



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 12:32 PM EDT

PDB ID : 5S5P
Title : Tubulin-Z53825177-complex
Authors : Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.79 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
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)	:	2.20

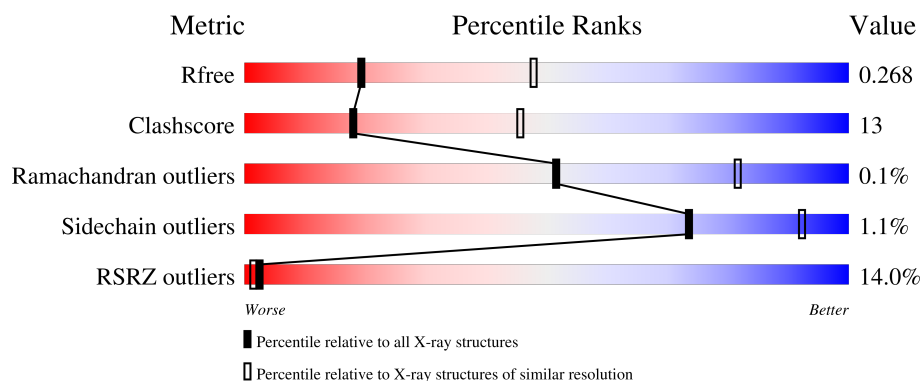
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	<div> <div>9%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
1	C	451	<div> <div>3%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
2	B	445	<div> <div>15%</div> <div>67%</div> <div>27%</div> <div>5%</div> </div>
2	D	445	<div> <div>14%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
3	E	143	<div> <div>10%</div> <div>67%</div> <div>19%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div></div><div></div><div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17752 atoms, of which 10 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	15	1	0
			3349	2103	575	644	27			
2	D	429	Total	C	N	O	S	6	0	0
			3358	2107	573	651	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7 | A | 2 | Total Ca
2 2 | 0 | 0 |
| 7 | B | 1 | Total Ca
1 1 | 0 | 0 |
| 7 | C | 1 | Total Ca
1 1 | 0 | 0 |

-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including atoms N1, N2, N3, N7, C2, C4, C5, C6, and C8. The ribose sugar is a five-membered ring with carbons C1', C2', C3', C4', and C5'. The two phosphate groups are represented by phosphorus atoms (P) and their associated oxygen atoms (O). The structure is labeled with various atom identifiers: N1, N2, N3, N7, C2, C4, C5, C6, C8, C1'(R), C2'(R), C3'(S), C4'(R), C5', O1A, O2A, O3A, O3B, O3C, O4', O5', O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792

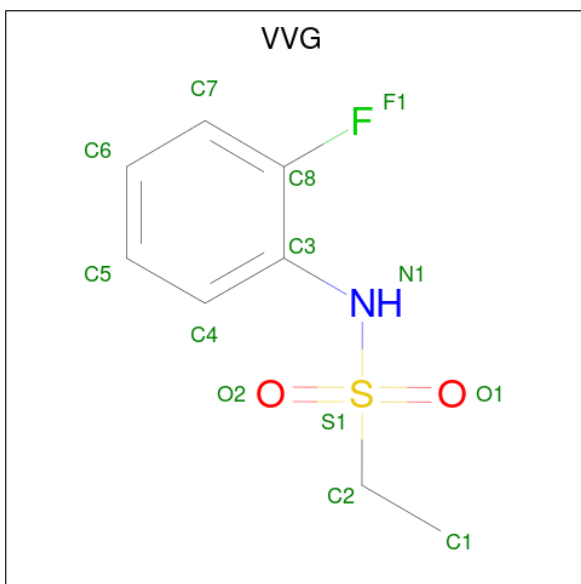
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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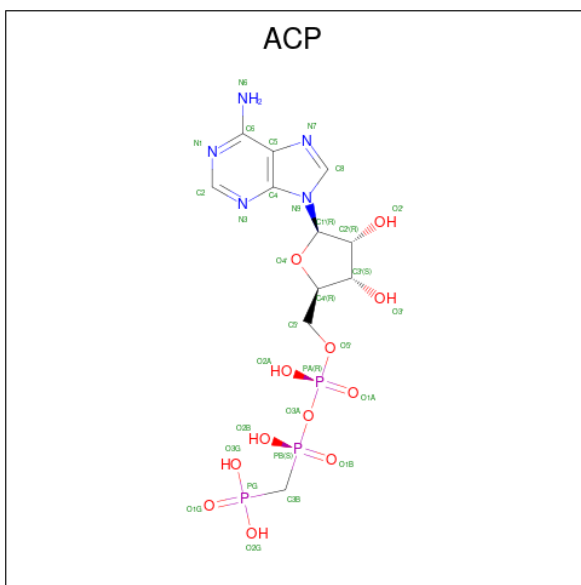
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is N-(2-fluorophenyl)ethanesulfonamide (three-letter code: VVG) (formula: $C_8H_{10}FNO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	C	1	Total	C	F	H	N	O	S	0	0
			23	8	1	10	1	2	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

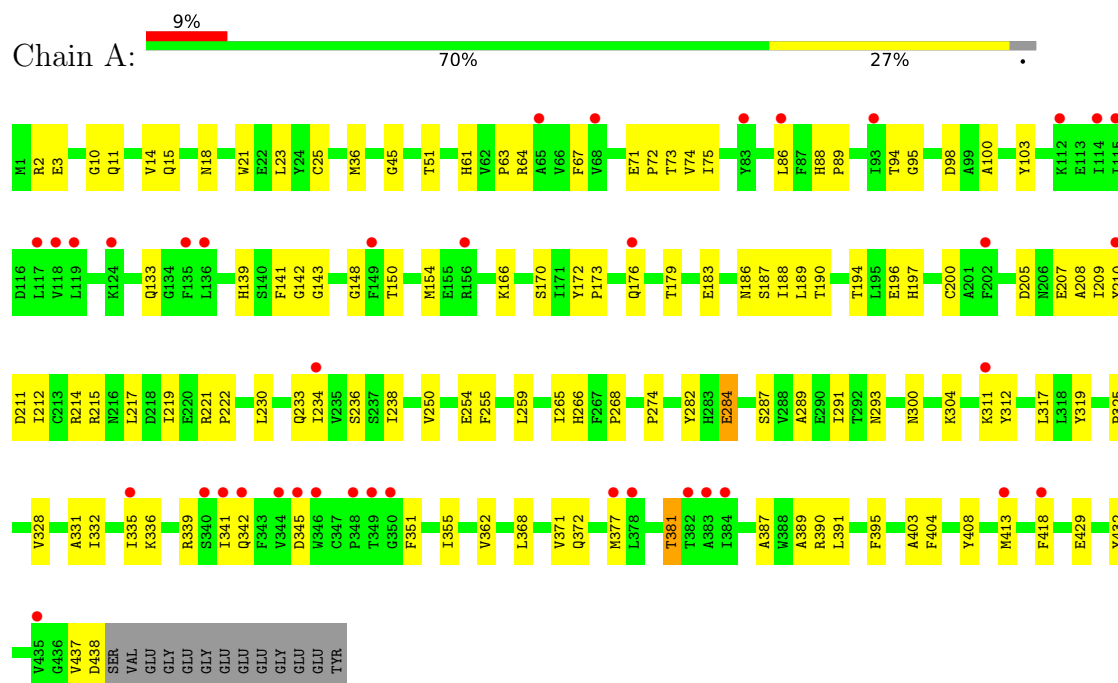
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	9	Total O 9 9	0	0
12	B	26	Total O 26 26	0	0
12	C	56	Total O 56 56	0	0
12	D	4	Total O 4 4	0	0
12	E	2	Total O 2 2	0	0
12	F	1	Total O 1 1	0	0

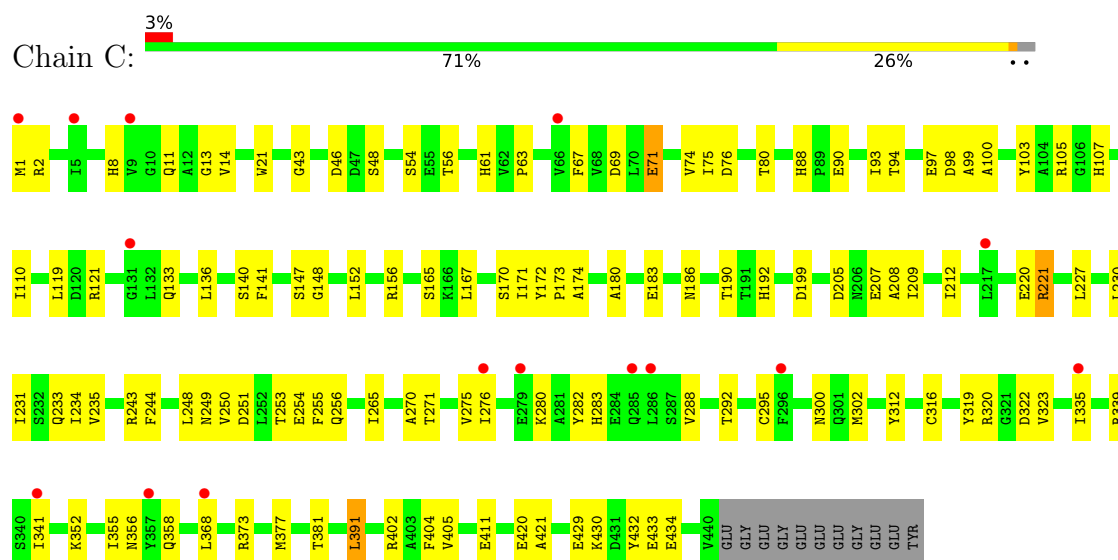
3 Residue-property plots

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.

