



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:05 AM UTC

PDB ID : 6H9B / pdb_00006h9b
Title : 1,1-Diheterocyclic Ethylenes Derived from Quinaldine and Carbazole as New Tubulin Polymerization Inhibitors: Synthesis, Metabolism, and Biological Evaluation
Authors : Varela, P.F.; Gigant, B.
Deposited on : 2018-08-03
Resolution : 2.75 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:

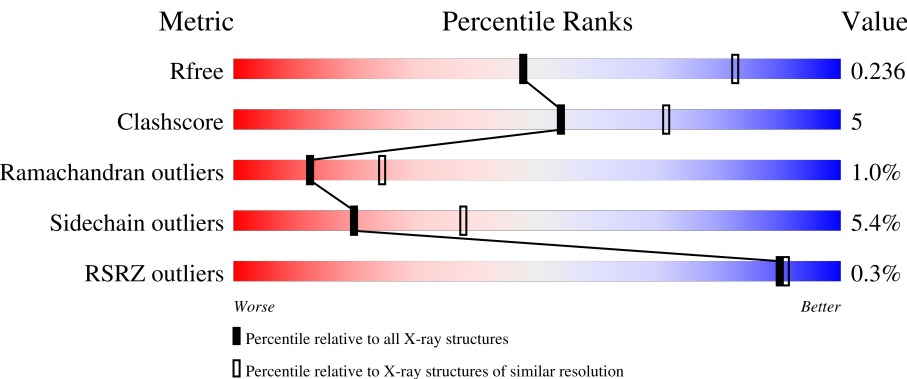
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	433	87%11%.
1	C	433	85%13%.
2	B	431	78%19%..
2	D	431	80%16%..

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Mol	Chain	Length	Quality of chain
3	E	142	% 77% 16% ...

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15148 atoms, of which 40 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3380	2141	574	643	22			
1	C	433	Total	C	N	O	S	0	0	0
			3393	2149	576	646	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3393	2128	580	658	27			
2	D	427	Total	C	N	O	S	0	0	0
			3356	2105	572	652	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	136	Total	C	N	O	S	0	0	0
			1125	691	209	221	4			

There are 3 discrepancies between the modelled and reference sequences:

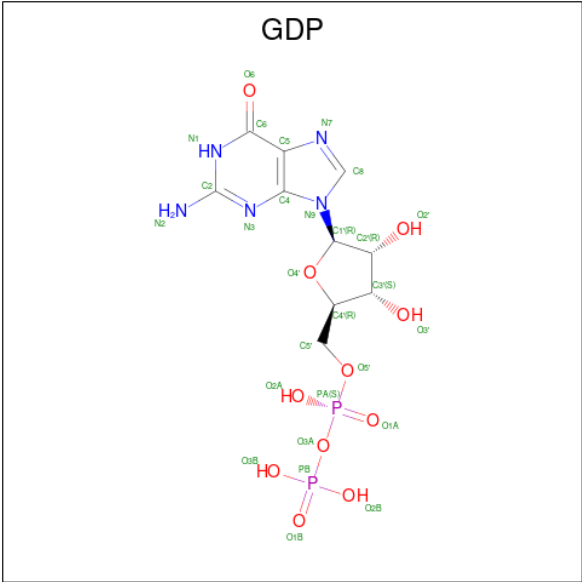
Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	SER	conflict	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- 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	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	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		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	H	N	0	0
			47	25	20	2		

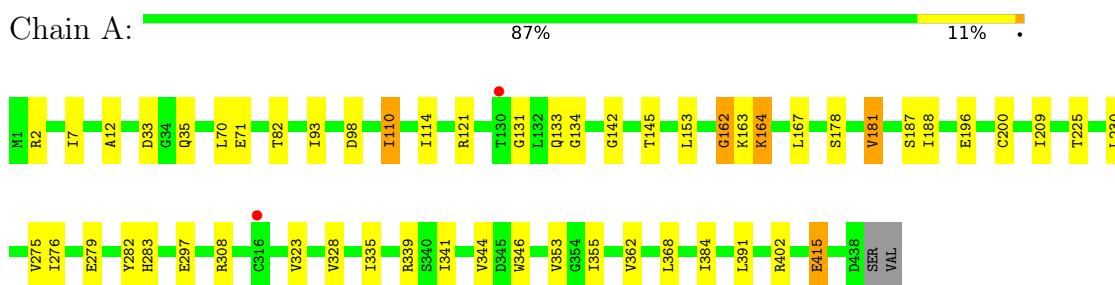
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	51	Total	O	0	0
			51	51		
9	B	43	Total	O	0	0
			43	43		
9	C	57	Total	O	0	0
			57	57		
9	D	64	Total	O	0	0
			64	64		
9	E	15	Total	O	0	0
			15	15		

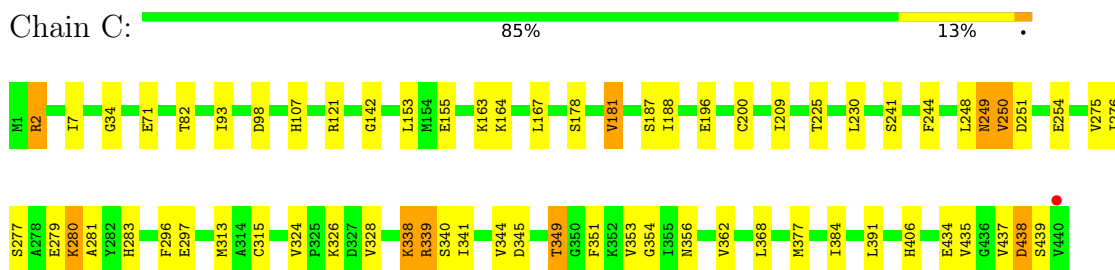
3 Residue-property plots

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.

