Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:33 PM EDT

PDB ID	:	6TDE
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:

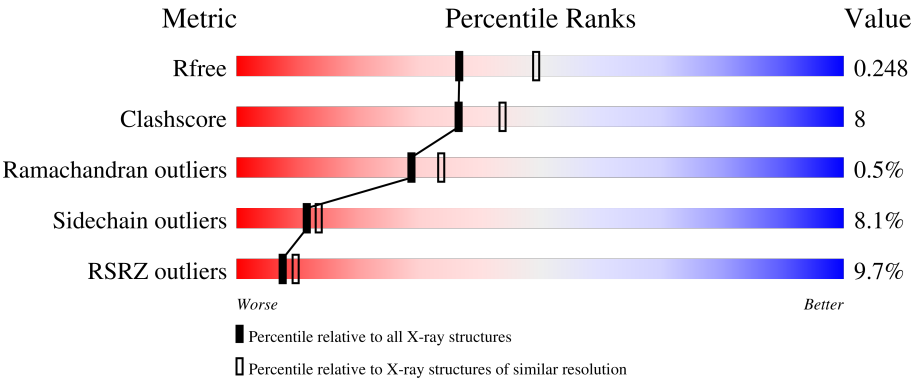
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 <=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	11% 76% 17%
1	C	451	6% 79% 16%
2	B	445	12% 74% 19%
2	D	445	5% 77% 18%
3	E	143	21% 74% 16% 8%

2 Entry composition (i)

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			

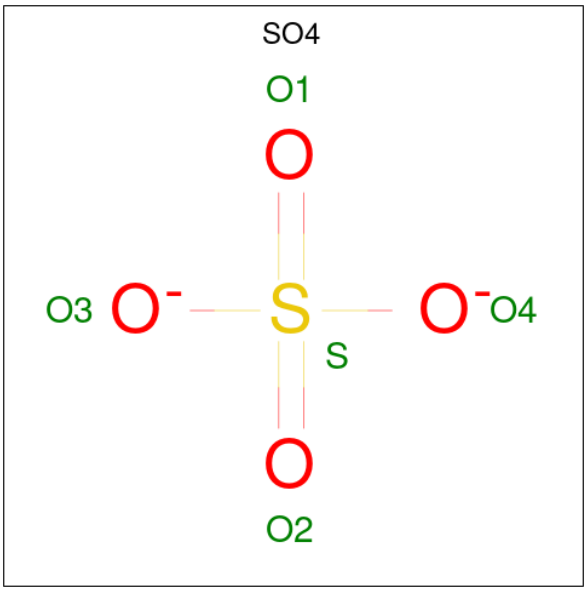
- Molecule 3 is a protein called Stathmin-4.

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:

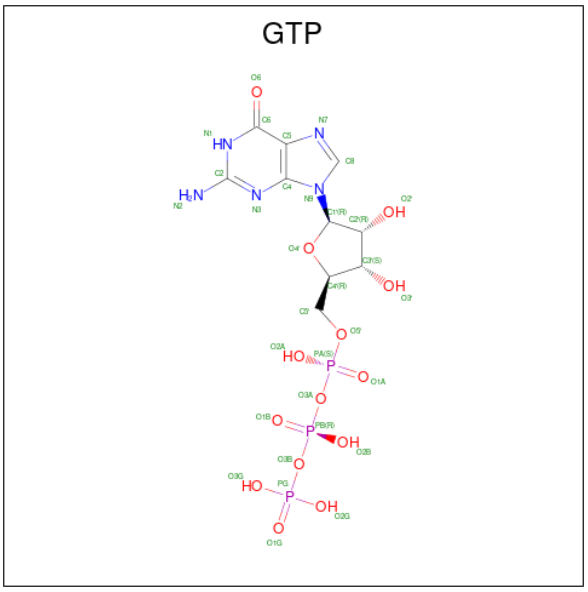
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ACE	-	acetylation	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

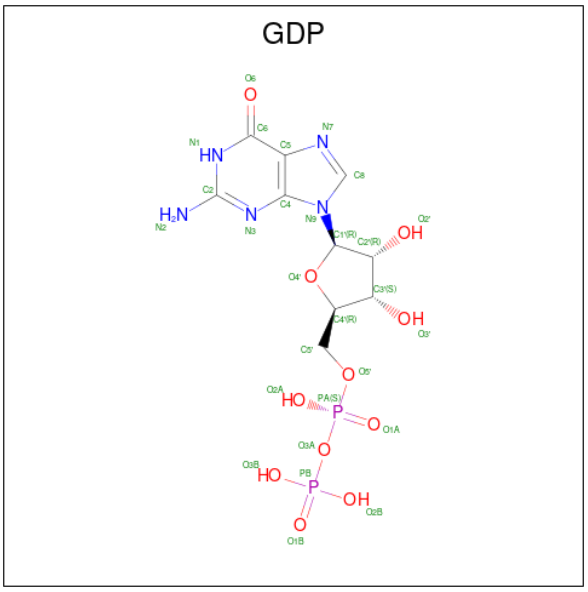


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

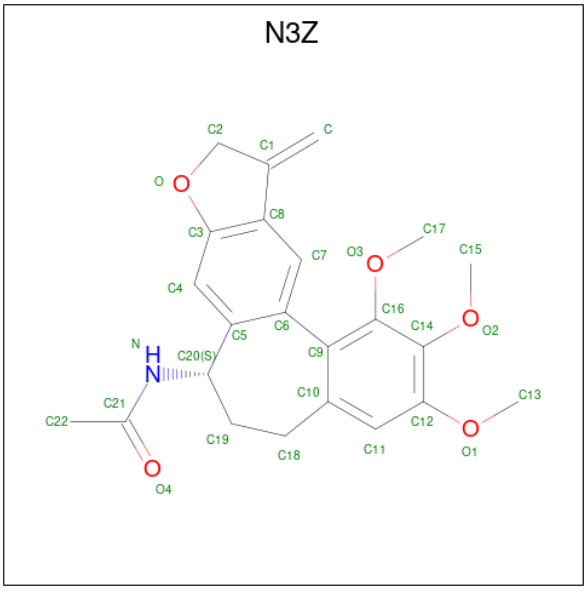
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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 (three-letter code: N3Z) (formula: $C_{23}H_{25}NO_5$) (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.

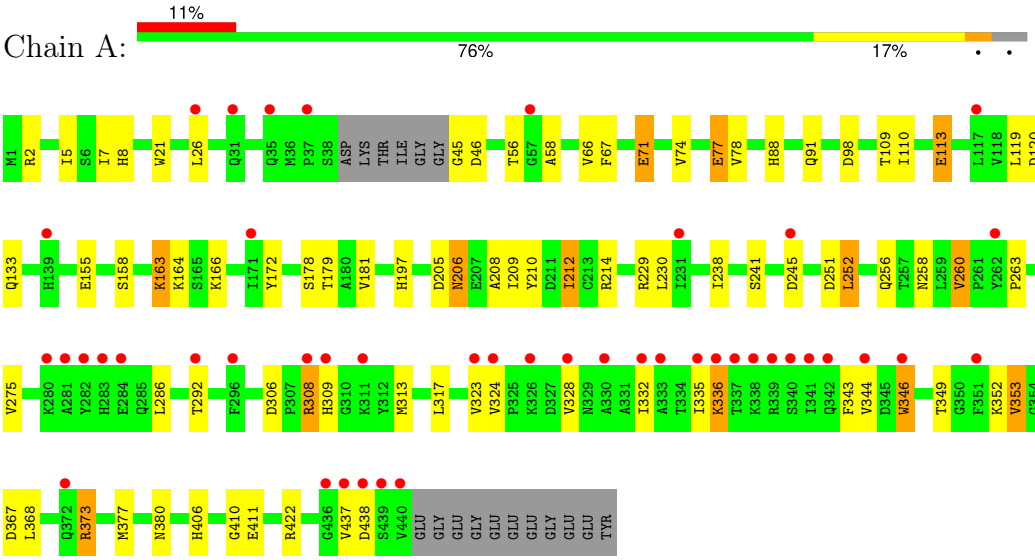
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	39	Total	O	0	0
			39	39		
9	B	31	Total	O	0	0
			31	31		
9	C	54	Total	O	0	0
			54	54		
9	D	34	Total	O	0	0
			34	34		
9	E	15	Total	O	0	0
			15	15		

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.

