C5'-O5'-PA-O3A
5	C	504	GTP	C5'-O5'-PA-O1A
5	C	504	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
5	C	504	GTP	PB-O3B-PG-O2G
7	B	503	GDP	PB-O3A-PA-O1A
5	A	502	GTP	PB-O3A-PA-O2A
5	C	504	GTP	PB-O3A-PA-O2A
7	B	503	GDP	PB-O3A-PA-O2A

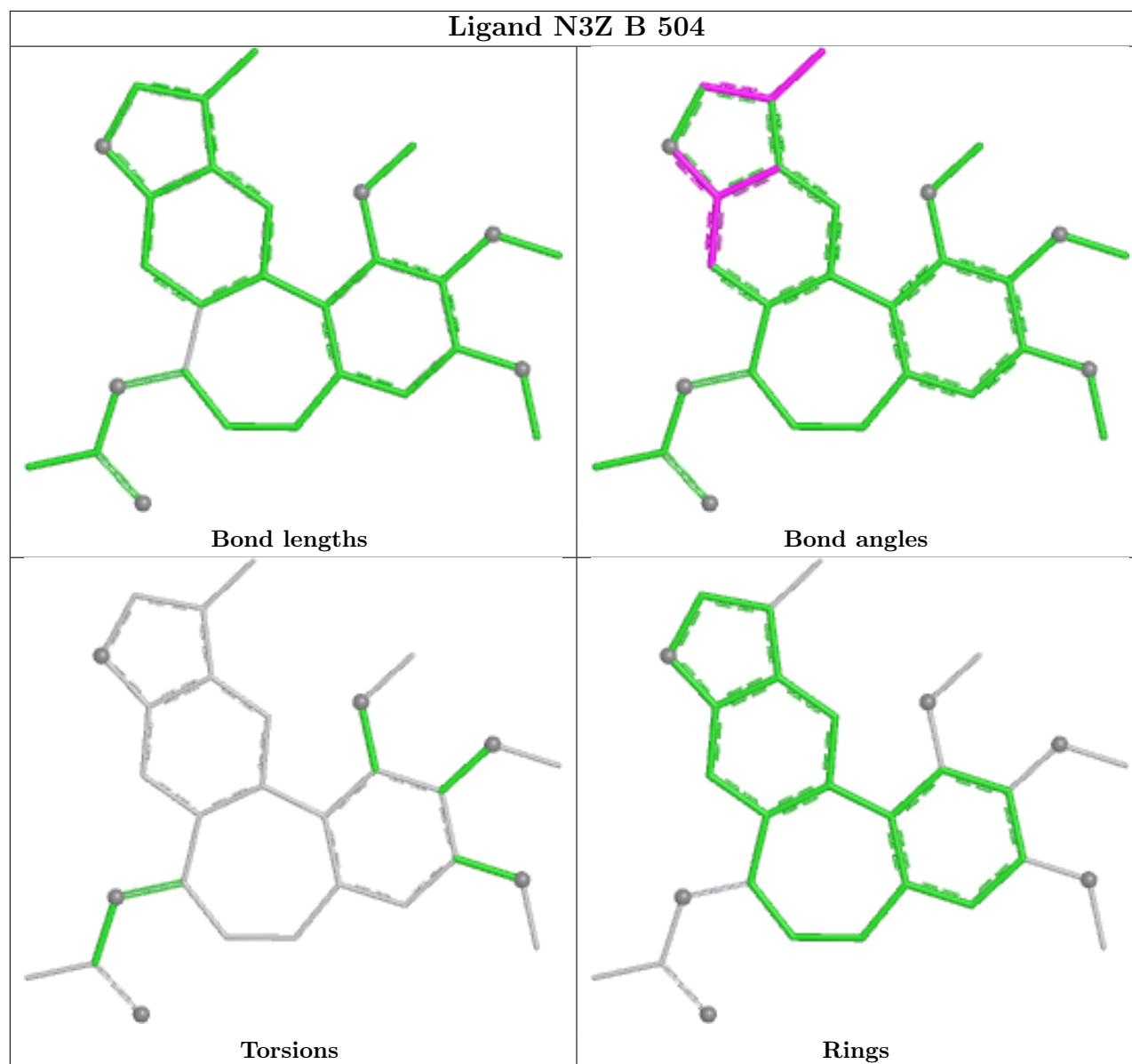
There are no ring outliers.