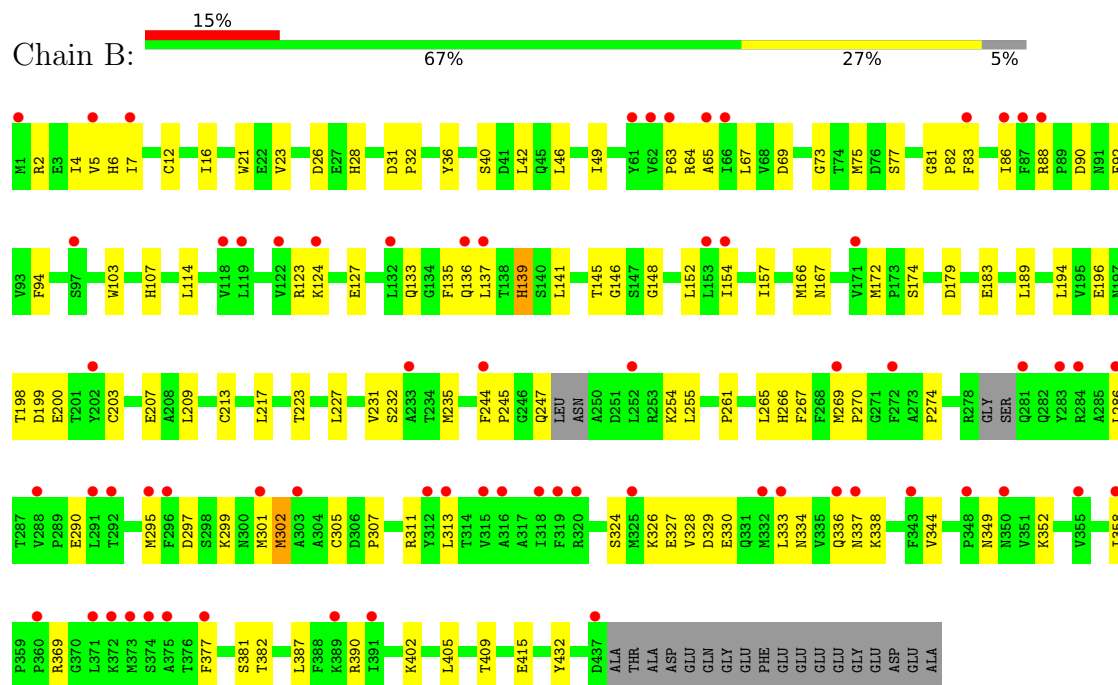
• Molecule 1: Tubulin alpha-1B chain



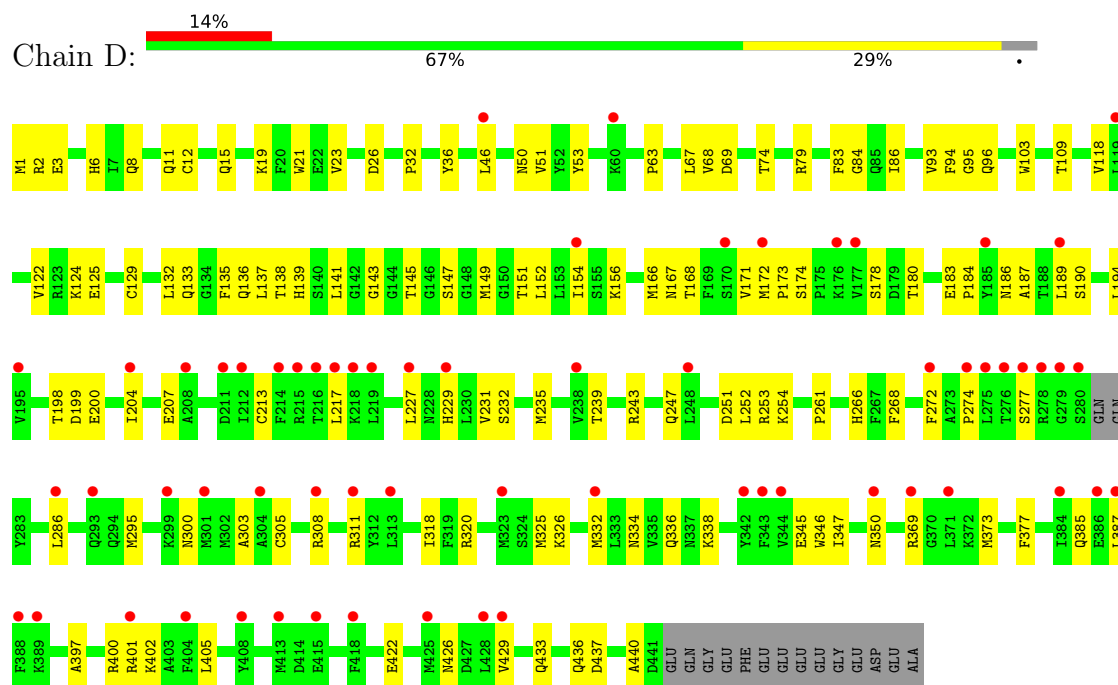
• Molecule 1: Tubulin alpha-1B chain



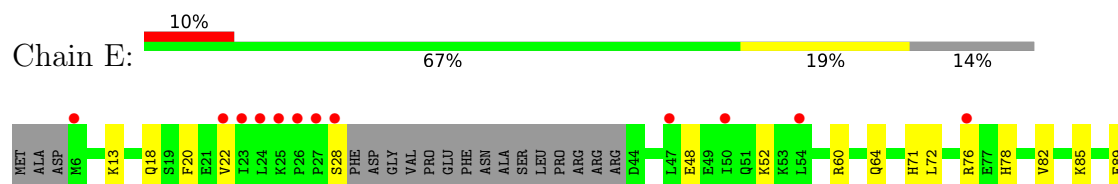
- Molecule 2: Tubulin beta-2B chain



- Molecule 2: Tubulin beta-2B chain

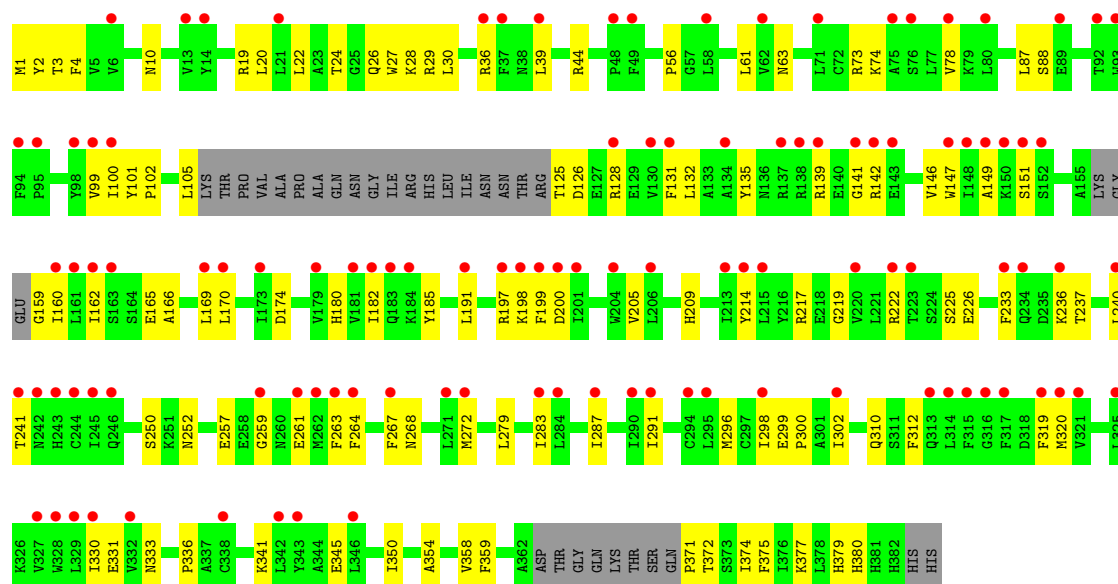


- Molecule 3: Stathmin-4





● Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.71Å 160.63Å 179.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.32 – 2.79 91.03 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (80.32-2.79) 99.2 (91.03-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.265 0.226 , 0.268	Depositor DCC
R_{free} test set	3715 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17752	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: ACP, CA, MG, GDP, MES, VVG, 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	0.25	0/3502	0.41	0/4754
1	C	0.26	0/3515	0.43	0/4772
2	B	0.26	0/3422	0.42	0/4630
2	D	0.25	0/3431	0.41	0/4647
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17836	0.41	0/24137

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 [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	3424	0	3334	90	0
1	C	3437	0	3348	103	0
2	B	3349	0	3230	87	0
2	D	3358	0	3231	99	0
3	E	1014	0	1029	22	0
4	F	2877	0	2839	83	0
5	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	2	0
8	D	28	0	12	5	0
9	B	12	0	12	2	0
10	C	13	10	0	3	0
11	F	31	0	14	3	0
12	A	9	0	0	1	0
12	B	26	0	0	2	0
12	C	56	0	0	2	0
12	D	4	0	0	1	0
12	E	2	0	0	0	0
12	F	1	0	0	0	0
All	All	17742	10	17085	467	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 13.

