



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 01:36 pm BST

PDB ID : 9H32 / pdb_00009h32
Title : T2R-TTL-PROTAC3 complex
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Deposited on : 2024-10-15
Resolution : 2.31 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

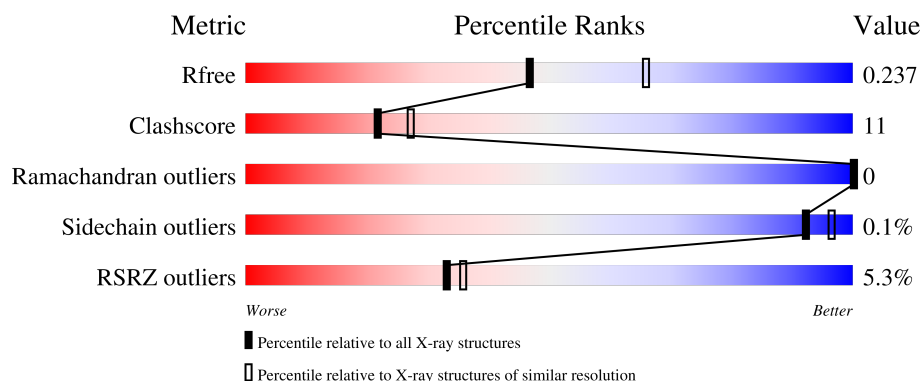
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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>4%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	451	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div>
2	D	445	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>.</div> </div> </div>
3	E	143	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>22%</div> <div>15%</div> </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> <div><div>9%</div><div>67%</div><div>22%</div><div>11%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17946 atoms, of which 63 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	1	0
			3443	2178	585	657	23			

- 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	0	1	0
			3345	2102	572	644	27			
2	D	425	Total	C	N	O	S	0	1	0
			3346	2100	570	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	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

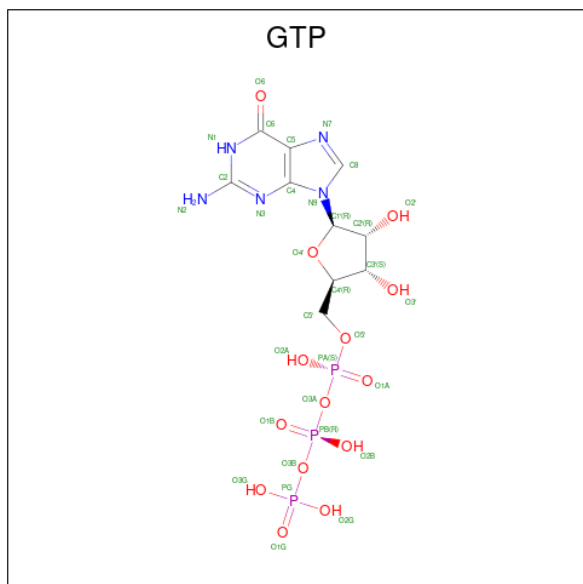
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	0	0
			2793	1792	477	510	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: 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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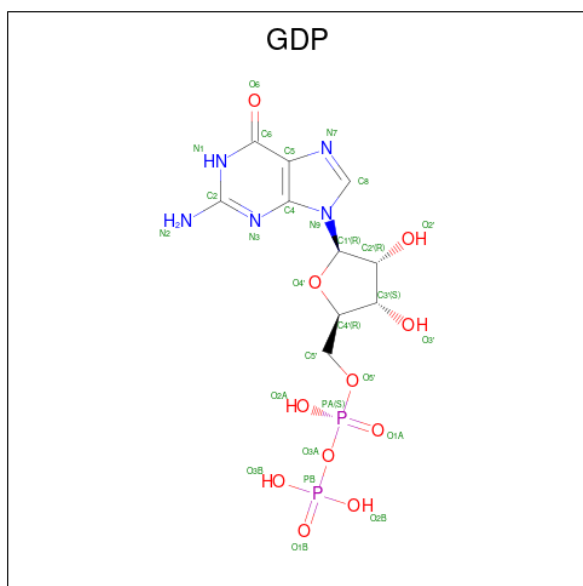
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

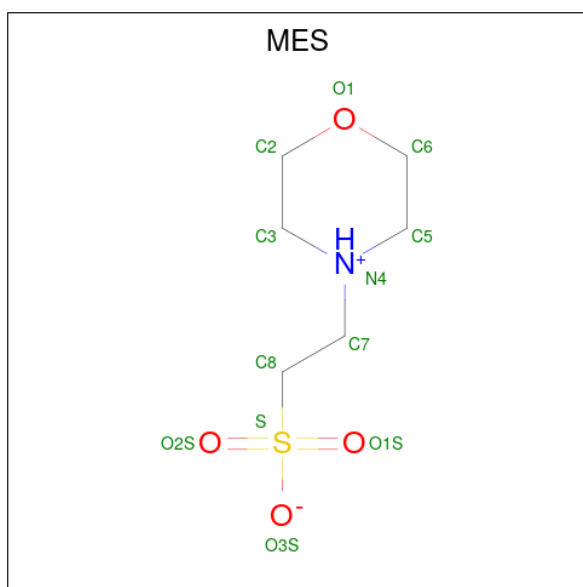
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



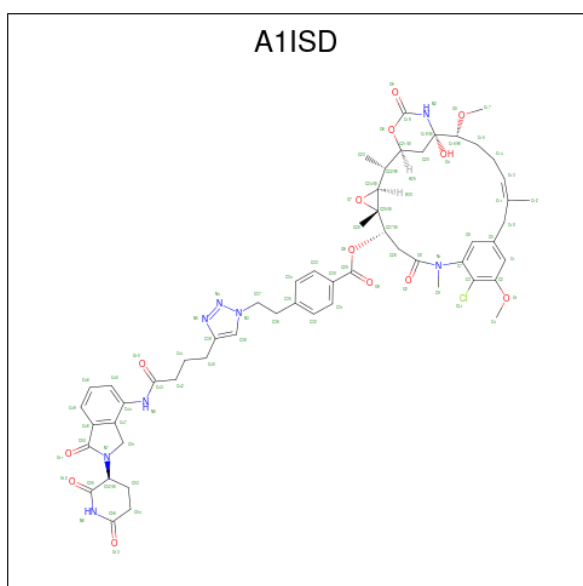
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is (1S,2R,3S,5S,6S,16E,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16-tetraen-6-yl 4-(2-{4-[4-({2-[(3S)-2,6-dioxopiperidin-3-yl]-1-oxo-2,3-dihydro-1H-isindol-4-yl}amino)-4-oxobutyl]-1H-1,2,3-triazol-1-yl}ethyl)benzoate (CCD ID: A1ISD) (formula: C₅₆H₆₅ClN₈O₁₃) (labeled as "Ligand of Interest" by depositor).



- # ACP
-
- The chemical structure of Adenosine 3'-phosphate (ACP) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a triphosphate chain. The adenosine moiety is represented by a blue-colored structure, with the adenine base and ribose sugar. The triphosphate chain is represented by a red-colored structure, showing the three phosphate groups. The structure is labeled with atom names and numbers, indicating the specific atoms involved in the reaction. The triphosphate chain is shown in a 3D representation, with the phosphate groups connected by oxygen atoms. The structure is labeled with atom names and numbers, indicating the specific atoms involved in the reaction.

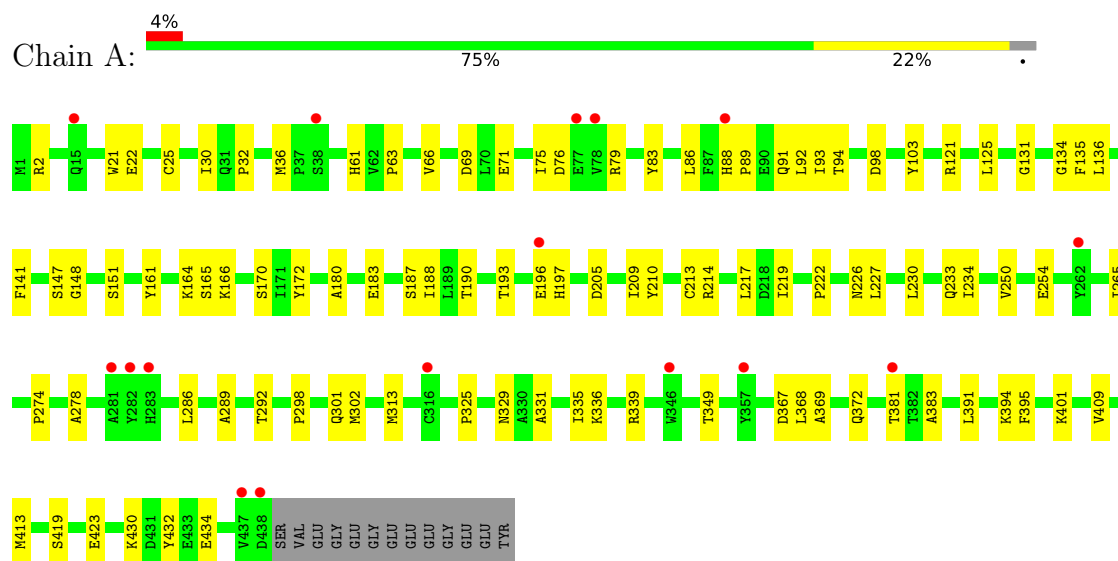
- Molecule 12 is water.