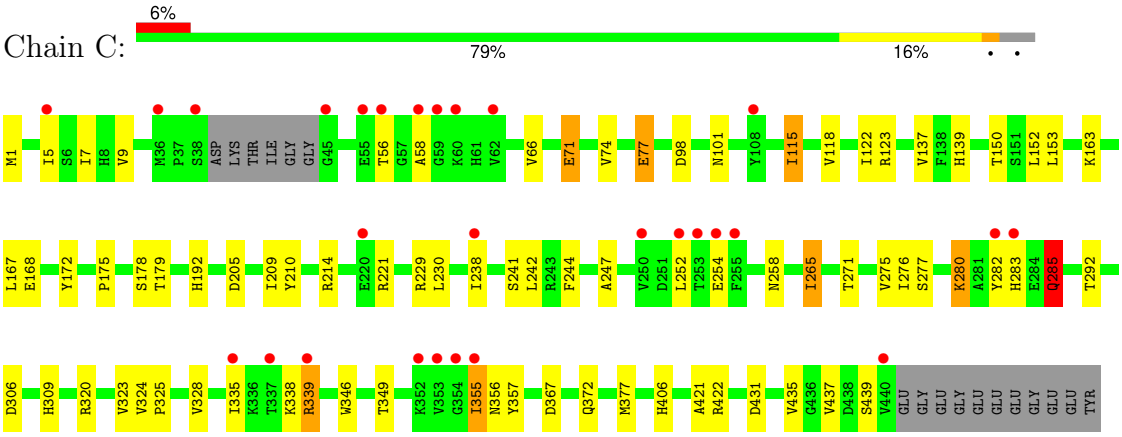
• Molecule 1: Tubulin alpha chain

Chain A:



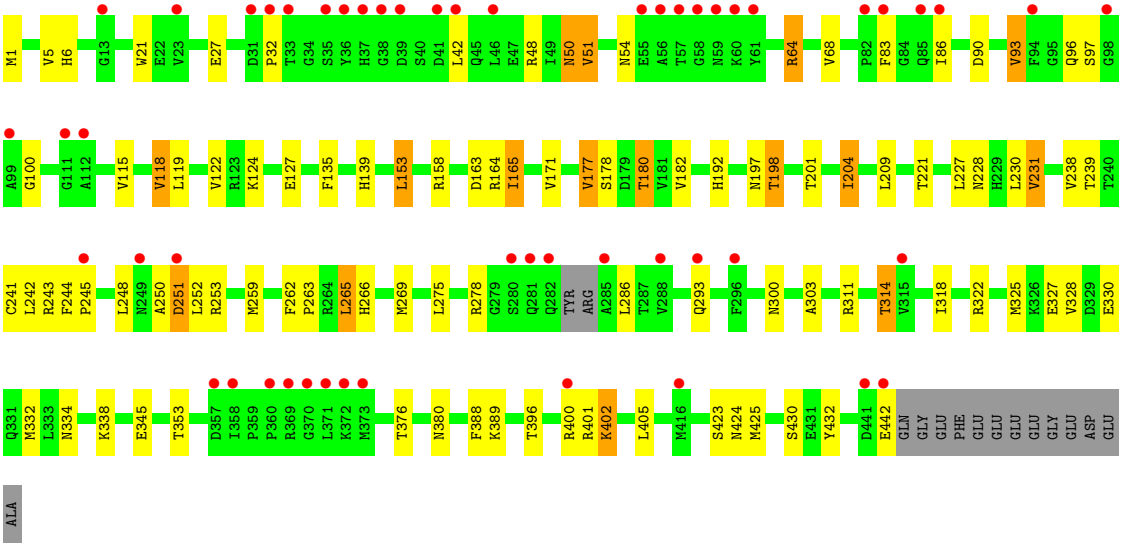
• Molecule 1: Tubulin alpha chain

Chain C:

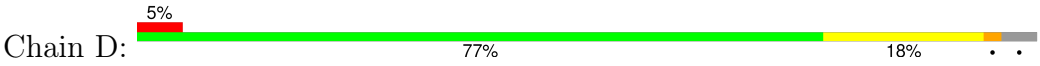


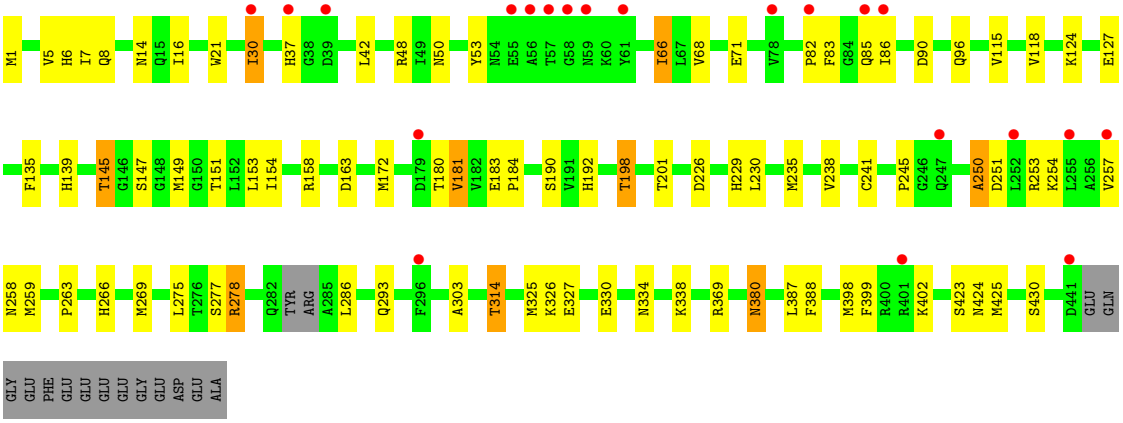
• Molecule 2: Tubulin beta chain

Chain B:

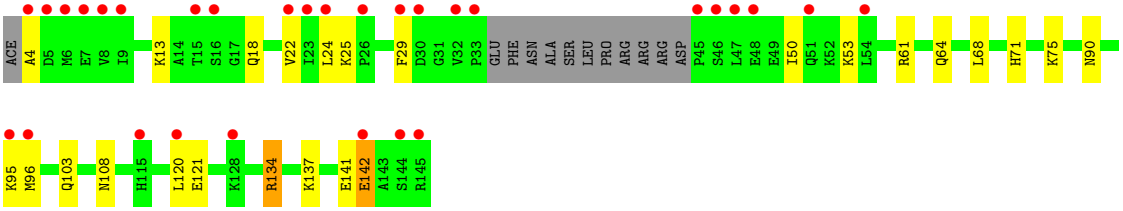


• Molecule 2: Tubulin beta chain





• Molecule 3: Stathmin-4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.48Å 128.14Å 251.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.29 44.98 – 2.29	Depositor EDS
% Data completeness (in resolution range)	51.9 (45.00-2.29) 51.9 (44.98-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (23-SEP-2019)	Depositor
R, R_{free}	0.198 , 0.232 0.212 , 0.248	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 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GTP, GDP, N3Z, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/3466	0.59	0/4705
1	C	0.40	0/3474	0.57	0/4716
2	B	0.44	0/3448	0.61	0/4669
2	D	0.45	0/3460	0.62	0/4686
3	E	0.37	0/1086	0.52	0/1444
All	All	0.42	0/14934	0.59	0/20220

There are no bond length outliers.

There are no bond angle outliers.

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	55	0
1	C	3397	0	3307	53	0
2	B	3375	0	3249	68	0
2	D	3387	0	3258	57	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	229	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 (229) 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	0.94
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: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
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:D:388:PHE:HD1	2:D:425:MET:HE3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
2:B:259:MET:HE3	2:B:314:THR:HG23	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:B:388:PHE:HD1	2:B:425:MET:HE3	1.63	0.62
2:D:192:HIS:HD2	2:D:424:ASN:ND2	1.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:PHE:HD1	2:D:425:MET:CE	2.14	0.60
2:D:192:HIS:CD2	2:D:424:ASN:HD22	2.02	0.60
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
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: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: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
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
1:C:9:VAL:HG13	1:C:139:HIS:CB	2.37	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
2:D:388:PHE:CD1	2:D:425:MET:HE3	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.44	0.52
1:A:308:ARG:NE	1:A:309:HIS:CD2	2.77	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:C:325:PRO:HA	1:C:328:VAL:HG22	1.92	0.51
1:A:158:SER:HB2	1:A:166:LYS:HZ1	1.76	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
2:B:388:PHE:CD1	2:B:425:MET:HE3	2.44	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
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
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:CG	2:D:37:HIS:O	2.67	0.47
2:D:68:VAL:CG1	2:D:149:MET:HE1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:O	1:A:266:HIS:HD2	1.98	0.47
2:D:259:MET:HE3	2:D:314:THR:HG23	1.97	0.47
2:D:42:LEU:HD22	2:D:245:PRO:HG2	1.97	0.46
2:D:259:MET:HE3	2:D:259:MET:HB3	1.84	0.46
2:B:165:ILE:HD11	2:B:252:LEU:HD23	1.97	0.46
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.36	0.46
2:B:163:ASP:O	2:B:253:ARG:NH2	2.49	0.46
2:B:259:MET:HE3	2:B:314:THR:CG2	2.43	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
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
2:D:184:PRO:HD2	2:D:398:MET:HE1	1.98	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:D:334:ASN:O	2:D:338:LYS:HG2	2.17	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:259:MET:CE	2:D:314:THR:HG23	2.48	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:D:16:ILE:HD12	2:D:235:MET:HE1	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	430/451 (95%)	419 (97%)	9 (2%)	2 (0%)	29	34
1	C	430/451 (95%)	417 (97%)	9 (2%)	4 (1%)	17	18
2	B	426/445 (96%)	415 (97%)	10 (2%)	1 (0%)	47	57
2	D	428/445 (96%)	415 (97%)	11 (3%)	2 (0%)	29	34
3	E	127/143 (89%)	123 (97%)	4 (3%)	0	100	100
All	All	1841/1935 (95%)	1789 (97%)	43 (2%)	9 (0%)	29	34

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	366/379 (97%)	336 (92%)	30 (8%)	11 13
1	C	367/379 (97%)	348 (95%)	19 (5%)	23 30
2	B	371/383 (97%)	333 (90%)	38 (10%)	7 7
2	D	373/383 (97%)	342 (92%)	31 (8%)	11 12
3	E	115/125 (92%)	104 (90%)	11 (10%)	8 9
All	All	1592/1649 (96%)	1463 (92%)	129 (8%)	11 13

