



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:10 AM UTC

PDB ID : 5S5Y / pdb_00005s5y
Title : Tubulin-Z26781952-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

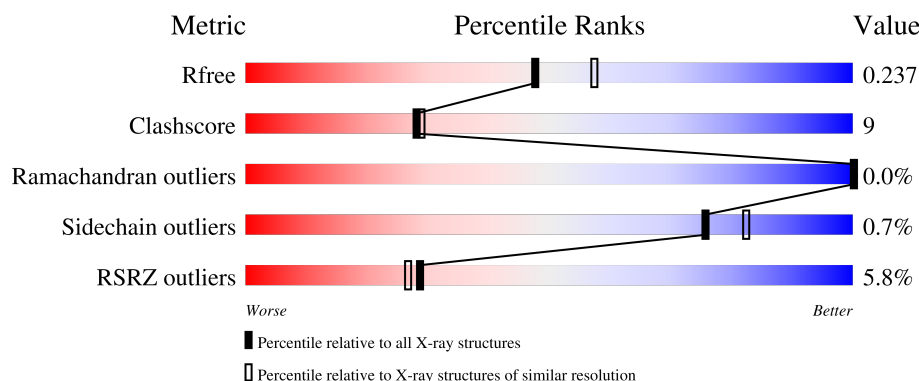
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	4% 78% 19% .
1	C	451	4% 78% 20% .
2	B	445	5% 76% 19% .
2	D	445	6% 75% 22% .
3	E	143	9% 73% 13% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	8% 72% 19% 9%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18024 atoms, of which 15 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	425	Total	C	N	O	S	2	0	0
			3348	2103	573	645	27			
2	D	428	Total	C	N	O	S	5	0	0
			3353	2104	572	650	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

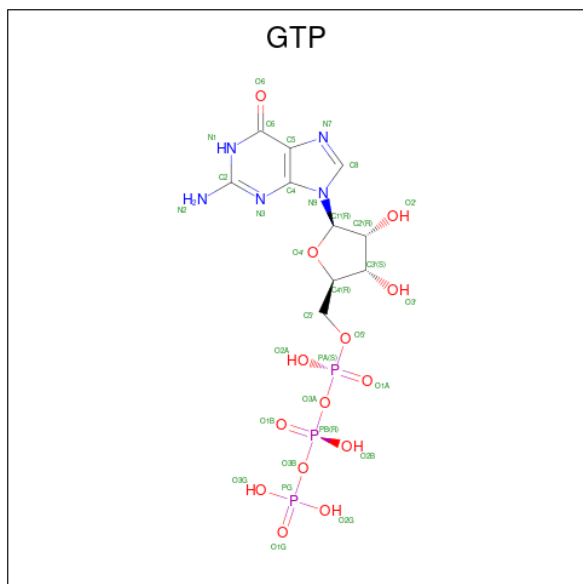
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2863	1835	492	522	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 (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		

Continued on next page...

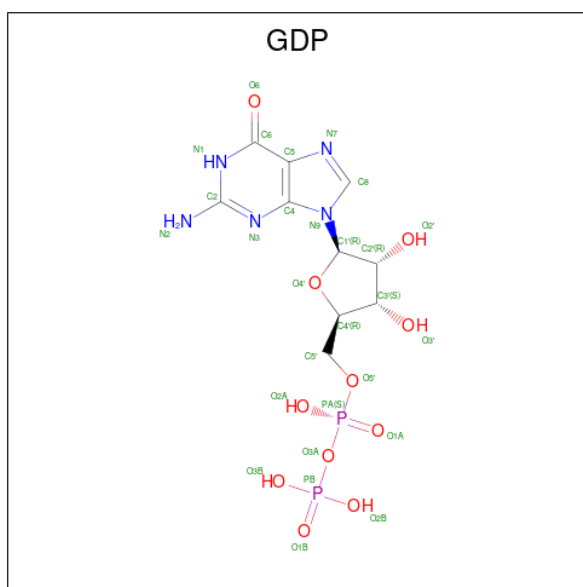
Continued from previous page...

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).

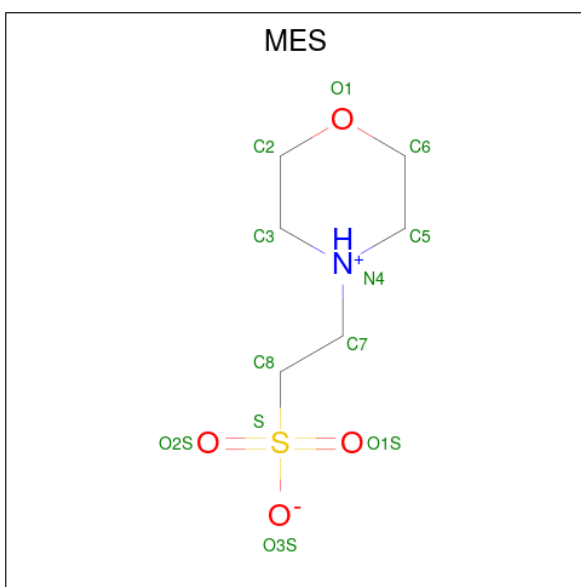
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



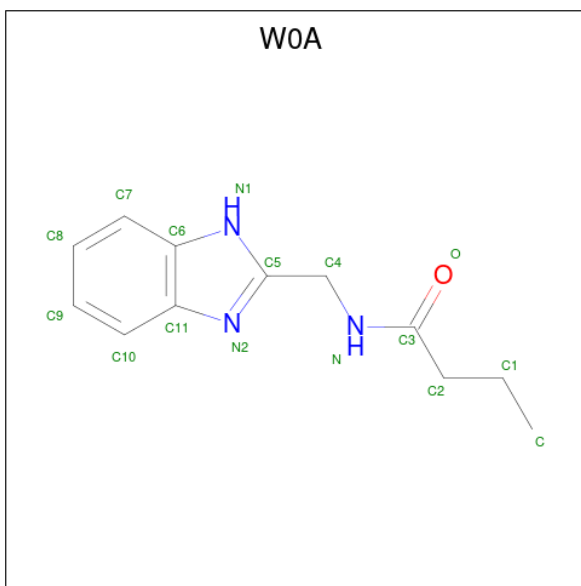
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