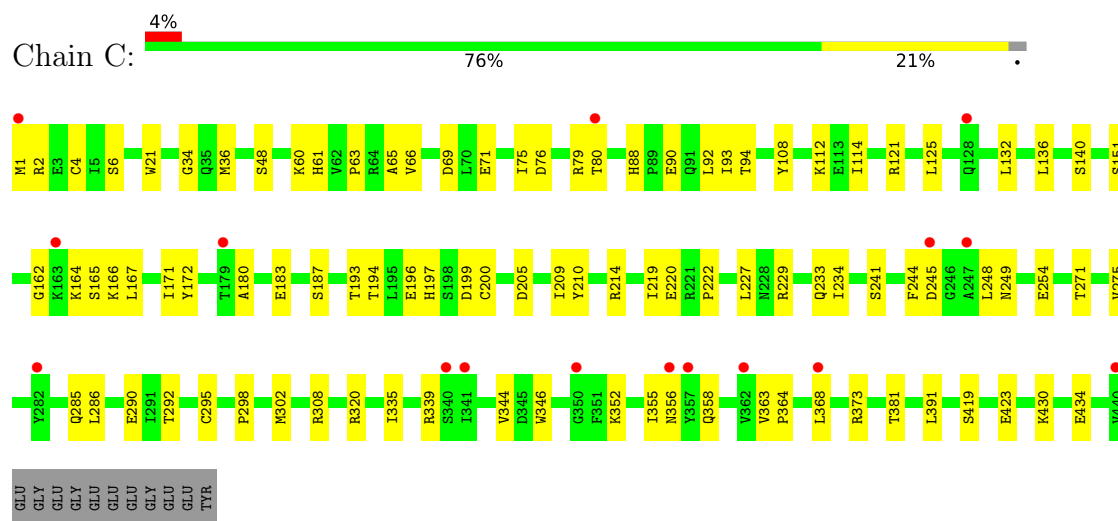
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha-1B chain

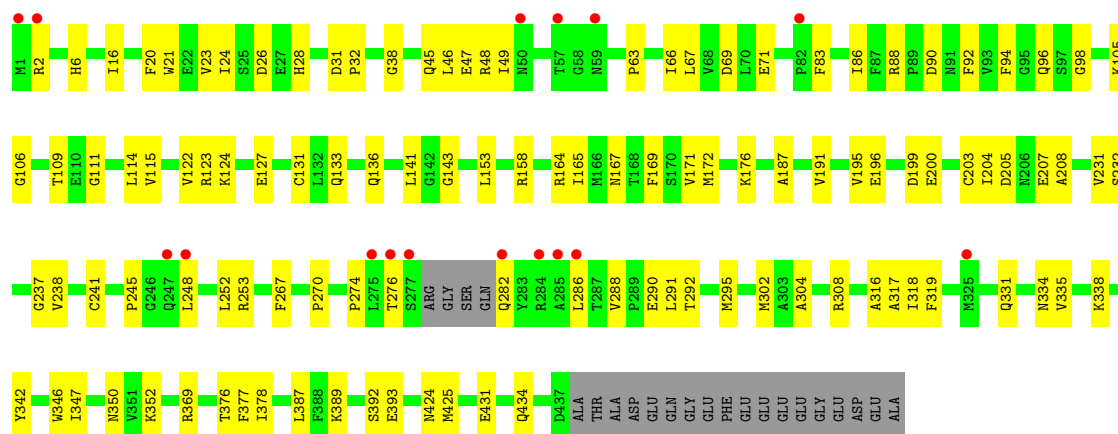


• Molecule 1: Tubulin alpha-1B chain

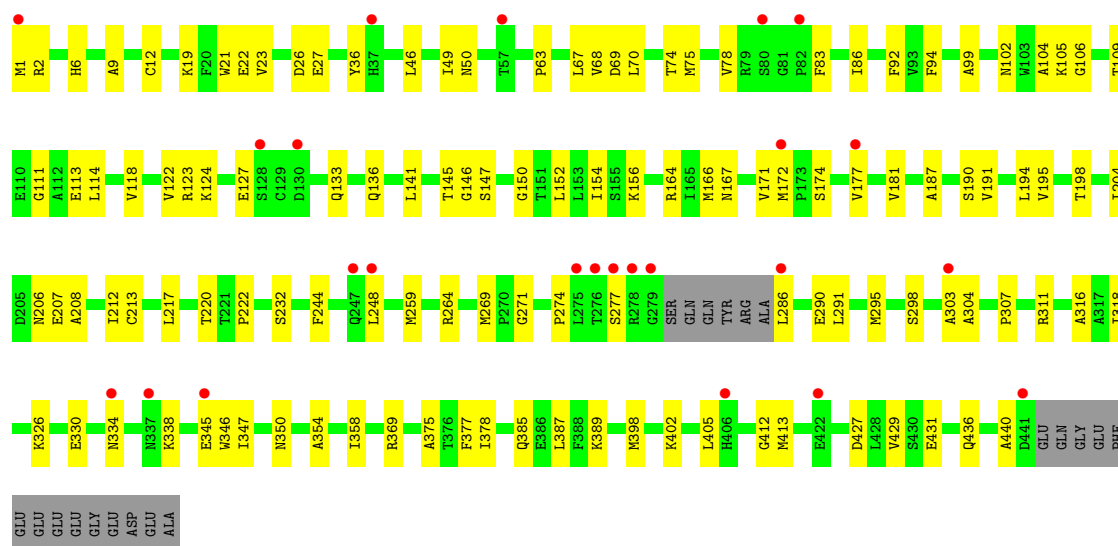


• Molecule 2: Tubulin beta-2B chain

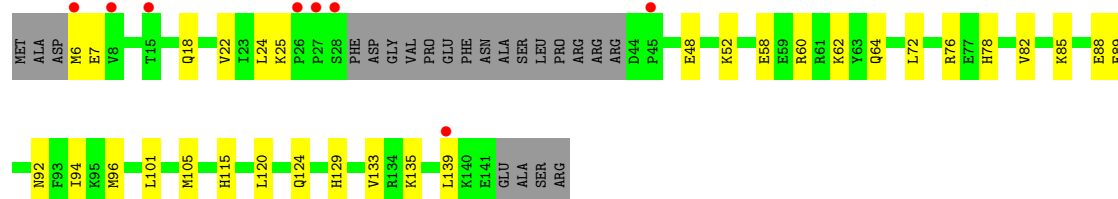




• Molecule 2: Tubulin beta-2B chain

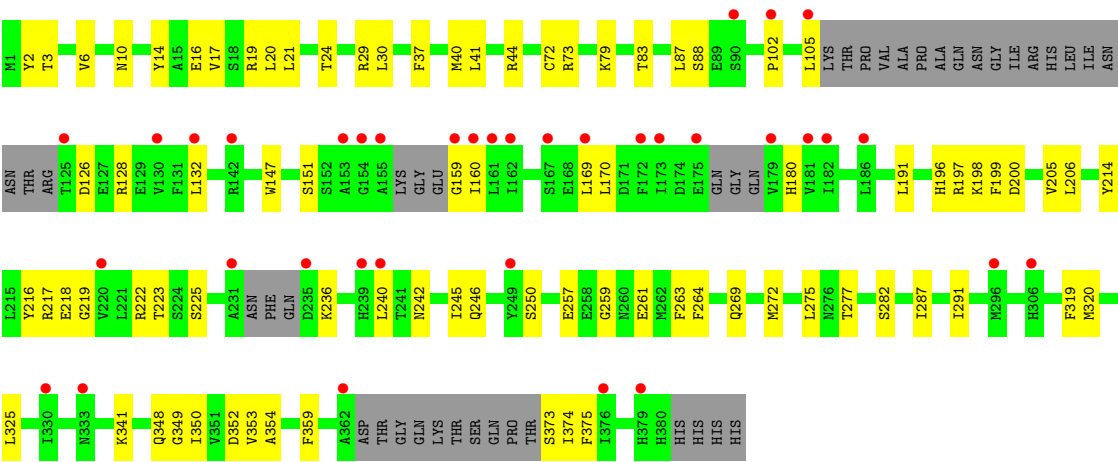


• Molecule 3: Stathmin-4



• 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	105.03Å 157.92Å 181.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.31 48.05 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.05-2.31) 99.9 (48.05-2.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.211 , 0.235 0.213 , 0.237	Depositor DCC
R_{free} test set	6639 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	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	0.95	EDS
Total number of atoms	17946	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: A1ISD, GDP, MG, GTP, MES, CA, ACP

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	0.07	0/3502	0.21	0/4754
1	C	0.08	0/3521	0.23	0/4780
2	B	0.07	0/3419	0.22	0/4629
2	D	0.06	0/3419	0.20	0/4630
3	E	0.06	0/1008	0.14	0/1337
4	F	0.05	0/2854	0.19	0/3853
All	All	0.07	0/17723	0.21	0/23983