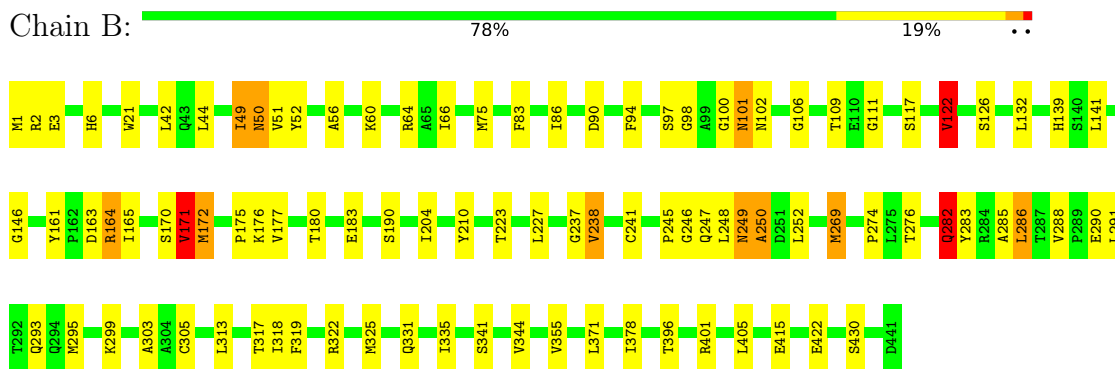
• Molecule 1: Tubulin alpha chain



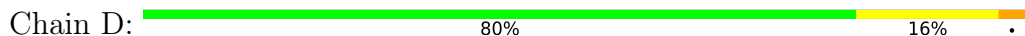
• Molecule 1: Tubulin alpha chain

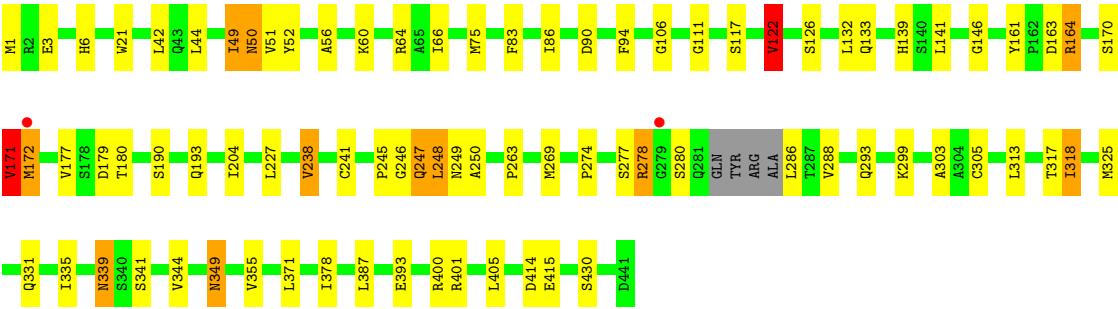


• Molecule 2: Tubulin beta chain

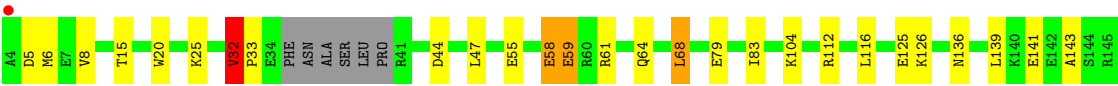
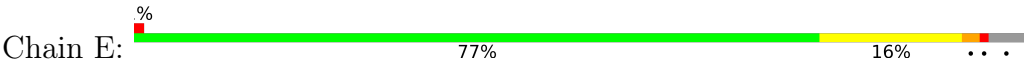