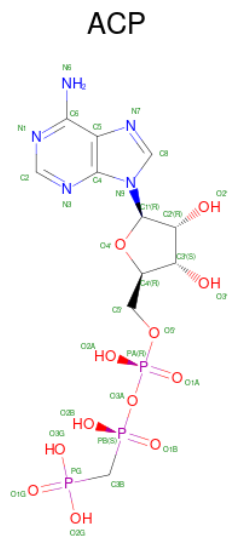
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is N-[(1H-benzimidazol-2-yl)methyl]butanamide (CCD ID: W0A) (formula: $C_{12}H_{15}N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	H	N	O	0	0
			31	12	15	3	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: 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

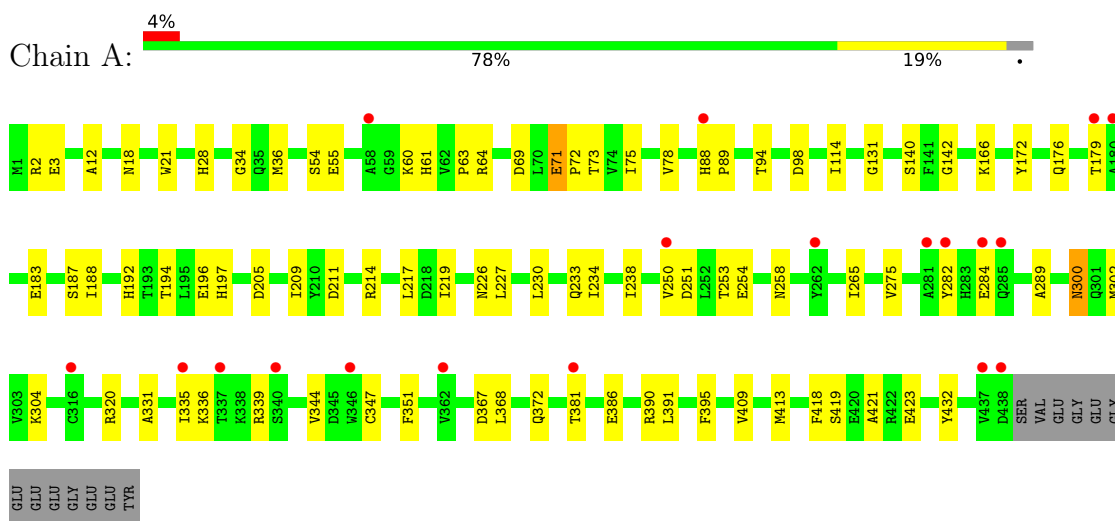
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	61	Total O 61 61	0	0
12	B	82	Total O 82 82	0	0
12	C	186	Total O 186 186	0	0
12	D	27	Total O 27 27	0	0
12	E	8	Total O 8 8	0	0
12	F	12	Total O 12 12	0	0

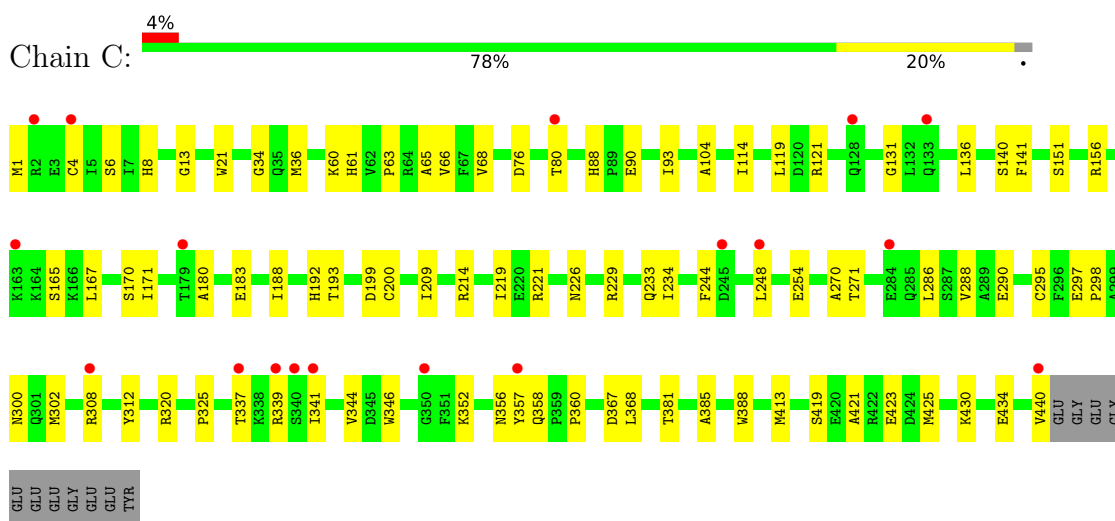
3 Residue-property plots [i](#)

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.