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	70	0
1	C	3443	0	3352	66	0
2	B	3345	0	3227	79	0
2	D	3346	0	3222	83	0
3	E	1000	0	1018	20	0
4	F	2793	0	2766	59	0
5	A	32	0	12	1	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	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	12	0	13	1	0
10	D	78	63	0	0	0
11	F	31	0	14	0	0
12	A	50	0	0	2	0
12	B	68	0	0	3	0
12	C	115	0	0	3	0
12	D	26	0	0	2	0
12	E	8	0	0	1	0
12	F	15	0	0	1	0
All	All	17883	63	16994	367	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 11.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.46	0.98
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.46	0.96
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.48	0.94
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.56	0.88
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.56	0.87
1:A:381:THR:HG22	1:A:383:ALA:H	1.44	0.83
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.65	0.78
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.52	0.74
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.71	0.73
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.71
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.73	0.70
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.72	0.69
2:D:136:GLN:HA	2:D:167:ASN:O	1.93	0.69
1:C:76:ASP:O	1:C:80:THR:HG22	1.92	0.69
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.22	0.69
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.73	0.69
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.23	0.68
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.26	0.68
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.26	0.67
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.67
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.09	0.67
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.77	0.67
2:B:136:GLN:HA	2:B:167:ASN:O	1.94	0.66
2:D:181:VAL:HG22	2:D:398:MET:SD	2.36	0.66
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.76	0.66
2:B:276:THR:HG21	2:B:282:GLN:HA	1.75	0.66
1:A:71:GLU:O	12:A:601:HOH:O	2.15	0.65
4:F:246:GLN:O	4:F:250:SER:HB3	1.97	0.64
1:C:209:ILE:HD11	1:C:302:MET:CE	2.28	0.64
2:D:83:PHE:O	2:D:86:ILE:HG22	1.97	0.64
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.77	0.64
1:C:180:ALA:O	1:C:183:GLU:HG3	1.97	0.64
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.80	0.64
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.80	0.64
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.38	0.63
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.79	0.63
3:E:85:LYS:NZ	3:E:89:GLU:OE2	2.30	0.62
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.80	0.62
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.82	0.62
2:D:147:SER:HB2	2:D:190:SER:OG	2.00	0.62
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.81	0.62
3:E:129:HIS:O	3:E:133:VAL:HG23	2.00	0.61
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.82	0.61
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.83	0.61
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.82	0.61
2:D:311:ARG:NH1	2:D:436:GLN:O	2.34	0.61
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.37	0.60
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.60
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.37	0.60
2:D:298:SER:HB3	2:D:307:PRO:HD2	1.84	0.60
2:D:269:MET:HG3	2:D:303:ALA:CB	2.31	0.59
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:GLU:HG2	2:B:245:PRO:CG	2.29	0.59
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.38	0.59
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.18	0.59
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.85	0.58
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.58
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.84	0.58
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.03	0.58
1:A:430:LYS:O	1:A:434:GLU:HG3	2.02	0.58
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.34	0.58
2:B:2:ARG:O	2:B:133:GLN:NE2	2.29	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.05	0.57
2:B:123:ARG:O	2:B:127:GLU:HG3	2.05	0.57
4:F:199:PHE:CB	4:F:223:THR:HG22	2.34	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.57
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.87	0.57
2:B:187:ALA:O	2:B:191:VAL:HG23	2.05	0.57
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.40	0.56
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.87	0.56
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.21	0.56
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.35	0.56
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.04	0.56
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.41	0.56
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.88	0.56
1:A:394:LYS:NZ	12:A:602:HOH:O	2.39	0.56
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.06	0.56
2:B:389:LYS:O	2:B:393:GLU:HG3	2.05	0.56
1:A:214:ARG:HG2	1:A:219:ILE:O	2.06	0.56
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.88	0.55
1:A:83:TYR:HB3	1:A:86:LEU:HD12	1.89	0.55
2:B:2:ARG:HE	2:B:133:GLN:HG2	1.71	0.55
2:B:69:ASP:O	2:B:94:PHE:HA	2.06	0.55
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.87	0.55
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.87	0.55
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.06	0.55
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.40	0.55
3:E:115:HIS:HB3	12:E:308:HOH:O	2.06	0.55
1:C:419:SER:O	1:C:423:GLU:HG3	2.07	0.55
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.88	0.55
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.89	0.54
2:D:69:ASP:O	2:D:94:PHE:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.89	0.54
1:C:48:SER:OG	1:C:245:ASP:HB2	2.07	0.54
2:D:109:THR:O	2:D:113:GLU:HG2	2.07	0.54
2:B:196:GLU:HG2	12:B:664:HOH:O	2.08	0.54
2:D:152:LEU:O	2:D:156:LYS:HG2	2.08	0.54
2:B:115:VAL:HG23	2:B:153:LEU:HD23	1.89	0.54
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.89	0.54
1:A:69:ASP:O	1:A:94:THR:HA	2.07	0.54
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.08	0.54
4:F:159:GLY:C	4:F:160:ILE:HD12	2.32	0.54
1:C:271:THR:HG21	1:C:295:CYS:O	2.07	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.53
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.91	0.53
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.44	0.53
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.90	0.53
4:F:72:CYS:O	4:F:73:ARG:HD2	2.09	0.53
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.39	0.53
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.44	0.53
2:B:141:LEU:HD12	2:B:172:MET:SD	2.48	0.53
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.42	0.53
1:C:1:MET:HE3	1:C:2:ARG:HH21	1.74	0.53
1:C:220:GLU:HB3	2:D:326:LYS:HD2	1.91	0.52
2:D:191:VAL:O	2:D:195:VAL:HG23	2.09	0.52
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.91	0.52
2:D:217:LEU:HA	2:D:277:SER:HB3	1.89	0.52
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.52
1:A:419:SER:O	1:A:423:GLU:HG3	2.10	0.52
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.91	0.52
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.92	0.52
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.44	0.52
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.24	0.52
2:D:145:THR:HB	8:D:501:GDP:O2B	2.09	0.52
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.52
2:D:427:ASP:O	2:D:431:GLU:HG3	2.10	0.52
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.90	0.52
1:C:285:GLN:HE21	1:C:373:ARG:HH22	1.56	0.51
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.45	0.51
4:F:259:GLY:O	4:F:261:GLU:HG3	2.09	0.51
2:D:106:GLY:O	2:D:111:GLY:HA3	2.10	0.51
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:20:LEU:O	4:F:24:THR:HG23	2.10	0.51
1:C:335:ILE:HG23	1:C:339:ARG:CG	2.41	0.51
2:D:75:MET:N	12:D:601:HOH:O	2.23	0.51
1:C:166:LYS:NZ	12:C:602:HOH:O	2.44	0.51
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.10	0.51
3:E:72:LEU:O	3:E:76:ARG:HG2	2.10	0.51
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.46	0.51
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.21	0.51
2:B:317:ALA:C	2:B:318:ILE:HD12	2.36	0.50
2:B:392:SER:HB2	2:B:425:MET:HE3	1.93	0.50
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.93	0.50
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.47	0.50
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.50
2:B:253[A]:ARG:NH1	9:B:504:MES:O1S	2.41	0.50
1:C:151:SER:HB2	1:C:193:THR:CG2	2.42	0.50
2:D:141:LEU:HD12	2:D:172:MET:SD	2.51	0.50
2:D:187:ALA:O	2:D:191:VAL:HG23	2.11	0.50
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.93	0.50
2:D:46:LEU:HA	2:D:49:ILE:HB	1.94	0.50
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.46	0.50
2:B:164:ARG:HD2	12:B:617:HOH:O	2.11	0.50
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.93	0.50
2:B:124:LYS:HD3	2:B:124:LYS:C	2.37	0.49
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.12	0.49
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.94	0.49
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.94	0.49
2:D:104:ALA:HB2	2:D:413:MET:SD	2.53	0.49
2:D:387:LEU:HD23	2:D:387:LEU:C	2.37	0.49
2:B:71:GLU:HG3	2:B:98:GLY:HA2	1.94	0.49
2:B:191:VAL:O	2:B:195:VAL:HG23	2.12	0.49
2:D:123:ARG:O	2:D:127:GLU:HG3	2.12	0.49
2:B:114:LEU:O	2:B:114:LEU:HG	2.11	0.49
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.12	0.49
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.43	0.49
2:D:291:LEU:HG	2:D:375:ALA:HB2	1.95	0.49
3:E:101:LEU:O	3:E:105:MET:HG2	2.12	0.49
1:A:22:GLU:HG3	1:A:83:TYR:HE2	1.78	0.49
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.46	0.49
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.94	0.49
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.78	0.49
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.47	0.49
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.48	0.49
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.48
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.93	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.52	0.48
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.53	0.48
1:C:196:GLU:HG2	12:C:631:HOH:O	2.12	0.48
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.77	0.48
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.49	0.48
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.48
2:B:48:ARG:NH2	2:B:241:CYS:O	2.47	0.48
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.95	0.48
4:F:199:PHE:HB2	4:F:223:THR:HG22	1.96	0.48
2:D:141:LEU:HA	2:D:147:SER:HB3	1.96	0.47
2:B:115:VAL:HG23	2:B:153:LEU:CD2	2.42	0.47
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.96	0.47
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.49	0.47
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.49	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.14	0.47
3:E:92:ASN:O	3:E:96:MET:HG2	2.14	0.47
4:F:160:ILE:HD12	4:F:160:ILE:N	2.29	0.47
1:A:187:SER:CB	1:A:391:LEU:HD21	2.44	0.47
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.47	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.49	0.47
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.97	0.47
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.95	0.47
4:F:6:VAL:HB	4:F:29:ARG:NH2	2.30	0.47
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.44	0.47
4:F:349:GLY:O	4:F:353:VAL:HG22	2.14	0.47
1:A:75:ILE:HB	1:A:94:THR:CG2	2.45	0.47
2:D:295:MET:CE	2:D:377:PHE:HB2	2.42	0.47
2:B:431:GLU:O	2:B:434:GLN:HG2	2.14	0.47
2:D:9:ALA:HA	2:D:68:VAL:O	2.15	0.46
1:A:134:GLY:HA3	1:A:165:SER:O	2.16	0.46
4:F:17:VAL:O	4:F:21:LEU:HG	2.14	0.46
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.50	0.46
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.51	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HG2	1:C:219:ILE:O	2.16	0.46
2:D:208:ALA:O	2:D:212:ILE:HG13	2.15	0.46
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.97	0.46
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.98	0.46
1:A:75:ILE:HB	1:A:94:THR:HG21	1.97	0.46
1:A:298:PRO:HA	1:A:301:GLN:CD	2.40	0.46
4:F:200:ASP:OD2	4:F:222:ARG:NH2	2.48	0.46
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.51	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.46
2:D:23:VAL:O	2:D:27:GLU:HG3	2.16	0.46
1:A:25:CYS:HB3	1:A:30:ILE:O	2.16	0.46
2:B:295:MET:CG	2:B:377:PHE:HB2	2.45	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.51	0.46
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.16	0.45
2:B:424:ASN:HB3	12:B:602:HOH:O	2.16	0.45
3:E:7:GLU:O	3:E:22:VAL:HA	2.16	0.45
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.98	0.45
2:D:208:ALA:HB2	2:D:304:ALA:HB2	1.98	0.45
1:C:285:GLN:NE2	1:C:373:ARG:HH22	2.14	0.45
2:D:75:MET:SD	2:D:94:PHE:HB3	2.56	0.45
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.96	0.45
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.46	0.45
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.47	0.45
2:B:318:ILE:HD12	2:B:318:ILE:N	2.32	0.45
4:F:269:GLN:HA	4:F:272:MET:HE2	1.99	0.45
2:D:164:ARG:HD2	12:D:625:HOH:O	2.15	0.45
4:F:16:GLU:O	4:F:20:LEU:HG	2.15	0.45
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.98	0.45
1:A:331:ALA:O	1:A:335:ILE:HG13	2.17	0.45
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.99	0.45
1:C:229:ARG:NH1	12:C:608:HOH:O	2.50	0.45
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.17	0.45
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.52	0.45
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.99	0.45
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.52	0.45
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.99	0.45
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.98	0.45
2:B:387:LEU:C	2:B:387:LEU:HD23	2.41	0.44
4:F:350:ILE:O	4:F:354:ALA:HB3	2.17	0.44
2:B:143:GLY:HA3	8:B:501:GDP:O3A	2.18	0.44
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:CE	2:D:50:ASN:HB2	2.32	0.44
2:D:67:LEU:N	2:D:67:LEU:HD12	2.33	0.44
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.46	0.44
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.99	0.44
4:F:3:THR:HB	4:F:30:LEU:HD11	1.99	0.44
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.81	0.44
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.53	0.44
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.48	0.44
2:B:46:LEU:HA	2:B:49:ILE:HB	2.00	0.44
2:D:74:THR:O	2:D:78:VAL:HG23	2.18	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.44
3:E:120:LEU:O	3:E:124:GLN:HG3	2.18	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.44
4:F:151:SER:HB3	4:F:180:HIS:CG	2.53	0.43
1:A:234:ILE:HD12	1:A:234:ILE:N	2.33	0.43
2:D:102:ASN:ND2	2:D:105:LYS:HG3	2.33	0.43
4:F:373:SER:N	12:F:504:HOH:O	2.51	0.43
1:A:166:LYS:HE2	1:A:197:HIS:O	2.17	0.43
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.00	0.43
1:C:241:SER:HA	1:C:249:ASN:OD1	2.18	0.43
1:A:135:PHE:O	1:A:136:LEU:HD23	2.19	0.43
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.99	0.43
1:A:180:ALA:O	1:A:183:GLU:HG3	2.18	0.43
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.43
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.01	0.43
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.99	0.43
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.19	0.43
2:B:199:ASP:C	2:B:200:GLU:HG3	2.43	0.43
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.00	0.43
2:D:2:ARG:HB3	2:D:133:GLN:HG2	2.00	0.43
1:A:151:SER:HB2	1:A:193:THR:OG1	2.19	0.43
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.84	0.43
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.01	0.43
2:D:124:LYS:C	2:D:124:LYS:HD3	2.44	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
2:D:174:SER:OG	2:D:207:GLU:OE1	2.30	0.43
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.54	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.43
2:B:67:LEU:N	2:B:67:LEU:HD12	2.34	0.43
1:C:187:SER:CB	1:C:391:LEU:HD21	2.48	0.43
4:F:87:LEU:O	4:F:88:SER:OG	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:128:ARG:O	4:F:132:LEU:HG	2.19	0.42
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.54	0.42
1:A:2:ARG:HB3	1:A:131:GLY:O	2.19	0.42
2:B:2:ARG:HA	2:B:131:CYS:O	2.19	0.42
2:D:412:GLY:C	3:E:133:VAL:HG13	2.45	0.42
1:C:69:ASP:O	1:C:94:THR:HA	2.19	0.42
1:C:132:LEU:HG	1:C:164:LYS:HD3	2.02	0.42
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.00	0.42
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.19	0.42
4:F:272:MET:HG2	4:F:277:THR:O	2.19	0.42
1:A:302:MET:HE2	1:A:302:MET:HA	2.00	0.42
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.50	0.42
3:E:88:GLU:OE1	3:E:88:GLU:HA	2.19	0.42
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.20	0.42
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.49	0.42
1:C:194:THR:O	1:C:194:THR:HG22	2.19	0.42
2:D:114:LEU:HG	2:D:114:LEU:O	2.20	0.42
2:D:220:THR:C	2:D:222:PRO:HD3	2.44	0.42
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.42
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.42
1:C:75:ILE:HB	1:C:94:THR:HG21	2.01	0.42
2:D:385:GLN:O	2:D:389:LYS:HG3	2.20	0.42
2:B:295:MET:HE1	2:B:319:PHE:CZ	2.55	0.42
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.02	0.42
2:B:158:ARG:NH1	2:B:196:GLU:O	2.53	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.55	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.01	0.41
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.02	0.41
2:D:146:GLY:O	2:D:150:GLY:HA3	2.20	0.41
4:F:19:ARG:HD2	4:F:19:ARG:O	2.20	0.41
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.56	0.41
4:F:225:SER:HG	4:F:250:SER:HG	1.61	0.41
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.54	0.41
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.20	0.41
4:F:79:LYS:O	4:F:83:THR:OG1	2.35	0.41
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.50	0.41
1:C:21:TRP:CZ2	1:C:65:ALA:HB2	2.56	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.41
3:E:135:LYS:O	3:E:139:LEU:HG	2.19	0.41
1:C:108:TYR:O	1:C:112:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:VAL:O	2:D:122:VAL:HG23	2.21	0.41
2:B:248:LEU:HD21	2:B:352:LYS:HB3	2.03	0.41
2:B:295:MET:HG3	2:B:377:PHE:HB2	2.03	0.41
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.01	0.41
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.02	0.41
2:D:326:LYS:O	2:D:330:GLU:HG3	2.21	0.41
3:E:78:HIS:O	3:E:82:VAL:HG23	2.19	0.41
4:F:128:ARG:HH12	4:F:170:LEU:HB3	1.84	0.41
1:A:349:THR:HB	3:E:25:LYS:HB3	2.03	0.41
1:A:213:CYS:O	1:A:217:LEU:HB2	2.21	0.40
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.21	0.40
1:C:165:SER:HA	1:C:199:ASP:OD2	2.21	0.40
1:C:234:ILE:HD12	1:C:234:ILE:N	2.36	0.40
2:D:259:MET:HE2	2:D:378:ILE:HG22	2.02	0.40
2:D:271:GLY:HA3	2:D:377:PHE:HB3	2.02	0.40
1:A:32:PRO:HA	1:A:83:TYR:CD1	2.56	0.40
2:B:171:VAL:HA	2:B:204:ILE:O	2.21	0.40
1:A:325:PRO:HD3	3:E:18:GLN:NE2	2.36	0.40
1:C:363:VAL:CG1	1:C:364:PRO:HD2	2.51	0.40
2:B:96:GLN:CB	1:C:1:MET:HE2	2.40	0.40
4:F:275:LEU:HD22	4:F:275:LEU:N	2.37	0.40
1:A:289:ALA:HA	1:A:331:ALA:CB	2.51	0.40
1:A:329:ASN:HB3	3:E:6:MET:CE	2.51	0.40
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.56	0.40
1:C:6:SER:O	1:C:65:ALA:HA	2.22	0.40
2:D:213:CYS:HA	2:D:217:LEU:HD12	2.03	0.40
4:F:19:ARG:HD2	4:F:19:ARG:C	2.45	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	436/451 (97%)	423 (97%)	13 (3%)	0	100	100
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	420/445 (94%)	410 (98%)	10 (2%)	0	100	100
2	D	422/445 (95%)	412 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	330/384 (86%)	319 (97%)	11 (3%)	0	100	100
All	All	2164/2319 (93%)	2110 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	369 (100%)	0	100	100
1	C	372/379 (98%)	370 (100%)	2 (0%)	86	93
2	B	368/383 (96%)	368 (100%)	0	100	100
2	D	368/383 (96%)	368 (100%)	0	100	100
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	306/342 (90%)	306 (100%)	0	100	100
All	All	1892/1993 (95%)	1890 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	71	GLU
1	C	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	393	HIS
2	B	136	GLN
2	B	192	HIS
2	B	193	GLN
2	B	331	GLN
2	B	349	ASN
2	B	434	GLN
1	C	285	GLN
1	C	372	GLN
1	C	393	HIS
2	D	6	HIS
2	D	50	ASN
2	D	136	GLN
2	D	247	GLN
2	D	331	GLN
2	D	339	ASN
3	E	18	GLN
3	E	92	ASN
3	E	115	HIS
3	E	136	ASN
4	F	242	ASN
4	F	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)
10	A1ISD	D	503	-	84,86,86	2.78	28 (33%)	102,127,127	2.24	31 (30%)
9	MES	B	504	-	12,12,12	1.14	1 (8%)	14,16,16	0.92	1 (7%)
11	ACP	F	401	6	27,33,33	2.32	3 (11%)	32,52,52	1.19	4 (12%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.46	6 (18%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.44	5 (15%)
8	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)