• Molecule 2: Tubulin beta chain





● 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	64.94Å 128.48Å 251.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 2.75 47.65 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.65-2.75) 99.9 (47.65-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.73Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.172 , 0.216 0.190 , 0.236	Depositor DCC
R_{free} test set	2789 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 119.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15148	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: FWH, SO4, MG, GDP, 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	0.79	1/3457 (0.0%)	1.24	9/4693 (0.2%)
1	C	0.84	0/3470	1.27	9/4711 (0.2%)
2	B	0.91	5/3468 (0.1%)	1.37	16/4697 (0.3%)
2	D	0.93	4/3429 (0.1%)	1.36	15/4643 (0.3%)
3	E	0.87	1/1136 (0.1%)	1.44	3/1510 (0.2%)
All	All	0.87	11/14960 (0.1%)	1.32	52/20254 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	269	MET	SD-CE	-6.91	1.62	1.79
2	D	172	MET	SD-CE	6.22	1.95	1.79
2	B	172	MET	CA-C	-6.11	1.46	1.53
2	B	295	MET	SD-CE	-5.96	1.64	1.79
2	D	288	VAL	CA-CB	5.95	1.57	1.54
3	E	32	VAL	CA-C	5.88	1.59	1.52
1	A	323	VAL	C-N	5.66	1.37	1.32
2	B	288	VAL	CA-CB	5.66	1.57	1.54
2	B	109	THR	CA-C	5.42	1.55	1.52
2	D	249	ASN	CA-C	-5.17	1.47	1.53
2	D	278	ARG	CA-C	5.10	1.59	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	247	GLN	CA-C-N	11.82	142.98	121.70
2	D	247	GLN	C-N-CA	11.82	142.98	121.70
1	C	340	SER	N-CA-C	-8.24	100.27	110.41
2	D	349	ASN	CA-CB-CG	7.49	120.08	112.60
3	E	59	GLU	CB-CG-CD	6.64	123.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	GLY	CA-C-N	6.63	134.20	121.54
2	B	246	GLY	C-N-CA	6.63	134.20	121.54
2	B	285	ALA	CA-C-N	6.53	134.02	121.54
2	B	285	ALA	C-N-CA	6.53	134.02	121.54
2	D	249	ASN	N-CA-C	-6.51	95.68	107.60
2	B	282	GLN	CA-C-N	6.51	133.42	121.70
2	B	282	GLN	C-N-CA	6.51	133.42	121.70
1	C	297	GLU	CB-CG-CD	6.47	123.59	112.60
1	A	142	GLY	N-CA-C	6.24	120.75	112.77
2	B	101	ASN	CA-CB-CG	6.16	118.76	112.60
2	D	415	GLU	CA-C-N	6.14	128.51	120.28
2	D	415	GLU	C-N-CA	6.14	128.51	120.28
1	A	145	THR	CA-C-N	6.07	126.83	120.03
1	A	145	THR	C-N-CA	6.07	126.83	120.03
1	C	345	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	297	GLU	CB-CG-CD	6.00	122.80	112.60
3	E	47	LEU	CA-C-N	5.95	128.18	120.44
3	E	47	LEU	C-N-CA	5.95	128.18	120.44
2	B	249	ASN	N-CA-C	-5.95	98.13	110.80
2	D	163	ASP	CA-CB-CG	5.85	118.45	112.60
2	B	163	ASP	CA-CB-CG	5.84	118.44	112.60
2	D	339	ASN	CA-CB-CG	5.83	118.43	112.60
2	B	415	GLU	CA-C-N	5.77	128.01	120.28
2	B	415	GLU	C-N-CA	5.77	128.01	120.28
2	B	288	VAL	N-CA-CB	5.71	114.91	110.45
2	B	122	VAL	N-CA-CB	5.71	118.31	110.54
2	D	171	VAL	N-CA-CB	5.71	117.89	111.21
2	D	122	VAL	N-CA-CB	5.64	118.21	110.54
2	B	171	VAL	N-CA-CB	5.48	117.62	111.21
1	A	162	GLY	CA-C-N	5.46	131.97	121.54
1	A	162	GLY	C-N-CA	5.46	131.97	121.54
2	D	313	LEU	N-CA-C	-5.38	104.84	111.40
1	C	250	VAL	N-CA-CB	5.34	120.05	111.23
2	D	414	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	102	ASN	CA-CB-CG	5.34	117.94	112.60
2	D	179	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	251	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	249	ASN	CA-C-O	-5.23	114.90	121.02
2	D	288	VAL	N-CA-CB	5.21	114.51	110.45
1	C	142	GLY	N-CA-C	5.21	120.35	113.37
2	D	3	GLU	N-CA-C	5.21	117.77	109.96
1	C	34	GLY	CA-C-N	-5.17	114.48	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	GLY	C-N-CA	-5.17	114.48	122.59
1	A	114	ILE	N-CA-CB	-5.16	106.19	112.33
1	A	344	VAL	CA-C-N	5.12	127.39	120.38
1	A	344	VAL	C-N-CA	5.12	127.39	120.38
2	B	313	LEU	N-CA-C	-5.09	105.19	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3380	0	3290	22	0
1	C	3393	0	3304	36	0
2	B	3393	0	3270	49	0
2	D	3356	0	3234	35	0
3	E	1125	0	1134	13	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
4	E	5	0	0	0	0
5	A	32	0	12	0	0
5	C	32	0	12	1	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	0	0
8	B	27	20	0	2	0
8	D	27	20	0	3	0
9	A	51	0	0	2	0
9	B	43	0	0	0	0
9	C	57	0	0	0	0
9	D	64	0	0	1	0
9	E	15	0	0	0	0
All	All	15108	40	14280	144	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 (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.03	1.10
2:B:282:GLN:HB2	2:B:283:TYR:HA	1.48	0.94
1:C:296:PHE:CZ	1:C:377:MET:HE1	2.06	0.91
1:C:244:PHE:HB2	1:C:356:ASN:ND2	1.87	0.88
1:A:181:VAL:HG13	8:B:505:FWH:C22	2.14	0.77
2:B:98:GLY:H	1:C:2:ARG:NH1	1.85	0.74
2:B:282:GLN:HB2	2:B:283:TYR:CA	2.16	0.74
1:C:313:MET:SD	1:C:435:VAL:HG11	2.27	0.73
3:E:32:VAL:HB	3:E:33:PRO:CD	2.19	0.73
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.71	0.72
2:D:56:ALA:HB3	2:D:60:LYS:HG3	1.73	0.71
3:E:58:GLU:HG2	3:E:61:ARG:NH2	2.06	0.70
1:C:277:SER:HB3	1:C:280:LYS:HG3	1.79	0.64
1:C:244:PHE:CB	1:C:356:ASN:HD21	1.94	0.63
1:C:313:MET:SD	1:C:435:VAL:CG1	2.86	0.63
2:B:269:MET:HE3	2:B:305:CYS:HB2	1.81	0.62
3:E:64:GLN:O	3:E:68:LEU:HD12	2.00	0.61
1:C:181:VAL:HG13	8:D:505:FWH:C22	2.31	0.61
2:B:237:GLY:O	2:B:318:ILE:HD12	2.01	0.60
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.82	0.60
2:B:331:GLN:O	2:B:335:ILE:HG12	2.02	0.60
2:D:331:GLN:O	2:D:335:ILE:HG12	2.02	0.60
2:B:401:ARG:HH22	1:C:438:ASP:H	1.49	0.59
2:D:1:MET:SD	2:D:133:GLN:HA	2.44	0.58
2:D:247:GLN:HE22	2:D:325:MET:HE1	1.68	0.57
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.86	0.57
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.35	0.57
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.86	0.57
2:D:400:ARG:HH12	2:D:401:ARG:HH11	1.53	0.57
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.88	0.56
3:E:136:ASN:HA	3:E:139:LEU:HD12	1.89	0.55
2:B:161:TYR:HB3	2:B:164:ARG:HG3	1.88	0.55
2:B:269:MET:CE	2:B:305:CYS:HB2	2.37	0.55
3:E:8:VAL:HG23	3:E:20:TRP:CD1	2.42	0.55
2:D:51:VAL:HG23	2:D:52:TYR:CD2	2.42	0.55
1:C:248:LEU:O	1:C:354:GLY:HA2	2.07	0.54
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:LEU:O	2:D:49:ILE:HG13	2.08	0.54
2:B:51:VAL:HG23	2:B:52:TYR:CD2	2.42	0.54
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.90	0.54
2:B:44:LEU:O	2:B:49:ILE:HG13	2.07	0.53
2:B:101:ASN:HB3	2:B:180:THR:HG21	1.90	0.53
2:D:269:MET:HE3	2:D:305:CYS:HB2	1.90	0.52
1:A:308:ARG:CZ	1:A:339:ARG:HD3	2.40	0.52
1:C:437:VAL:O	1:C:438:ASP:HB2	2.09	0.52
2:B:50:ASN:O	2:B:64:ARG:NH2	2.41	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.10	0.51
2:B:42:LEU:HD23	2:B:245:PRO:HG2	1.92	0.50
2:D:241:CYS:SG	2:D:318:ILE:HD13	2.51	0.50
1:C:296:PHE:HZ	1:C:377:MET:HE1	1.70	0.50
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.42	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.49
1:A:355:ILE:HD11	3:E:20:TRP:HH2	1.78	0.49
2:B:282:GLN:CB	2:B:283:TYR:HA	2.32	0.49
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.95	0.49
2:D:50:ASN:O	2:D:64:ARG:NH2	2.40	0.49
2:D:238:VAL:HG22	2:D:378:ILE:HG12	1.95	0.49
2:B:286:LEU:HA	2:B:290:GLU:OE1	2.12	0.49
2:B:180:THR:HG23	2:B:183:GLU:HG3	1.95	0.48
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.48
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.95	0.48
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.95	0.48
2:B:223:THR:HG23	1:C:326:LYS:HE2	1.96	0.48
2:B:317:THR:HG22	2:B:319:PHE:CE1	2.49	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
2:B:175:PRO:HB3	1:C:349:THR:HG23	1.96	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.47
2:D:139:HIS:HD2	2:D:146:GLY:O	1.96	0.47
2:B:401:ARG:HH11	1:C:439:SER:HB2	1.79	0.47
1:C:434:GLU:HA	1:C:437:VAL:HG23	1.96	0.47
1:A:402:ARG:HD2	1:A:415:GLU:OE1	2.15	0.47
2:B:2:ARG:HG3	2:B:3:GLU:OE2	2.15	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.15	0.47
1:A:134:GLY:HA2	1:A:164:LYS:HG2	1.96	0.47
3:E:58:GLU:HG2	3:E:61:ARG:HH22	1.79	0.47
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.97	0.46
2:B:249:ASN:O	2:B:250:ALA:CB	2.63	0.46
2:D:139:HIS:HE1	2:D:170:SER:OG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.97	0.46
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.96	0.46
3:E:32:VAL:HB	3:E:33:PRO:HD2	1.95	0.46
2:B:325:MET:HE2	2:B:355:VAL:HB	1.97	0.46
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.97	0.46
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.97	0.46
2:B:139:HIS:HE1	2:B:170:SER:OG	1.99	0.46
1:A:12:ALA:HB3	9:A:602:HOH:O	2.16	0.46
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.97	0.46
1:A:98:ASP:HB2	9:A:603:HOH:O	2.15	0.46
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.97	0.46
1:C:98:ASP:HB2	5:C:502:GTP:O1G	2.16	0.46
2:D:269:MET:CE	2:D:305:CYS:HB2	2.45	0.46
2:B:126:SER:HB2	2:B:132:LEU:HD22	1.98	0.45
2:B:317:THR:CG2	2:B:319:PHE:CE1	2.99	0.45
2:B:139:HIS:HD2	2:B:146:GLY:O	2.00	0.45
2:B:238:VAL:HG22	2:B:378:ILE:HG12	1.98	0.45
2:B:97:SER:HA	1:C:2:ARG:HD3	1.97	0.45
2:B:249:ASN:O	2:B:250:ALA:HB3	2.16	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.45
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.69	0.45
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.97	0.45
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.97	0.45
2:B:141:LEU:HD22	2:B:190:SER:HB3	1.98	0.45
1:C:315:CYS:O	1:C:351:PHE:HA	2.16	0.45
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.51	0.45
2:B:98:GLY:H	1:C:2:ARG:HH11	1.59	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.97	0.45
2:D:241:CYS:HB2	8:D:505:FWH:C3	2.47	0.45
2:D:274:PRO:HB3	2:D:286:LEU:HD13	1.98	0.45
2:B:176:LYS:HD3	2:B:210:TYR:CD2	2.52	0.45
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.99	0.44
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.00	0.44
1:C:338:LYS:HE2	1:C:339:ARG:HH22	1.83	0.44
2:B:172:MET:HE2	2:B:172:MET:HB2	1.81	0.44
2:B:241:CYS:HB2	8:B:505:FWH:C3	2.47	0.44
2:B:83:PHE:O	2:B:86:ILE:HG22	2.17	0.44
1:C:241:SER:HB3	1:C:249:ASN:O	2.17	0.44
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.44
2:D:325:MET:HE2	2:D:355:VAL:HB	2.00	0.44
2:D:393:GLU:HB2	9:D:609:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.43
3:E:79:GLU:O	3:E:83:ILE:HD12	2.19	0.43
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.99	0.43
1:C:276:ILE:HG23	1:C:280:LYS:HD2	2.01	0.43
2:B:396:THR:HG22	2:B:422:GLU:OE2	2.18	0.43
3:E:141:GLU:C	3:E:143:ALA:H	2.27	0.43
1:C:338:LYS:HE2	1:C:339:ARG:HH12	1.84	0.42
2:D:126:SER:HB2	2:D:132:LEU:HD22	2.01	0.42
2:D:400:ARG:HH12	2:D:401:ARG:NH1	2.16	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.42
1:A:276:ILE:HG21	1:A:283:HIS:CE1	2.54	0.42
2:B:75:MET:HE2	2:B:94:PHE:HD2	1.85	0.42
1:A:33:ASP:OD1	1:A:35:GLN:HG2	2.20	0.41
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.01	0.41
3:E:55:GLU:O	3:E:59:GLU:HG2	2.20	0.41
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.41
2:D:42:LEU:HD23	2:D:245:PRO:HG2	2.02	0.41
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.02	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.02	0.41
2:B:100:GLY:HA2	1:C:254:GLU:HG3	2.02	0.41
2:D:246:GLY:HA2	2:D:247:GLN:HA	1.83	0.41
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.86	0.40
2:D:250:ALA:HB1	8:D:505:FHW:C6	2.52	0.40
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.40
2:D:193:GLN:HE22	3:E:126:LYS:HE2	1.86	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	427/433 (99%)	412 (96%)	10 (2%)	5 (1%)	10 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	429/433 (99%)	402 (94%)	21 (5%)	6 (1%)	9	17
2	B	429/431 (100%)	410 (96%)	16 (4%)	3 (1%)	18	34
2	D	423/431 (98%)	411 (97%)	10 (2%)	2 (0%)	24	43
3	E	132/142 (93%)	125 (95%)	4 (3%)	3 (2%)	5	9
All	All	1840/1870 (98%)	1760 (96%)	61 (3%)	19 (1%)	12	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	247	GLN
2	B	250	ALA
2	B	286	LEU
1	C	281	ALA
1	C	349	THR
3	E	32	VAL
1	A	162	GLY
2	D	248	LEU
2	D	278	ARG
1	C	280	LYS
3	E	5	ASP
1	A	282	TYR
1	C	250	VAL
3	E	44	ASP
1	A	163	LYS
1	A	341	ILE
1	C	438	ASP
1	A	131	GLY
1	C	341	ILE