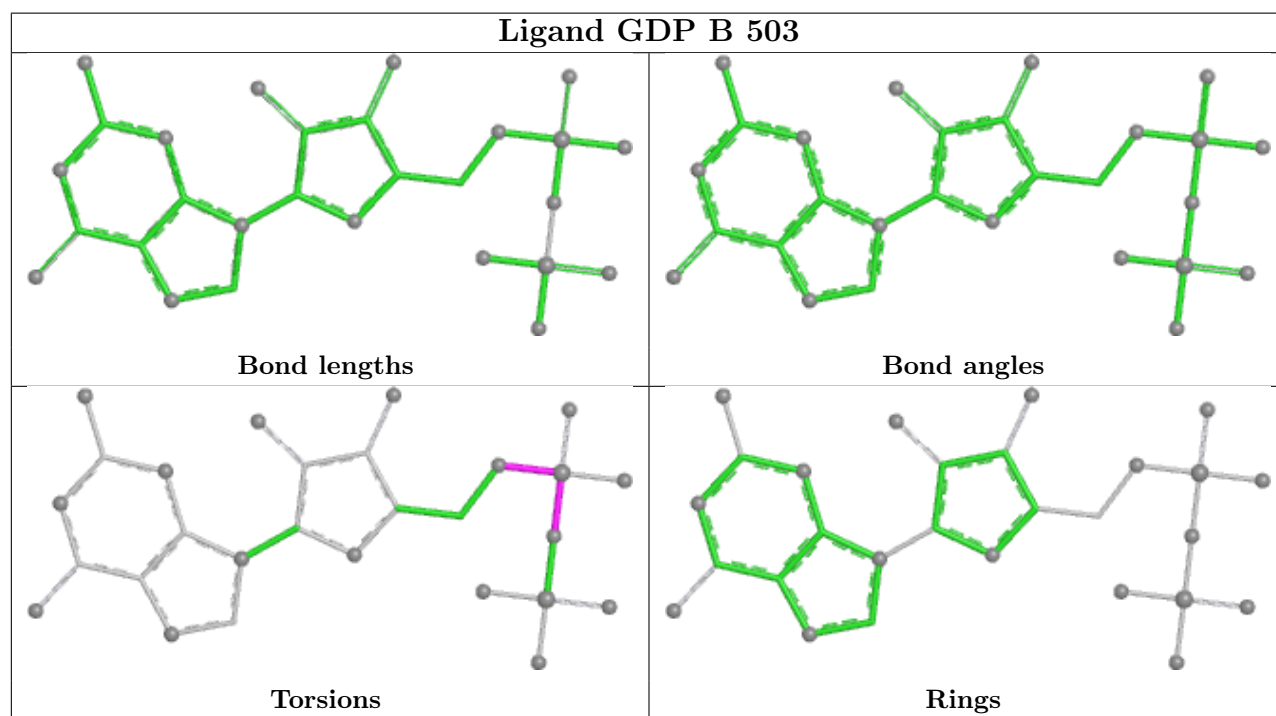
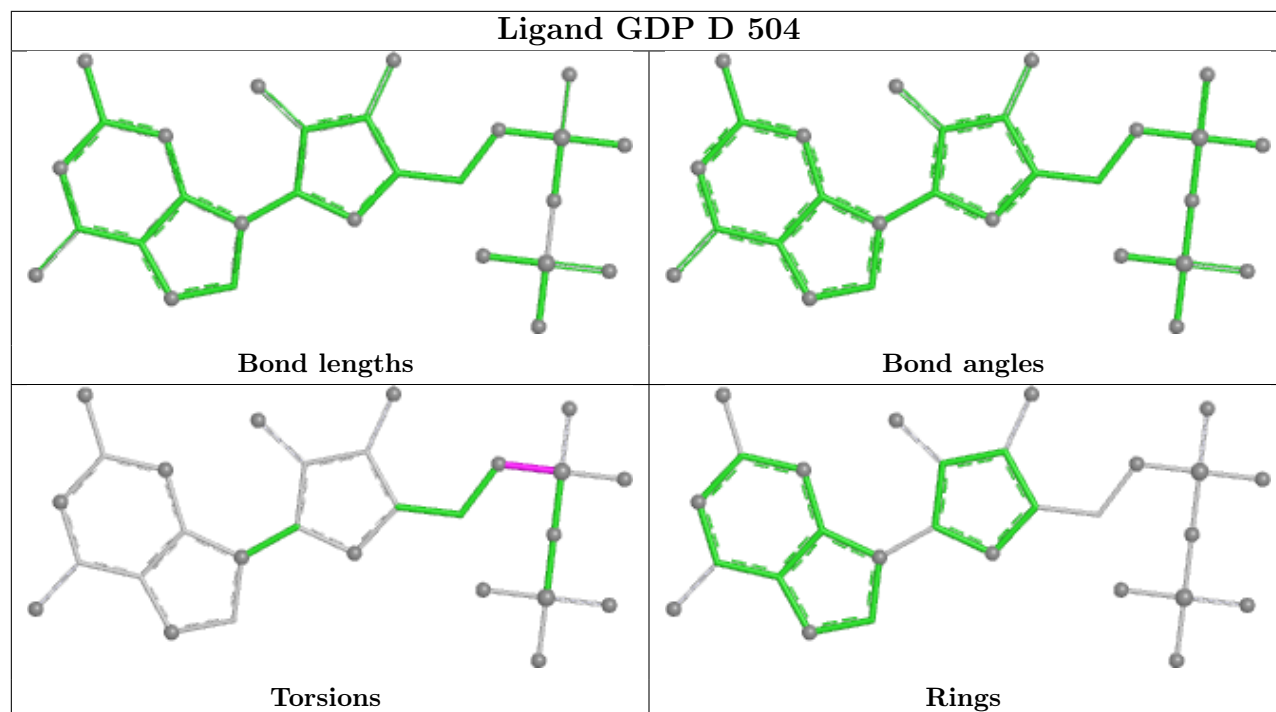
3 monomers are involved in 4 short contacts:

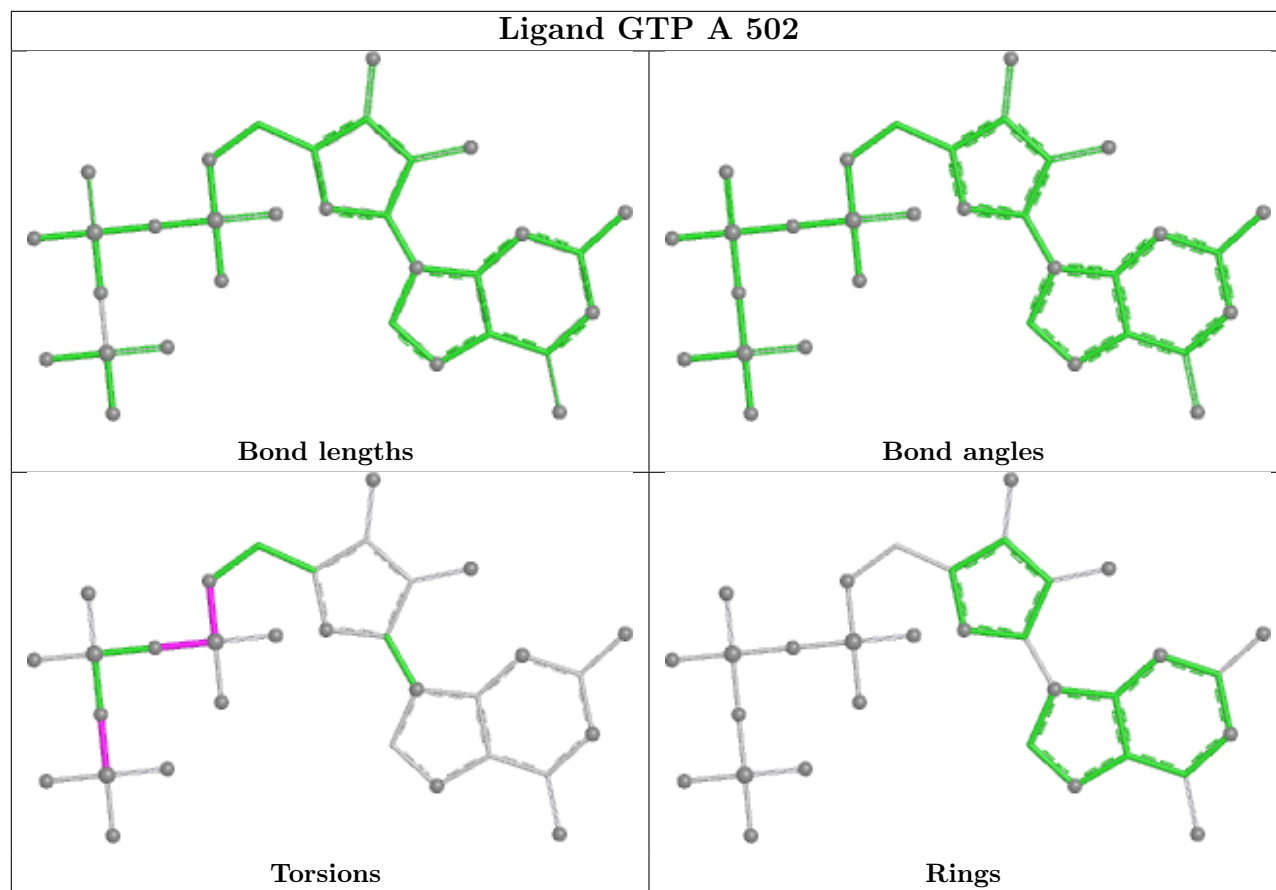
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	SO4	1	0
7	D	504	GDP	2	0
5	A	502	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