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	B	501	6	-	3/12/32/32	0/3/3/3
10	A1ISD	D	503	-	-	14/70/120/120	0/7/9/9
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
11	ACP	F	401	6	-	6/15/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	A1ISD	C50-N7	11.26	1.47	1.36
11	F	401	ACP	PB-O3A	10.93	1.70	1.58
10	D	503	A1ISD	O11-C50	9.21	1.40	1.22
10	D	503	A1ISD	C8-N1	6.79	1.49	1.35
10	D	503	A1ISD	C51-N7	6.00	1.51	1.46
10	D	503	A1ISD	C43-N6	5.48	1.47	1.35
10	D	503	A1ISD	C15-C14	-5.42	1.35	1.53
10	D	503	A1ISD	C55-N8	5.10	1.46	1.37
10	D	503	A1ISD	C51-C47	5.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	A1ISD	C56-N8	4.79	1.45	1.37
10	D	503	A1ISD	O8-C29	4.01	1.42	1.34
5	C	501	GTP	C5-C6	-3.99	1.39	1.47
10	D	503	A1ISD	C7-N1	3.97	1.49	1.44
10	D	503	A1ISD	C10-C11	3.93	1.56	1.51
5	A	501	GTP	C5-C6	-3.90	1.39	1.47
10	D	503	A1ISD	C39-N5	3.55	1.38	1.34
10	D	503	A1ISD	O8-C27	-3.31	1.40	1.46
10	D	503	A1ISD	C44-N6	3.15	1.47	1.41
10	D	503	A1ISD	C48-C47	3.09	1.45	1.39
10	D	503	A1ISD	C38-N3	3.06	1.38	1.35
10	D	503	A1ISD	C25-C24	3.05	1.51	1.47
9	B	504	MES	C8-S	3.04	1.81	1.77
10	D	503	A1ISD	O1-C2	2.88	1.41	1.37
10	D	503	A1ISD	O6-C21	-2.74	1.42	1.46
10	D	503	A1ISD	C10-C5	2.73	1.56	1.51
10	D	503	A1ISD	C20-C21	2.72	1.58	1.52
10	D	503	A1ISD	C28-C8	2.62	1.56	1.51
8	D	501	GDP	C6-N1	-2.35	1.34	1.37
10	D	503	A1ISD	C30-C29	2.32	1.55	1.50
8	B	501	GDP	C6-N1	-2.30	1.34	1.37
11	F	401	ACP	PB-O2B	-2.20	1.51	1.56
5	C	501	GTP	C2-N3	2.19	1.38	1.33
5	A	501	GTP	C2-N3	2.16	1.38	1.33
10	D	503	A1ISD	O5-C19	2.14	1.25	1.21
11	F	401	ACP	C8-N7	-2.08	1.31	1.34
10	D	503	A1ISD	O12-C55	-2.06	1.19	1.23
10	D	503	A1ISD	C38-C39	2.02	1.39	1.36
10	D	503	A1ISD	O10-C43	-2.01	1.19	1.23