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	365/367 (100%)	352 (96%)	13 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	367/367 (100%)	349 (95%)	18 (5%)	22	43
2	B	374/374 (100%)	352 (94%)	22 (6%)	18	33
2	D	371/374 (99%)	346 (93%)	25 (7%)	15	28
3	E	120/125 (96%)	111 (92%)	9 (8%)	12	24
All	All	1597/1607 (99%)	1510 (95%)	87 (5%)	20	38

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	THR
1	A	110	ILE
1	A	164	LYS
1	A	178	SER
1	A	181	VAL
1	A	188	ILE
1	A	196	GLU
1	A	225	THR
1	A	279	GLU
1	A	335	ILE
1	A	362	VAL
1	A	384	ILE
1	A	415	GLU
2	B	1	MET
2	B	49	ILE
2	B	50	ASN
2	B	90	ASP
2	B	117	SER
2	B	122	VAL
2	B	164	ARG
2	B	171	VAL
2	B	177	VAL
2	B	227	LEU
2	B	238	VAL
2	B	248	LEU
2	B	276	THR
2	B	282	GLN
2	B	293	GLN
2	B	299	LYS
2	B	322	ARG
2	B	341	SER
2	B	344	VAL

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Mol	Chain	Res	Type
2	B	371	LEU
2	B	405	LEU
2	B	430	SER
1	C	2	ARG
1	C	71	GLU
1	C	82	THR
1	C	163	LYS
1	C	164	LYS
1	C	178	SER
1	C	181	VAL
1	C	188	ILE
1	C	196	GLU
1	C	225	THR
1	C	279	GLU
1	C	283	HIS
1	C	324	VAL
1	C	338	LYS
1	C	339	ARG
1	C	344	VAL
1	C	362	VAL
1	C	384	ILE
2	D	49	ILE
2	D	50	ASN
2	D	90	ASP
2	D	117	SER
2	D	122	VAL
2	D	164	ARG
2	D	171	VAL
2	D	177	VAL
2	D	180	THR
2	D	227	LEU
2	D	238	VAL
2	D	248	LEU
2	D	277	SER
2	D	280	SER
2	D	293	GLN
2	D	299	LYS
2	D	317	THR
2	D	318	ILE
2	D	339	ASN
2	D	341	SER
2	D	344	VAL

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Mol	Chain	Res	Type
2	D	349	ASN
2	D	371	LEU
2	D	405	LEU
2	D	430	SER
3	E	6	MET
3	E	15	THR
3	E	25	LYS
3	E	58	GLU
3	E	68	LEU
3	E	104	LYS
3	E	112	ARG
3	E	116	LEU
3	E	125	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	283	HIS
1	A	372	GLN
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	136	GLN
2	B	139	HIS
2	B	167	ASN
2	B	282	GLN
2	B	385	GLN
2	B	436	GLN
1	C	31	GLN
1	C	107	HIS
1	C	258	ASN
1	C	293	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	8	GLN
2	D	14	ASN
2	D	101	ASN
2	D	136	GLN
2	D	139	HIS

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Mol	Chain	Res	Type
2	D	167	ASN
2	D	193	GLN
2	D	247	GLN
2	D	281	GLN
2	D	349	ASN
3	E	78	HIS
3	E	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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
8	FWH	D	505	-	31,31,31	0.43	0	46,46,46	0.80	2 (4%)
4	SO4	D	502	-	4,4,4	0.19	0	6,6,6	0.29	0
4	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.16	0
4	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.20	0
4	SO4	C	501	-	4,4,4	0.31	0	6,6,6	0.10	0
5	GTP	A	503	6	33,34,34	0.53	0	50,54,54	0.74	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	502	6	33,34,34	0.48	0	50,54,54	0.72	1 (2%)
7	GDP	D	504	-	29,30,30	0.58	0	45,47,47	0.72	2 (4%)
8	FWH	B	505	-	31,31,31	0.36	0	46,46,46	0.88	2 (4%)
4	SO4	A	501	-	4,4,4	0.31	0	6,6,6	0.26	0
4	SO4	D	501	-	4,4,4	0.38	0	6,6,6	0.27	0
4	SO4	D	503	-	4,4,4	0.19	0	6,6,6	0.56	0
4	SO4	E	201	-	4,4,4	0.24	0	6,6,6	0.15	0
4	SO4	B	501	-	4,4,4	0.20	0	6,6,6	0.22	0
7	GDP	B	504	-	29,30,30	0.52	0	45,47,47	0.76	2 (4%)
4	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.33	0
4	SO4	C	504	-	4,4,4	0.30	0	6,6,6	0.12	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
8	FWH	D	505	-	-	1/8/8/8	0/5/5/5
7	GDP	D	504	-	-	5/16/32/32	0/3/3/3
5	GTP	A	503	6	-	8/22/38/38	0/3/3/3
5	GTP	C	502	6	-	8/22/38/38	0/3/3/3
8	FWH	B	505	-	-	1/8/8/8	0/5/5/5
7	GDP	B	504	-	-	6/16/32/32	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	505	FWH	C9-C16-C11	-3.86	113.34	118.22
8	B	505	FWH	C9-C16-C24	3.47	125.58	120.15
8	D	505	FWH	C9-C16-C11	-3.32	114.02	118.22
8	D	505	FWH	C9-C16-C24	3.17	125.10	120.15
7	B	504	GDP	O2A-PA-O5'	2.74	119.97	107.57
5	A	503	GTP	O3G-PG-O3B	2.32	112.41	104.64
7	B	504	GDP	O2B-PB-O3A	2.26	112.22	104.64
5	C	502	GTP	O3A-PA-O1A	-2.21	104.05	110.70
7	D	504	GDP	O2A-PA-O3A	2.11	112.99	107.27
7	D	504	GDP	O2B-PB-O3A	2.08	111.61	104.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	GTP	C5'-O5'-PA-O3A
5	A	503	GTP	C5'-O5'-PA-O1A
5	A	503	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
7	B	504	GDP	C5'-O5'-PA-O3A
7	B	504	GDP	C5'-O5'-PA-O1A
7	B	504	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	505	FWH	C10-C11-C16-C9
8	D	505	FWH	C10-C11-C16-C9
5	A	503	GTP	PB-O3A-PA-O1A
7	B	504	GDP	PB-O3A-PA-O1A
7	D	504	GDP	PB-O3A-PA-O1A
5	C	502	GTP	C3'-C4'-C5'-O5'
5	A	503	GTP	PG-O3B-PB-O3A
5	C	502	GTP	PB-O3B-PG-O1G
5	C	502	GTP	PB-O3B-PG-O2G
5	C	502	GTP	O4'-C4'-C5'-O5'
7	D	504	GDP	PB-O3A-PA-O2A
7	B	504	GDP	C4'-C5'-O5'-PA
5	A	503	GTP	PG-O3B-PB-O1B
5	A	503	GTP	PG-O3B-PB-O2B
5	A	503	GTP	PB-O3A-PA-O2A
7	B	504	GDP	PB-O3A-PA-O2A