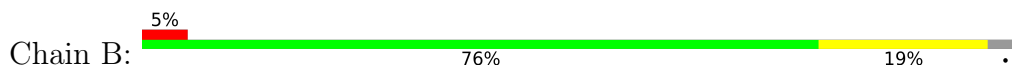
- Molecule 1: Tubulin alpha-1B chain

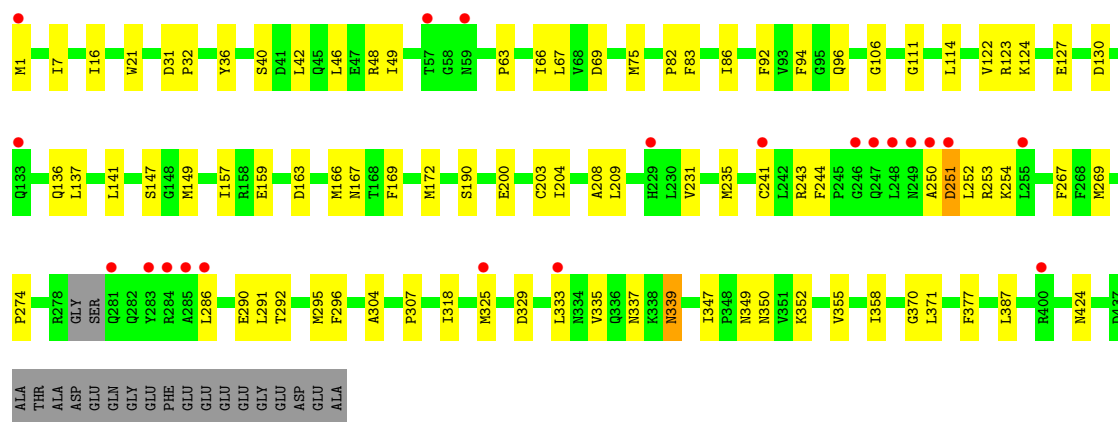


- Molecule 1: Tubulin alpha-1B chain

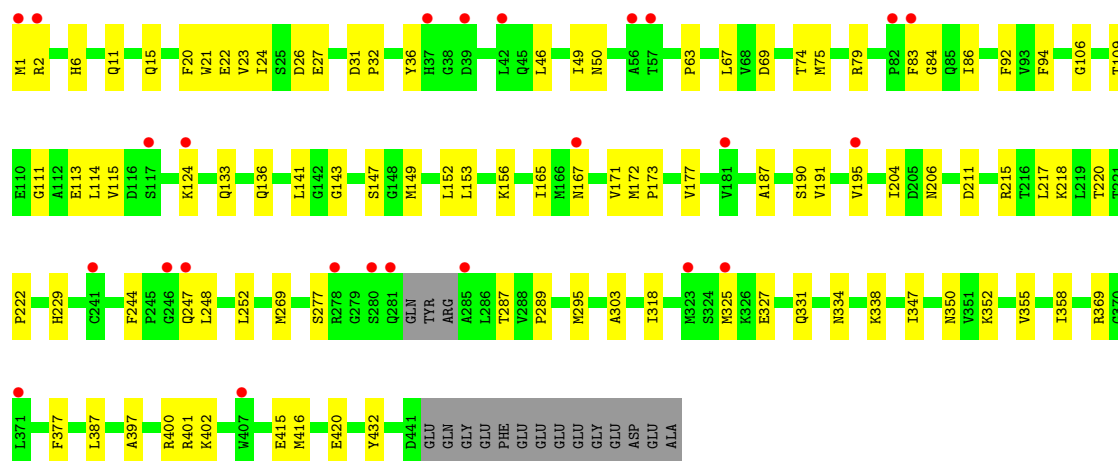
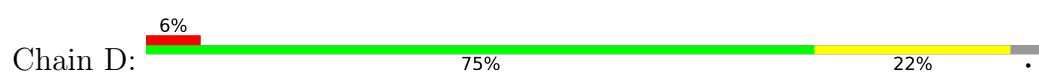


- Molecule 2: Tubulin beta-2B chain

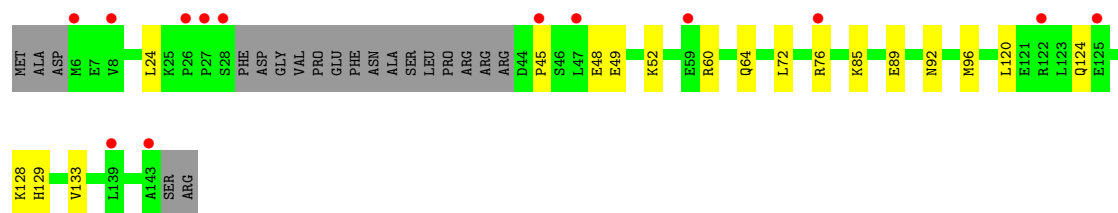
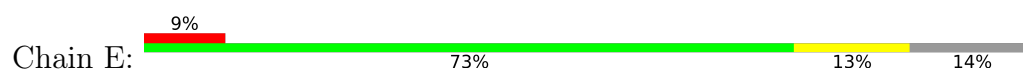




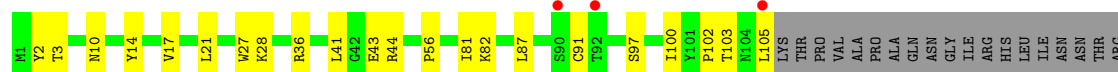
• Molecule 2: Tubulin beta-2B chain

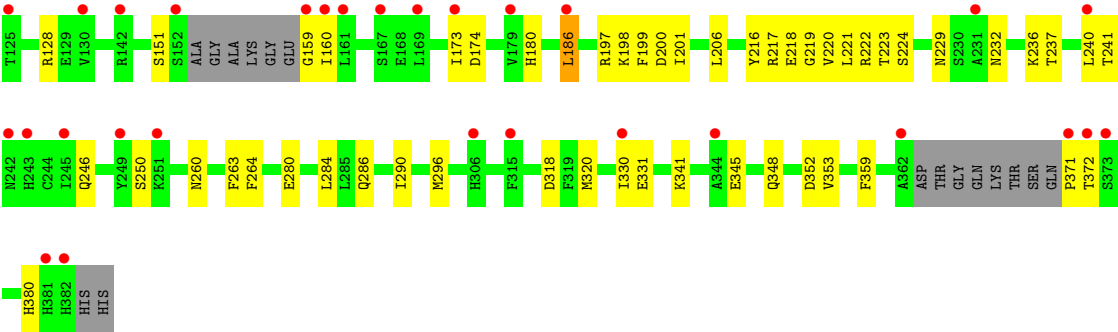


• Molecule 3: Stathmin-4



• 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	104.96Å 158.75Å 179.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.31 – 2.26 63.31 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.31-2.26) 99.9 (63.31-2.26)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.202 , 0.231 0.207 , 0.237	Depositor DCC
R_{free} test set	6901 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18024	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, W0A, GTP, MES, ACP, CA, GDP

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	0.11	0/3502	0.28	0/4754
1	C	0.14	0/3521	0.32	0/4780
2	B	0.12	0/3422	0.29	0/4633
2	D	0.10	0/3426	0.27	0/4640
3	E	0.10	0/1022	0.23	0/1356
4	F	0.09	0/2930	0.27	0/3959
All	All	0.11	0/17823	0.28	0/24122

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	63	1
1	C	3443	0	3352	53	1
2	B	3348	0	3223	64	0
2	D	3353	0	3229	70	0
3	E	1014	0	1029	13	0
4	F	2863	0	2826	56	0
5	A	32	0	12	1	0

Continued on next page...

Continued from previous page...

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	0	0
8	D	28	0	12	1	0
9	B	12	0	12	0	0
10	C	16	15	0	0	0
11	F	31	0	14	3	0
12	A	61	0	0	2	0
12	B	82	0	0	2	0
12	C	186	0	0	3	0
12	D	27	0	0	2	0
12	E	8	0	0	0	0
12	F	12	0	0	1	0
All	All	18009	15	17067	309	1

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 9.