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	A1ISD	C51-N7-C50	-9.10	109.38	113.12
10	D	503	A1ISD	O8-C29-C30	5.25	120.40	111.92
10	D	503	A1ISD	C48-C50-N7	5.11	109.46	106.44
10	D	503	A1ISD	C26-C25-C24	-4.93	109.88	121.05
10	D	503	A1ISD	C47-C51-N7	4.81	103.33	101.79
10	D	503	A1ISD	C56-N8-C55	-4.78	119.95	126.61
10	D	503	A1ISD	C25-O7-C24	4.70	63.62	60.79
10	D	503	A1ISD	O7-C25-C26	-4.12	108.25	114.17
10	D	503	A1ISD	O7-C25-C27	3.75	122.00	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	A1ISD	O1-C2-C3	3.64	119.85	115.53
11	F	401	ACP	O1G-PG-C3B	-3.63	103.41	111.24
10	D	503	A1ISD	O6-C19-O5	-3.59	112.65	117.87
8	D	501	GDP	PA-O3A-PB	-3.52	120.76	132.83
10	D	503	A1ISD	N5-N4-N3	3.48	109.94	107.31
5	A	501	GTP	PA-O3A-PB	-3.21	121.81	132.83
5	A	501	GTP	C5-C6-N1	3.19	119.59	113.95
5	C	501	GTP	PA-O3A-PB	-3.15	122.03	132.83
10	D	503	A1ISD	C49-C46-C45	3.13	124.69	120.25
5	C	501	GTP	C5-C6-N1	3.13	119.48	113.95
10	D	503	A1ISD	C53-C52-N7	-3.11	110.75	114.11
5	C	501	GTP	C8-N7-C5	3.04	108.79	102.99
10	D	503	A1ISD	C38-C39-N5	-3.04	106.83	111.34
5	C	501	GTP	PB-O3B-PG	-3.03	122.43	132.83
10	D	503	A1ISD	C54-C56-N8	3.02	120.05	116.65
5	A	501	GTP	C8-N7-C5	3.02	108.74	102.99
8	D	501	GDP	C3'-C2'-C1'	2.82	105.22	100.98
11	F	401	ACP	O2B-PB-O1B	2.82	119.48	110.07
5	A	501	GTP	C2-N1-C6	-2.78	119.98	125.10
8	B	501	GDP	PA-O3A-PB	-2.74	123.42	132.83
10	D	503	A1ISD	C14-C13-C11	-2.71	121.14	127.66
5	C	501	GTP	C2-N1-C6	-2.70	120.12	125.10
9	B	504	MES	O2S-S-C8	-2.68	103.68	106.92
5	A	501	GTP	PB-O3B-PG	-2.68	123.64	132.83
10	D	503	A1ISD	C28-C8-N1	2.64	121.87	118.89
10	D	503	A1ISD	O6-C19-N2	2.61	123.64	118.78
10	D	503	A1ISD	C42-C43-N6	2.60	119.18	114.59
10	D	503	A1ISD	C27-O8-C29	-2.57	112.96	117.55
10	D	503	A1ISD	C52-C55-N8	2.57	119.70	116.25
10	D	503	A1ISD	O1-C2-C1	-2.52	119.79	124.12
10	D	503	A1ISD	C4-O1-C2	-2.38	113.93	117.53
10	D	503	A1ISD	C14-C15-C16	2.37	119.13	113.90
8	D	501	GDP	C8-N7-C5	2.37	107.50	102.99
10	D	503	A1ISD	C53-C54-C56	-2.35	109.96	114.12
8	B	501	GDP	C8-N7-C5	2.33	107.43	102.99
8	B	501	GDP	C5-C6-N1	2.33	118.06	113.95
8	D	501	GDP	C5-C6-N1	2.27	117.95	113.95
10	D	503	A1ISD	C45-C44-C47	2.25	123.46	120.68
11	F	401	ACP	PB-O3A-PA	-2.23	125.50	132.56
10	D	503	A1ISD	C47-C48-C50	-2.16	106.71	108.39
5	A	501	GTP	O6-C6-C5	-2.08	120.30	124.37
11	F	401	ACP	O3G-PG-O2G	2.08	114.16	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	A1ISD	O7-C24-C25	-2.06	58.36	59.83
10	D	503	A1ISD	O8-C29-O9	-2.02	120.23	123.53
10	D	503	A1ISD	O7-C25-C24	-2.02	58.02	59.38

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
10	D	503	A1ISD	C3-C2-O1-C4
10	D	503	A1ISD	C25-C27-O8-C29
10	D	503	A1ISD	C53-C52-N7-C51
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
10	D	503	A1ISD	C1-C2-O1-C4
10	D	503	A1ISD	C28-C27-O8-C29
10	D	503	A1ISD	O8-C29-C30-C33
10	D	503	A1ISD	O8-C29-C30-C31
10	D	503	A1ISD	O9-C29-C30-C31
10	D	503	A1ISD	O9-C29-C30-C33
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
10	D	503	A1ISD	C53-C52-N7-C50
10	D	503	A1ISD	C55-C52-N7-C51
11	F	401	ACP	PB-C3B-PG-O3G
10	D	503	A1ISD	C20-C21-C22-C23
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A

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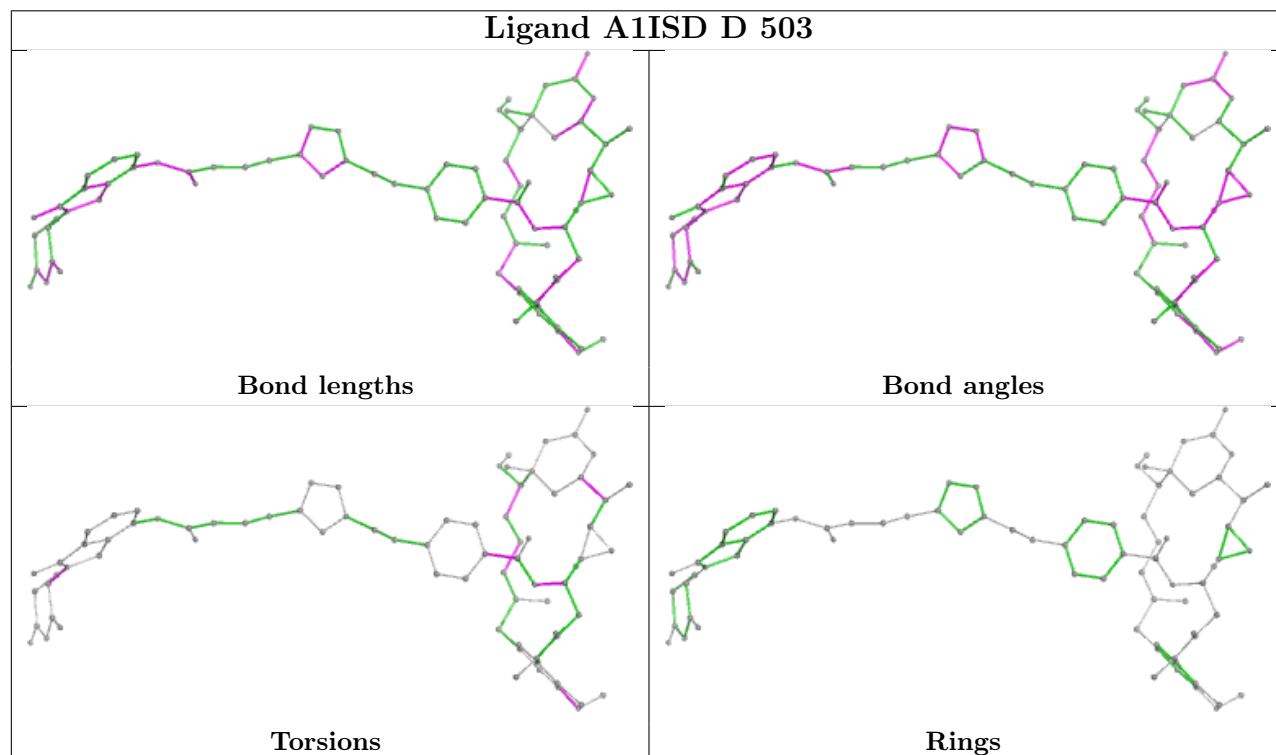
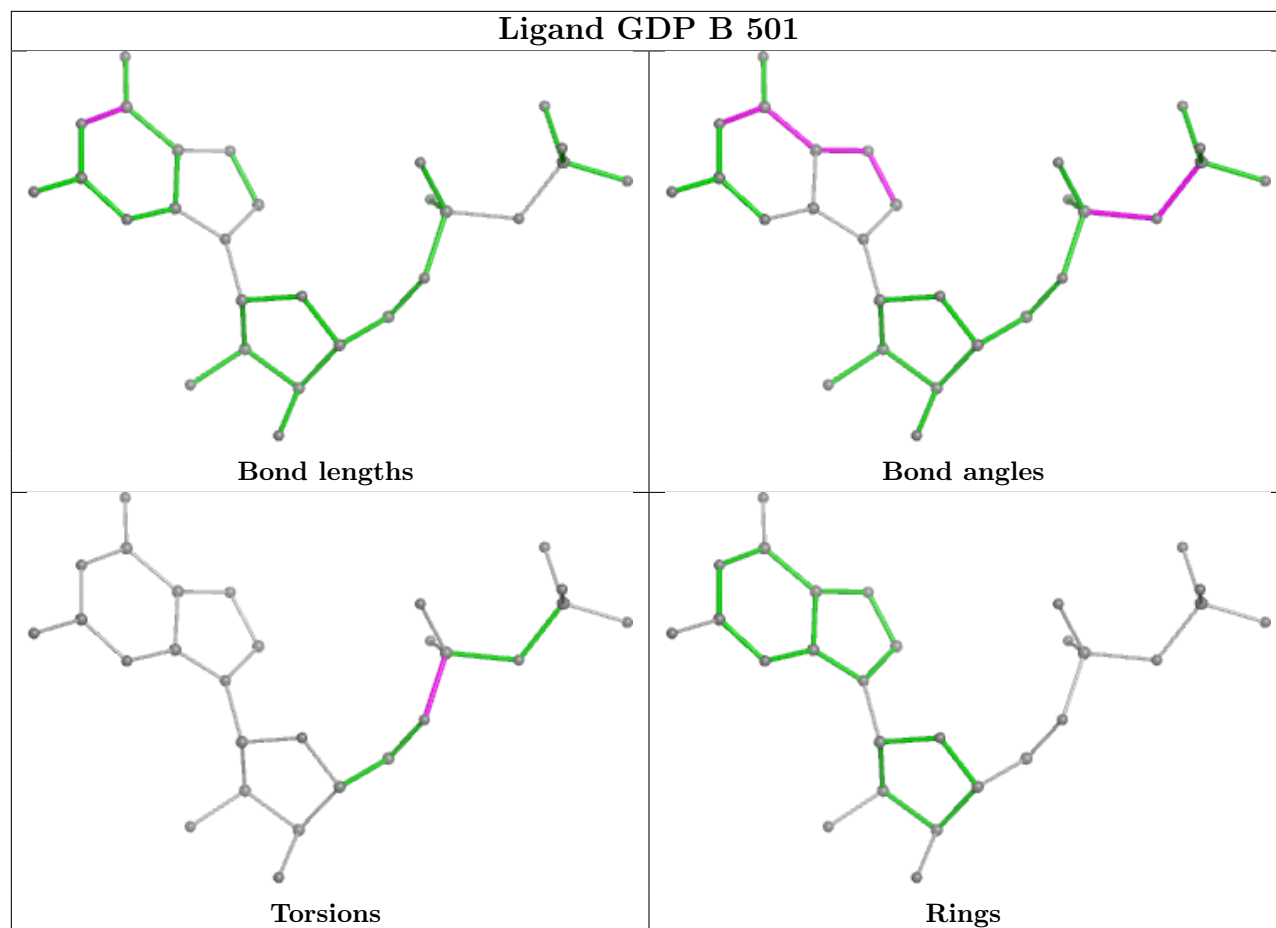
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3A-PA-O1A
10	D	503	A1ISD	C11-C13-C14-C15
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
10	D	503	A1ISD	C14-C15-C16-O3

There are no ring outliers.