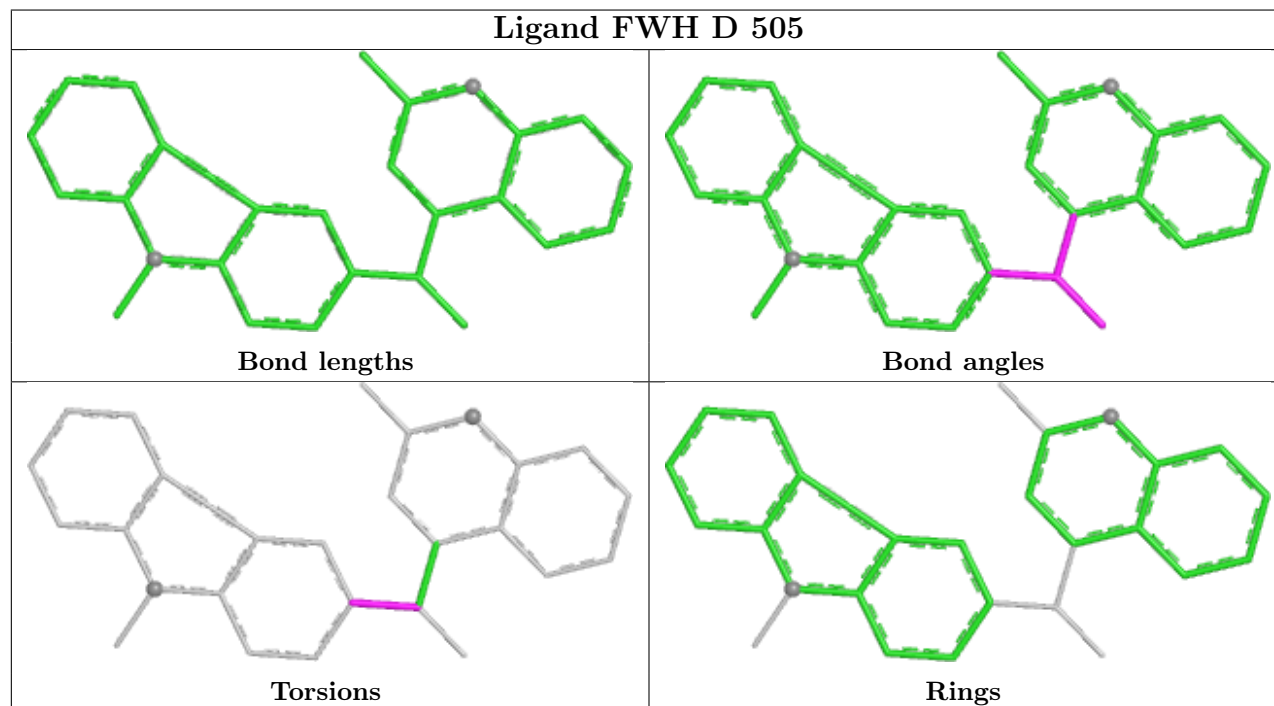
There are no ring outliers.

3 monomers are involved in 6 short contacts:

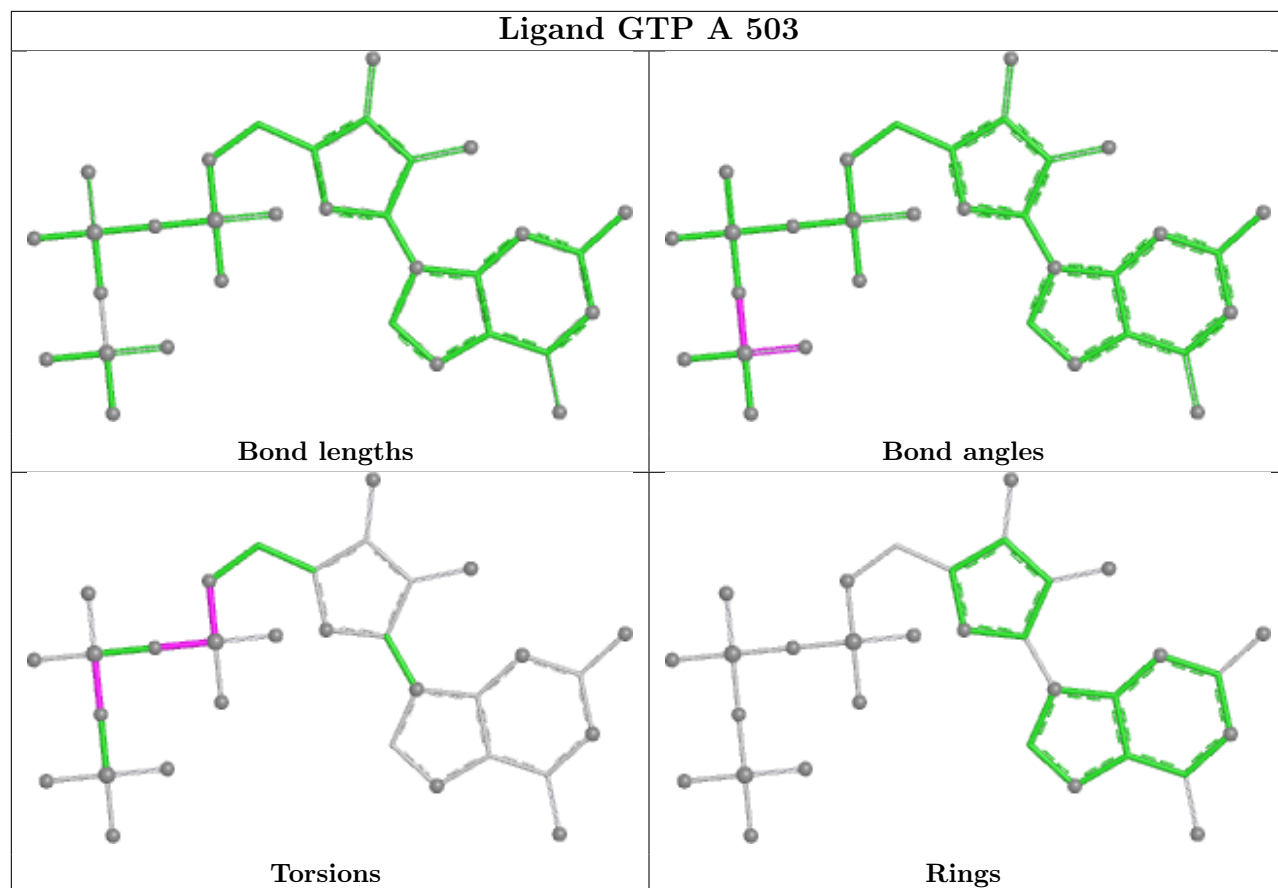
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	505	FWH	3	0
5	C	502	GTP	1	0
8	B	505	FWH	2	0