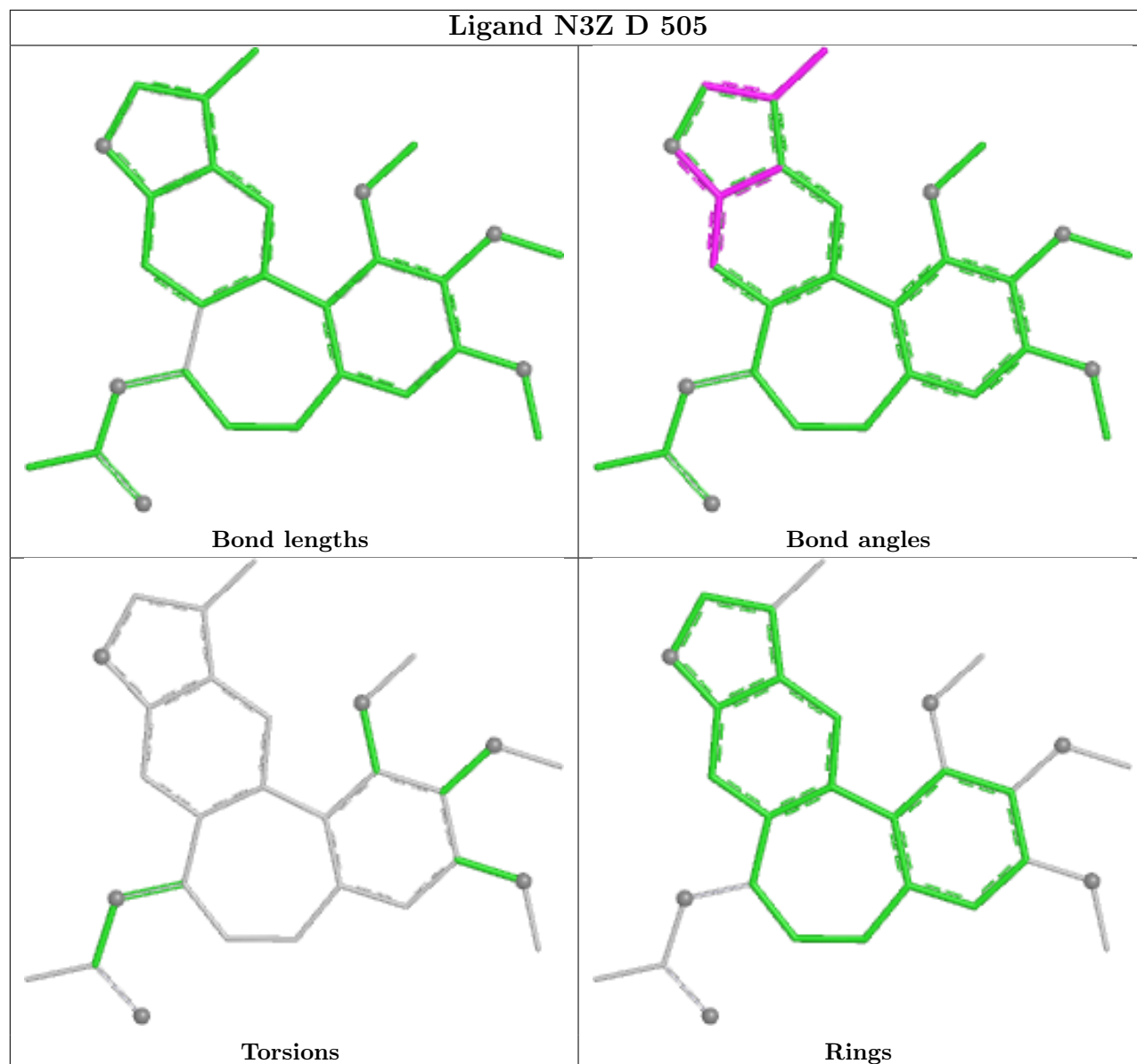
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