All (467) 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:A:2:ARG:HB2	1:A:133:GLN:HE21	1.27	0.97
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.48	0.93
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.50	0.91
2:D:217:LEU:HA	2:D:277:SER:HB3	1.55	0.87
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.60	0.83
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.64	0.80
2:D:147:SER:HB2	2:D:190:SER:OG	1.81	0.80
2:D:397:ALA:O	2:D:401:ARG:NH1	2.15	0.79
2:B:209:LEU:HD21	2:B:302:MET:HG2	1.63	0.78
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.68	0.76
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.68	0.76
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.66	0.76
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:HD23	1:C:167:LEU:HB3	1.69	0.74
2:D:136:GLN:HA	2:D:167:ASN:O	1.88	0.73
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.14	0.73
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.69	0.73
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.71	0.71
1:C:136:LEU:CD2	1:C:167:LEU:HD13	2.21	0.71
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.21	0.70
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.57	0.69
1:C:76:ASP:O	1:C:80:THR:HG22	1.93	0.69
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.74	0.69
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.56	0.69
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.25	0.69
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.75	0.69
2:B:196:GLU:OE2	3:E:71:HIS:NE2	2.26	0.68
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.75	0.68
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.76	0.68
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.29	0.68
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.75	0.68
1:C:69:ASP:OD2	12:C:601:HOH:O	2.12	0.68
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.29	0.67
1:A:408:TYR:HB3	1:A:413:MET:HE1	1.76	0.67
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.23	0.67
2:B:83:PHE:O	2:B:86:ILE:HG22	1.94	0.67
1:A:328:VAL:O	1:A:332:ILE:HG13	1.93	0.67
2:B:174:SER:OG	2:B:207:GLU:HB2	1.96	0.66
1:A:141:PHE:HB3	1:A:187:SER:OG	1.95	0.66
2:B:69:ASP:O	2:B:94:PHE:HA	1.95	0.66
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.77	0.66
2:D:174:SER:OG	2:D:207:GLU:OE1	2.13	0.66
2:B:88:ARG:NH1	2:B:90:ASP:OD2	2.28	0.66
2:D:433:GLN:NE2	2:D:437:ASP:OD2	2.28	0.66
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.77	0.65
2:D:11:GLN:HA	2:D:74:THR:HG21	1.77	0.65
1:C:271:THR:HG21	1:C:295:CYS:O	1.96	0.65
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.79	0.65
1:C:256:GLN:NE2	10:C:504:VVG:O1	2.29	0.65
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.78	0.64
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.32	0.64
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.80	0.64
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.80	0.64
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:14:VAL:HG23	1.98	0.63
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.81	0.63
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.33	0.63
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.32	0.62
1:A:408:TYR:HB3	1:A:413:MET:CE	2.29	0.62
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.08	0.62
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.00	0.62
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.35	0.61
2:B:40:SER:OG	2:B:42:LEU:HD13	2.00	0.61
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.65	0.61
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.30	0.61
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.16	0.61
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.35	0.61
1:C:165:SER:HA	1:C:199:ASP:OD2	2.00	0.61
1:C:74:VAL:HB	12:C:608:HOH:O	2.01	0.60
4:F:371:PRO:HA	4:F:372:THR:C	2.20	0.60
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.37	0.60
1:A:404:PHE:CE1	2:B:261:PRO:HB3	2.37	0.60
1:A:312:TYR:CD2	1:A:381:THR:HG23	2.36	0.59
1:A:187:SER:CB	1:A:391:LEU:HD21	2.33	0.59
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.85	0.59
2:B:141:LEU:HD12	2:B:172:MET:SD	2.42	0.59
4:F:225:SER:O	4:F:252:ASN:HB2	2.03	0.59
4:F:146:VAL:HG11	4:F:233:PHE:CZ	2.38	0.58
1:C:192:HIS:CG	1:C:421:ALA:HA	2.38	0.58
2:D:180:THR:O	2:D:183:GLU:HG3	2.03	0.58
2:B:324:SER:O	2:B:328:VAL:HG23	2.04	0.58
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.36	0.58
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.39	0.58
2:B:145:THR:HB	8:B:501:GDP:O2B	2.04	0.58
1:C:136:LEU:HD22	1:C:167:LEU:HD22	1.85	0.58
2:D:180:THR:HB	2:D:183:GLU:HG3	1.85	0.58
3:E:135:LYS:O	3:E:139:LEU:HG	2.04	0.58
1:A:45:GLY:HA3	12:A:605:HOH:O	2.02	0.58
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.84	0.58
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.86	0.58
2:D:198:THR:HG1	2:D:266:HIS:HE2	1.51	0.58
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.84	0.57
1:A:214:ARG:HG2	1:A:219:ILE:O	2.04	0.57
2:D:251:ASP:OD1	2:D:254:LYS:N	2.29	0.57
1:A:287:SER:O	1:A:291:ILE:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.87	0.57
2:D:311:ARG:NH1	2:D:436:GLN:O	2.37	0.57
2:D:83:PHE:O	2:D:86:ILE:HG22	2.05	0.57
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.87	0.57
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.17	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.05	0.57
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.85	0.57
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.21	0.56
1:A:387:ALA:HA	1:A:390:ARG:HD3	1.87	0.56
3:E:137:LYS:HE2	3:E:141:GLU:OE2	2.04	0.56
1:A:2:ARG:O	1:A:51:THR:HG22	2.05	0.56
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.38	0.56
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.56
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.87	0.56
1:C:99:ALA:O	1:C:105:ARG:HD3	2.06	0.56
1:C:429:GLU:O	1:C:433:GLU:HG3	2.06	0.56
2:D:320:ARG:O	2:D:373:MET:HA	2.06	0.56
3:E:78:HIS:O	3:E:82:VAL:HG23	2.05	0.56
2:B:136:GLN:HA	2:B:167:ASN:O	2.05	0.56
2:B:297:ASP:OD2	2:B:299:LYS:NZ	2.38	0.56
1:C:320:ARG:HA	1:C:356:ASN:O	2.05	0.56
2:D:152:LEU:O	2:D:156:LYS:HG2	2.05	0.55
4:F:371:PRO:HA	4:F:372:THR:HB	1.87	0.55
2:B:305:CYS:O	2:B:307:PRO:HD3	2.06	0.55
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.37	0.55
2:B:311:ARG:O	2:B:382:THR:HG23	2.06	0.55
2:D:68:VAL:HA	2:D:93:VAL:O	2.07	0.55
4:F:371:PRO:HA	4:F:372:THR:O	2.06	0.55
1:A:234:ILE:O	1:A:238:ILE:HG13	2.07	0.55
1:C:322:ASP:OD2	1:C:373:ARG:NH2	2.37	0.55
2:D:69:ASP:O	2:D:94:PHE:HA	2.07	0.55
2:D:93:VAL:HG11	2:D:118:VAL:HG22	1.87	0.55
2:B:223:THR:O	2:B:227:LEU:HD13	2.07	0.55
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.07	0.55
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.88	0.55
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.42	0.54
4:F:159:GLY:C	4:F:160:ILE:HD12	2.27	0.54
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.38	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.54
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.89	0.54
1:C:250:VAL:HB	1:C:255:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.08	0.54
2:D:231:VAL:O	2:D:235:MET:HG3	2.08	0.54
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.43	0.53
2:B:334:ASN:O	2:B:338:LYS:HG3	2.08	0.53
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.90	0.53
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.90	0.53
2:D:141:LEU:HA	2:D:147:SER:HB3	1.89	0.53
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.90	0.53
2:D:239:THR:O	2:D:243:ARG:HG3	2.08	0.53
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.07	0.53
2:B:326:LYS:O	2:B:330:GLU:HG3	2.09	0.53
1:C:136:LEU:HD22	1:C:167:LEU:HD13	1.90	0.53
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.08	0.53
3:E:72:LEU:O	3:E:76:ARG:HG2	2.08	0.53
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.91	0.53
1:A:284:GLU:CD	1:A:284:GLU:H	2.11	0.53
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.53
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.44	0.53
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.90	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.52
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.90	0.52
1:C:186:ASN:O	1:C:190:THR:HG22	2.10	0.52
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.25	0.52
2:B:6:HIS:HD2	2:B:65:ALA:HB1	1.73	0.52
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.10	0.52
2:D:95:GLY:O	2:D:96:GLN:NE2	2.42	0.52
2:D:124:LYS:C	2:D:124:LYS:HD3	2.30	0.52
3:E:48:GLU:O	3:E:52:LYS:HG3	2.09	0.52
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.44	0.52
2:B:46:LEU:HA	2:B:49:ILE:HB	1.92	0.52
1:C:172:TYR:CE1	1:C:391:LEU:HD22	2.44	0.52
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.40	0.52
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.45	0.52
3:E:13:LYS:HG2	3:E:18:GLN:OE1	2.09	0.52
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.52
1:C:174:ALA:HB2	1:C:207:GLU:N	2.24	0.51
1:A:289:ALA:HA	1:A:331:ALA:CB	2.40	0.51
1:C:172:TYR:CZ	1:C:391:LEU:HD13	2.46	0.51
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.92	0.51
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.39	0.51
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.10	0.51
1:A:141:PHE:HB2	1:A:173:PRO:HD3	1.93	0.50
1:C:172:TYR:HE1	1:C:391:LEU:HD22	1.77	0.50
2:B:270:PRO:HA	2:B:377:PHE:O	2.10	0.50
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.41	0.50
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.46	0.50
1:C:276:ILE:HD11	1:C:280:LYS:HB3	1.93	0.50
4:F:268:ASN:O	4:F:272:MET:HG3	2.11	0.50
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.27	0.50
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.76	0.50
2:D:11:GLN:HB3	8:D:501:GDP:O2A	2.12	0.50
2:D:133:GLN:OE1	2:D:252:LEU:N	2.36	0.50
4:F:19:ARG:HD2	4:F:19:ARG:O	2.12	0.50
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.43	0.50
2:B:231:VAL:O	2:B:235:MET:HG3	2.11	0.50
2:D:1:MET:CE	2:D:50:ASN:HB2	2.42	0.50
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.47	0.49
1:C:180:ALA:HB3	1:C:183:GLU:CG	2.42	0.49
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.27	0.49
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.47	0.49
1:C:8:HIS:HB3	1:C:13:GLY:O	2.12	0.49
2:D:200:GLU:HB2	2:D:268:PHE:CE2	2.46	0.49
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.46	0.49
4:F:320:MET:CG	4:F:330:ILE:HD11	2.42	0.49
2:B:4:ILE:O	2:B:64:ARG:HD2	2.13	0.49
2:D:295:MET:CE	2:D:377:PHE:HB2	2.39	0.49
3:E:128:LYS:O	3:E:128:LYS:HD3	2.13	0.49
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.42	0.49
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.93	0.49
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.43	0.49
1:C:288:VAL:CG2	1:C:323:VAL:HG22	2.41	0.49
2:D:141:LEU:HD12	2:D:172:MET:SD	2.52	0.49
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.47	0.49
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.47	0.49
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.95	0.49
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.93	0.49
1:A:317:LEU:HD13	1:A:319:TYR:OH	2.13	0.49
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.94	0.49
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.94	0.48
1:C:312:TYR:CD2	1:C:341:ILE:HG23	2.48	0.48
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ILE:HB	2:B:166:MET:HE3	1.94	0.48
10:C:504:VVG:O1	10:C:504:VVG:F1	2.21	0.48
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.95	0.48
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.42	0.48
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.49	0.48
1:A:319:TYR:HB2	1:A:355:ILE:HG12	1.96	0.48
2:B:124:LYS:HD3	2:B:124:LYS:C	2.34	0.48
2:D:11:GLN:O	2:D:15:GLN:HG2	2.13	0.48
2:D:145:THR:HB	8:D:501:GDP:O2B	2.12	0.48
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.49	0.48