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

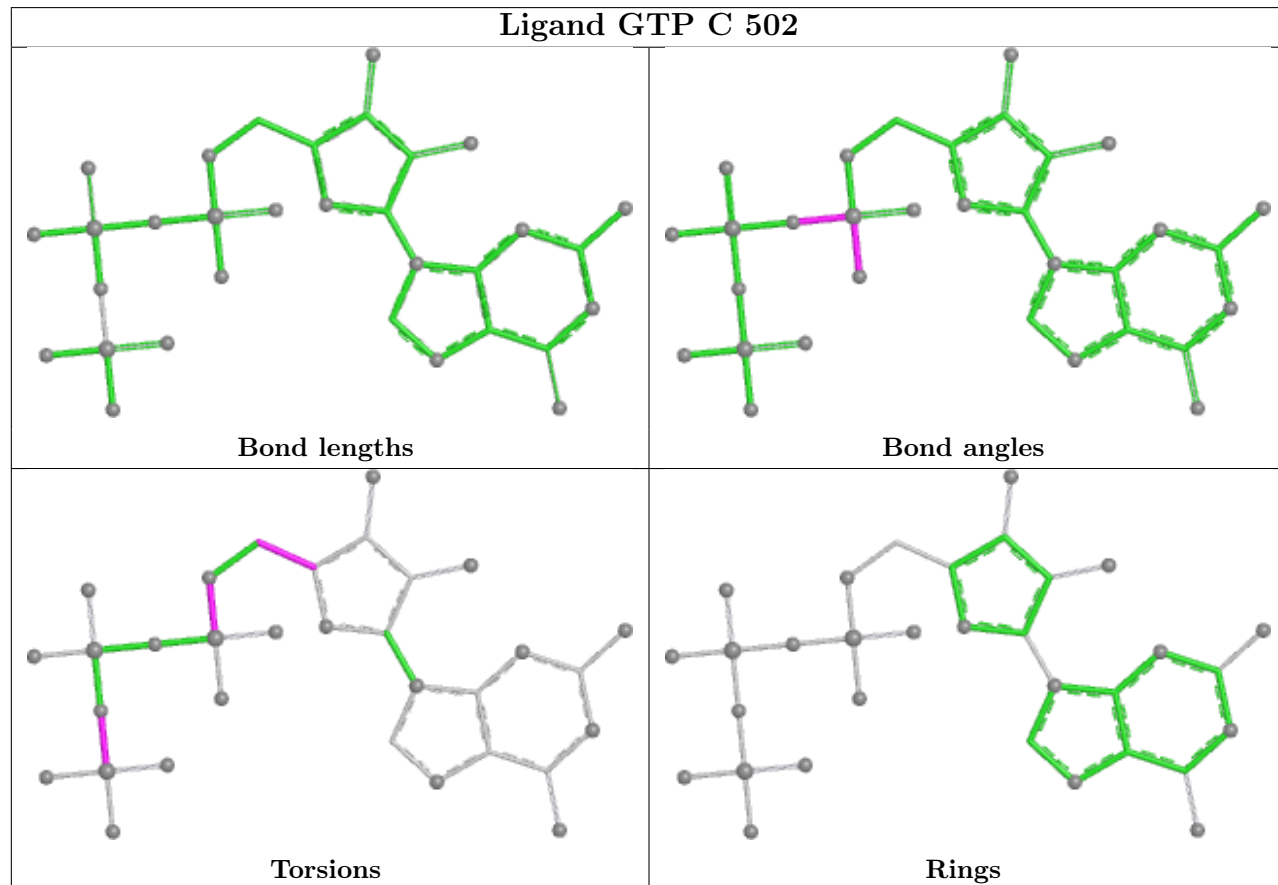
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

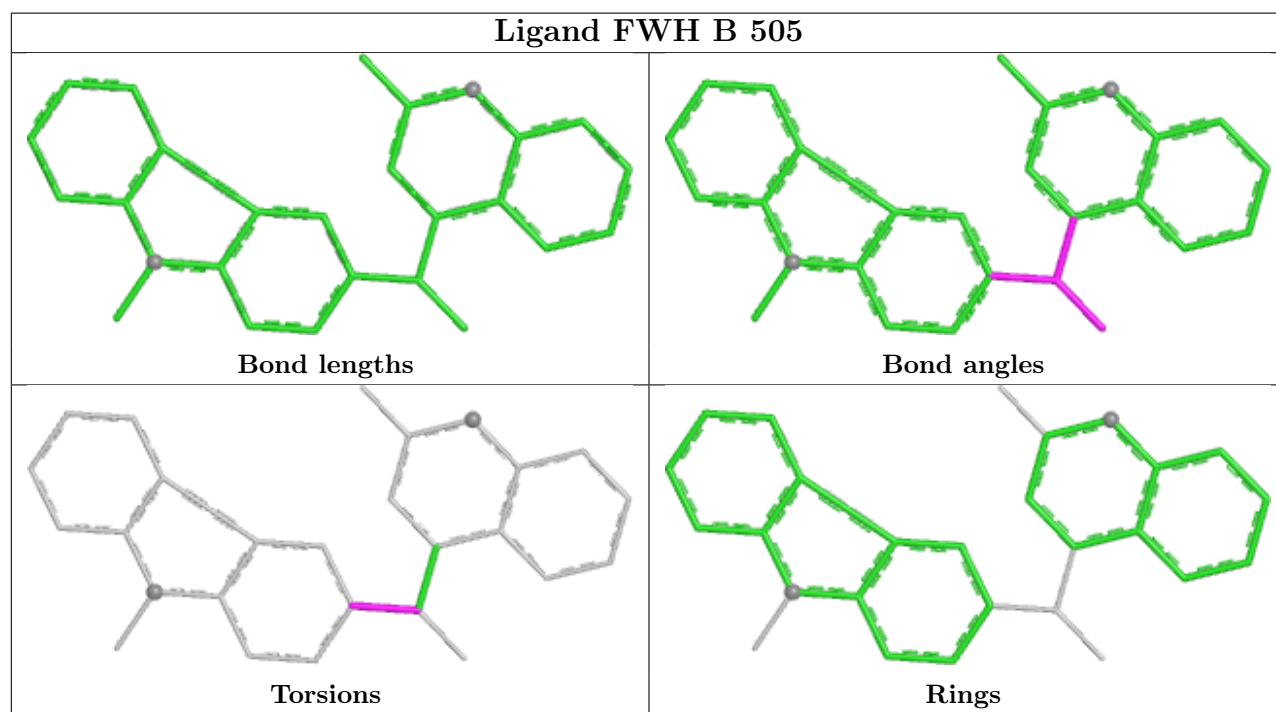
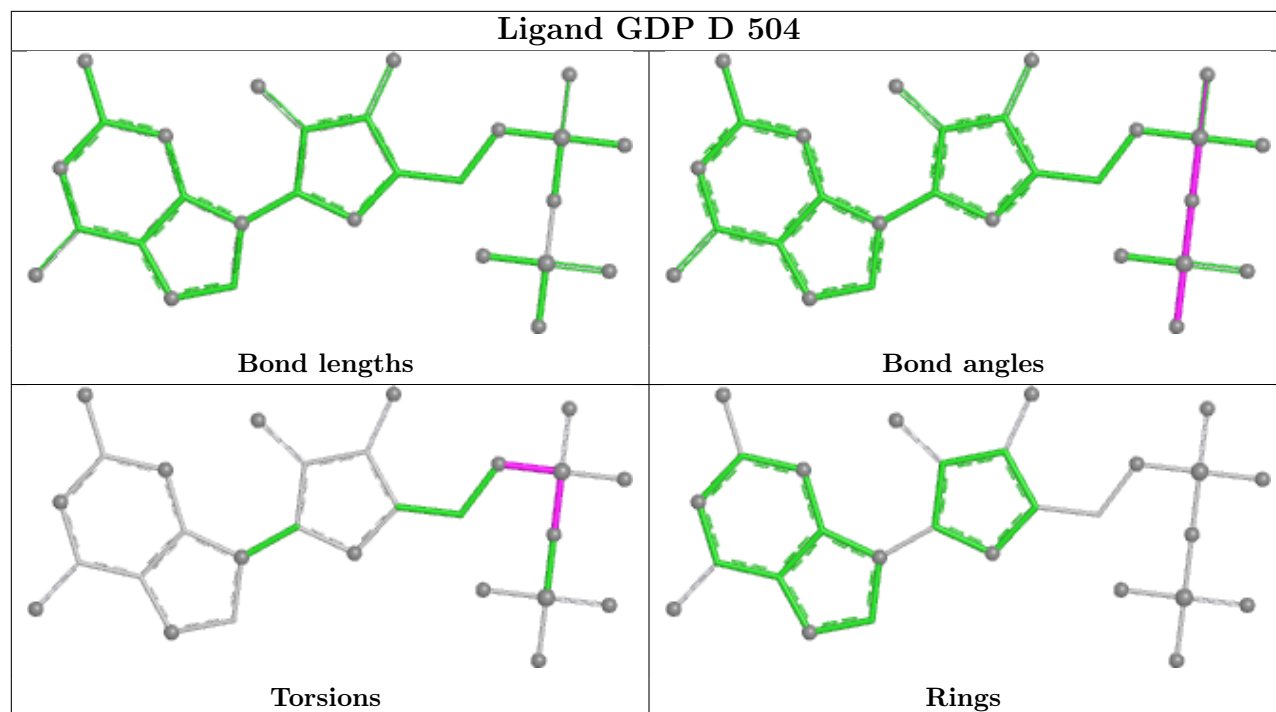