All (309) 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)
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.57	0.85
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.60	0.84
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.43	0.83
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.62	0.82
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.62	0.81
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.98	0.80
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.63	0.79
2:D:397:ALA:O	2:D:401:ARG:NH1	2.16	0.78
1:C:76:ASP:O	1:C:80:THR:HG22	1.84	0.78
2:B:83:PHE:O	2:B:86:ILE:HG22	1.85	0.76
1:A:179:THR:HA	2:B:352:LYS:HD2	1.68	0.75
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.69	0.74
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.22	0.73
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.71	0.72
2:D:83:PHE:O	2:D:86:ILE:HG22	1.88	0.72
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.72	0.71
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.05	0.71
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.56	0.70
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.72	0.69
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.75	0.69
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.67
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.94	0.67
2:B:241:CYS:HB3	2:B:250:ALA:CB	2.24	0.67
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.78	0.66
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.31	0.65
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.14	0.65
1:C:270:ALA:O	1:C:302:MET:HG2	1.96	0.65
1:A:28:HIS:O	1:A:36:MET:HE3	1.96	0.65
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.79	0.65
4:F:371:PRO:HA	4:F:372:THR:O	1.98	0.64
2:D:432:TYR:OH	12:D:601:HOH:O	2.14	0.64
2:D:325:MET:HE2	2:D:355:VAL:HG21	1.80	0.64
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.80	0.63
1:A:214:ARG:HG2	1:A:219:ILE:O	1.98	0.63
2:B:424:ASN:HB3	12:B:602:HOH:O	1.97	0.63
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.34	0.63
2:D:215:ARG:O	2:D:218:LYS:HE3	1.99	0.63
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.62
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.62
4:F:371:PRO:HA	4:F:372:THR:HB	1.80	0.62
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.80	0.62
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.30	0.61
2:B:69:ASP:O	2:B:94:PHE:HA	2.01	0.60
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.35	0.60
4:F:159:GLY:C	4:F:160:ILE:HD12	2.27	0.60
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.32	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.02	0.59
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.19	0.59
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.67	0.59
1:C:209:ILE:HD11	1:C:302:MET:CE	2.31	0.59
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.03	0.59
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.18	0.59
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.38	0.59
2:B:141:LEU:HD12	2:B:172:MET:SD	2.43	0.58
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.85	0.58
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.33	0.58
3:E:72:LEU:O	3:E:76:ARG:HG2	2.04	0.58
4:F:371:PRO:HA	4:F:372:THR:C	2.27	0.58
2:D:217:LEU:HA	2:D:277:SER:HB3	1.86	0.58
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.14	0.58
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.04	0.58
4:F:371:PRO:CA	4:F:372:THR:HB	2.34	0.57
2:D:327:GLU:O	2:D:331:GLN:HG2	2.03	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.03	0.57
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.19	0.57
1:A:300:ASN:HB3	12:A:602:HOH:O	2.04	0.57
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.86	0.57
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.57
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.04	0.57
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.40	0.56
1:C:419:SER:O	1:C:423:GLU:HG3	2.05	0.56
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.38	0.56
2:B:124:LYS:HD3	2:B:124:LYS:C	2.30	0.56
1:A:209:ILE:HD11	1:A:302:MET:SD	2.45	0.56
2:B:169:PHE:CD1	2:B:235:MET:HE3	2.40	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.40	0.56
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.41	0.56
4:F:91:CYS:HA	12:F:511:HOH:O	2.04	0.56
2:B:167:ASN:OD1	2:B:200:GLU:HB2	2.05	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.88	0.56
1:C:234:ILE:HG12	1:C:302:MET:CE	2.35	0.56
1:C:180:ALA:O	1:C:183:GLU:HG3	2.05	0.56
2:D:106:GLY:O	2:D:111:GLY:HA3	2.06	0.55
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.88	0.55
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.42	0.55
2:D:152:LEU:O	2:D:156:LYS:HG2	2.05	0.55
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.06	0.55
4:F:246:GLN:O	4:F:250:SER:HB3	2.06	0.55
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.89	0.55
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.07	0.55
2:B:96:GLN:CB	1:C:1:MET:HE2	2.37	0.55
2:D:124:LYS:C	2:D:124:LYS:HD3	2.31	0.55
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.89	0.54
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.90	0.54
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.42	0.54
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.90	0.53
1:A:187:SER:CB	1:A:391:LEU:HD21	2.37	0.53
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.89	0.53
2:D:11:GLN:HA	2:D:74:THR:HG21	1.91	0.53
1:C:271:THR:HG21	1:C:295:CYS:O	2.09	0.52
2:D:187:ALA:O	2:D:191:VAL:HG23	2.09	0.52
2:B:123:ARG:O	2:B:127:GLU:HG3	2.09	0.52
2:B:147:SER:HG	2:B:190:SER:HG	1.57	0.52
2:D:318:ILE:HG12	12:D:611:HOH:O	2.08	0.52
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.41	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.51
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.92	0.51
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.51
1:A:320:ARG:HD2	12:A:652:HOH:O	2.11	0.51
2:B:251:ASP:O	2:B:254:LYS:N	2.44	0.51
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.45	0.51
2:D:67:LEU:N	2:D:67:LEU:HD12	2.25	0.51
3:E:92:ASN:O	3:E:96:MET:HG2	2.11	0.51
2:B:295:MET:CG	2:B:377:PHE:HB2	2.40	0.51
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.75	0.51
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.92	0.51
2:D:69:ASP:O	2:D:94:PHE:HA	2.11	0.50
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.11	0.50
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.47	0.50
2:B:82:PRO:O	12:B:601:HOH:O	2.20	0.50
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.93	0.50
2:B:46:LEU:HA	2:B:49:ILE:HB	1.93	0.50
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.93	0.50
1:A:54:SER:O	1:A:61:HIS:HA	2.11	0.50
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.93	0.50
2:D:1:MET:HE2	2:D:50:ASN:CB	2.38	0.50
2:D:1:MET:HG3	2:D:50:ASN:CB	2.42	0.50
2:D:220:THR:O	2:D:222:PRO:HD3	2.10	0.50
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.47	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.50
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.46	0.50
1:C:165:SER:HA	1:C:199:ASP:OD2	2.12	0.50
3:E:129:HIS:O	3:E:133:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.12	0.49
1:C:214:ARG:HG2	1:C:219:ILE:O	2.12	0.49
2:D:211:ASP:O	2:D:215:ARG:HB2	2.13	0.49
2:B:40:SER:OG	2:B:42:LEU:HD13	2.13	0.49
2:D:191:VAL:O	2:D:195:VAL:HG23	2.12	0.49
2:D:387:LEU:HD23	2:D:387:LEU:C	2.36	0.49
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.41	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.49
3:E:120:LEU:O	3:E:124:GLN:HG3	2.13	0.49
2:D:1:MET:CE	2:D:50:ASN:HB2	2.38	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.49
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.95	0.49
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.94	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.12	0.49
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.95	0.48