1:C:147:SER:HB2	1:C:190:THR:HB	1.95	0.48
2:D:199:ASP:O	2:D:266:HIS:HB2	2.13	0.48
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.35	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.48	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.48
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.48
1:C:234:ILE:HG12	1:C:302:MET:CE	2.43	0.48
2:D:3:GLU:OE1	2:D:129:CYS:HB3	2.14	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.29	0.48
4:F:141:GLY:O	4:F:142:ARG:HB2	2.14	0.48
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.49	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.48
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.48	0.48
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.43	0.48
2:B:313:LEU:HD23	2:B:344:VAL:HG11	1.96	0.47
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.95	0.47
1:A:266:HIS:O	1:A:268:PRO:HD3	2.14	0.47
1:C:48:SER:HB3	1:C:243:ARG:O	2.14	0.47
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.95	0.47
1:C:1:MET:O	1:C:2:ARG:HB2	2.13	0.47
1:C:271:THR:HG21	1:C:295:CYS:HA	1.96	0.47
2:D:53:TYR:CE2	2:D:63:PRO:HG3	2.49	0.47
1:A:200:CYS:HA	1:A:266:HIS:HB2	1.96	0.47
1:A:413:MET:HE3	1:A:418:PHE:CE2	2.50	0.47
2:B:329:ASP:O	2:B:333:LEU:HG	2.15	0.47
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.97	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.15	0.47
4:F:29:ARG:O	4:F:30:LEU:HD23	2.14	0.47
4:F:259:GLY:O	4:F:261:GLU:HG3	2.14	0.47
2:B:333:LEU:O	2:B:337:ASN:ND2	2.48	0.47
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:88:SER:OG	2.24	0.47
1:C:271:THR:CG2	1:C:295:CYS:HA	2.45	0.47
1:C:271:THR:HG23	1:C:300:ASN:O	2.15	0.47
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.97	0.47
1:C:174:ALA:HB2	1:C:207:GLU:H	1.80	0.46
2:D:145:THR:O	2:D:149:MET:HB3	2.15	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
4:F:2:TYR:O	4:F:27:TRP:HA	2.16	0.46
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.79	0.46
2:D:303:ALA:O	2:D:305:CYS:N	2.49	0.46
4:F:237:THR:HG21	4:F:250:SER:HA	1.97	0.46
2:B:409:THR:HG21	12:B:614:HOH:O	2.15	0.46
1:C:167:LEU:C	1:C:167:LEU:HD23	2.36	0.46
3:E:85:LYS:O	3:E:89:GLU:HG3	2.16	0.46
1:C:43:GLY:HA2	1:C:56:THR:O	2.15	0.46
1:C:97:GLU:O	1:C:110:ILE:HG21	2.15	0.46
2:D:79:ARG:O	2:D:84:GLY:HA3	2.15	0.46
2:D:308:ARG:NH1	12:D:1102:HOH:O	2.48	0.46
1:A:103:TYR:CD1	1:A:189:LEU:HD13	2.51	0.46
2:B:199:ASP:OD1	9:B:504:MES:H62	2.16	0.46
4:F:24:THR:O	4:F:26:GLN:HG3	2.16	0.46
1:C:1:MET:HG3	1:C:2:ARG:H	1.81	0.46
1:C:173:PRO:HB3	1:C:183:GLU:OE1	2.16	0.46
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.46
2:D:32:PRO:HA	2:D:83:PHE:CD2	2.51	0.46
2:D:132:LEU:HD21	2:D:135:PHE:CZ	2.51	0.46
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.98	0.46
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.16	0.46
2:B:179:ASP:N	2:B:183:GLU:OE2	2.42	0.46
1:C:192:HIS:CD2	1:C:421:ALA:HA	2.51	0.46
4:F:63:ASN:HA	4:F:312:PHE:O	2.16	0.46
1:A:208:ALA:O	1:A:212:ILE:HG13	2.16	0.46
4:F:209:HIS:HB2	4:F:310:GLN:OE1	2.16	0.46
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.97	0.45
1:A:255:PHE:O	1:A:259:LEU:HB2	2.16	0.45
1:C:404:PHE:CD1	2:D:261:PRO:HA	2.51	0.45
1:A:3:GLU:HG2	1:A:64:ARG:NH1	2.31	0.45
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.51	0.45
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.15	0.45
2:D:145:THR:N	8:D:501:GDP:O2B	2.49	0.45
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:274:PRO:HB3	2:D:286:LEU:CD2	2.46	0.45
4:F:10:ASN:HB3	4:F:44:ARG:HH22	1.81	0.45
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.33	0.45
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.45
1:C:192:HIS:NE2	1:C:420:GLU:HG2	2.32	0.45
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.20	0.45
2:D:387:LEU:HD23	2:D:387:LEU:C	2.37	0.45
3:E:132:GLU:HA	3:E:135:LYS:HB3	1.99	0.45
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.41	0.45
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.17	0.45
1:C:11:GLN:HE22	2:D:247:GLN:CD	2.19	0.45
3:E:109:LYS:O	3:E:109:LYS:HG2	2.17	0.45
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.99	0.45
2:B:336:GLN:OE1	4:F:36:ARG:NH2	2.49	0.45
1:C:80:THR:O	1:C:80:THR:OG1	2.35	0.45
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.98	0.45
2:B:199:ASP:O	2:B:266:HIS:HB2	2.17	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.99	0.45
4:F:345:GLU:HG2	4:F:374:ILE:HD12	1.99	0.45
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.52	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.16	0.45
3:E:127:ASP:O	3:E:131:GLU:HG2	2.17	0.45
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.51	0.45
2:B:387:LEU:C	2:B:387:LEU:HD23	2.38	0.44
1:C:133:GLN:HE21	1:C:253:THR:HG21	1.82	0.44
2:B:77:SER:O	2:B:81:GLY:N	2.51	0.44
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.18	0.44
1:C:270:ALA:O	1:C:302:MET:HG2	2.17	0.44
4:F:151:SER:HB3	4:F:180:HIS:CG	2.52	0.44
4:F:162:ILE:HD13	4:F:185:TYR:CE1	2.52	0.44
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.45	0.44
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.16	0.44
4:F:3:THR:HA	4:F:28:LYS:O	2.17	0.44
1:C:105:ARG:NH1	1:C:411:GLU:OE2	2.50	0.44
1:A:179:THR:HA	2:B:352:LYS:HD2	2.00	0.44
2:B:139:HIS:ND1	2:B:146:GLY:O	2.44	0.44
4:F:22:LEU:HD23	4:F:27:TRP:O	2.18	0.44
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.00	0.44
1:C:46:ASP:N	1:C:46:ASP:OD1	2.49	0.44
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.44
1:A:207:GLU:OE2	1:A:304:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.17	0.44
2:B:114:LEU:O	2:B:114:LEU:HG	2.18	0.44
4:F:101:TYR:N	4:F:126:ASP:OD1	2.40	0.44
4:F:240:LEU:HD12	4:F:240:LEU:N	2.33	0.44
1:C:231:ILE:O	1:C:235:VAL:HG23	2.17	0.44
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.53	0.44
4:F:160:ILE:HD12	4:F:160:ILE:N	2.33	0.44
1:A:72:PRO:HD3	1:A:95:GLY:O	2.18	0.43
2:B:295:MET:CG	2:B:377:PHE:HB2	2.47	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.18	0.43
2:B:67:LEU:N	2:B:67:LEU:HD12	2.33	0.43
1:C:69:ASP:O	1:C:94:THR:HA	2.18	0.43
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.43
2:D:272:PHE:O	2:D:300:ASN:HB3	2.18	0.43
2:B:174:SER:CB	2:B:207:GLU:HB2	2.49	0.43
10:C:504:VVG:F1	10:C:504:VVG:S1	2.66	0.43
1:A:154:MET:HG3	1:A:194:THR:HG23	1.99	0.43
2:B:107:HIS:ND1	2:B:152:LEU:HB2	2.34	0.43
2:B:265:LEU:HD22	2:B:432:TYR:CZ	2.54	0.43
2:B:301:MET:HE1	2:B:377:PHE:CZ	2.54	0.43
1:C:107:HIS:O	1:C:152:LEU:HD22	2.18	0.43
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.58	0.43
1:A:289:ALA:HA	1:A:331:ALA:HB2	2.00	0.43
2:D:332:MET:O	2:D:336:GLN:HG3	2.19	0.43
2:D:422:GLU:HG2	2:D:426:ASN:HD21	1.84	0.43
2:B:63:PRO:CD	2:B:86:ILE:HG12	2.49	0.43
2:B:244:PHE:HB3	2:B:245:PRO:HD2	2.00	0.43
1:C:402:ARG:C	1:C:405:VAL:HG23	2.39	0.43
2:D:173:PRO:HG3	2:D:187:ALA:HB2	2.01	0.43
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.34	0.43
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.49	0.43
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.54	0.43
1:C:319:TYR:HB2	1:C:355:ILE:HG12	2.01	0.43
2:D:251:ASP:OD1	2:D:253:ARG:N	2.52	0.43
4:F:125:THR:HB	4:F:126:ASP:H	1.66	0.43
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.54	0.43
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.81	0.43
1:A:351:PHE:O	3:E:22:VAL:HG12	2.19	0.43
4:F:61:LEU:HD12	4:F:310:GLN:O	2.18	0.43
2:D:2:ARG:O	2:D:51:VAL:HG13	2.20	0.42
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:HE21	4:F:56:PRO:HB3	1.83	0.42
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.02	0.42
1:C:234:ILE:HD12	1:C:234:ILE:H	1.84	0.42
2:D:227:LEU:O	2:D:231:VAL:HG23	2.19	0.42
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.38	0.42
2:B:338:LYS:HZ1	4:F:1:MET:HB3	1.83	0.42
1:C:282:TYR:O	1:C:283:HIS:HB2	2.18	0.42
4:F:296:MET:SD	4:F:380:HIS:HB2	2.58	0.42
2:B:402:LYS:CB	2:B:405:LEU:HD12	2.49	0.42
4:F:209:HIS:CE1	4:F:358:VAL:HG22	2.55	0.42
2:B:269:MET:HE3	2:B:301:MET:SD	2.60	0.42
1:C:234:ILE:HD12	1:C:234:ILE:N	2.34	0.42
2:D:124:LYS:HD3	2:D:125:GLU:N	2.34	0.42
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.18	0.42
1:A:71:GLU:HG2	1:A:73:THR:H	1.83	0.42
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.53	0.42
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.54	0.42
2:D:109:THR:HG21	3:E:137:LYS:HZ3	1.85	0.42
2:D:345:GLU:H	2:D:345:GLU:HG2	1.68	0.42
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.42
4:F:350:ILE:O	4:F:354:ALA:HB3	2.18	0.42
1:C:180:ALA:HB3	1:C:183:GLU:HG2	2.01	0.42
1:A:312:TYR:CE2	1:A:381:THR:HG23	2.55	0.42
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.55	0.42
1:C:180:ALA:O	1:C:183:GLU:HG3	2.20	0.42
1:C:339:ARG:O	1:C:341:ILE:HD12	2.20	0.42
2:B:324:SER:HB3	2:B:327:GLU:CB	2.50	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.42
3:E:128:LYS:HD3	3:E:128:LYS:C	2.40	0.42
4:F:78:VAL:HG11	4:F:99:VAL:HG23	2.01	0.42
4:F:225:SER:HB2	4:F:252:ASN:O	2.20	0.42
2:B:390:ARG:NH1	12:B:604:HOH:O	2.53	0.41
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.54	0.41
2:D:53:TYR:HE2	2:D:63:PRO:HG3	1.85	0.41
1:A:186:ASN:O	1:A:190:THR:HG22	2.20	0.41
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.55	0.41
2:D:8:GLN:HB3	2:D:138:THR:OG1	2.21	0.41
1:C:147:SER:OG	1:C:186:ASN:HB3	2.20	0.41
2:D:1:MET:HE2	2:D:50:ASN:HB2	2.02	0.41
3:E:129:HIS:O	3:E:133:VAL:HG23	2.19	0.41
1:A:437:VAL:HG12	1:A:438:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:HIS:ND1	2:B:49:ILE:HD12	2.36	0.41
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.56	0.41
1:A:75:ILE:HB	1:A:94:THR:HG21	2.03	0.41
1:A:311:LYS:HA	1:A:342:GLN:O	2.20	0.41
2:B:123:ARG:O	2:B:127:GLU:HG3	2.21	0.41
1:C:136:LEU:HD21	1:C:167:LEU:HD13	2.02	0.41
1:C:220:GLU:HB3	2:D:326:LYS:HD2	2.02	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.38	0.41
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.41
2:B:194:LEU:HA	2:B:198:THR:HG23	2.03	0.41
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.55	0.41
1:A:71:GLU:OE2	2:B:2:ARG:NH2	2.54	0.41
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.56	0.41
1:A:389:ALA:HA	1:A:429:GLU:OE2	2.21	0.41
2:B:5:VAL:HB	2:B:135:PHE:CD1	2.56	0.41
2:D:183:GLU:N	2:D:184:PRO:CD	2.84	0.41
4:F:4:PHE:HB3	4:F:39:LEU:HB3	2.03	0.41
4:F:198:LYS:HG2	4:F:199:PHE:N	2.36	0.41
4:F:333:ASN:HB2	4:F:336:PRO:HB3	2.03	0.41
1:A:293:ASN:HA	1:A:335:ILE:CD1	2.50	0.41
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.56	0.41
9:B:504:MES:H81	9:B:504:MES:H51	1.85	0.41
1:C:11:GLN:NE2	2:D:247:GLN:OE1	2.50	0.41
2:D:23:VAL:HG21	2:D:232:SER:HB2	2.03	0.41
1:A:154:MET:HE3	1:A:166:LYS:HE2	2.03	0.40
1:C:54:SER:O	1:C:61:HIS:HA	2.21	0.40
4:F:149:ALA:O	4:F:160:ILE:HG23	2.20	0.40
1:A:403:ALA:O	1:A:404:PHE:HB2	2.22	0.40
2:B:235:MET:HB3	2:B:235:MET:HE2	1.94	0.40
1:C:172:TYR:OH	1:C:391:LEU:HD13	2.21	0.40
1:C:270:ALA:HB3	1:C:302:MET:HG3	2.03	0.40
1:C:275:VAL:O	1:C:275:VAL:HG12	2.19	0.40
1:C:209:ILE:HD11	1:C:302:MET:HE3	2.02	0.40
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.51	0.40
4:F:298:ILE:HD12	4:F:302:ILE:HD13	2.03	0.40
4:F:377:LYS:HE2	4:F:379:HIS:CD2	2.57	0.40
1:C:221:ARG:HG3	2:D:325:MET:CG	2.46	0.40
1:C:316:CYS:O	1:C:377:MET:HA	2.22	0.40
2:D:147:SER:O	2:D:151:THR:HG23	2.22	0.40
1:A:75:ILE:HB	1:A:94:THR:CG2	2.51	0.40
1:A:289:ALA:HA	1:A:331:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ALA:O	1:C:212:ILE:HG13	2.22	0.40
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.56	0.40
4:F:191:LEU:HA	4:F:197:ARG:O	2.21	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	436/451 (97%)	418 (96%)	17 (4%)	1 (0%)	47	78
1	C	438/451 (97%)	419 (96%)	19 (4%)	0	100	100
2	B	418/445 (94%)	394 (94%)	22 (5%)	2 (0%)	29	61
2	D	425/445 (96%)	408 (96%)	17 (4%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	318 (92%)	26 (8%)	0	100	100
All	All	2180/2319 (94%)	2075 (95%)	102 (5%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
2	B	73	GLY
2	B	82	PRO