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	26	LEU
1	A	71	GLU
1	A	77	GLU
1	A	78	VAL
1	A	113	GLU
1	A	120	ASP
1	A	123	ARG
1	A	163	LYS
1	A	179	THR
1	A	181	VAL
1	A	206	ASN
1	A	212	ILE
1	A	229	ARG
1	A	238	ILE
1	A	241	SER
1	A	252	LEU
1	A	260	VAL
1	A	308	ARG
1	A	317	LEU
1	A	324	VAL
1	A	336	LYS
1	A	346	TRP

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Mol	Chain	Res	Type
1	A	353	VAL
1	A	355	ILE
1	A	367	ASP
1	A	373	ARG
1	A	422	ARG
1	A	437	VAL
1	A	438	ASP
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	139	HIS
2	B	153	LEU
2	B	158	ARG
2	B	164	ARG
2	B	165	ILE
2	B	177	VAL
2	B	180	THR
2	B	182	VAL
2	B	198	THR
2	B	204	ILE
2	B	221	THR
2	B	230	LEU
2	B	231	VAL
2	B	238	VAL
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	322	ARG
2	B	345	GLU
2	B	389	LYS
2	B	402	LYS

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Mol	Chain	Res	Type
2	B	423	SER
2	B	430	SER
2	B	442	GLU
1	C	1	MET
1	C	5	ILE
1	C	71	GLU
1	C	77	GLU
1	C	115	ILE
1	C	123	ARG
1	C	229	ARG
1	C	238	ILE
1	C	241	SER
1	C	265	ILE
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	355	ILE
1	C	367	ASP
1	C	422	ARG
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	139	HIS
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	230	LEU
2	D	238	VAL

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Mol	Chain	Res	Type
2	D	275	LEU
2	D	277	SER
2	D	278	ARG
2	D	286	LEU
2	D	293	GLN
2	D	314	THR
2	D	325	MET
2	D	369	ARG
2	D	380	ASN
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	95	LYS
3	E	103	GLN
3	E	108	ASN
3	E	120	LEU
3	E	121	GLU
3	E	134	ARG
3	E	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	101	ASN
1	A	107	HIS
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	393	HIS
2	B	192	HIS
2	B	197	ASN
2	B	331	GLN
2	B	406	HIS
1	C	31	GLN
1	C	101	ASN
1	C	256	GLN
1	C	258	ASN
1	C	356	ASN

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Mol	Chain	Res	Type
2	D	14	ASN
2	D	85	GLN
2	D	192	HIS
2	D	380	ASN
2	D	426	ASN
3	E	51	GLN
3	E	64	GLN
3	E	129	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	503	-	4,4,4	0.32	0	6,6,6	0.27	0
5	GTP	A	502	6	29,34,34	0.90	2 (6%)	35,54,54	0.72	0
8	N3Z	D	505	-	31,32,32	0.29	0	42,47,47	0.75	3 (7%)
7	GDP	D	504	-	25,30,30	0.87	1 (4%)	30,47,47	0.84	0
4	SO4	C	501	-	4,4,4	0.32	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	C	502	-	4,4,4	0.26	0	6,6,6	0.13	0
7	GDP	B	503	-	25,30,30	0.90	1 (4%)	30,47,47	0.79	0
5	GTP	C	504	6	29,34,34	0.87	2 (6%)	35,54,54	0.69	0
4	SO4	A	501	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	D	501	-	4,4,4	0.26	0	6,6,6	0.16	0
4	SO4	D	502	-	4,4,4	0.29	0	6,6,6	0.23	0
8	N3Z	B	504	-	31,32,32	0.21	0	42,47,47	0.73	3 (7%)
4	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.22	0
4	SO4	C	503	-	4,4,4	0.36	0	6,6,6	0.07	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
5	GTP	A	502	6	-	5/18/38/38	0/3/3/3
8	N3Z	D	505	-	-	0/10/32/32	0/4/4/4
7	GDP	D	504	-	-	3/12/32/32	0/3/3/3
7	GDP	B	503	-	-	5/12/32/32	0/3/3/3
5	GTP	C	504	6	-	5/18/38/38	0/3/3/3
8	N3Z	B	504	-	-	0/10/32/32	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	504	GTP	C5-C4	-2.33	1.37	1.43
5	C	504	GTP	C8-N7	-2.26	1.31	1.34
7	B	503	GDP	C8-N7	-2.17	1.31	1.34
5	A	502	GTP	C5-C4	-2.14	1.37	1.43
5	A	502	GTP	C8-N7	-2.14	1.31	1.34
7	D	504	GDP	C8-N7	-2.14	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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.

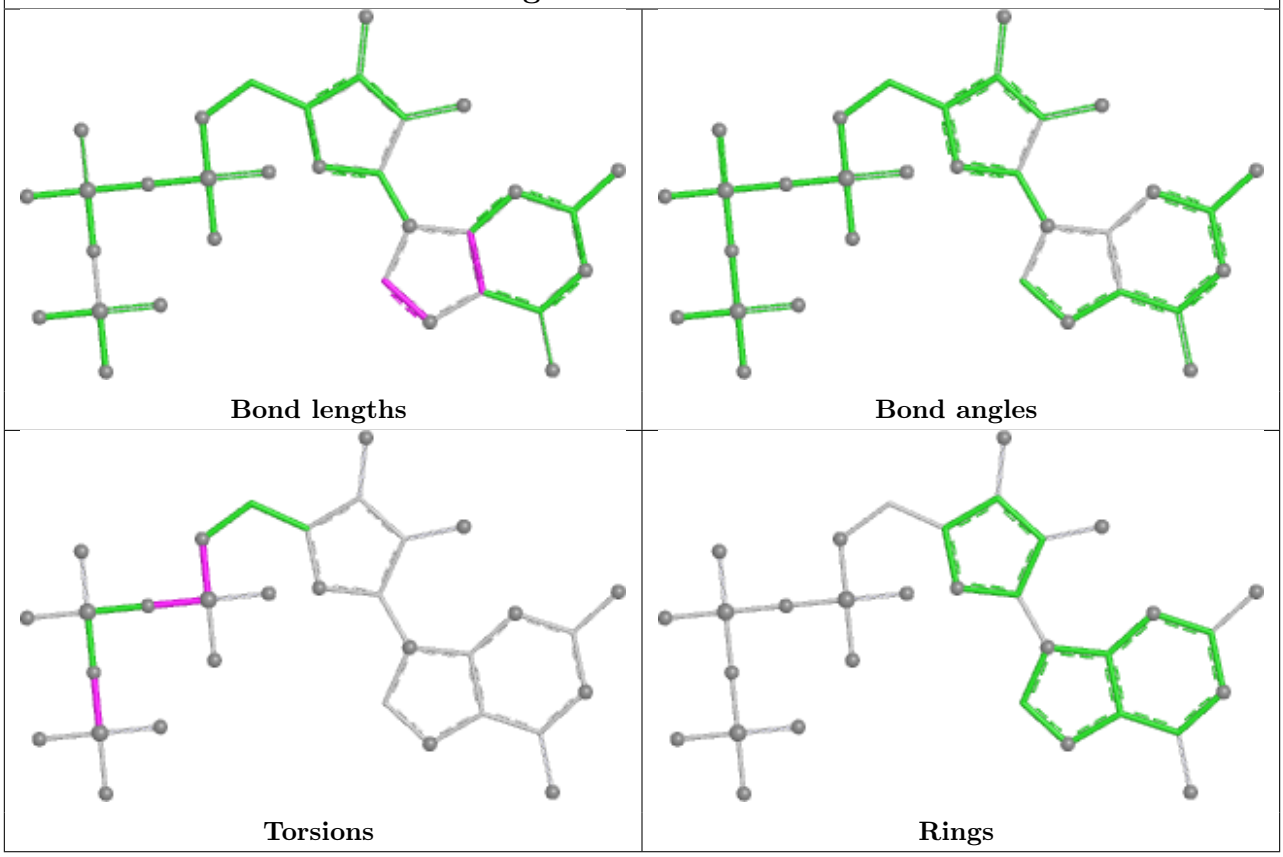
3 monomers are involved in 4 short contacts:

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

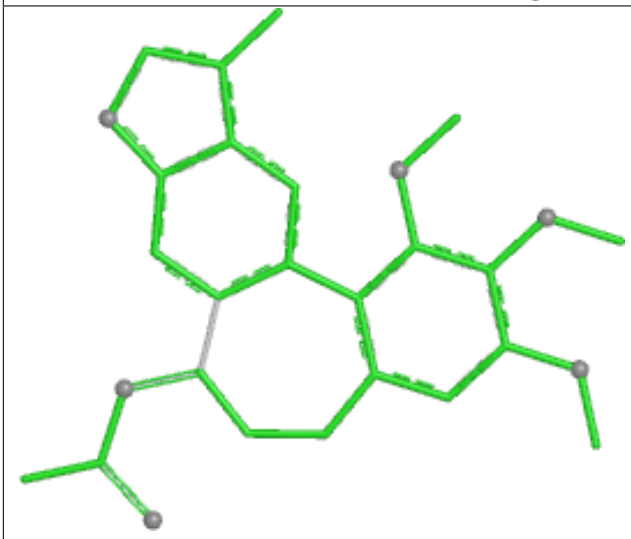
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