2:B:387:LEU:C	2:B:387:LEU:HD23	2.38	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.48
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.24	0.48
3:E:60:ARG:O	3:E:64:GLN:HG3	2.13	0.48
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.94	0.48
2:D:46:LEU:HA	2:D:49:ILE:HB	1.95	0.48
2:D:114:LEU:HD23	2:D:149:MET:HE1	1.95	0.48
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.48	0.48
1:A:419:SER:O	1:A:423:GLU:HG3	2.13	0.48
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.43	0.48
2:B:329:ASP:O	2:B:333:LEU:HG	2.14	0.48
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.94	0.48
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.96	0.48
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.79	0.48
2:B:163:ASP:O	2:B:253:ARG:NH1	2.46	0.48
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.43	0.48
4:F:371:PRO:HA	4:F:372:THR:CB	2.42	0.48
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.49	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.14	0.47
2:B:318:ILE:N	2:B:318:ILE:HD12	2.29	0.47
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.96	0.47
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.96	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.95	0.47
2:B:169:PHE:CE1	2:B:235:MET:HE3	2.50	0.47
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.30	0.47
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.46
2:B:231:VAL:O	2:B:235:MET:HG3	2.15	0.46
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.97	0.46
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.42	0.46
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.44	0.46
4:F:17:VAL:O	4:F:21:LEU:HG	2.16	0.46
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.96	0.46
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.15	0.46
1:A:284:GLU:CD	1:A:284:GLU:H	2.24	0.46
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.51	0.46
1:C:229:ARG:NH1	12:C:706:HOH:O	2.49	0.46
1:A:409:VAL:HA	1:A:413:MET:O	2.16	0.46
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.98	0.46
2:B:48:ARG:HB2	2:B:243:ARG:O	2.16	0.45
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.16	0.45
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.34	0.45
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.98	0.45
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.98	0.45
1:C:440:VAL:HG12	1:C:440:VAL:O	2.15	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.51	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.52	0.45
4:F:237:THR:O	4:F:246:GLN:NE2	2.44	0.45
1:A:55:GLU:HA	1:A:60:LYS:O	2.17	0.45
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.16	0.45
2:B:325:MET:HE2	2:B:355:VAL:HG11	1.99	0.45
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.99	0.45
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.45
4:F:320:MET:CG	4:F:330:ILE:HD11	2.47	0.45
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.47	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.44
2:D:23:VAL:O	2:D:27:GLU:HG3	2.17	0.44
1:C:8:HIS:HB3	1:C:13:GLY:O	2.17	0.44
2:D:416:MET:O	2:D:420:GLU:HG3	2.17	0.44
2:B:7:ILE:O	2:B:137:LEU:HD12	2.18	0.44
1:A:12:ALA:CB	1:A:140:SER:HB3	2.48	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.44
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.53	0.44
1:A:289:ALA:HA	1:A:331:ALA:CB	2.48	0.44
4:F:197:ARG:HB2	4:F:224:SER:O	2.18	0.44
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:296:MET:SD	4:F:380:HIS:HB2	2.57	0.44
1:A:166:LYS:HE2	1:A:197:HIS:O	2.18	0.44
1:C:66:VAL:HG12	1:C:68:VAL:HG23	2.00	0.44
1:C:288:VAL:HG23	12:C:835:HOH:O	2.16	0.44
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.16	0.44
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.53	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.46	0.43
2:B:335:VAL:O	2:B:339:ASN:ND2	2.51	0.43
2:D:11:GLN:O	2:D:15:GLN:HG2	2.18	0.43
2:D:220:THR:C	2:D:222:PRO:HD3	2.43	0.43
2:B:370:GLY:O	2:B:371:LEU:HD23	2.18	0.43
2:D:147:SER:HB2	2:D:190:SER:OG	2.18	0.43
2:B:159:GLU:HB2	3:E:72:LEU:HD13	2.01	0.43
1:C:1:MET:HE3	1:C:131:GLY:HA3	2.01	0.43
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.54	0.43
4:F:222:ARG:O	4:F:241:THR:HB	2.18	0.43
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.43
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.91	0.43
1:C:234:ILE:HD12	1:C:234:ILE:N	2.34	0.43
3:E:85:LYS:O	3:E:89:GLU:HG3	2.18	0.43
4:F:198:LYS:HG2	4:F:199:PHE:H	1.84	0.43
2:B:42:LEU:N	2:B:42:LEU:HD12	2.34	0.42
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.54	0.42
2:D:173:PRO:HG3	2:D:187:ALA:HB2	2.01	0.42
4:F:3:THR:HA	4:F:28:LYS:O	2.18	0.42
4:F:206:LEU:HD23	4:F:353:VAL:CG2	2.49	0.42
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.49	0.42
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.01	0.42
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.50	0.42
2:D:248:LEU:HD21	2:D:352:LYS:HB3	2.01	0.42
1:A:114:ILE:HG12	1:A:114:ILE:O	2.20	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.20	0.42
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.42
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.54	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.83	0.42
2:D:79:ARG:O	2:D:84:GLY:HA3	2.20	0.42
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.20	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.42
1:C:320:ARG:HG3	1:C:360:PRO:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.55	0.42
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.41
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.54	0.41
2:D:141:LEU:HD12	2:D:172:MET:SD	2.60	0.41
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.20	0.41
2:B:349:ASN:O	2:B:352:LYS:HE2	2.21	0.41
1:C:104:ALA:HB2	1:C:413:MET:SD	2.60	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.41
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.03	0.41
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.02	0.41
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.21	0.41
2:B:251:ASP:O	2:B:252:LEU:C	2.62	0.41
2:D:109:THR:O	2:D:113:GLU:HG2	2.20	0.41
2:D:177:VAL:HG21	2:D:206:ASN:HB3	2.02	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.56	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.61	0.41
1:C:325:PRO:HD2	12:C:807:HOH:O	2.21	0.41
4:F:160:ILE:HD12	4:F:160:ILE:N	2.35	0.41
4:F:229:ASN:ND2	4:F:232:ASN:HB3	2.36	0.41
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.43	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.41
1:A:386:GLU:O	1:A:390:ARG:HG3	2.21	0.41
4:F:223:THR:O	4:F:260:ASN:HB3	2.21	0.41
4:F:341:LYS:HG2	4:F:341:LYS:O	2.21	0.41
2:B:1:MET:HB2	2:B:130:ASP:OD2	2.21	0.41
2:B:67:LEU:HD12	2:B:67:LEU:N	2.36	0.41
1:C:151:SER:HB2	1:C:193:THR:CG2	2.51	0.41
2:D:2:ARG:HB3	2:D:133:GLN:HG3	2.01	0.41
4:F:2:TYR:HB3	4:F:27:TRP:CZ3	2.55	0.41
4:F:240:LEU:HD12	4:F:240:LEU:N	2.36	0.41
1:A:2:ARG:HB3	1:A:131:GLY:O	2.20	0.41
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.56	0.41
1:A:234:ILE:O	1:A:238:ILE:HG13	2.21	0.40
1:C:192:HIS:CG	1:C:421:ALA:HA	2.56	0.40
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.54	0.40
4:F:186:LEU:HD12	4:F:320:MET:HB3	2.04	0.40
4:F:286:GLN:O	4:F:290:ILE:HG13	2.21	0.40
1:A:194:THR:O	1:A:194:THR:HG22	2.20	0.40
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.43	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.03	0.40
1:A:251:ASP:OD1	1:A:253:THR:HB	2.22	0.40
1:C:6:SER:O	1:C:65:ALA:HA	2.21	0.40
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.03	0.40
1:C:297:GLU:HB3	1:C:300:ASN:HD22	1.85	0.40
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.56	0.40
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.52	0.40
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.57	0.40
4:F:82:LYS:NZ	4:F:97:SER:O	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:NE2	1:C:337:THR:O[3_555]	2.16	0.04