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	369/379 (97%)	362 (98%)	7 (2%)	57	85
1	C	371/379 (98%)	366 (99%)	5 (1%)	69	91
2	B	368/383 (96%)	363 (99%)	5 (1%)	67	90
2	D	368/383 (96%)	366 (100%)	2 (0%)	88	96
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	314 (100%)	1 (0%)	92	98
All	All	1901/1993 (95%)	1881 (99%)	20 (1%)	73	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	A	362	VAL
1	A	381	THR
2	B	139	HIS
2	B	247	GLN
2	B	302	MET
2	B	349	ASN
2	B	381	SER
1	C	71	GLU
1	C	221	ARG
1	C	251	ASP
1	C	381	THR
1	C	391	LEU
2	D	139	HIS
2	D	229	HIS
4	F	73	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
2	B	15	GLN

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Mol	Chain	Res	Type
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
2	B	300	ASN
2	B	349	ASN
2	B	406	HIS
1	C	11	GLN
1	C	85	GLN
1	C	133	GLN
1	C	256	GLN
2	D	96	GLN
2	D	167	ASN
2	D	294	GLN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

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 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	GDP	D	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.92	8 (25%)
9	MES	B	504	-	12,12,12	2.30	1 (8%)	14,16,16	1.98	5 (35%)
11	ACP	F	401	6	27,33,33	1.38	5 (18%)	32,52,52	1.50	4 (12%)
8	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.93	8 (25%)
10	VVG	C	504	-	13,13,13	0.75	1 (7%)	15,18,18	0.56	0
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.75	6 (18%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.79	8 (24%)

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	GDP	D	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
8	GDP	B	501	6	-	2/12/32/32	0/3/3/3
10	VVG	C	504	-	-	3/8/8/8	0/1/1/1
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.69	1.66	1.77
8	B	501	GDP	C6-C5	4.19	1.48	1.41
8	D	501	GDP	C6-C5	4.14	1.48	1.41
5	C	501	GTP	C6-N1	3.31	1.38	1.33
5	A	501	GTP	C6-N1	3.12	1.38	1.33
11	F	401	ACP	PG-O3G	2.90	1.61	1.54
11	F	401	ACP	PG-O2G	2.89	1.61	1.54
11	F	401	ACP	PB-O3A	2.62	1.61	1.58
11	F	401	ACP	C5-C4	2.55	1.47	1.40
8	D	501	GDP	C5-C4	2.46	1.47	1.40
8	B	501	GDP	C5-C4	2.34	1.47	1.40
11	F	401	ACP	PB-O2B	2.26	1.61	1.56
10	C	504	VVG	C2-S1	2.24	1.79	1.76

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.41	120.00	127.22
5	C	501	GTP	N3-C2-N1	-5.26	120.20	127.22
8	B	501	GDP	C2-N3-C4	5.22	121.32	115.36
8	D	501	GDP	C2-N3-C4	4.90	120.95	115.36
5	A	501	GTP	C2-N3-C4	4.50	120.50	115.36
11	F	401	ACP	PA-O3A-PB	-4.29	118.95	132.56
8	D	501	GDP	C5-C6-N1	-4.13	117.78	123.43
9	B	504	MES	C5-N4-C3	4.07	117.98	108.83
5	C	501	GTP	C2-N3-C4	4.00	119.92	115.36
8	D	501	GDP	C6-N1-C2	3.99	122.27	115.93
8	B	501	GDP	C6-N1-C2	3.82	122.00	115.93
8	B	501	GDP	C5-C6-N1	-3.71	118.35	123.43
8	B	501	GDP	C6-C5-C4	-3.70	117.27	120.80
5	C	501	GTP	PA-O3A-PB	-3.56	120.61	132.83
11	F	401	ACP	C3'-C2'-C1'	3.52	106.28	100.98
8	B	501	GDP	N3-C2-N1	-3.41	122.67	127.22
8	D	501	GDP	PA-O3A-PB	-3.40	121.15	132.83
8	D	501	GDP	C6-C5-C4	-3.37	117.58	120.80
5	C	501	GTP	C5-C6-N1	-3.24	119.00	123.43
8	D	501	GDP	N3-C2-N1	-3.19	122.96	127.22
11	F	401	ACP	N3-C2-N1	-3.17	123.72	128.68
9	B	504	MES	C6-C5-N4	-3.12	105.37	110.10
8	B	501	GDP	PA-O3A-PB	-2.89	122.91	132.83
5	A	501	GTP	PA-O3A-PB	-2.88	122.95	132.83
8	B	501	GDP	C4-C5-N7	-2.88	106.40	109.40
8	D	501	GDP	C4-C5-N7	-2.80	106.49	109.40
5	A	501	GTP	C5-C6-N1	-2.79	119.61	123.43
5	C	501	GTP	C6-N1-C2	2.68	120.19	115.93
5	C	501	GTP	PB-O3B-PG	-2.65	123.74	132.83
11	F	401	ACP	C4-C5-N7	-2.58	106.71	109.40
5	A	501	GTP	PB-O3B-PG	-2.56	124.06	132.83
9	B	504	MES	O3S-S-C8	2.51	109.83	105.77
5	A	501	GTP	C6-N1-C2	2.50	119.90	115.93
8	B	501	GDP	C3'-C2'-C1'	2.39	104.58	100.98
9	B	504	MES	O1S-S-C8	2.35	109.74	106.92
8	D	501	GDP	C3'-C2'-C1'	2.16	104.24	100.98
9	B	504	MES	C7-N4-C5	2.16	116.76	111.23
5	A	501	GTP	C3'-C2'-C1'	2.10	104.14	100.98
5	A	501	GTP	N2-C2-N1	2.01	120.38	117.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

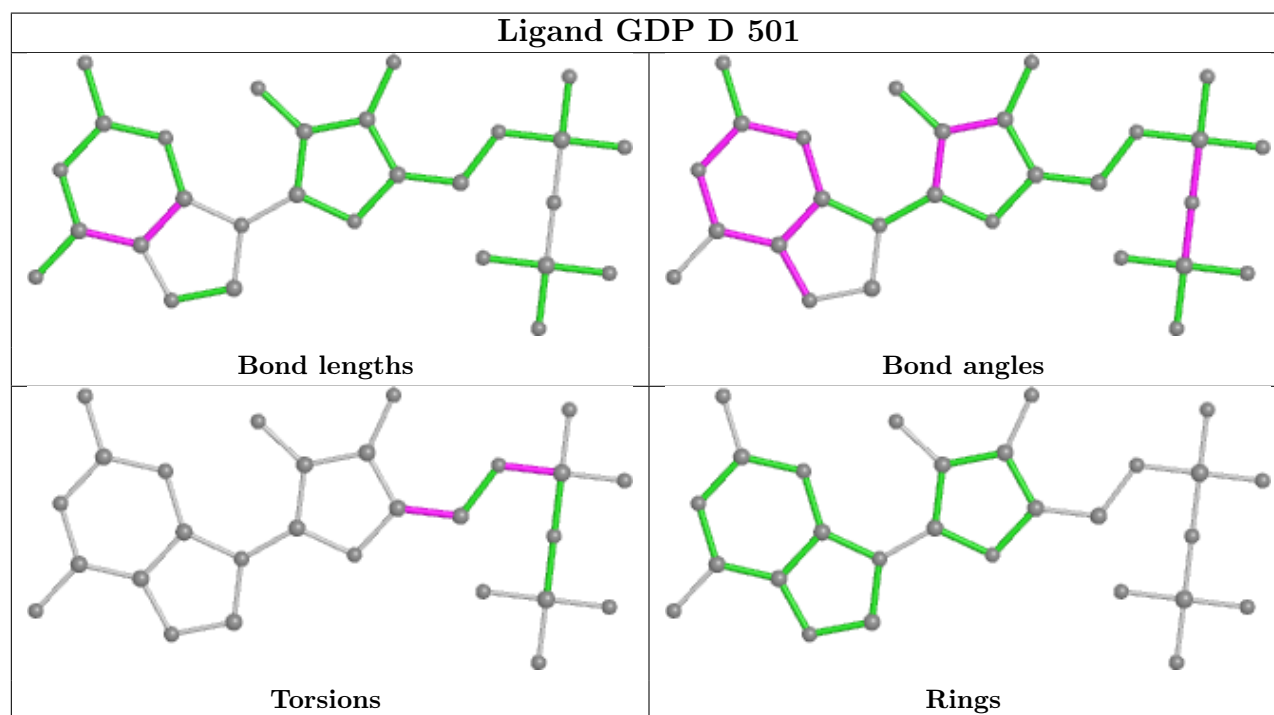
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
10	C	504	VVG	C4-C3-N1-S1
10	C	504	VVG	C8-C3-N1-S1
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O3S
5	C	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A
8	D	501	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	O4'-C4'-C5'-O5'
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
10	C	504	VVG	C1-C2-S1-O2
5	A	501	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

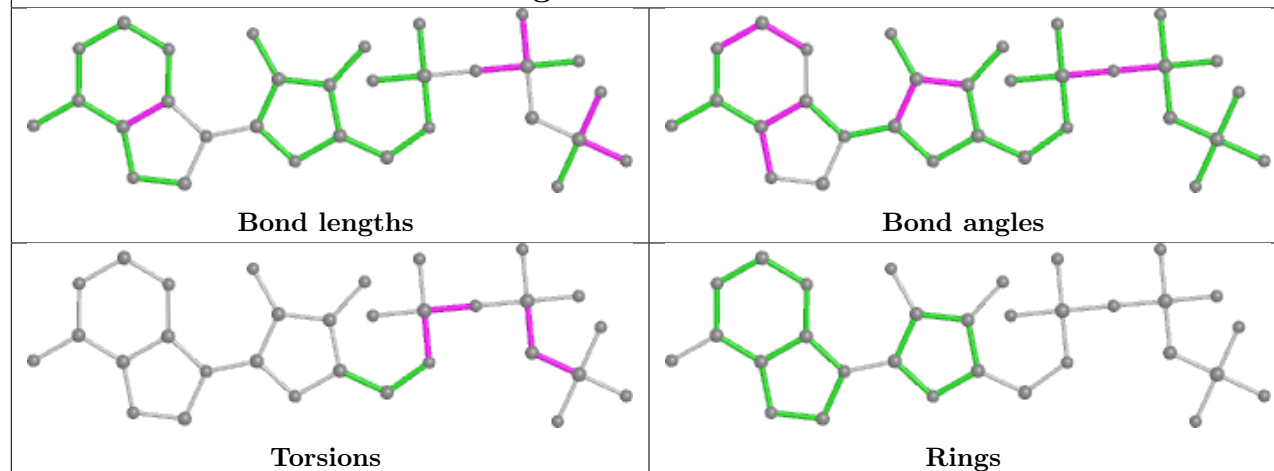
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	5	0
9	B	504	MES	2	0
11	F	401	ACP	3	0
8	B	501	GDP	2	0
10	C	504	VVG	3	0
5	A	501	GTP	3	0

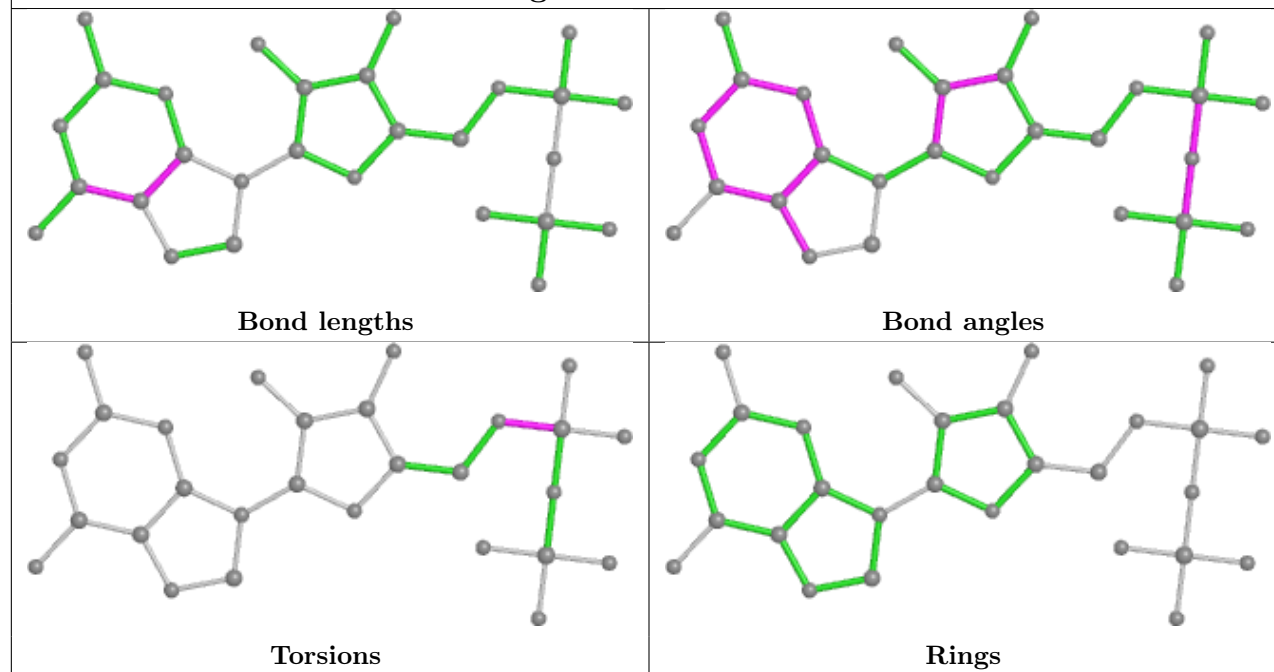
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