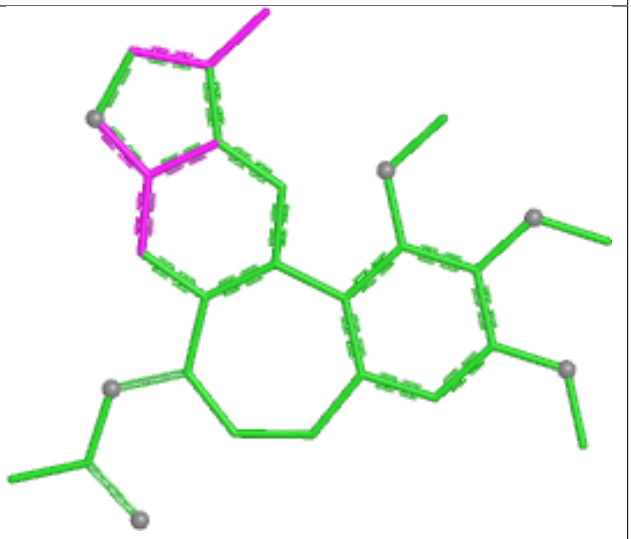
Ligand GTP A 502



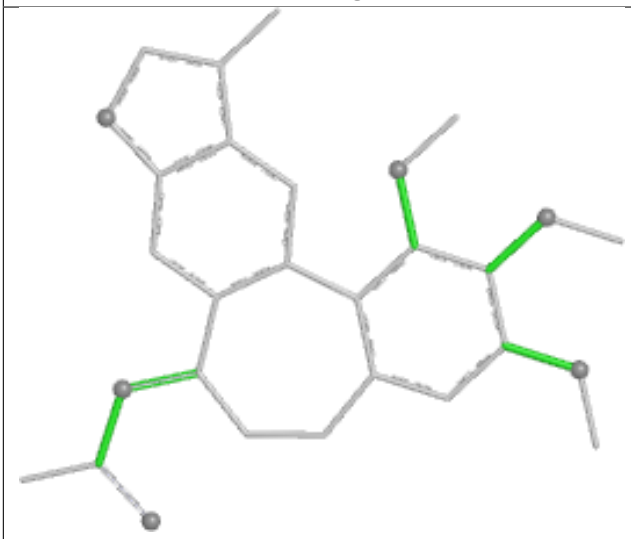
Ligand N3Z D 505



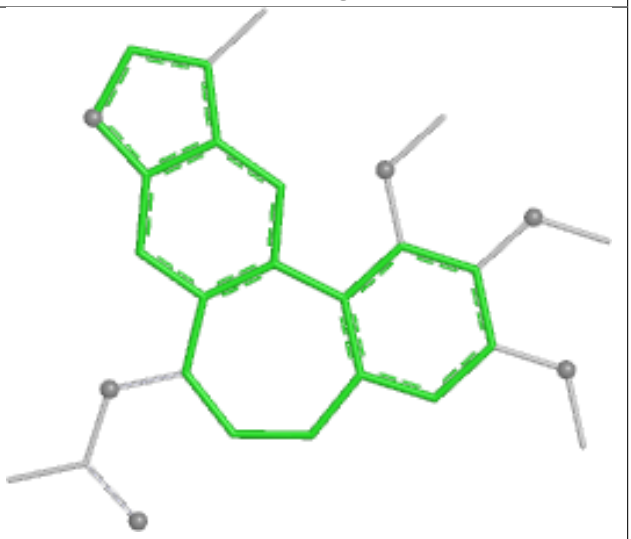
Bond lengths



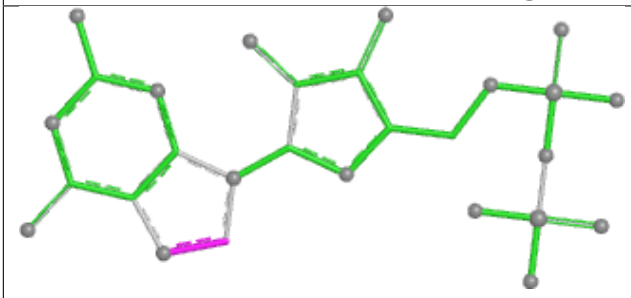
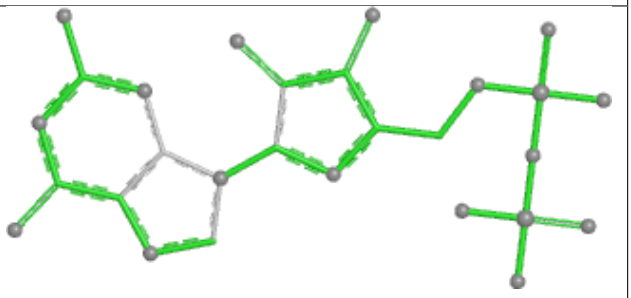
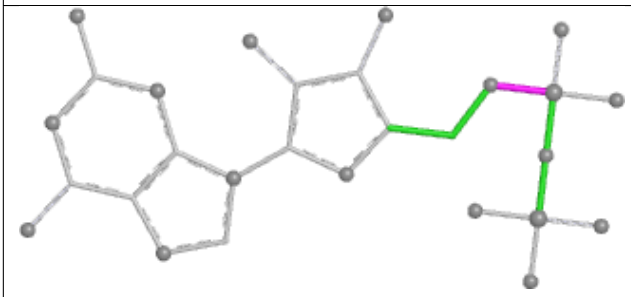
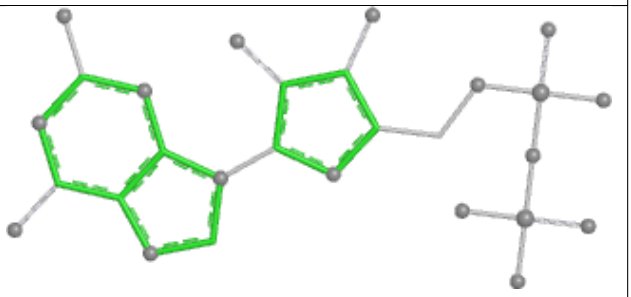
Bond angles

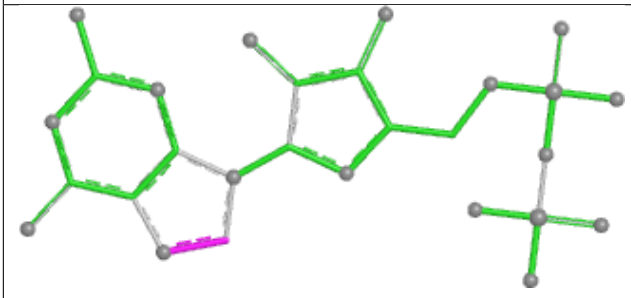
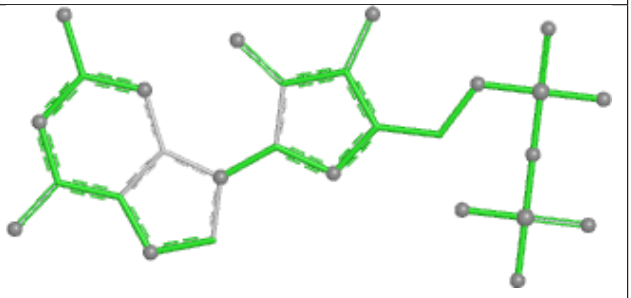
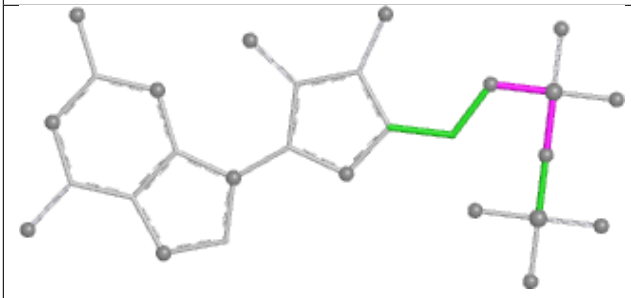
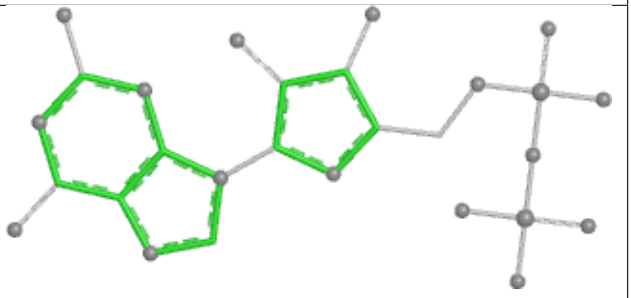