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%)	422 (97%)	14 (3%)	0	100	100
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	421/445 (95%)	406 (96%)	15 (4%)	0	100	100
2	D	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	341/384 (89%)	327 (96%)	13 (4%)	1 (0%)	36	40
All	All	2180/2319 (94%)	2114 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	186	LEU

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%)	365 (99%)	4 (1%)	65	75
1	C	372/379 (98%)	370 (100%)	2 (0%)	81	87
2	B	367/383 (96%)	364 (99%)	3 (1%)	73	80
2	D	368/383 (96%)	366 (100%)	2 (0%)	81	87
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	79
4	F	315/342 (92%)	314 (100%)	1 (0%)	86	90
All	All	1901/1993 (95%)	1888 (99%)	13 (1%)	76	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	282	TYR
1	A	300	ASN
1	A	381	THR
2	B	251	ASP
2	B	291	LEU
2	B	339	ASN
1	C	339	ARG
1	C	381	THR
2	D	229	HIS
2	D	247	GLN
3	E	128	LYS
4	F	43	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	HIS
1	A	101	ASN
1	A	301	GLN
2	B	15	GLN
2	B	167	ASN
2	B	192	HIS
2	B	193	GLN
2	B	282	GLN
2	B	294	GLN
2	B	331	GLN
2	B	349	ASN
2	B	434	GLN
1	C	11	GLN
1	C	256	GLN
1	C	300	ASN
1	C	309	HIS
2	D	294	GLN
2	D	331	GLN
3	E	115	HIS
3	E	136	ASN
4	F	196	HIS
4	F	269	GLN
4	F	306	HIS
4	F	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
9	MES	B	504	-	12,12,12	2.31	1 (8%)	15,16,16	1.93	3 (20%)
11	ACP	F	401	6	31,33,33	1.67	8 (25%)	47,52,52	1.87	10 (21%)
8	GDP	D	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
10	W0A	C	601	-	17,17,17	1.36	1 (5%)	21,22,22	1.20	1 (4%)
8	GDP	B	501	6	29,30,30	1.10	3 (10%)	45,47,47	1.72	7 (15%)
5	GTP	C	602	6	33,34,34	0.97	3 (9%)	50,54,54	1.51	8 (16%)
5	GTP	A	501	6	33,34,34	0.99	3 (9%)	50,54,54	1.53	8 (16%)