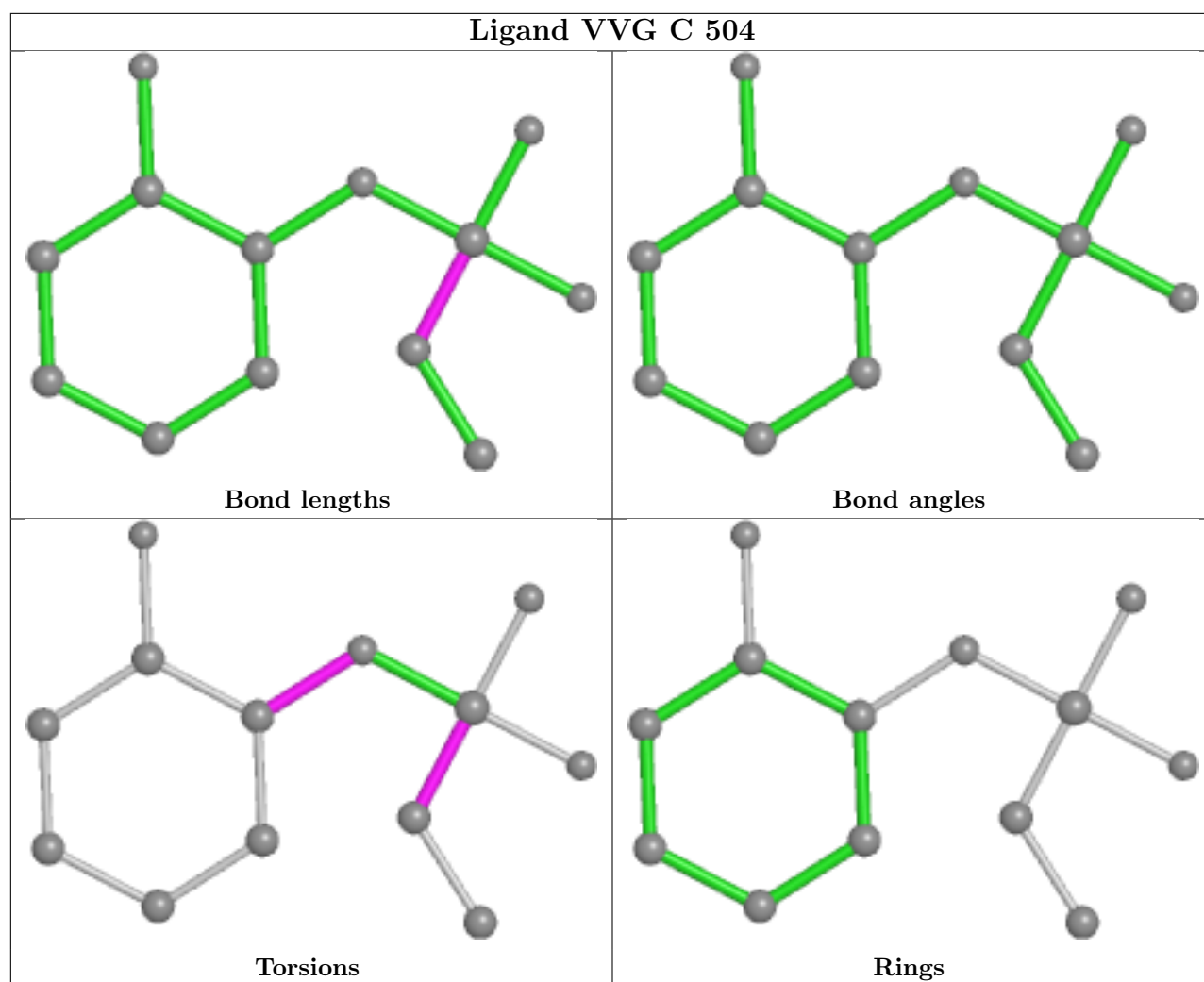


Ligand ACP F 401

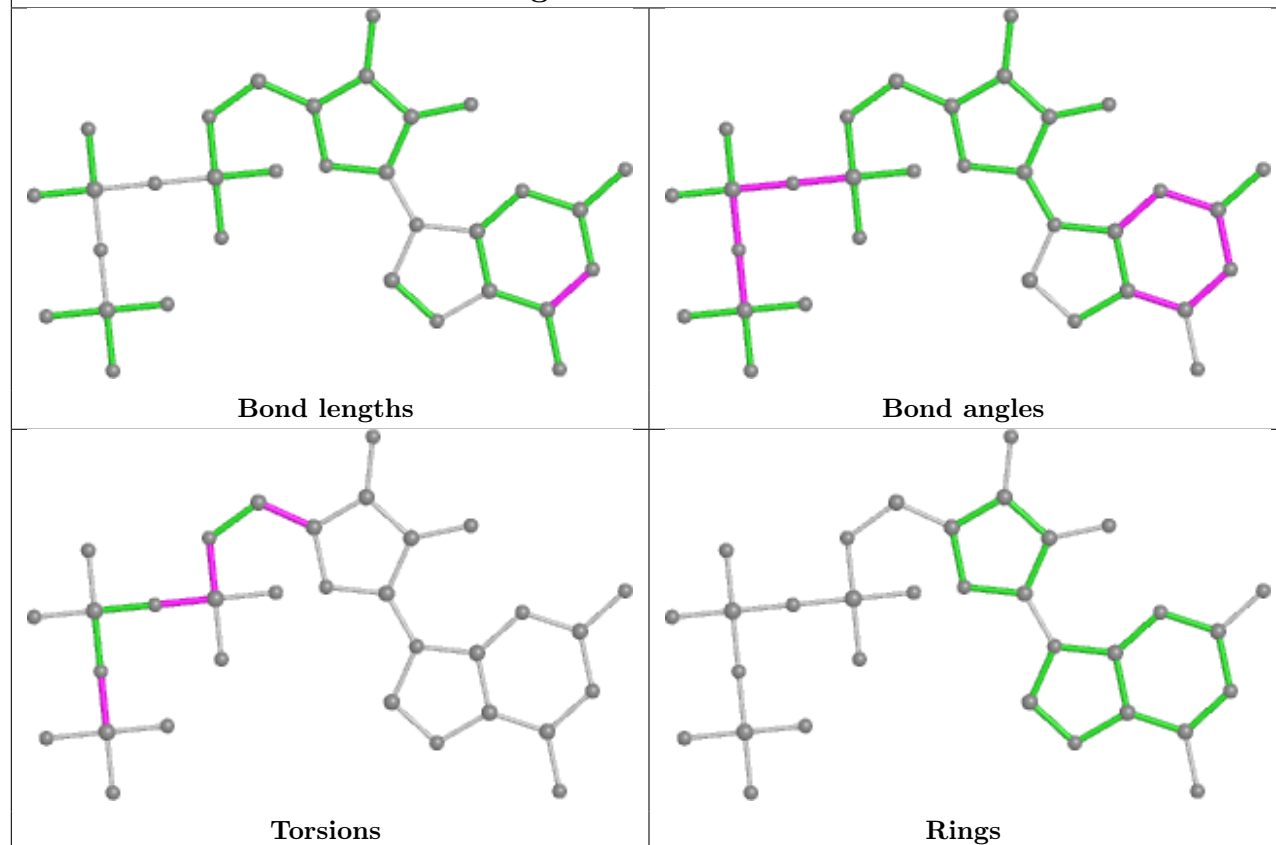


Ligand GDP B 501

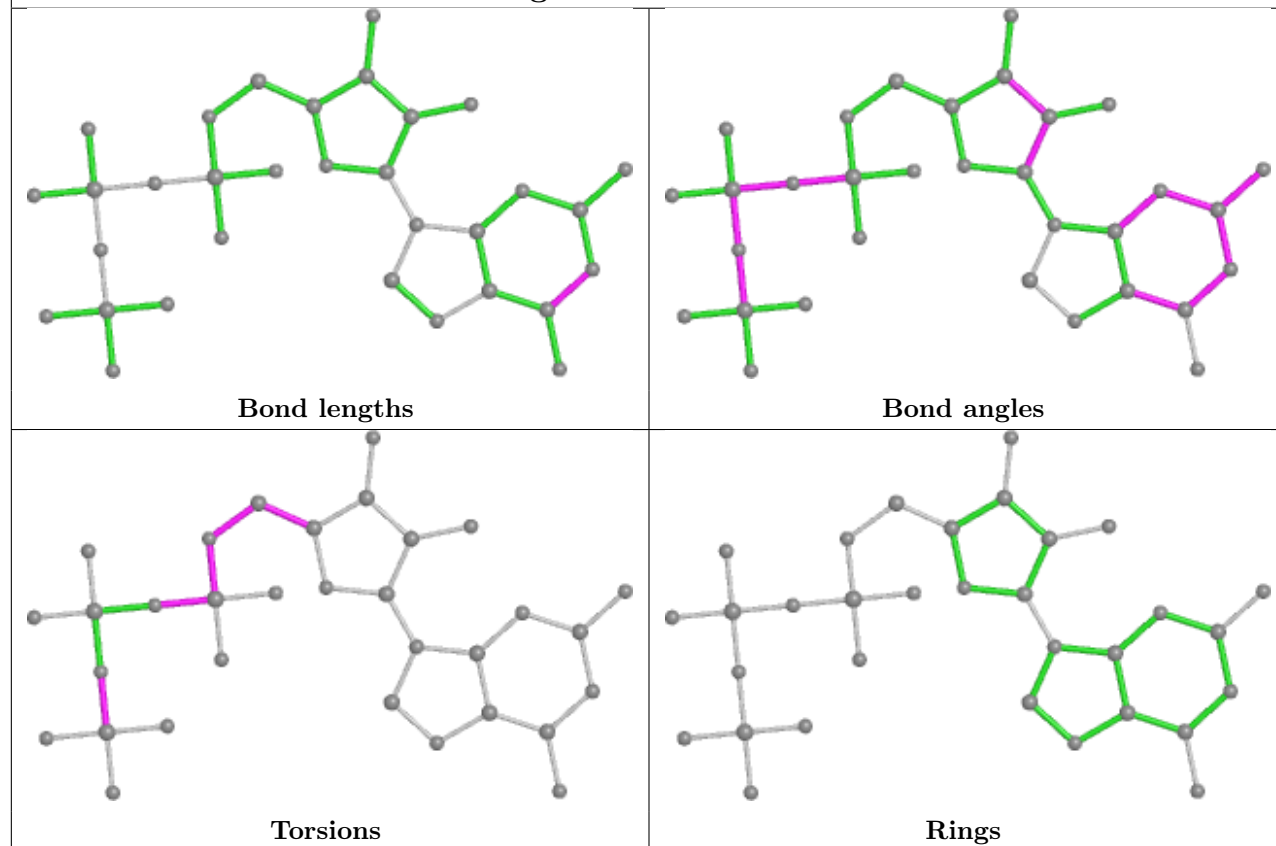




Ligand GTP C 501



Ligand GTP A 501



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	438/451 (97%)	0.69	39 (8%) 9 5	75, 102, 151, 213	0
1	C	440/451 (97%)	0.68	15 (3%) 45 35	64, 83, 113, 161	0
2	B	423/445 (95%)	0.95	67 (15%) 2 1	67, 97, 155, 200	4 (0%)
2	D	429/445 (96%)	0.93	63 (14%) 2 1	80, 112, 150, 199	4 (0%)
3	E	123/143 (86%)	0.84	14 (11%) 5 3	82, 117, 179, 207	0
4	F	352/384 (91%)	1.49	111 (31%) 0 0	100, 140, 194, 226	0
All	All	2205/2319 (95%)	0.92	309 (14%) 2 1	64, 106, 169, 226	8 (0%)