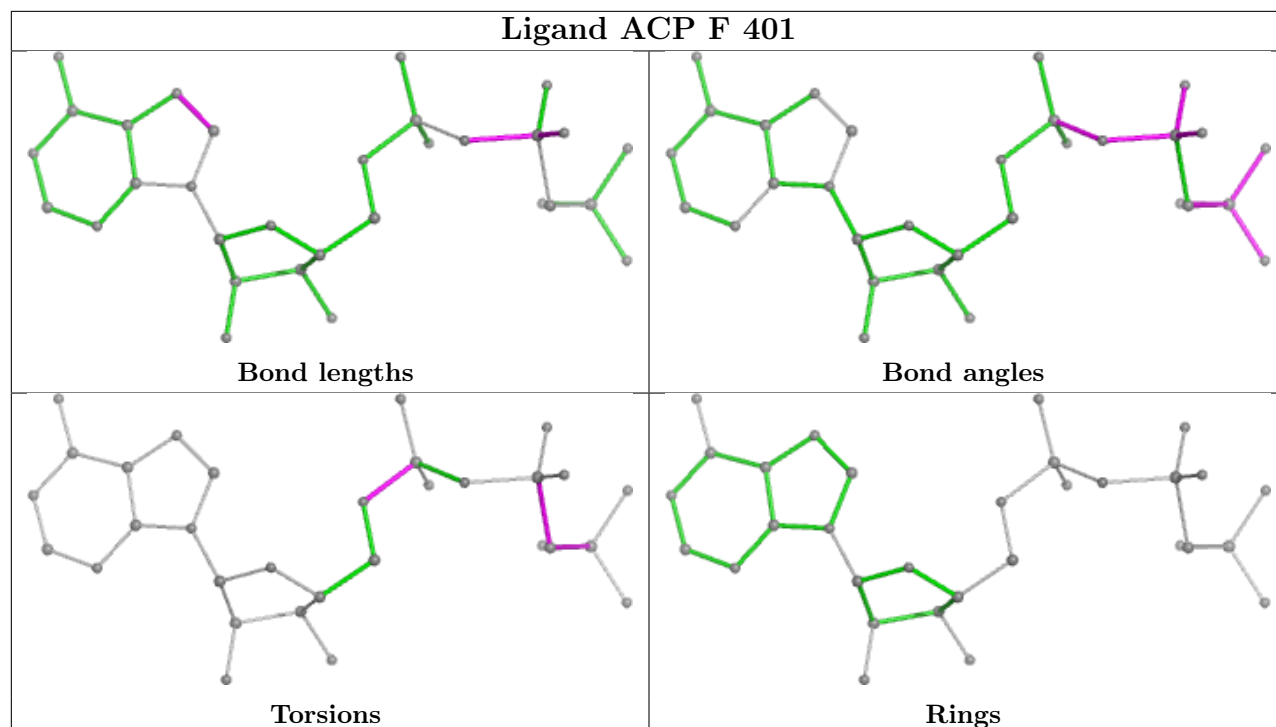
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
9	B	504	MES	1	0
5	A	501	GTP	1	0
8	D	501	GDP	2	0

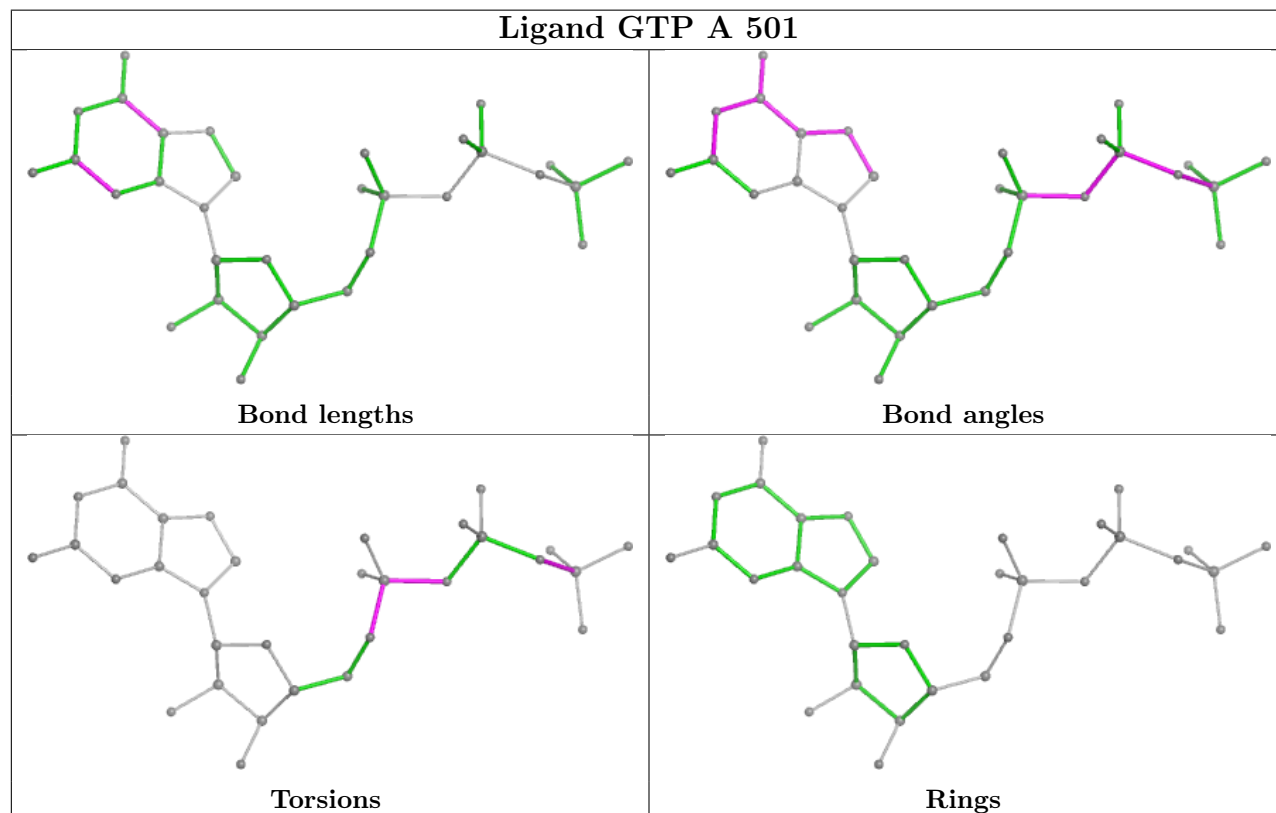
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