Torsions

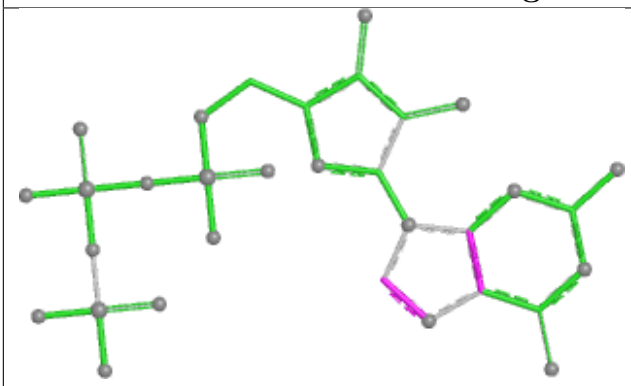


Rings

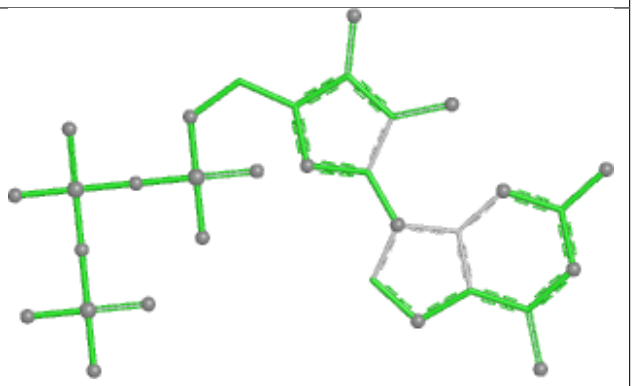
Ligand GDP D 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