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	11.0
2	D	277	SER	7.9
2	D	276	THR	7.8
2	D	215	ARG	7.7
4	F	142	ARG	7.1
2	D	278	ARG	6.7
4	F	98	TYR	6.5
4	F	182	ILE	6.4
2	B	333	LEU	6.1
4	F	134	ALA	6.0
4	F	169	LEU	5.9
4	F	330	ILE	5.9
3	E	25	LYS	5.8
3	E	24	LEU	5.7
2	D	429	VAL	5.7
4	F	234	GLN	5.7
2	D	217	LEU	5.6
1	A	350	GLY	5.6
4	F	162	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	5.5
1	A	349	THR	5.5
2	D	216	THR	5.5
2	D	212	ILE	5.1
4	F	320	MET	5.1
2	D	388	PHE	5.1
2	D	280	SER	5.1
2	D	279	GLY	5.0
4	F	204	TRP	5.0
4	F	143	GLU	4.9
2	B	288	VAL	4.9
2	D	218	LYS	4.9
2	D	219	LEU	4.8
3	E	6	MET	4.8
4	F	199	PHE	4.8
1	A	114	ILE	4.7
2	B	301	MET	4.6
4	F	342	LEU	4.6
2	D	275	LEU	4.5
4	F	327	VAL	4.5
2	B	332	MET	4.5
3	E	54	LEU	4.5
1	A	86	LEU	4.5
4	F	291	ILE	4.4
2	B	286	LEU	4.4
4	F	243	HIS	4.4
4	F	181	VAL	4.4
4	F	319	PHE	4.4
2	D	272	PHE	4.3
3	E	139	LEU	4.3
4	F	321	VAL	4.3
1	A	115	ILE	4.3
2	B	373	MET	4.3
3	E	26	PRO	4.2
4	F	58	LEU	4.2
4	F	329	LEU	4.2
2	D	387	LEU	4.1
2	D	311	ARG	4.1
1	A	340	SER	4.1
4	F	220	VAL	4.1
2	B	337	ASN	4.1
2	B	319	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	314	LEU	4.0
1	A	345	ASP	4.0
4	F	13	VAL	3.9
4	F	137	ARG	3.8
2	D	299	LYS	3.8
4	F	315	PHE	3.8
4	F	150	LYS	3.7
4	F	93	TRP	3.7
1	A	344	VAL	3.7
4	F	89	GLU	3.7
1	C	368	LEU	3.7
4	F	75	ALA	3.7
2	B	355	VAL	3.7
4	F	138	ARG	3.7
2	B	66	ILE	3.7
1	A	346	TRP	3.7
2	D	304	ALA	3.6
4	F	317	PHE	3.6
4	F	152	SER	3.6
2	D	425	MET	3.6
4	F	283	ILE	3.6
4	F	94	PHE	3.6
4	F	290	ILE	3.5
4	F	264	PHE	3.5
4	F	71	LEU	3.5
2	D	214	PHE	3.5
1	A	378	LEU	3.5
1	A	176	GLN	3.5
2	B	291	LEU	3.5
2	B	281	GLN	3.4
4	F	332	VAL	3.4
3	E	28	SER	3.4
2	D	195	VAL	3.4
4	F	343	TYR	3.4
2	D	418	PHE	3.4
4	F	197	ARG	3.4
1	C	335	ILE	3.3
4	F	287	ILE	3.3
4	F	241	THR	3.3
2	D	274	PRO	3.3
1	A	156	ARG	3.2
4	F	201	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	213	ILE	3.2
1	A	83	TYR	3.2
2	D	189	LEU	3.2
3	E	76	ARG	3.2
1	A	342	GLN	3.2
1	A	118	VAL	3.2
2	B	372	LYS	3.2
2	D	389	LYS	3.2
2	B	122	VAL	3.1
1	A	335	ILE	3.1
4	F	99	VAL	3.1
2	D	401	ARG	3.1
2	B	313	LEU	3.1
2	B	312	TYR	3.1
4	F	346	LEU	3.1
2	B	325	MET	3.1
2	D	248	LEU	3.1
1	A	377	MET	3.1
2	B	377	PHE	3.1
1	A	65	ALA	3.1
4	F	161	LEU	3.1
3	E	50	ILE	3.1
3	E	22	VAL	3.1
2	D	342	TYR	3.0
2	B	318	ILE	3.0
2	D	204	ILE	3.0
4	F	325	LEU	3.0
2	D	177	VAL	3.0
2	B	296	PHE	3.0
2	B	374	SER	3.0
4	F	206	LEU	3.0
2	B	358	ILE	2.9
2	D	323	MET	2.9
2	B	124	LYS	2.9
2	D	208	ALA	2.9
4	F	141	GLY	2.9
4	F	21	LEU	2.9
1	A	311	LYS	2.9
2	B	283	TYR	2.9
4	F	78	VAL	2.9
4	F	128	ARG	2.9
4	F	302	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	5	VAL	2.9
4	F	130	VAL	2.9
4	F	328	TRP	2.9
2	D	369	ARG	2.9
2	D	386	GLU	2.9
2	D	301	MET	2.8
2	D	172	MET	2.8
4	F	149	ALA	2.8
1	A	117	LEU	2.8
2	B	272	PHE	2.8
4	F	100	ILE	2.8
1	A	348	PRO	2.8
1	A	124	LYS	2.8
4	F	233	PHE	2.7
4	F	338	CYS	2.7
4	F	49	PHE	2.7
2	D	384	ILE	2.7
4	F	261	GLU	2.7
1	C	357	TYR	2.7
4	F	242	ASN	2.7
4	F	131	PHE	2.7
4	F	48	PRO	2.7
4	F	295	LEU	2.7
4	F	245	ILE	2.7
1	A	68	VAL	2.6
4	F	267	PHE	2.6
2	B	320	ARG	2.6
1	C	276	ILE	2.6
2	D	227	LEU	2.6
2	B	315	VAL	2.6
4	F	6	VAL	2.6
1	C	131	GLY	2.6
4	F	62	VAL	2.6
2	B	437	ASP	2.6
2	D	60	LYS	2.6
2	D	154	ILE	2.6
2	B	375	ALA	2.6
1	A	149	PHE	2.6
2	B	389	LYS	2.6
3	E	140	LYS	2.6
2	D	371	LEU	2.6
1	A	341	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	383	ALA	2.6
2	B	119	LEU	2.6
2	D	286	LEU	2.6
4	F	284	LEU	2.5
2	B	295	MET	2.5
4	F	36	ARG	2.5
2	B	87	PHE	2.5
4	F	236	LYS	2.5
1	C	217	LEU	2.5
2	B	83	PHE	2.5
4	F	160	ILE	2.5
1	A	435	VAL	2.5
1	C	286	LEU	2.5
1	A	135	PHE	2.5
2	B	336	GLN	2.5
4	F	271	LEU	2.5
4	F	184	LYS	2.5
1	C	1	MET	2.5
2	D	343	PHE	2.4
4	F	214	TYR	2.4
1	A	119	LEU	2.4
2	B	86	ILE	2.4
2	B	316	ALA	2.4
2	B	61	TYR	2.4
2	D	408	TYR	2.4
1	A	136	LEU	2.4
4	F	198	LYS	2.4
2	B	118	VAL	2.4
2	B	303	ALA	2.3
4	F	294	CYS	2.3
2	D	413	MET	2.3
2	B	65	ALA	2.3
3	E	47	LEU	2.3
2	B	391	ILE	2.3
2	D	185	TYR	2.3
2	D	428	LEU	2.3
4	F	259	GLY	2.3
2	B	292	THR	2.3
4	F	151	SER	2.3
1	A	210	TYR	2.3
1	C	341	ILE	2.3
2	B	88	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	360	PRO	2.3
2	D	229	HIS	2.3
4	F	246	GLN	2.3
4	F	14	TYR	2.3
1	A	93	ILE	2.3
2	B	154	ILE	2.3
4	F	173	ILE	2.3
4	F	313	GLN	2.2
4	F	215	LEU	2.2
4	F	222	ARG	2.2
1	A	418	PHE	2.2
2	B	7	ILE	2.2
2	B	62	VAL	2.2
4	F	76	SER	2.2
4	F	147	TRP	2.2
4	F	223	THR	2.2
1	C	296	PHE	2.2
1	A	234	ILE	2.2
4	F	298	ILE	2.2
2	B	153	LEU	2.2
2	B	202	TYR	2.2
4	F	263	PHE	2.2
4	F	316	GLY	2.2
2	B	252	LEU	2.2
2	D	308	ARG	2.2
2	D	313	LEU	2.2
2	B	244	PHE	2.2
2	B	132	LEU	2.2
4	F	244	CYS	2.2
2	D	293	GLN	2.2
1	C	66	VAL	2.2
2	D	46	LEU	2.2
4	F	191	LEU	2.2
2	B	233	ALA	2.2
4	F	179	VAL	2.2
4	F	183	GLN	2.2
1	A	413	MET	2.2
4	F	139	ARG	2.2
2	D	176	LYS	2.1
1	C	285	GLN	2.1
2	B	284	ARG	2.1
2	D	344	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	148	ILE	2.1
2	D	350	ASN	2.1
1	A	382	THR	2.1
2	B	343	PHE	2.1
4	F	37	PHE	2.1
4	F	170	LEU	2.1
2	B	63	PRO	2.1
2	B	269	MET	2.1
2	D	170	SER	2.1
4	F	163	SER	2.1
2	B	136	GLN	2.1
1	A	202	PHE	2.1
2	D	211	ASP	2.1
1	C	279	GLU	2.1
2	B	371	LEU	2.1
1	C	5	ILE	2.1
4	F	95	PRO	2.1
2	B	350	ASN	2.1
4	F	200	ASP	2.1
2	D	119	LEU	2.0
2	B	171	VAL	2.0
1	A	384	ILE	2.0
2	B	348	PRO	2.0
2	D	238	VAL	2.0
2	D	415	GLU	2.0
4	F	262	MET	2.0
4	F	80	LEU	2.0
3	E	23	ILE	2.0
2	B	97	SER	2.0
2	B	1	MET	2.0
2	D	332	MET	2.0
2	B	137	LEU	2.0
1	C	9	VAL	2.0
4	F	92	THR	2.0
2	D	404	PHE	2.0
4	F	272	MET	2.0
4	F	39	LEU	2.0
1	A	112	LYS	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 monosaccharides in this entry.