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
9	MES	B	504	-	-	5/6/14/14	0/1/1/1
11	ACP	F	401	6	-	11/19/38/38	0/3/3/3
8	GDP	D	501	6	-	6/16/32/32	0/3/3/3
10	W0A	C	601	-	-	0/8/8/8	0/2/2/2
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	602	6	-	9/22/38/38	0/3/3/3
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.72	1.66	1.77
11	F	401	ACP	C5-C4	4.76	1.47	1.39
10	C	601	W0A	C5-N2	3.55	1.38	1.32
8	D	501	GDP	C5-C4	3.13	1.47	1.38
8	B	501	GDP	C5-C4	2.99	1.46	1.38
11	F	401	ACP	PG-O3G	2.98	1.61	1.55
11	F	401	ACP	PG-O2G	2.98	1.61	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	2.70	1.61	1.58
11	F	401	ACP	C5-C6	2.66	1.48	1.41
5	A	501	GTP	PA-O3A	2.37	1.62	1.59
5	C	602	GTP	PA-O3A	2.35	1.62	1.59
8	D	501	GDP	C6-N1	-2.34	1.34	1.38
11	F	401	ACP	C8-N7	2.29	1.36	1.31
11	F	401	ACP	C5-N7	-2.25	1.35	1.39
5	A	501	GTP	PB-O3B	2.23	1.61	1.59
8	B	501	GDP	C6-N1	-2.19	1.34	1.38
11	F	401	ACP	PB-O2B	2.15	1.61	1.56
5	C	602	GTP	C2-N3	2.14	1.38	1.33
8	B	501	GDP	C5-N7	-2.09	1.34	1.39
5	C	602	GTP	PB-O3B	2.04	1.61	1.59
5	A	501	GTP	C2-N3	2.00	1.38	1.33
8	D	501	GDP	C5-N7	-2.00	1.35	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.03	118.79	128.39
11	F	401	ACP	C5-C4-N3	-5.83	118.69	126.72
8	B	501	GDP	C5-C4-N3	-5.68	119.34	128.39
9	B	504	MES	C5-N4-C3	5.27	120.19	108.84
8	B	501	GDP	C2-N3-C4	5.11	121.10	112.30
8	D	501	GDP	C2-N3-C4	5.05	120.99	112.30
5	C	602	GTP	C5-C4-N3	-4.73	120.86	128.39
11	F	401	ACP	N3-C4-N9	4.64	135.06	127.17
5	A	501	GTP	C2-N3-C4	4.62	120.25	112.30
5	A	501	GTP	C5-C4-N3	-4.60	121.07	128.39
8	D	501	GDP	N9-C4-N3	4.41	134.77	125.95
5	C	602	GTP	C2-N3-C4	4.39	119.87	112.30
8	B	501	GDP	N9-C4-N3	4.34	134.64	125.95
11	F	401	ACP	PB-O3A-PA	-3.95	119.48	132.37
11	F	401	ACP	C2-N3-C4	3.63	120.69	111.83
11	F	401	ACP	C4-C5-N7	-3.40	106.69	110.58
8	B	501	GDP	C6-C5-N7	3.40	136.47	130.29
8	D	501	GDP	C6-C5-N7	3.37	136.43	130.29
11	F	401	ACP	N3-C2-N1	-3.11	123.87	128.58
5	C	602	GTP	N9-C4-N3	3.03	132.01	125.95
5	A	501	GTP	N9-C8-N7	-2.84	108.14	113.40
5	C	602	GTP	C2-N1-C6	-2.83	119.98	125.11
5	C	602	GTP	N9-C8-N7	-2.81	108.19	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N9-C4-N3	2.76	131.47	125.95
5	A	501	GTP	C2-N1-C6	-2.72	120.18	125.11
9	B	504	MES	O1S-S-C8	2.68	110.78	106.73
11	F	401	ACP	C3'-C2'-C1'	2.64	106.47	101.46
8	D	501	GDP	C4-C5-N7	-2.64	106.49	110.67
10	C	601	W0A	N1-C5-N2	-2.62	109.53	112.72
8	B	501	GDP	O6-C6-C5	-2.59	119.70	126.53
11	F	401	ACP	C4-N9-C8	2.58	108.45	105.74
5	C	602	GTP	C8-N7-C5	2.57	108.85	104.26
5	A	501	GTP	C8-N7-C5	2.55	108.80	104.26
11	F	401	ACP	C5-N7-C8	2.47	107.33	103.45
5	A	501	GTP	C5-C6-N1	2.44	119.47	113.25
5	C	602	GTP	C5-C6-N1	2.38	119.30	113.25
5	C	602	GTP	O6-C6-C5	-2.32	120.40	126.53
8	B	501	GDP	C4-C5-N7	-2.31	107.01	110.67
5	A	501	GTP	O6-C6-C5	-2.31	120.45	126.53
9	B	504	MES	O2S-S-C8	2.28	110.17	106.73
8	D	501	GDP	O6-C6-C5	-2.17	120.81	126.53
8	B	501	GDP	C5-C6-N1	2.02	118.40	113.25
11	F	401	ACP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	602	GTP	C5'-O5'-PA-O3A
5	C	602	GTP	C5'-O5'-PA-O1A
5	C	602	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O2S
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-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	504	MES	C8-C7-N4-C3
9	B	504	MES	C7-C8-S-O1S
8	D	501	GDP	PA-O3A-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
9	B	504	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O1G
5	C	602	GTP	PB-O3B-PG-O1G
5	C	602	GTP	C4'-C5'-O5'-PA
5	C	602	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	602	GTP	PB-O3B-PG-O2G
5	C	602	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	602	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O1A

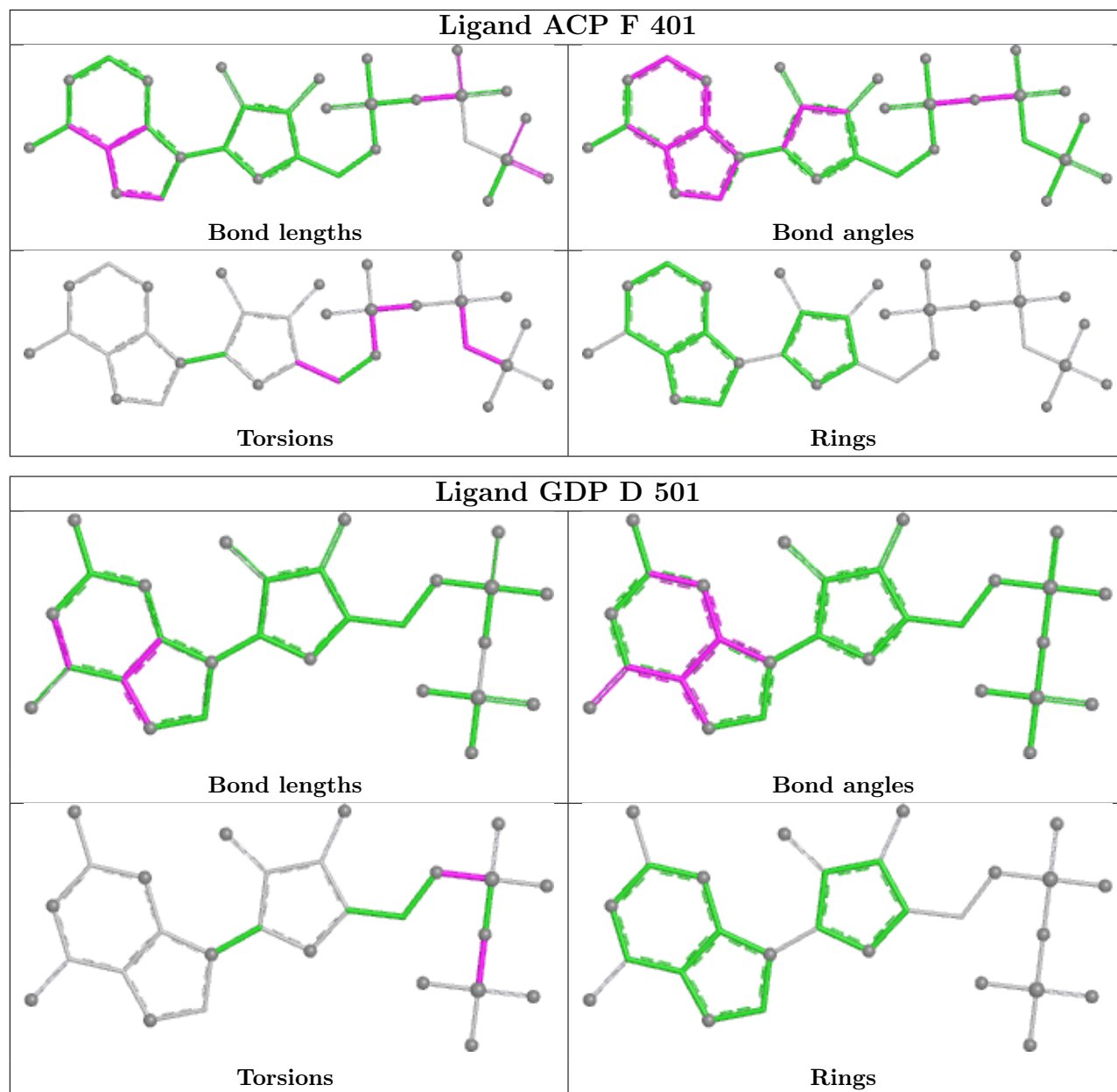
There are no ring outliers.