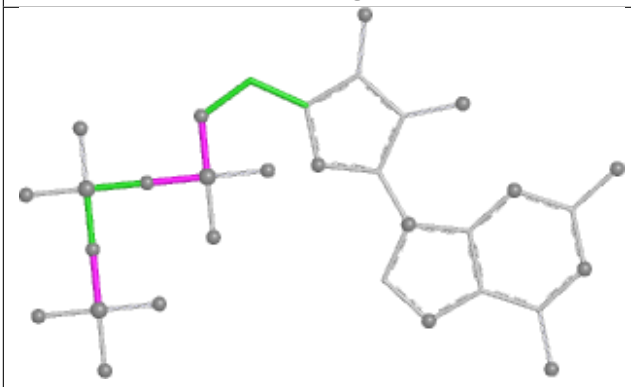
Ligand GTP C 504



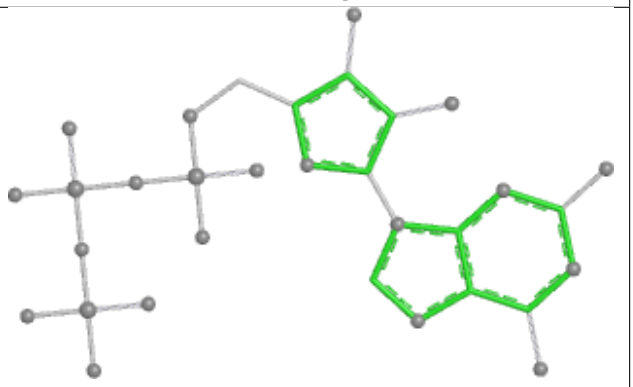
Bond lengths



Bond angles

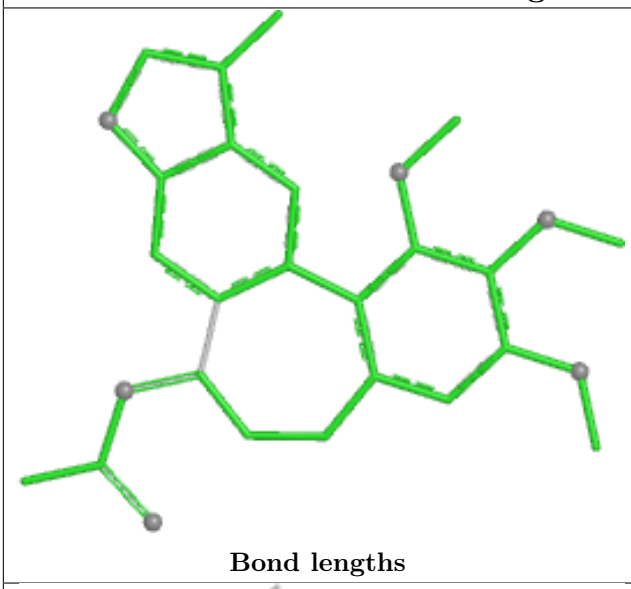


Torsions

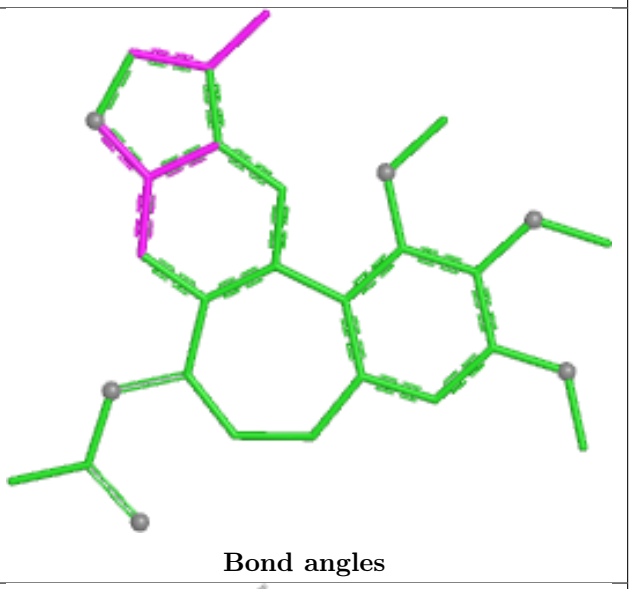


Rings

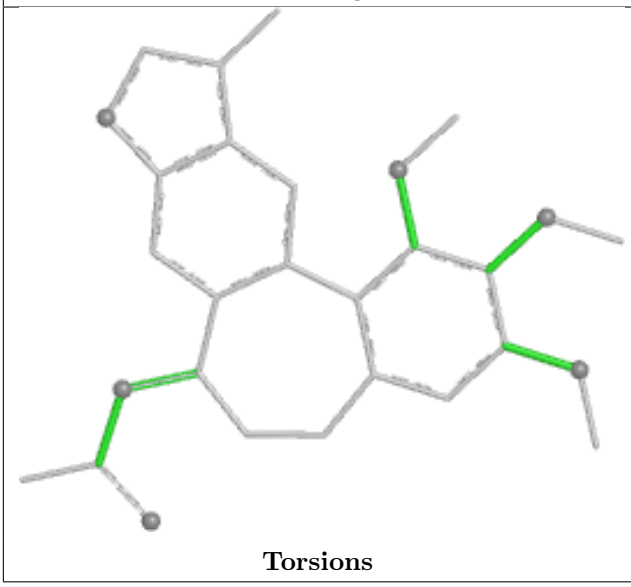
Ligand N3Z B 504



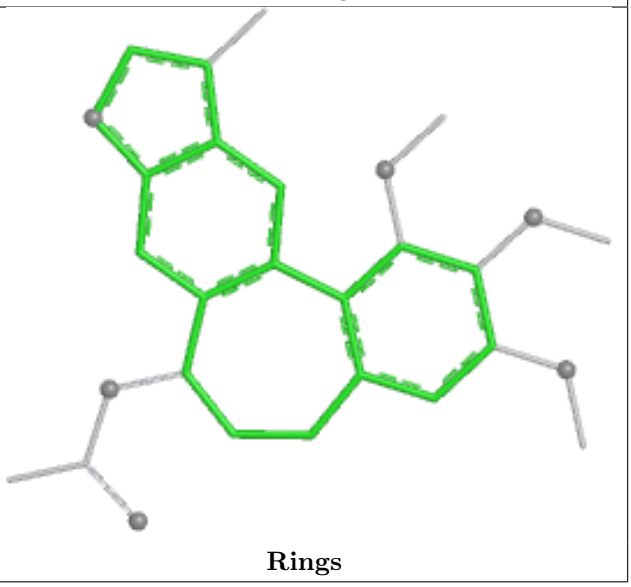
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	434/451 (96%)	0.72	49 (11%) 5 6	48, 81, 122, 142	0
1	C	434/451 (96%)	0.38	28 (6%) 18 23	41, 71, 103, 123	0
2	B	430/445 (96%)	0.74	52 (12%) 4 5	46, 71, 116, 149	0
2	D	429/445 (96%)	0.41	21 (4%) 29 35	45, 70, 107, 123	0
3	E	131/143 (91%)	1.42	30 (22%) 0 0	78, 106, 148, 165	0
All	All	1858/1935 (96%)	0.62	180 (9%) 7 10	41, 76, 120, 165	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	4	ALA	13.0
1	A	336	LYS	10.7
3	E	144	SER	10.2
3	E	33	PRO	10.0
1	A	335	ILE	9.4
1	A	439	SER	7.8
3	E	145	ARG	6.9
1	A	437	VAL	6.7
1	A	337	THR	6.7
1	A	440	VAL	6.6
3	E	32	VAL	6.4
1	A	436	GLY	6.1
1	A	438	ASP	6.0
1	A	282	TYR	5.9
3	E	30	ASP	5.8
2	B	61	TYR	5.6
2	B	371	LEU	5.5
2	B	373	MET	5.4
1	A	333	ALA	5.4
3	E	5	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
3	E	24	LEU	5.3
2	B	57	THR	5.3
1	A	357	TYR	5.2
3	E	8	VAL	5.2
2	B	281	GLN	5.2
3	E	45	PRO	5.2
2	B	360	PRO	4.8
2	B	441	ASP	4.8
3	E	6	MET	4.7
2	B	442	GLU	4.6
1	A	37	PRO	4.6
3	E	16	SER	4.6
1	C	62	VAL	4.5
1	A	346	TRP	4.4
2	B	37	HIS	4.3
2	D	57	THR	4.3
1	A	309	HIS	4.3
1	A	280	LYS	4.2
1	A	342	GLN	4.2
3	E	26	PRO	4.2
1	C	255	PHE	4.1
2	D	56	ALA	4.0
1	C	45	GLY	4.0
2	B	372	LYS	4.0
2	B	42	LEU	4.0
2	B	285	ALA	4.0
1	A	262	TYR	3.9
3	E	120	LEU	3.9
1	A	339	ARG	3.9
1	A	292	THR	3.9
2	D	37	HIS	3.9
2	D	58	GLY	3.8
1	A	281	ALA	3.8
2	B	280	SER	3.8
1	A	355	ILE	3.8
3	E	29	PHE	3.7
2	D	55	GLU	3.7
1	A	332	ILE	3.7
1	C	38	SER	3.7
2	B	32	PRO	3.7
2	B	245	PRO	3.7
2	D	82	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	338	LYS	3.6
2	B	59	ASN	3.5
1	C	36	MET	3.5
1	A	324	VAL	3.5
2	D	85	GLN	3.4
1	A	308	ARG	3.4
1	A	351	PHE	3.3
2	B	82	PRO	3.3
2	B	85	GLN	3.3
2	B	358	ILE	3.3
2	D	39	ASP	3.3
1	A	284	GLU	3.2
2	B	83	PHE	3.2
1	A	57	GLY	3.2
2	B	58	GLY	3.2
2	B	296	PHE	3.2
2	D	30	ILE	3.1
1	A	326	LYS	3.1
2	D	255	LEU	3.1
1	C	282	TYR	3.1
3	E	7	GLU	3.1
1	C	250	VAL	3.1
1	C	56	THR	3.1
3	E	54	LEU	3.1
1	A	283	HIS	3.0
2	B	56	ALA	3.0
3	E	15	THR	3.0
1	A	341	ILE	3.0
2	B	98	GLY	2.9
2	B	46	LEU	2.9
2	B	39	ASP	2.9
3	E	22	VAL	2.9
1	C	60	LYS	2.9
2	B	282	GLN	2.9
2	D	61	TYR	2.9
2	B	99	ALA	2.9
1	A	231	ILE	2.8
3	E	47	LEU	2.8
1	A	330	ALA	2.8
2	B	36	TYR	2.8
1	C	440	VAL	2.7
2	D	59	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	142	GLU	2.7
3	E	48	GLU	2.7
2	B	293	GLN	2.7
2	B	23	VAL	2.7
1	C	252	LEU	2.7
2	B	416	MET	2.7
3	E	128	LYS	2.6
2	D	252	LEU	2.6
2	D	296	PHE	2.6
2	B	370	GLY	2.6
3	E	95	LYS	2.6
1	A	311	LYS	2.6
2	B	86	ILE	2.6
2	B	315	VAL	2.5
1	C	335	ILE	2.5
2	D	441	ASP	2.5
1	C	354	GLY	2.5
3	E	51	GLN	2.5
2	B	60	LYS	2.4
1	A	344	VAL	2.4
2	B	288	VAL	2.4
2	B	13	GLY	2.4
2	B	31	ASP	2.4
1	A	323	VAL	2.4
2	B	33	THR	2.4
3	E	96	MET	2.4
1	A	340	SER	2.4
2	B	249	ASN	2.4
2	D	247	GLN	2.4
3	E	9	ILE	2.4
2	B	369	ARG	2.4
1	A	372	GLN	2.4
1	C	352	LYS	2.3
1	C	339	ARG	2.3
2	D	401	ARG	2.3
1	C	353	VAL	2.3
2	D	78	VAL	2.3
2	D	257	VAL	2.3
1	A	122	ILE	2.3
1	A	171	ILE	2.3
1	C	253	THR	2.3
2	B	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	112	ALA	2.3
3	E	46	SER	2.3
1	C	283	HIS	2.3
1	C	337	THR	2.2
2	D	179[A]	ASP	2.2
1	A	245	ASP	2.2
1	A	271	THR	2.2
2	B	41	ASP	2.2
1	A	31	GLN	2.2
1	C	55	GLU	2.2
1	C	59	GLY	2.2
2	D	86	ILE	2.2
1	A	26	LEU	2.2
1	A	35	GLN	2.2
1	A	296	PHE	2.1
1	C	108	TYR	2.1
2	B	357	ASP	2.1
1	C	254	GLU	2.1
3	E	23	ILE	2.1
2	B	251	ASP	2.1
1	A	328	VAL	2.1
2	B	111	GLY	2.1
1	C	5	ILE	2.1
3	E	115	HIS	2.1
1	C	238	ILE	2.1
1	C	355	ILE	2.1
1	A	139	HIS	2.1
1	C	220	GLU	2.0
2	B	55	GLU	2.0
2	B	94	PHE	2.0
1	A	117	LEU	2.0
1	C	58	ALA	2.0
2	B	38	GLY	2.0
2	B	400	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

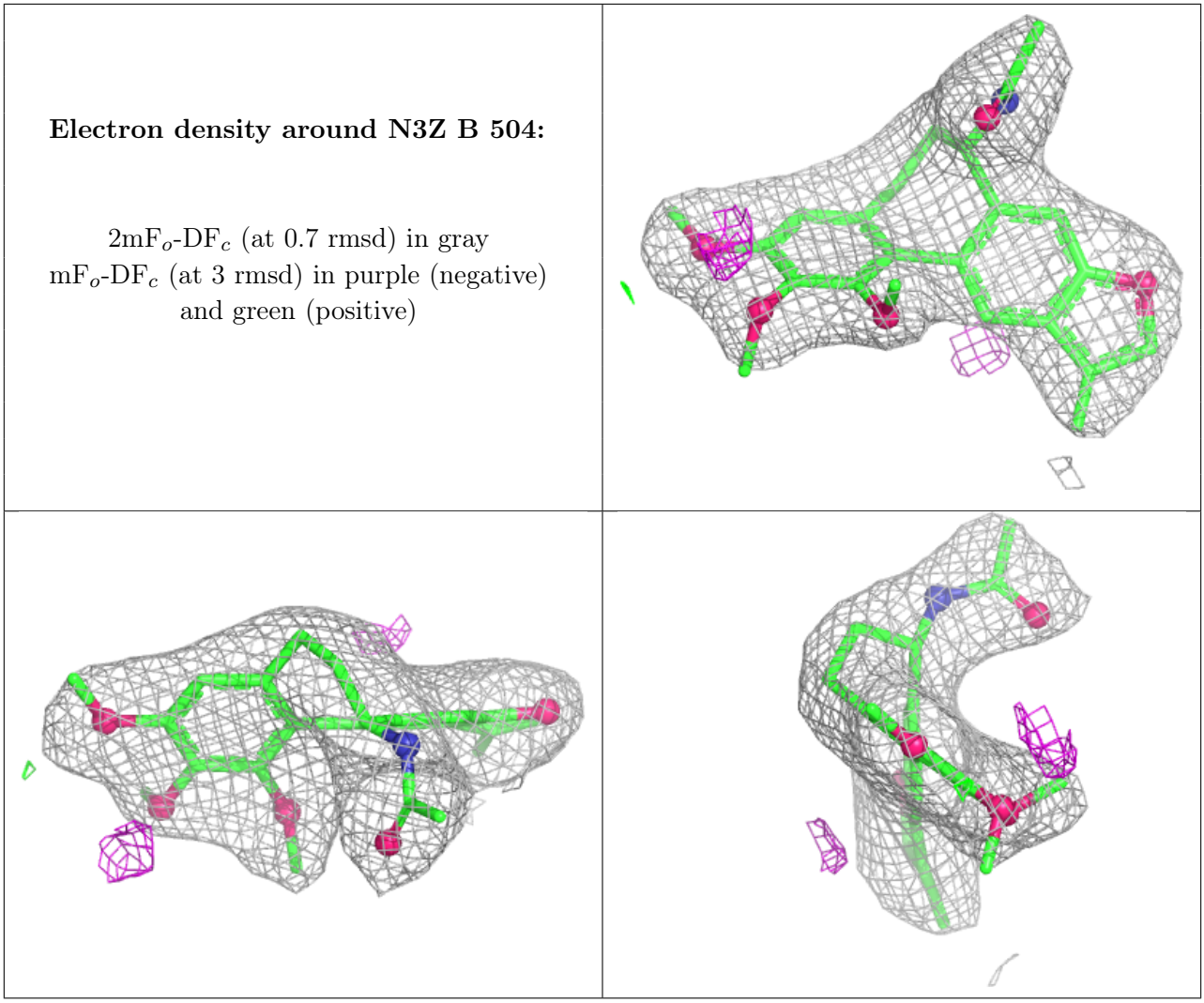
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	D	502	5/5	0.71	0.29	164,164,164,164	0
4	SO4	C	501	5/5	0.89	0.15	146,146,146,146	0
4	SO4	D	503	5/5	0.90	0.17	136,136,136,136	0
4	SO4	B	501	5/5	0.92	0.12	132,132,132,132	0
4	SO4	A	501	5/5	0.93	0.18	144,144,144,144	0
8	N3Z	B	504	29/29	0.93	0.17	68,68,69,69	0
4	SO4	B	502	5/5	0.94	0.07	187,187,187,187	0
4	SO4	C	503	5/5	0.94	0.17	151,151,151,151	0
4	SO4	D	501	5/5	0.94	0.15	120,121,121,121	0
6	MG	A	503	1/1	0.95	0.16	54,54,54,54	0
8	N3Z	D	505	29/29	0.95	0.15	59,61,62,62	0
4	SO4	C	502	5/5	0.97	0.20	146,146,146,146	0
7	GDP	B	503	28/28	0.97	0.19	57,59,59,60	0
7	GDP	D	504	28/28	0.98	0.12	59,62,65,66	0
5	GTP	A	502	32/32	0.98	0.18	50,52,53,54	0
5	GTP	C	504	32/32	0.98	0.15	53,54,55,56	0
6	MG	C	505	1/1	0.99	0.16	55,55,55,55	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.