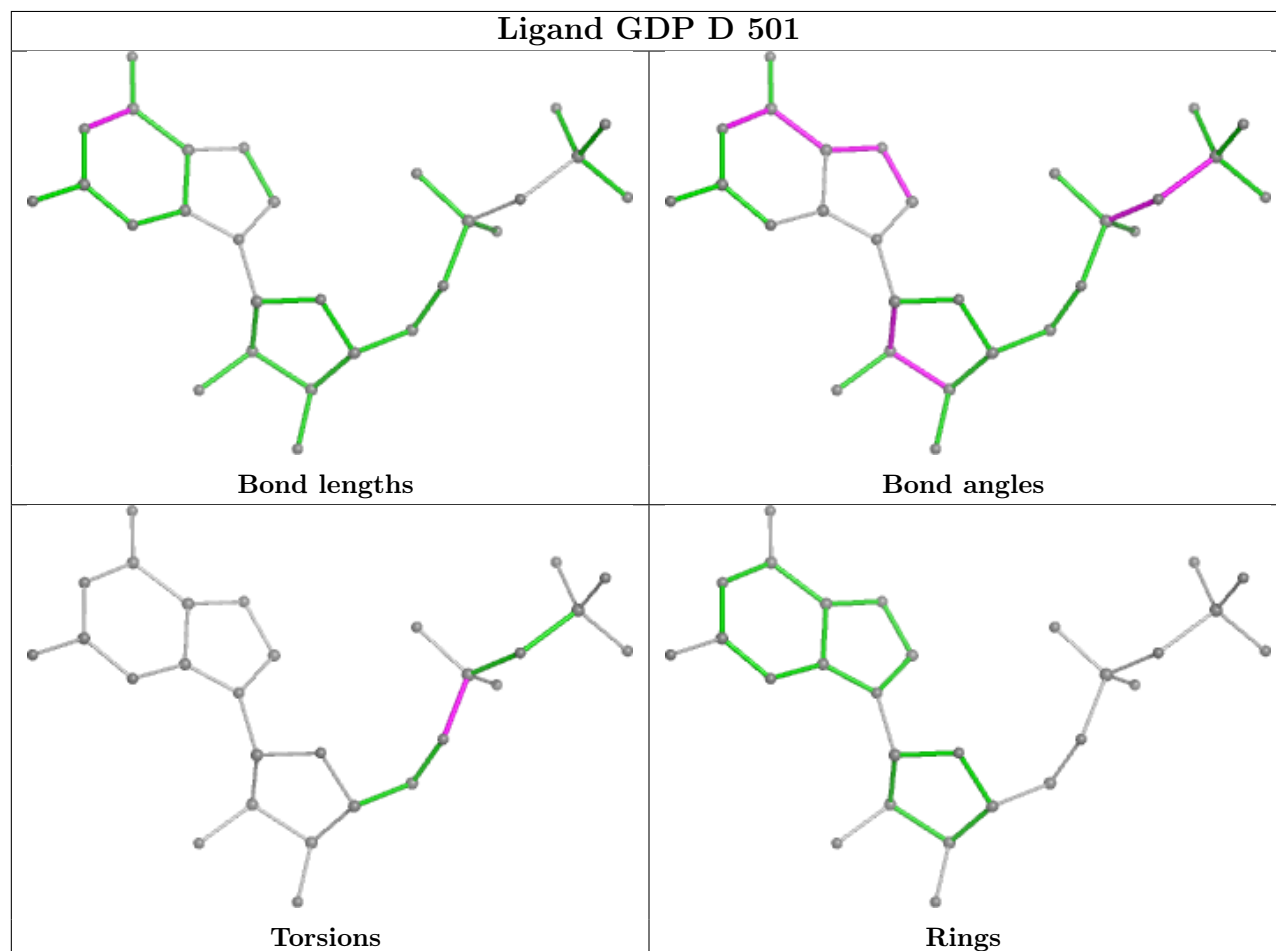
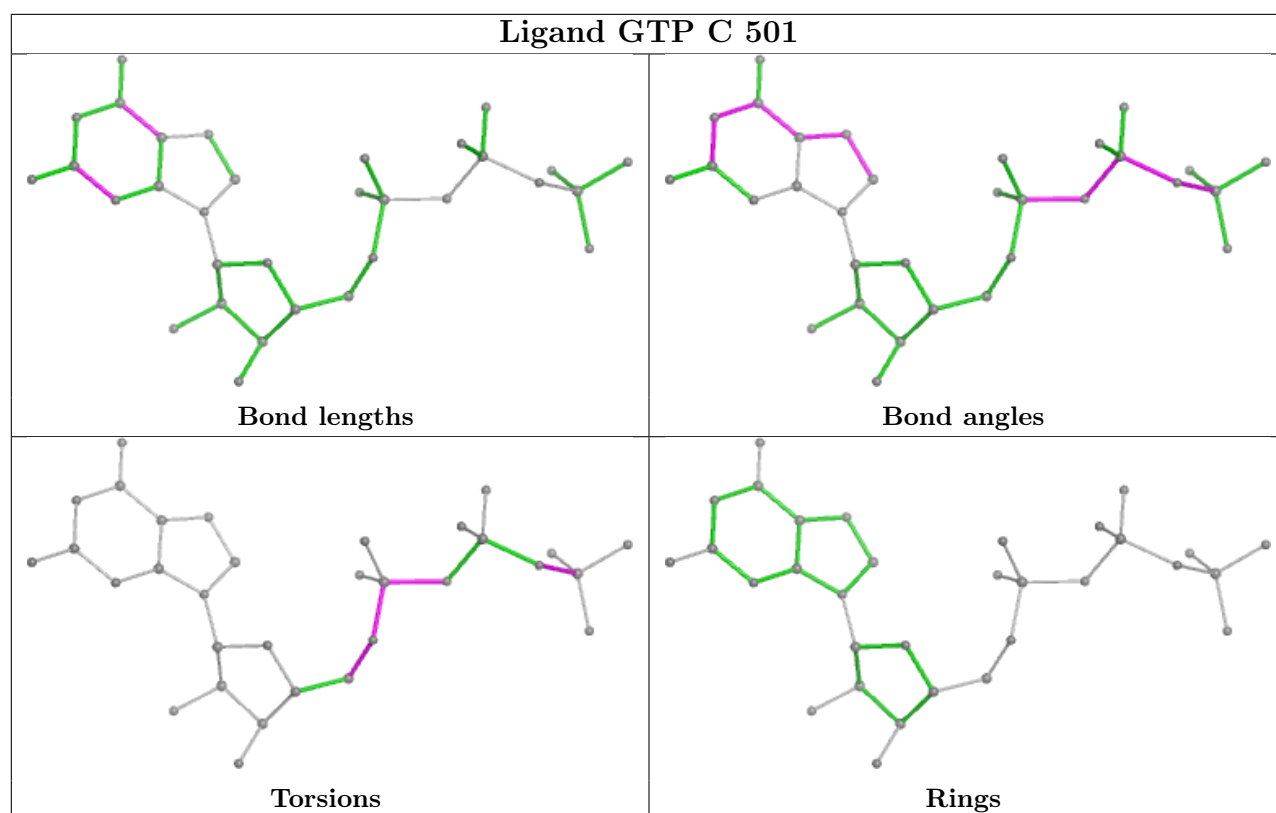


Ligand ACP F 401



Ligand 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%)	0.48	16 (3%)	45	48	50, 70, 98, 143	0
1	C	440/451 (97%)	0.19	16 (3%)	46	49	26, 56, 76, 104	1 (0%)
2	B	423/445 (95%)	0.41	16 (3%)	44	47	31, 64, 93, 125	1 (0%)
2	D	425/445 (95%)	0.62	24 (5%)	31	34	41, 79, 107, 140	1 (0%)
3	E	121/143 (84%)	0.81	8 (6%)	26	28	59, 80, 118, 125	0
4	F	342/384 (89%)	0.86	36 (10%)	13	15	63, 91, 151, 177	0
All	All	2189/2319 (94%)	0.51	116 (5%)	33	36	26, 72, 119, 177	3 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	7.1
2	D	279	GLY	6.7
2	B	1	MET	5.4
4	F	159	GLY	4.8
4	F	179	VAL	4.2
2	D	277	SER	4.0
4	F	231	ALA	4.0
1	A	282	TYR	3.8
4	F	125	THR	3.8
1	C	440	VAL	3.8
1	A	77	GLU	3.7
1	C	357	TYR	3.6
4	F	240	LEU	3.5
2	B	275	LEU	3.4
4	F	249	TYR	3.4
4	F	105	LEU	3.4
2	B	284	ARG	3.3
2	D	172	MET	3.2
2	B	276	THR	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	330	ILE	3.2
1	C	1	MET	3.2
2	D	303	ALA	3.2
4	F	181	VAL	3.1
4	F	153	ALA	3.1
4	F	161	LEU	3.0
1	A	281	ALA	3.0
1	C	341	ILE	2.9
2	B	285	ALA	2.9
1	A	381	THR	2.8
3	E	28	SER	2.8
1	C	163	LYS	2.8
4	F	173	ILE	2.8
2	D	128	SER	2.8
3	E	45	PRO	2.8
4	F	296	MET	2.7
2	D	422[A]	GLU	2.7
4	F	376	ILE	2.7
1	C	340	SER	2.7
1	C	245	ASP	2.7
4	F	130	VAL	2.7
2	D	406	HIS	2.7
2	B	57	THR	2.7
2	D	286	LEU	2.7
2	D	80	SER	2.7
2	D	278	ARG	2.6
2	B	82	PRO	2.6
2	D	276	THR	2.6
4	F	362	ALA	2.5
3	E	15	THR	2.5
1	C	362	VAL	2.5
4	F	220	VAL	2.5
3	E	139	LEU	2.5
4	F	186	LEU	2.5
4	F	162	ILE	2.4
4	F	169	LEU	2.4
4	F	379	HIS	2.4
2	D	57	THR	2.4
2	D	1	MET	2.4
1	C	282	TYR	2.4
2	B	59	ASN	2.4
1	A	88	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	239	HIS	2.4
2	B	248	LEU	2.4
2	D	345	GLU	2.3
4	F	175	GLU	2.3
1	A	262	TYR	2.3
1	A	196	GLU	2.3
1	C	179	THR	2.3
1	A	346	TRP	2.3
1	A	438	ASP	2.3
4	F	90	SER	2.3
2	D	247	GLN	2.3
2	B	286	LEU	2.3
3	E	6	MET	2.3
2	D	248	LEU	2.3
1	A	283	HIS	2.3
4	F	160	ILE	2.3
2	B	325	MET	2.2
1	C	356	ASN	2.2
4	F	172	PHE	2.2
2	B	247	GLN	2.2
4	F	102	PRO	2.2
2	D	130	ASP	2.2
1	C	368	LEU	2.2
1	C	80	THR	2.2
1	A	437	VAL	2.2
1	C	128	GLN	2.2
2	B	277	SER	2.2
4	F	182	ILE	2.2
1	C	247	ALA	2.2
3	E	8	VAL	2.1
4	F	142	ARG	2.1
2	B	50	ASN	2.1
2	D	275	LEU	2.1
2	D	334	ASN	2.1
2	D	337	ASN	2.1
1	A	15	GLN	2.1
1	A	78	VAL	2.1
2	D	441	ASP	2.1
4	F	235	ASP	2.1
4	F	167	SER	2.1
1	A	316	CYS	2.1
4	F	132	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	333	ASN	2.1
2	D	82	PRO	2.1
3	E	26	PRO	2.1
2	D	177	VAL	2.1
1	C	350	GLY	2.1
3	E	27	PRO	2.1
1	A	357	TYR	2.0
4	F	154	GLY	2.0
1	A	38	SER	2.0
2	B	282	GLN	2.0
2	B	2	ARG	2.0
2	D	37	HIS	2.0
4	F	306	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	402	1/1	0.31	0.24	107,107,107,107	0
7	CA	B	503	1/1	0.54	0.27	97,97,97,97	0
10	A1ISD	D	503	78/78	0.72	0.16	98,125,211,216	0
7	CA	E	201	1/1	0.73	0.15	106,106,106,106	0
6	MG	D	502	1/1	0.78	0.12	87,87,87,87	0
11	ACP	F	401	31/31	0.86	0.12	99,109,117,120	0
7	CA	A	503	1/1	0.91	0.07	92,92,92,92	0
8	GDP	D	501	28/28	0.91	0.12	75,80,86,94	0
9	MES	B	504	12/12	0.92	0.10	54,62,69,73	0
5	GTP	A	501	32/32	0.96	0.07	44,54,59,60	0

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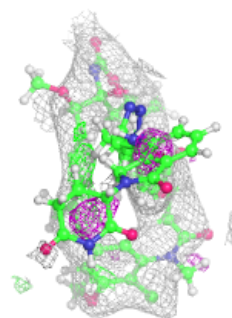
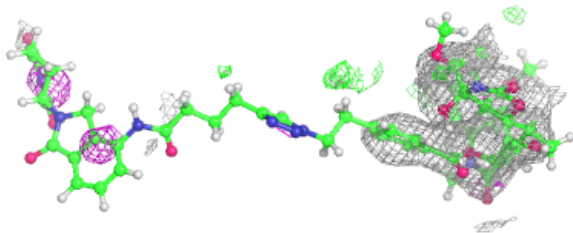
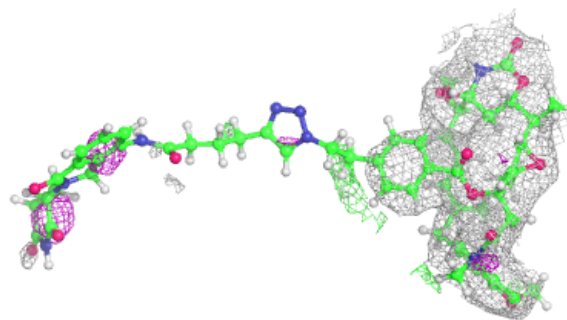
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	C	501	32/32	0.97	0.07	42,48,51,52	0
8	GDP	B	501	28/28	0.97	0.07	44,51,56,58	0
6	MG	B	502	1/1	0.99	0.03	43,43,43,43	0
7	CA	C	503	1/1	0.99	0.04	74,74,74,74	0
6	MG	C	502	1/1	1.00	0.03	48,48,48,48	0
6	MG	A	502	1/1	1.00	0.04	53,53,53,53	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.