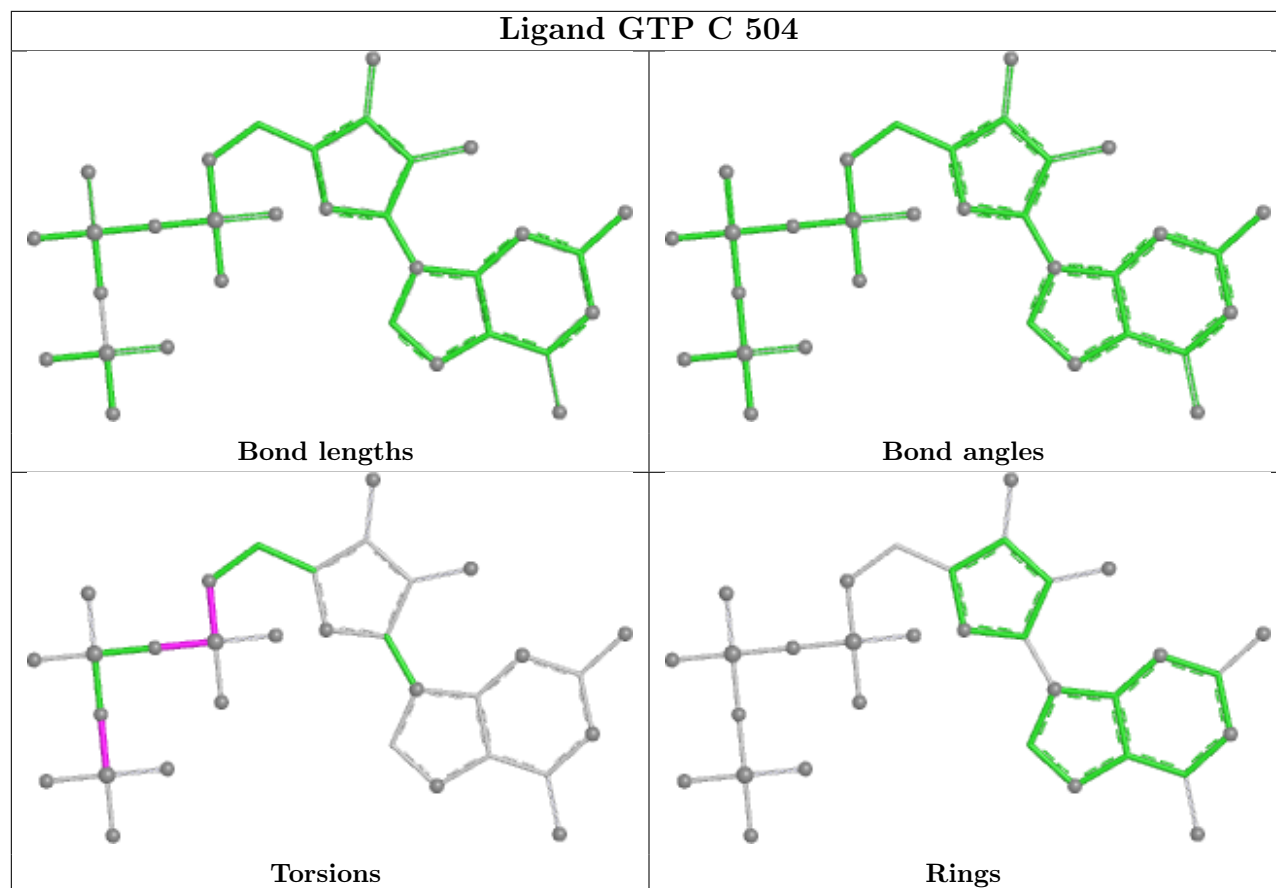






Ligand N3Z D 505





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	434/451 (96%)	0.54	21 (4%) 35 36	48, 81, 122, 142	0
1	C	434/451 (96%)	0.44	20 (4%) 37 38	41, 71, 103, 123	0
2	B	430/445 (96%)	0.49	21 (4%) 35 36	46, 71, 116, 149	0
2	D	429/445 (96%)	0.45	19 (4%) 39 40	32, 70, 107, 123	3 (0%)
3	E	131/143 (91%)	0.88	17 (12%) 7 8	78, 106, 148, 165	0
All	All	1858/1935 (96%)	0.51	98 (5%) 32 33	32, 76, 120, 165	3 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	5.5
1	C	350	GLY	4.9
3	E	32	VAL	4.7
2	B	296	PHE	4.2
1	A	292	THR	4.1
2	D	179[A]	ASP	4.0
2	D	66	ILE	3.9
1	A	440	VAL	3.8
2	D	172	MET	3.7
2	D	30	ILE	3.6
3	E	144	SER	3.4
2	D	296	PHE	3.2
1	C	38	SER	3.2
1	C	335	ILE	3.2
2	D	78	VAL	3.2
3	E	33	PRO	3.2
1	C	349	THR	3.2
1	C	351	PHE	3.1
1	A	332	ILE	3.1
1	A	341	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	122	ILE	3.0
1	C	255	PHE	2.9
3	E	22	VAL	2.9
2	B	371	LEU	2.8
2	D	248	LEU	2.8
1	C	238	ILE	2.8
1	C	360	PRO	2.8
1	C	362	VAL	2.8
3	E	24	LEU	2.8
2	D	57	THR	2.7
1	C	232	SER	2.7
3	E	54	LEU	2.7
1	A	282	TYR	2.7
1	A	252	LEU	2.7
1	A	38	SER	2.7
3	E	45	PRO	2.7
2	B	360	PRO	2.7
3	E	29	PHE	2.6
1	A	238	ILE	2.6
1	C	62	VAL	2.6
1	C	440	VAL	2.6
3	E	4	ALA	2.6
2	B	172	MET	2.6
2	D	83	PHE	2.6
1	A	66	VAL	2.5
1	C	108	TYR	2.5
2	B	52	TYR	2.5
2	B	61	TYR	2.5
1	A	351	PHE	2.5
1	C	5	ILE	2.5
1	A	436	GLY	2.4
2	B	100	GLY	2.4
3	E	120	LEU	2.4
2	D	37	HIS	2.4
2	B	202	TYR	2.3
1	C	137	VAL	2.3
2	B	94	PHE	2.3
2	D	399	PHE	2.3
2	B	249	ASN	2.3
2	B	295	MET	2.3
2	B	23	VAL	2.3
1	A	309	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	439	SER	2.3
2	D	68	VAL	2.3
2	D	61	TYR	2.2
3	E	140	LYS	2.2
2	B	358	ILE	2.2
2	B	248	LEU	2.2
1	C	135	PHE	2.2
2	B	74	THR	2.2
1	A	1	MET	2.1
2	D	325	MET	2.1
1	C	63	PRO	2.1
1	A	58	ALA	2.1
3	E	130	ALA	2.1
3	E	50	ILE	2.1
1	C	37	PRO	2.1
2	B	315	VAL	2.1
2	B	328	VAL	2.1
2	D	281	GLN	2.1
3	E	143	ALA	2.1
1	A	357	TYR	2.1
1	C	83	TYR	2.1
3	E	115	HIS	2.1
1	A	37	PRO	2.1
1	A	68	VAL	2.1
3	E	134	ARG	2.1
2	B	285	ALA	2.1
2	D	285	ALA	2.1
2	B	373	MET	2.1
2	D	70	LEU	2.1
1	C	346	TRP	2.1
1	A	363	VAL	2.0
2	B	118	VAL	2.0
3	E	8	VAL	2.0
2	B	377	PHE	2.0
2	D	282	GLN	2.0
2	D	119	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