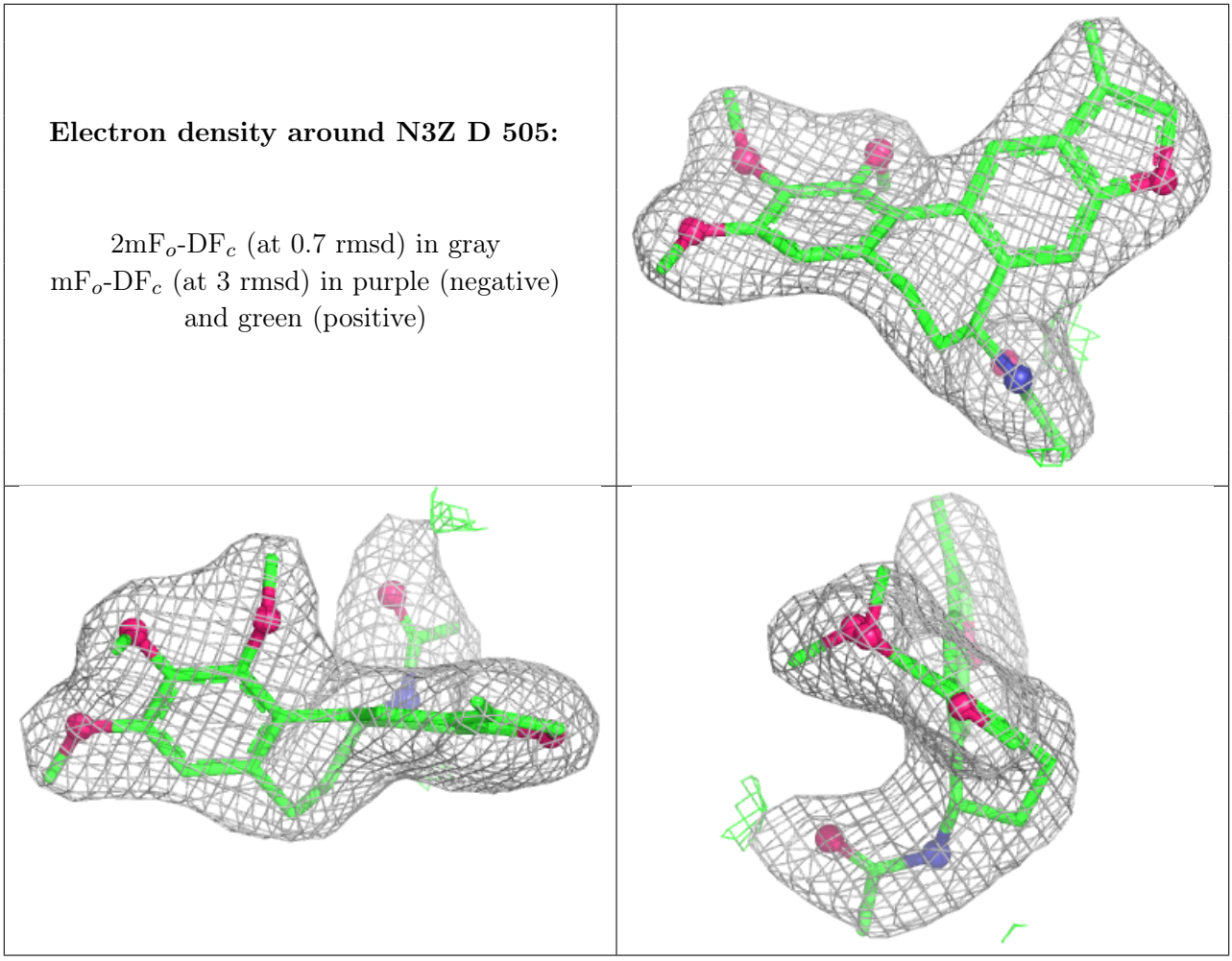
Electron density around N3Z B 504:

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



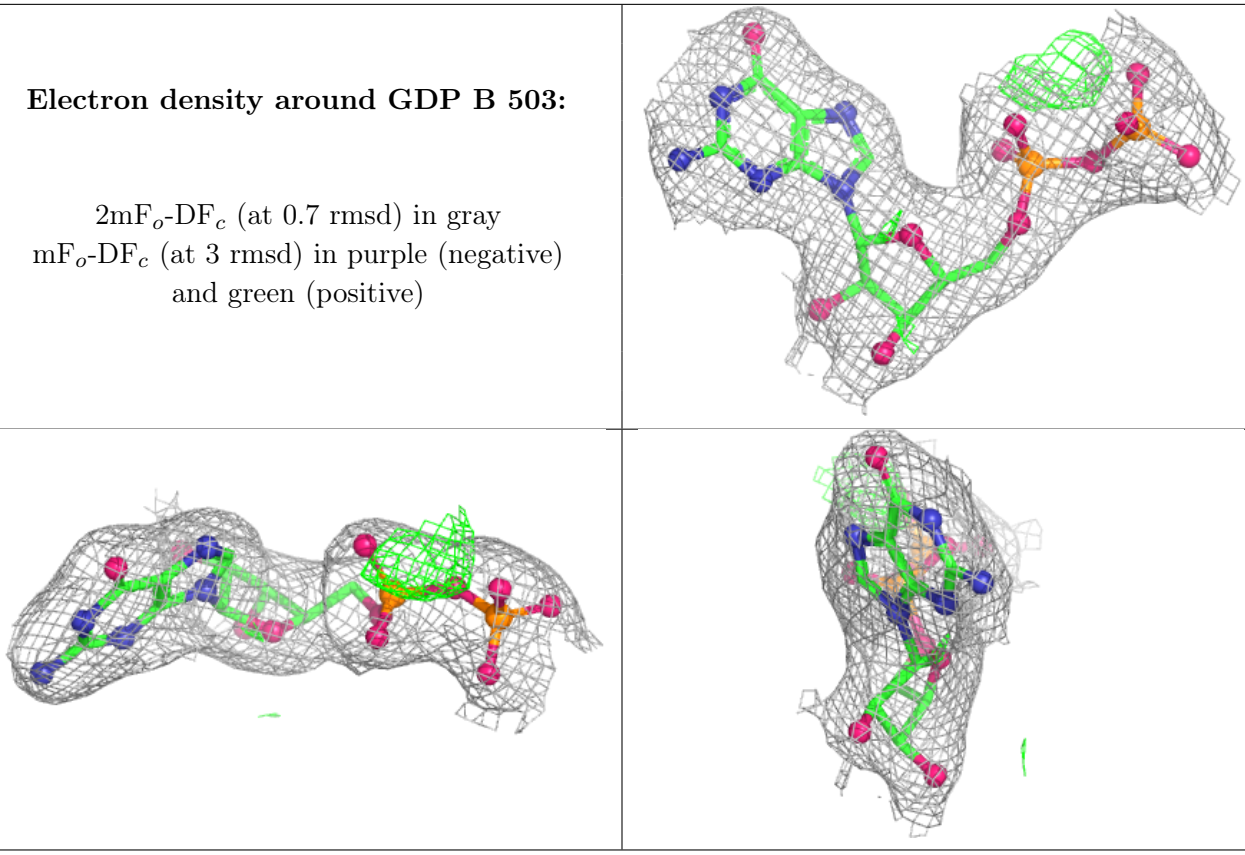
Electron density around N3Z D 505:

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



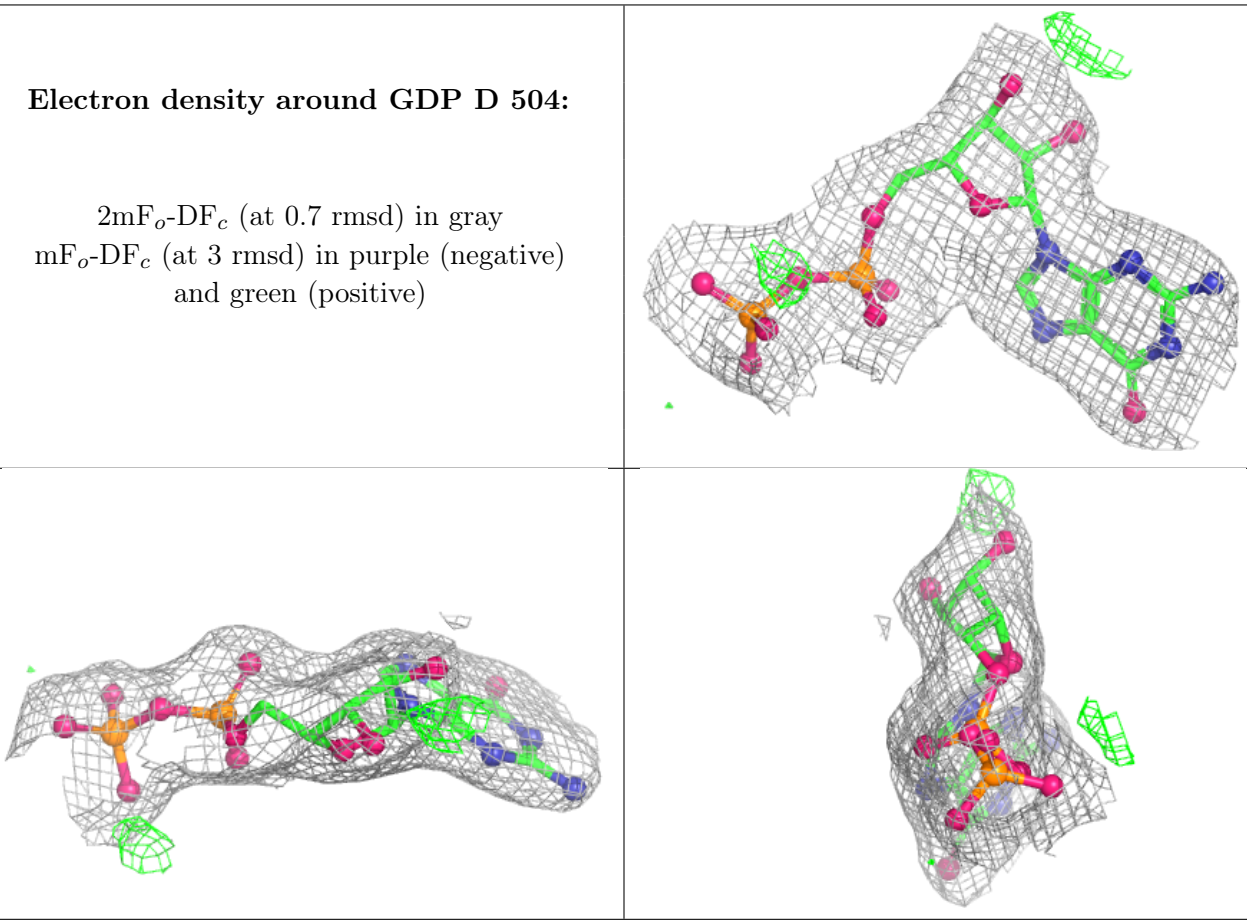
Electron density around GDP B 503:

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



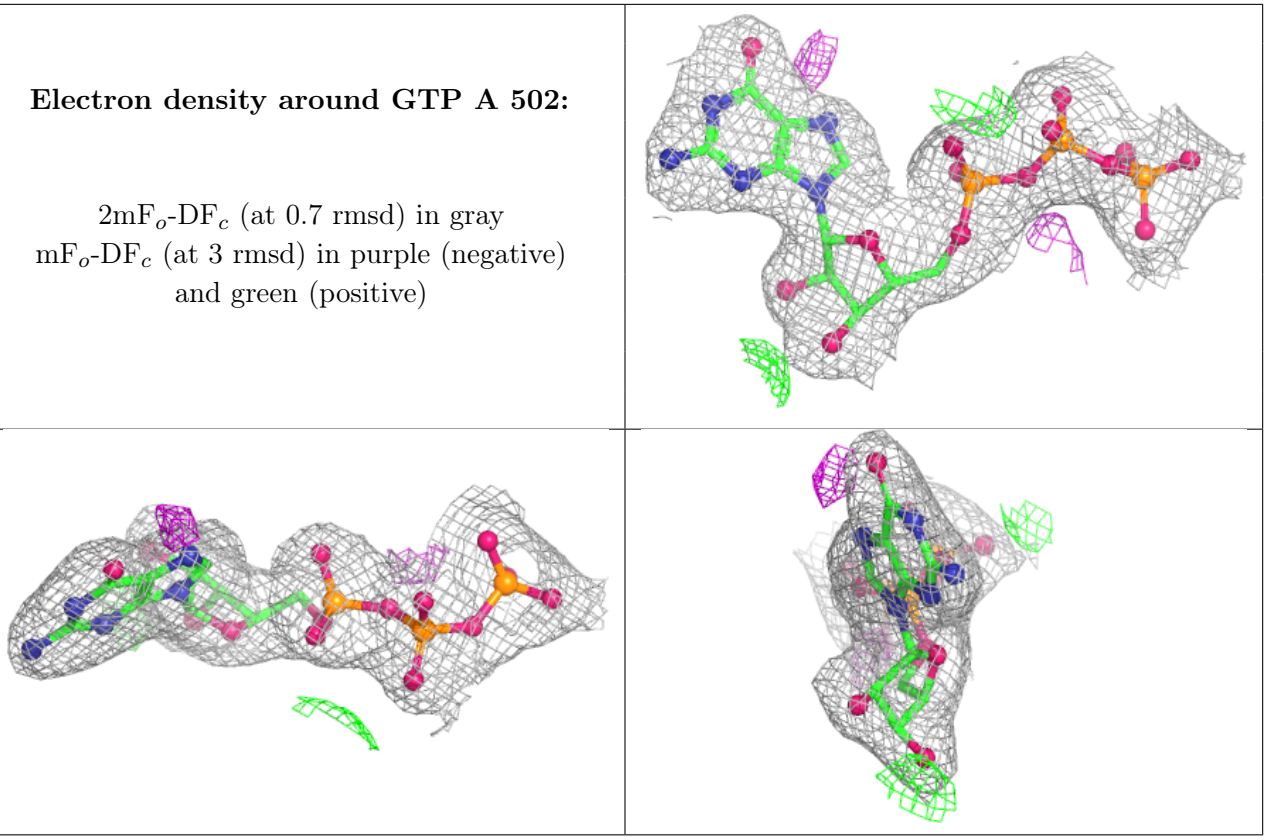
Electron density around GDP D 504:

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



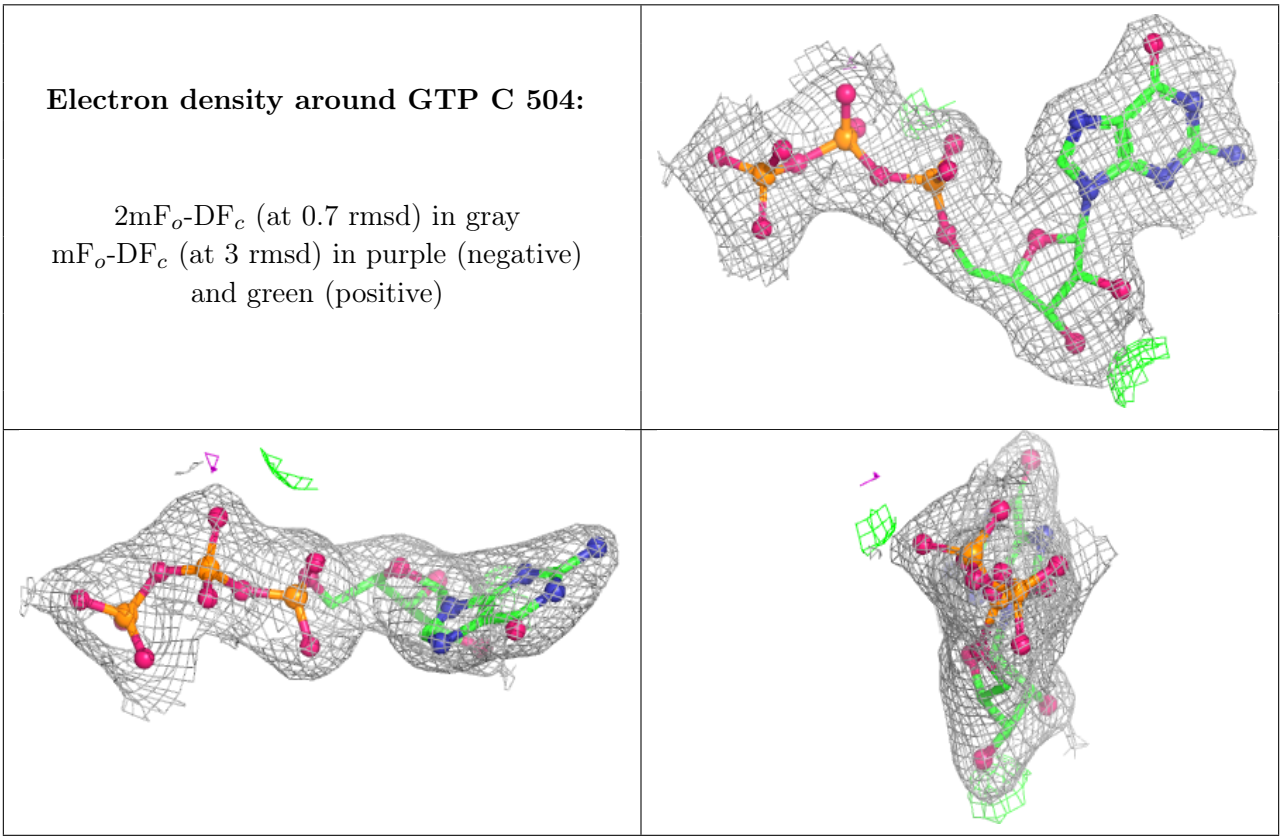
Electron density around GTP A 502:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.