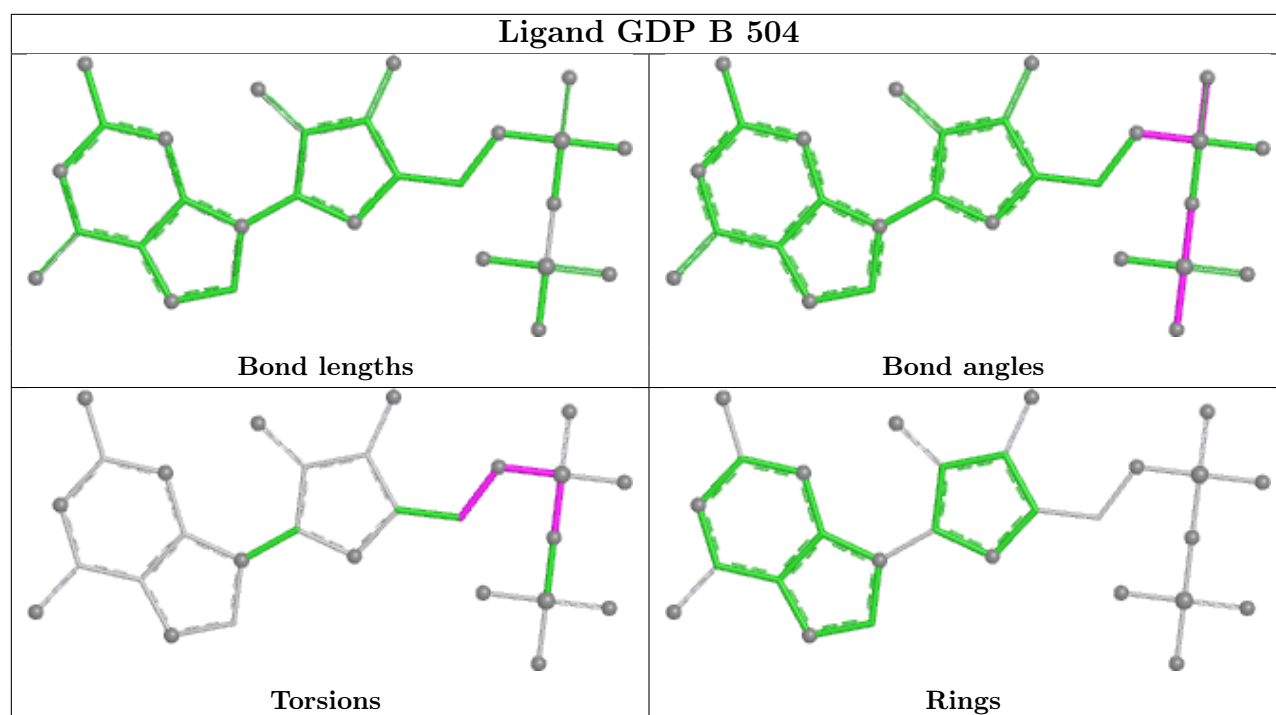
Ligand GTP A 503



Ligand GTP C 502







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	38:SER	C	46:ASP	N	10.49
1	A	38:SER	C	46:ASP	N	10.40

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/433 (99%)	-0.37	2 (0%) 87 87	79, 107, 150, 186	0
1	C	433/433 (100%)	-0.38	1 (0%) 91 92	71, 104, 147, 182	0
2	B	431/431 (100%)	-0.42	0 100 100	75, 102, 159, 191	0
2	D	427/431 (99%)	-0.37	2 (0%) 87 87	67, 93, 141, 171	0
3	E	136/142 (95%)	-0.42	1 (0%) 84 84	97, 132, 190, 200	0
All	All	1858/1870 (99%)	-0.39	6 (0%) 90 91	67, 105, 155, 200	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	CYS	2.7
1	A	130	THR	2.4
1	C	440	VAL	2.2
2	D	279	GLY	2.1
3	E	4	ALA	2.1
2	D	172	MET	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 ⓘ

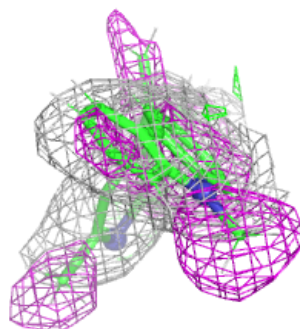
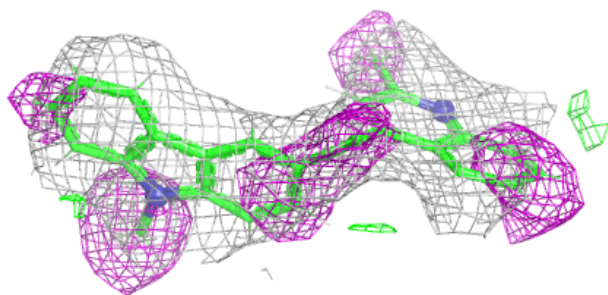
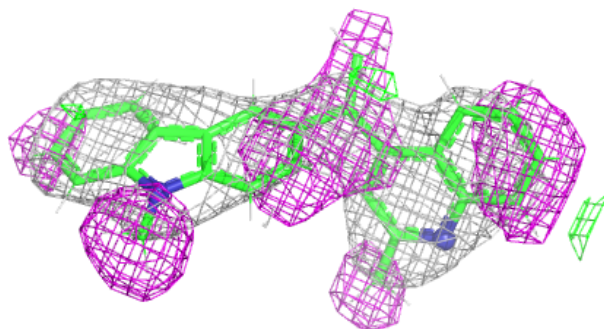
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	501	5/5	0.69	0.14	201,201,202,203	0
4	SO4	C	504	5/5	0.70	0.07	184,188,191,192	0
4	SO4	C	501	5/5	0.71	0.08	213,213,214,215	0
4	SO4	A	502	5/5	0.74	0.10	215,216,216,217	0
4	SO4	B	503	5/5	0.77	0.09	177,178,178,180	0
4	SO4	E	201	5/5	0.77	0.06	175,177,177,181	0
4	SO4	B	502	5/5	0.82	0.06	181,182,183,188	0
4	SO4	B	501	5/5	0.84	0.06	143,149,150,155	0
4	SO4	A	501	5/5	0.85	0.06	179,179,180,182	0
4	SO4	D	502	5/5	0.86	0.07	170,172,173,174	0
4	SO4	D	503	5/5	0.89	0.07	146,152,154,156	0
8	FWH	D	505	27/27	0.89	0.09	19,51,63,69	0
8	FWH	B	505	27/27	0.96	0.07	71,80,86,88	0
6	MG	A	504	1/1	0.97	0.04	86,86,86,86	0
7	GDP	B	504	28/28	0.97	0.06	85,94,101,104	0
7	GDP	D	504	28/28	0.97	0.06	71,82,92,95	0
5	GTP	A	503	32/32	0.97	0.06	89,96,107,111	0
5	GTP	C	502	32/32	0.97	0.06	85,92,98,100	0
6	MG	C	503	1/1	0.98	0.03	99,99,99,99	0

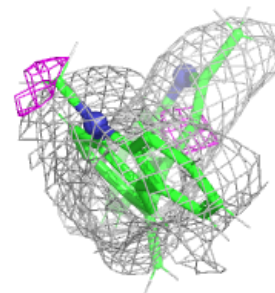
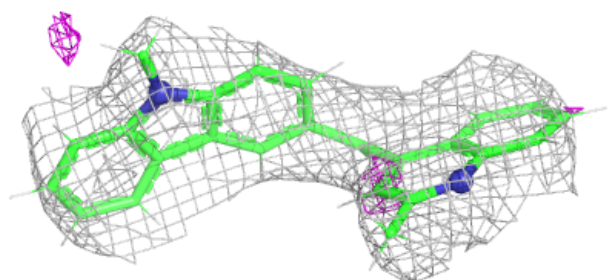
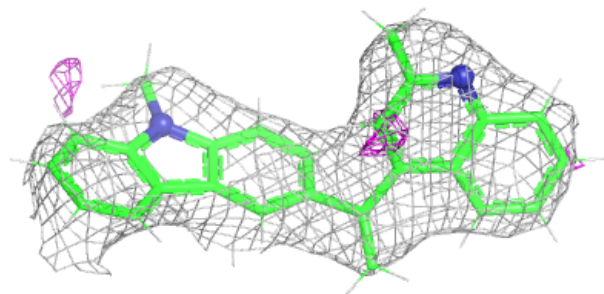
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FWH 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)