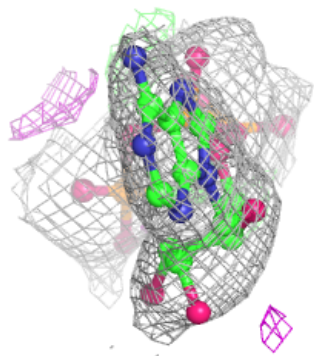
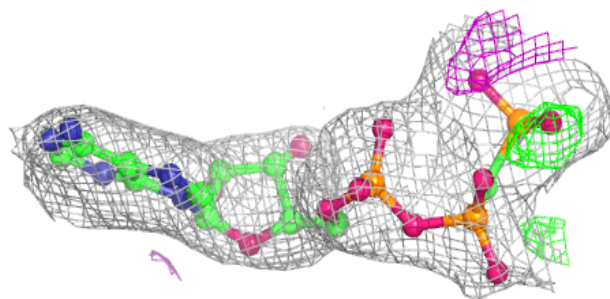
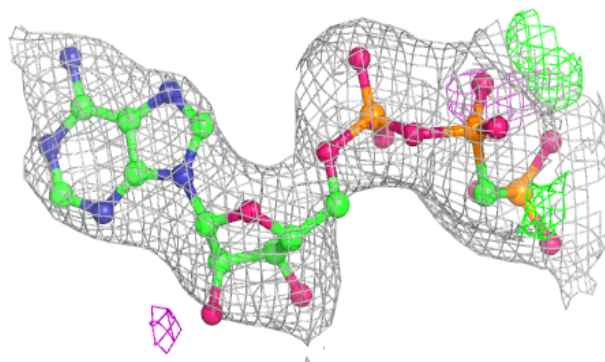
Electron density around A1ISD D 503:

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



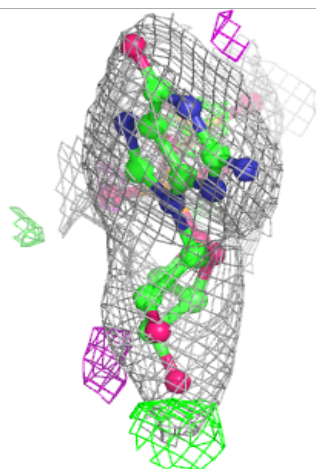
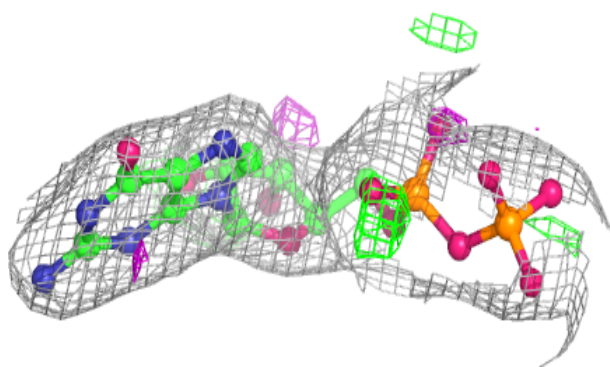
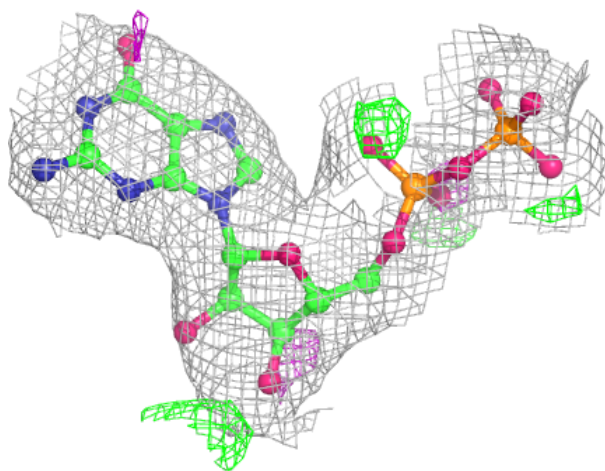
Electron density around ACP F 401:

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



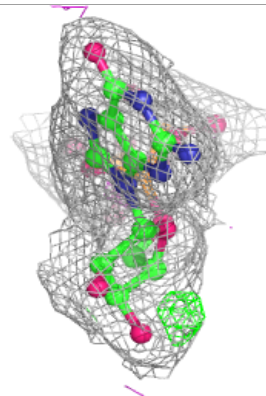
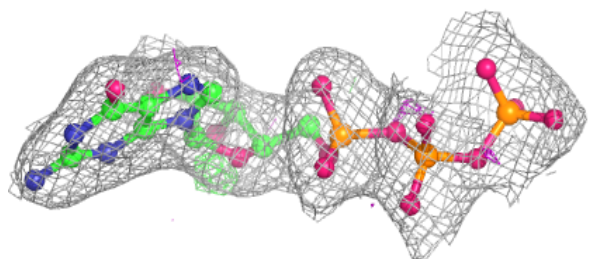
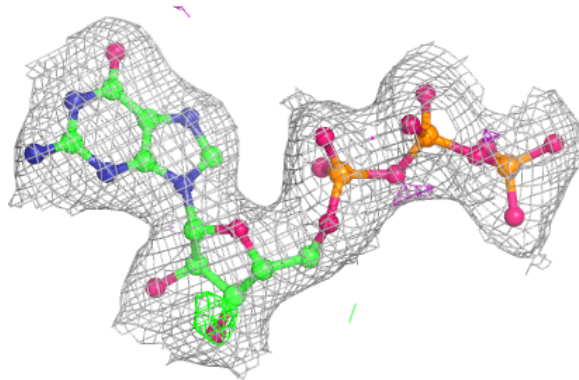
Electron density around GDP D 501:

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

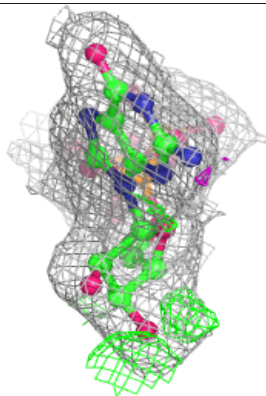
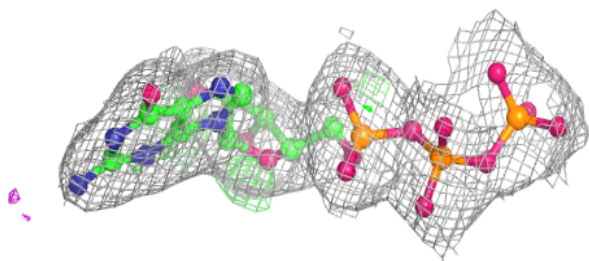
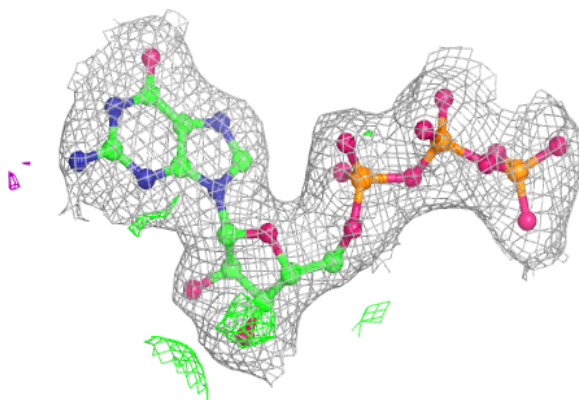


Electron density around GTP A 501:

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

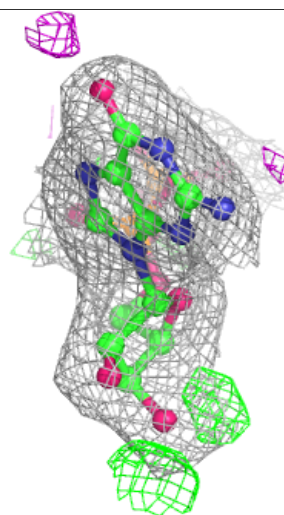
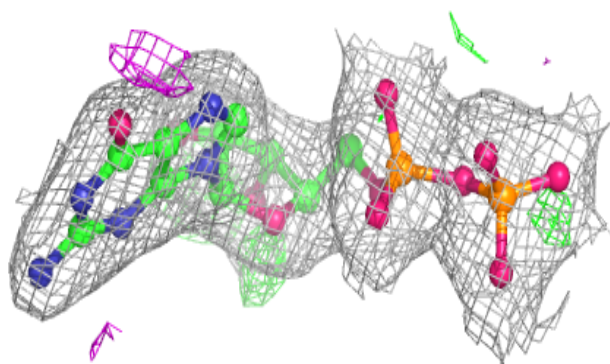
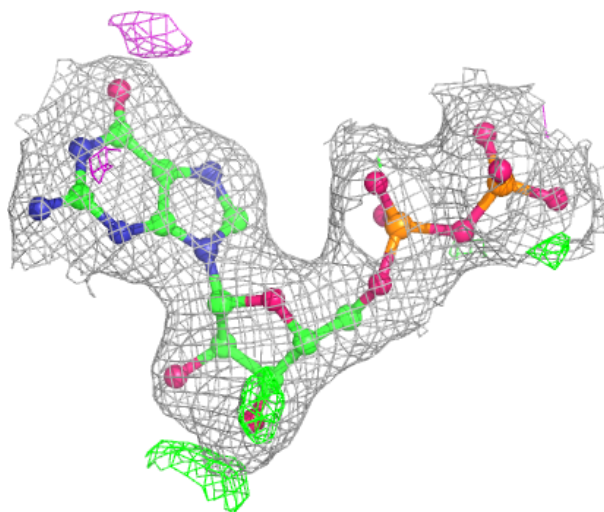
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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.