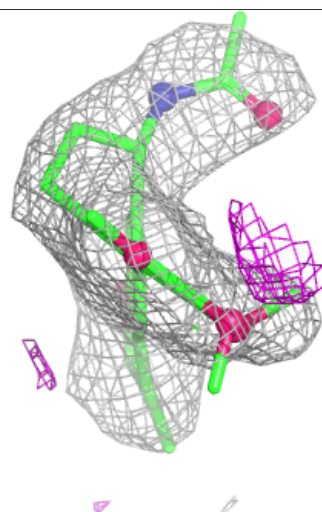
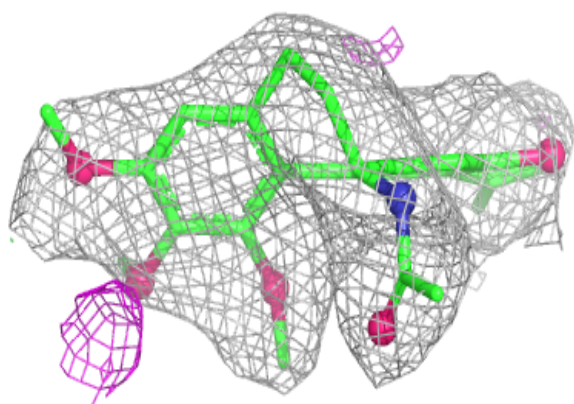
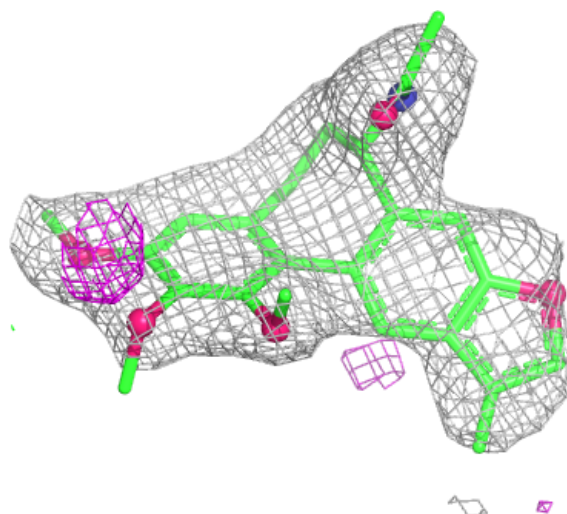
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	502	5/5	0.65	0.15	164,164,164,164	0
4	SO4	A	501	5/5	0.70	0.11	144,144,144,144	0
4	SO4	C	501	5/5	0.71	0.11	146,146,146,146	0
4	SO4	C	502	5/5	0.74	0.07	146,146,146,146	0
4	SO4	B	502	5/5	0.75	0.11	187,187,187,187	0
4	SO4	B	501	5/5	0.78	0.11	132,132,132,132	0
4	SO4	D	503	5/5	0.79	0.13	136,136,136,136	0
4	SO4	D	501	5/5	0.88	0.09	120,121,121,121	0
4	SO4	C	503	5/5	0.89	0.13	151,151,151,151	0
8	N3Z	B	504	29/29	0.93	0.11	68,68,69,69	0
8	N3Z	D	505	29/29	0.94	0.09	59,61,62,62	0
7	GDP	B	503	28/28	0.95	0.08	57,59,59,60	0
7	GDP	D	504	28/28	0.95	0.07	59,62,65,66	0
5	GTP	C	504	32/32	0.97	0.07	53,54,55,56	0
6	MG	C	505	1/1	0.97	0.12	55,55,55,55	0
5	GTP	A	502	32/32	0.97	0.06	50,52,53,54	0
6	MG	A	503	1/1	0.99	0.05	54,54,54,54	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.