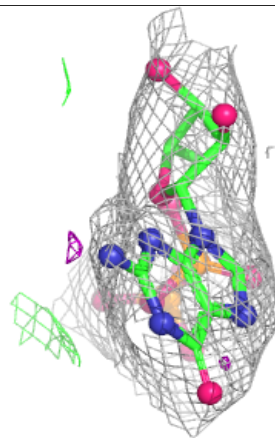
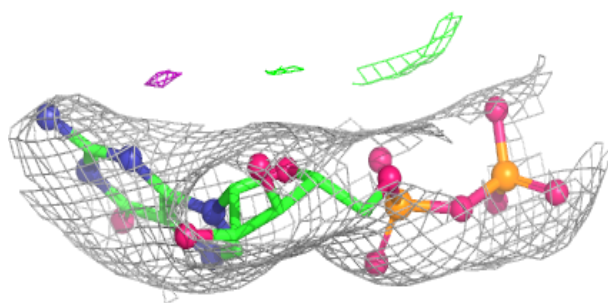
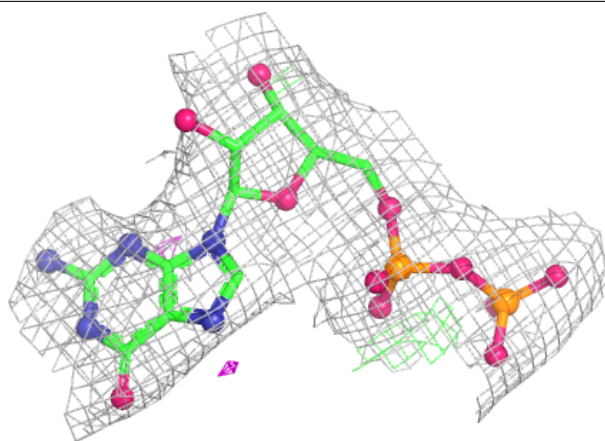
**Electron density around FWH B 505:**

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



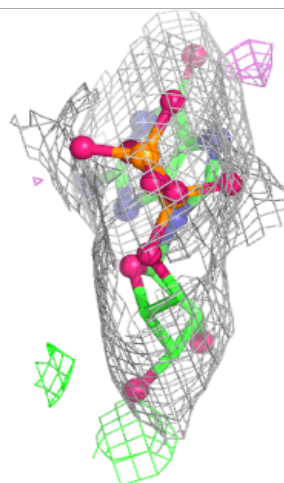
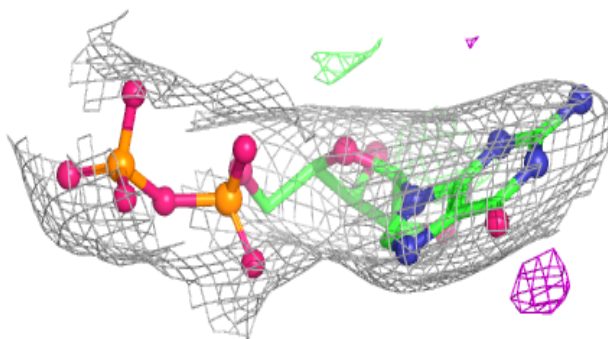
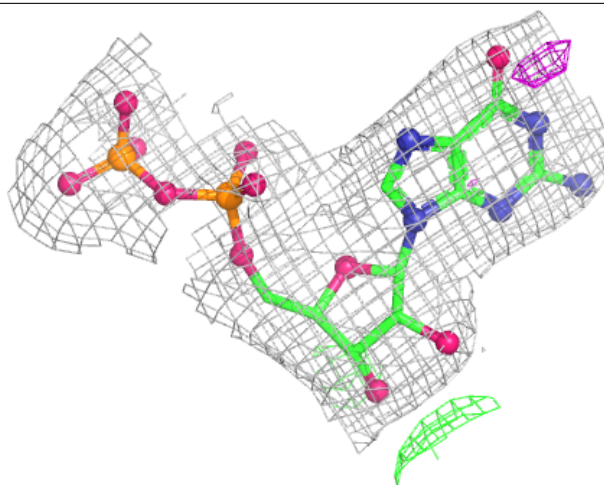
Electron density around GDP B 504:

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



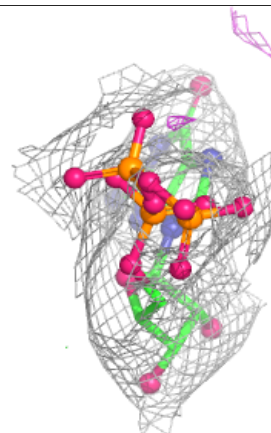
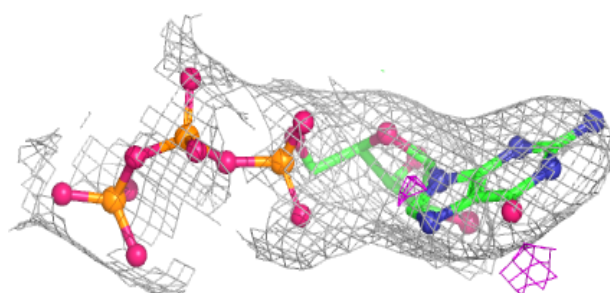
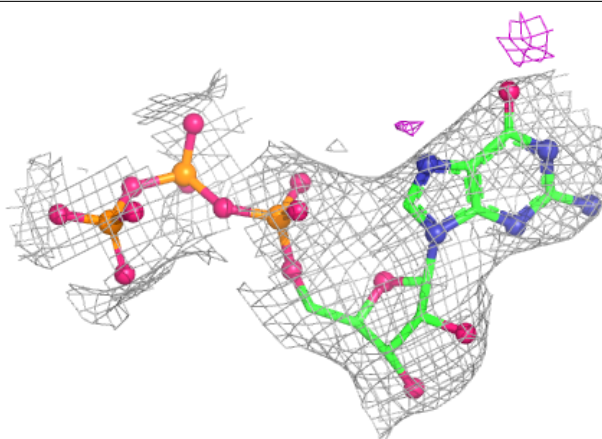
Electron density around GDP D 504:

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

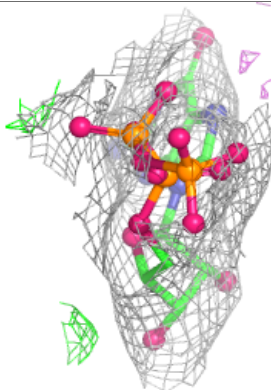
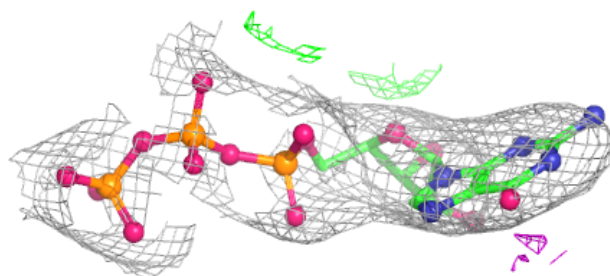
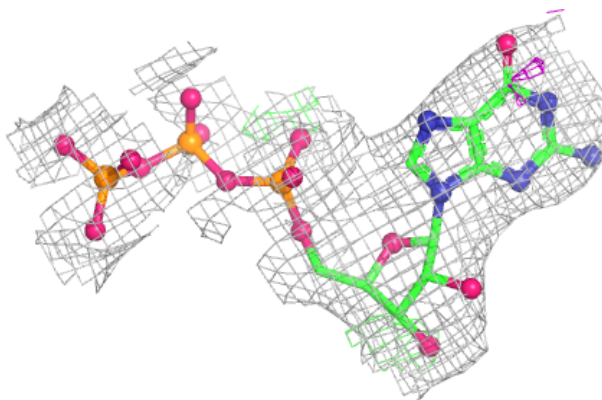


Electron density around GTP A 503:

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

**Electron density around GTP C 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.