6.4 Ligands ⓘ

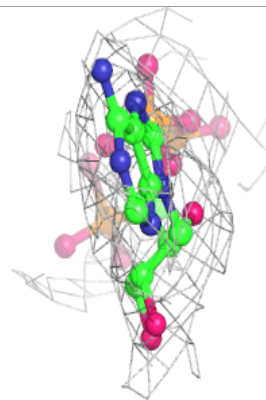
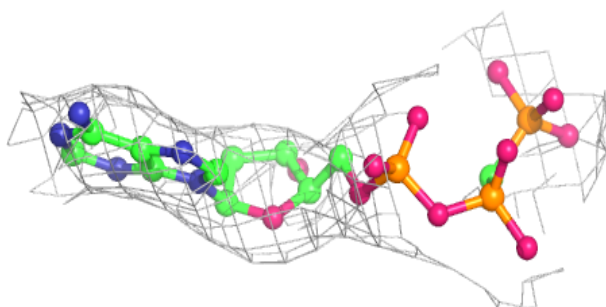
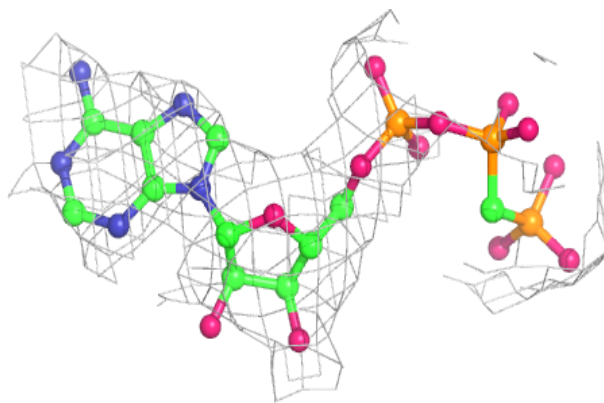
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.81	0.22	96,96,96,96	0
7	CA	A	504	1/1	0.83	0.14	119,119,119,119	0
11	ACP	F	401	31/31	0.86	0.21	133,149,157,159	0
7	CA	B	503	1/1	0.87	0.32	136,136,136,136	0
10	VVG	C	504	13/13	0.89	0.26	73,88,96,104	23
7	CA	A	503	1/1	0.91	0.16	142,142,142,142	0
6	MG	F	402	1/1	0.93	0.07	140,140,140,140	0
8	GDP	D	501	28/28	0.93	0.19	100,107,113,116	0
9	MES	B	504	12/12	0.95	0.15	107,114,128,134	0
5	GTP	A	501	32/32	0.96	0.16	71,78,85,94	0
5	GTP	C	501	32/32	0.97	0.20	64,74,81,86	0
6	MG	C	502	1/1	0.98	0.21	76,76,76,76	0
6	MG	B	502	1/1	0.98	0.20	73,73,73,73	0
7	CA	C	503	1/1	0.98	0.20	96,96,96,96	0
8	GDP	B	501	28/28	0.98	0.20	67,75,80,82	0
6	MG	A	502	1/1	0.99	0.18	86,86,86,86	0

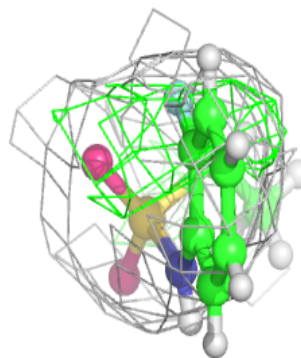
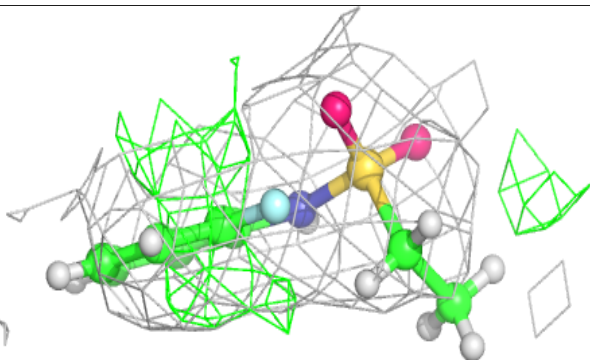
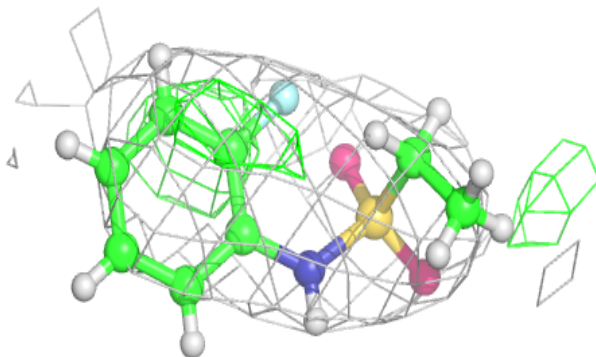
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

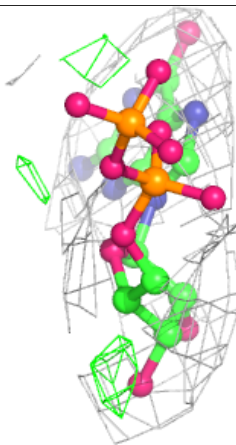
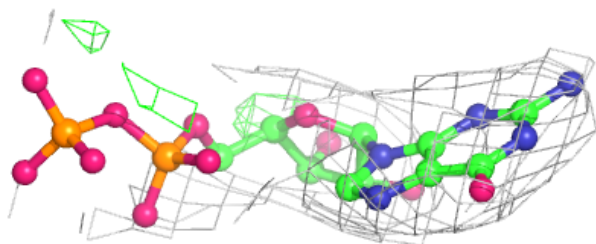
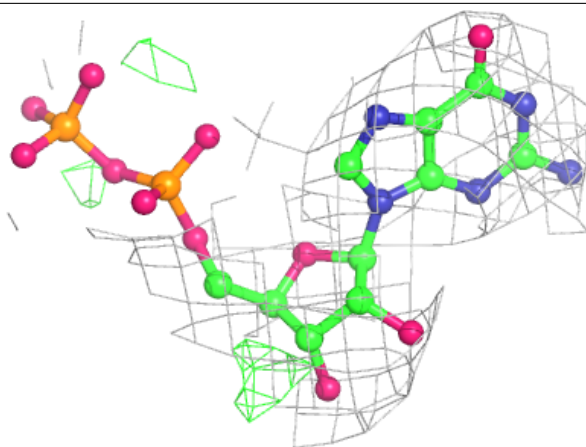
**Electron density around VVG C 504:**

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

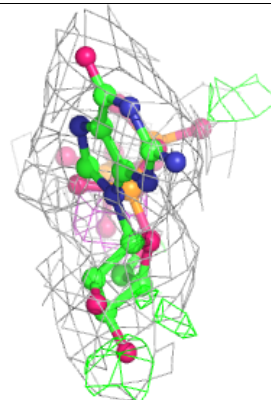
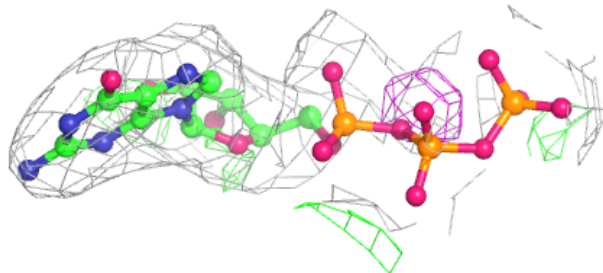
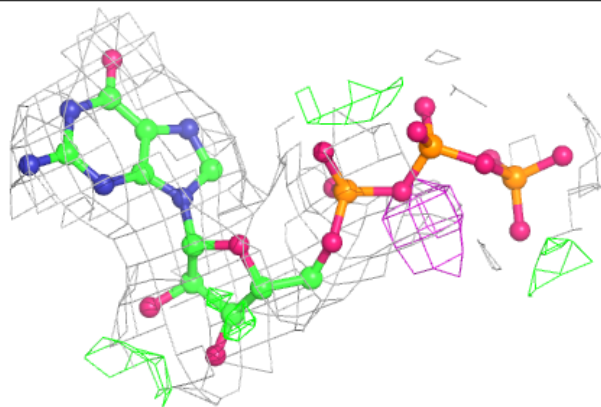


Electron density around GDP D 501:

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

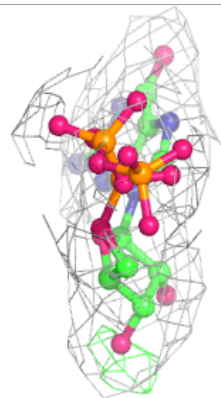
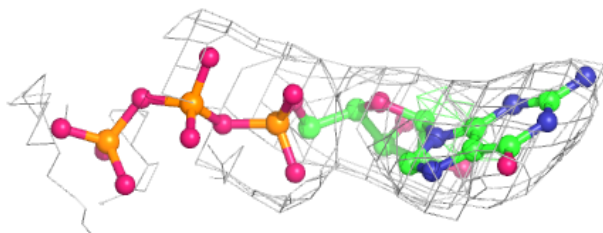
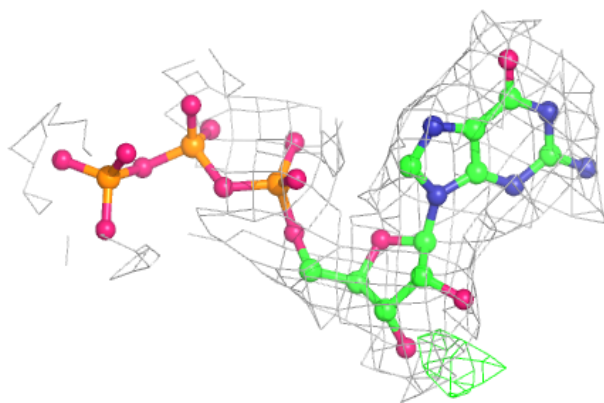
**Electron density around GTP A 501:**

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



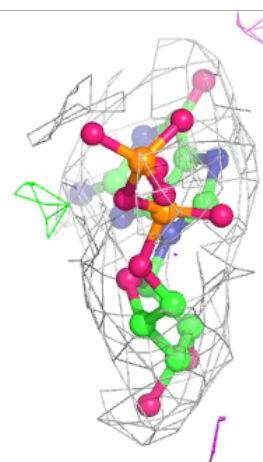
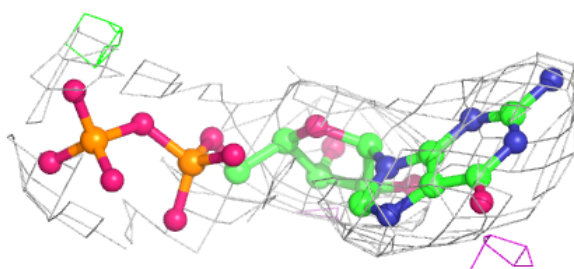
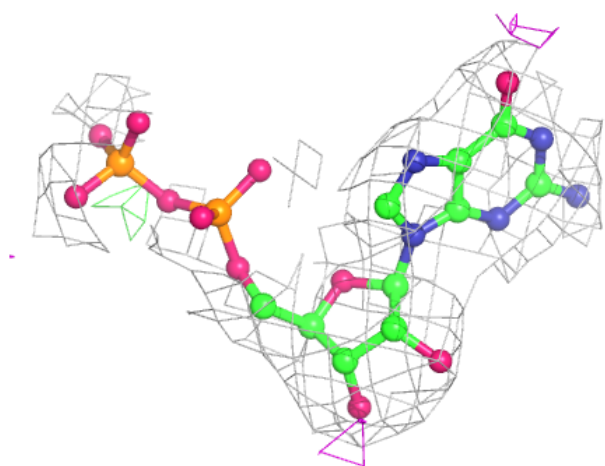
Electron density around GTP C 501:

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



Electron density around GDP B 501:

$2mF_o-DF_c$ (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.