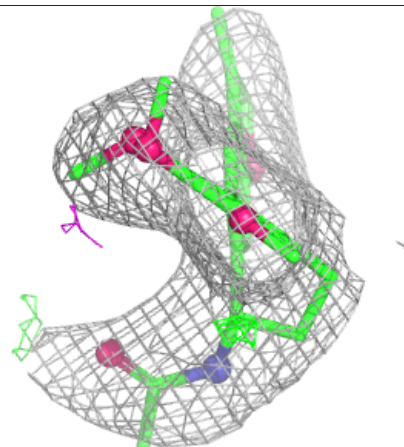
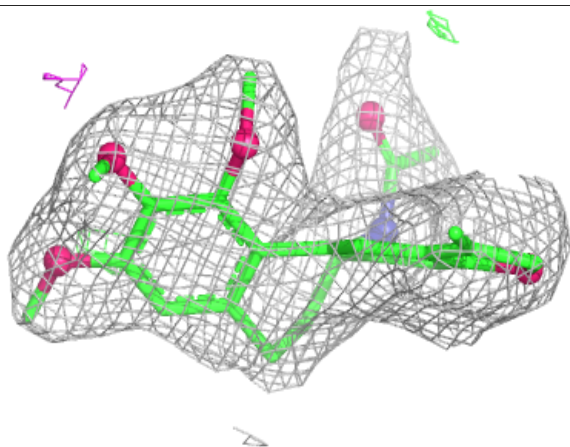
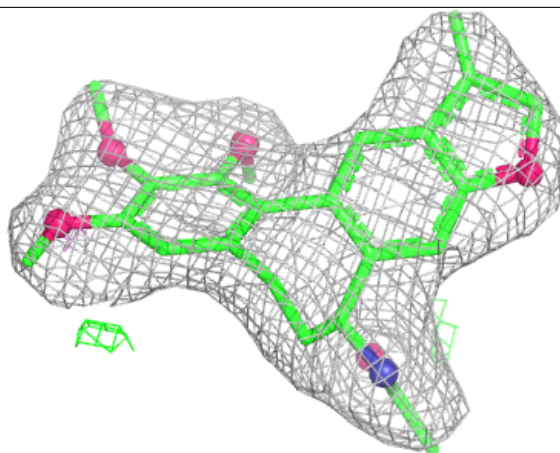
Electron density around N3Z B 504:

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

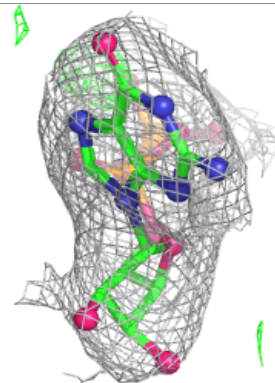
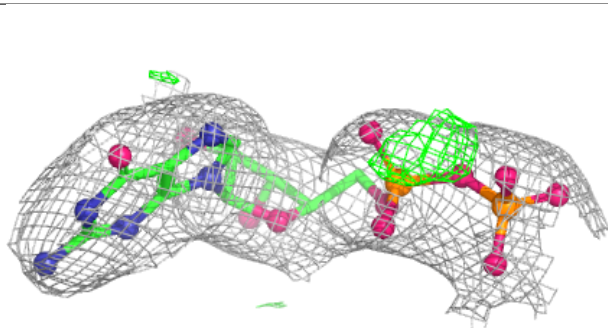
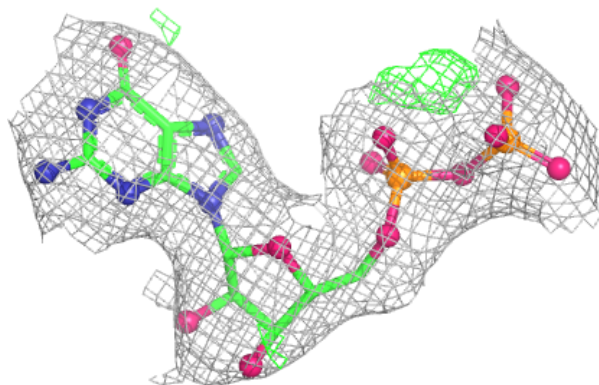


Electron density around N3Z D 505:

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

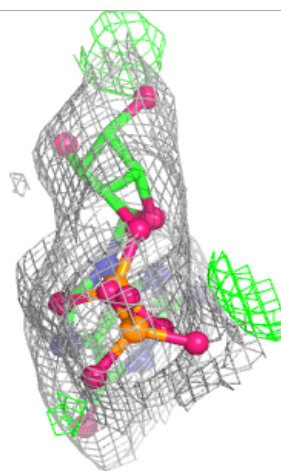
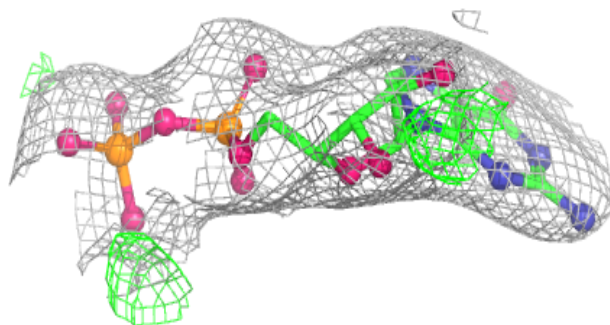
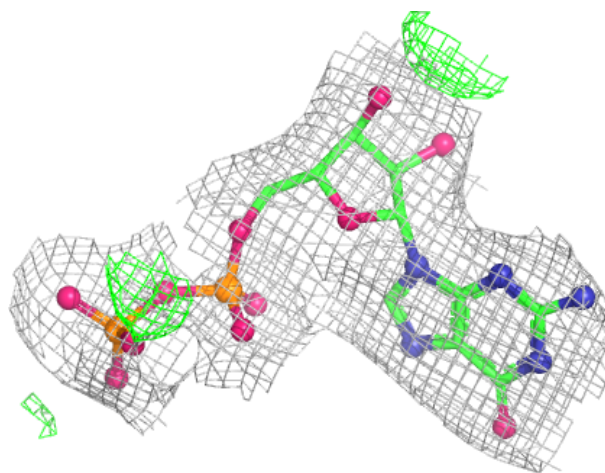
**Electron density around GDP B 503:**

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



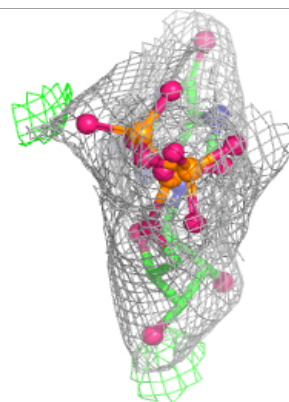
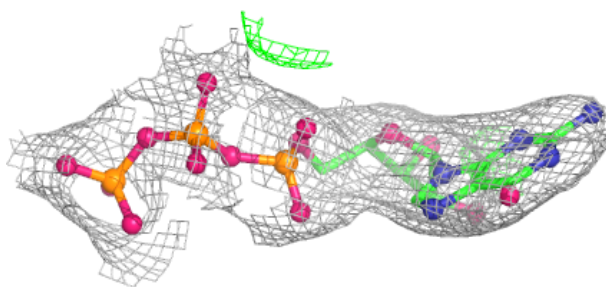
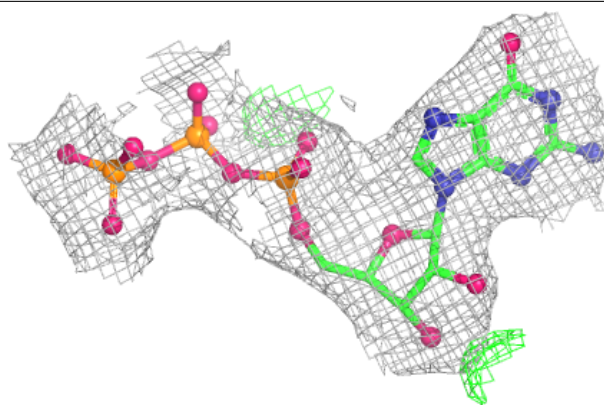
Electron density around GDP D 504:

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

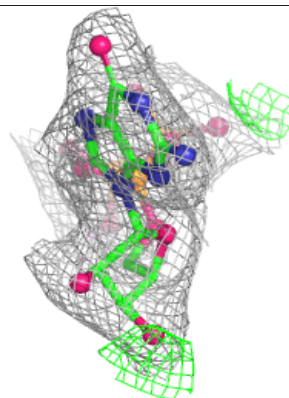
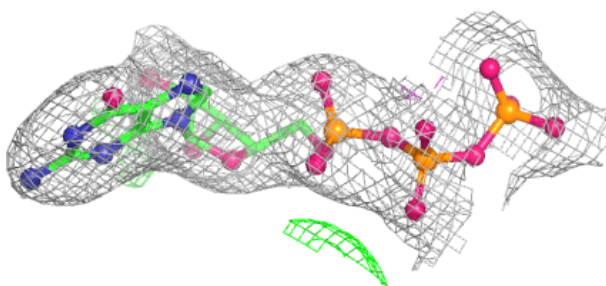
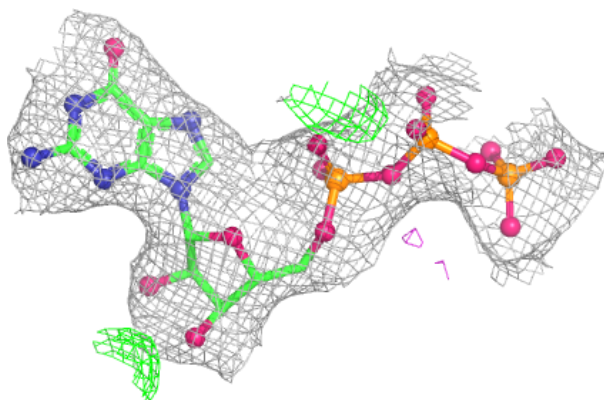


Electron density around GTP C 504:

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

**Electron density around GTP A 502:**

$2mF_o-DF_c$ (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.