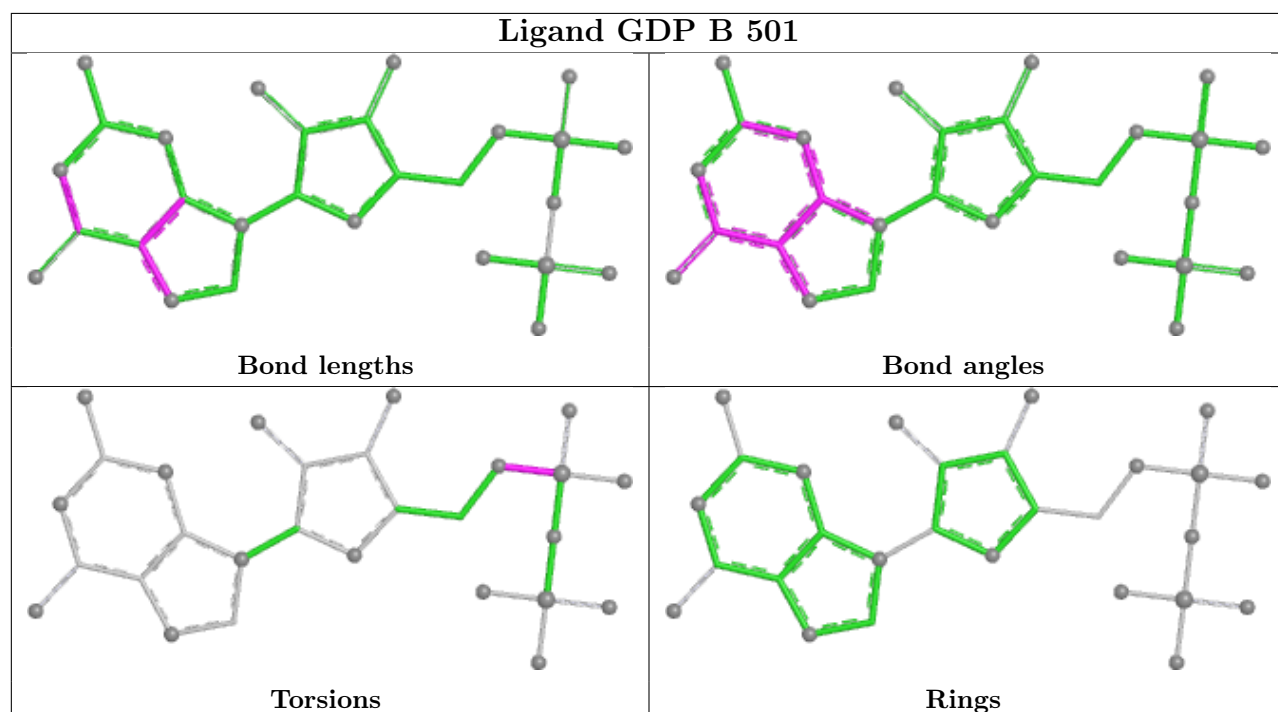
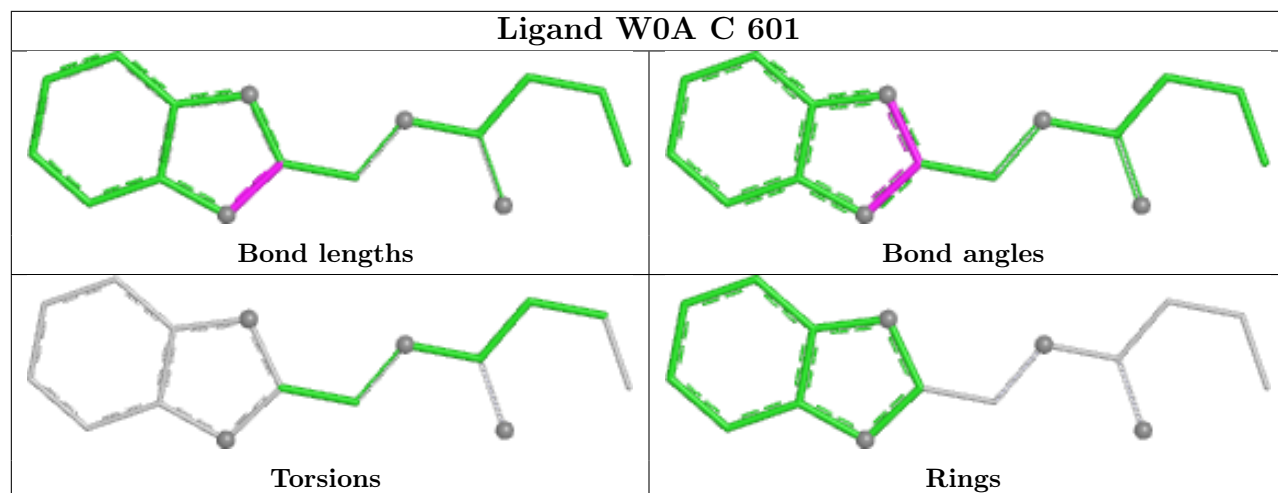
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	3	0
8	D	501	GDP	1	0
5	A	501	GTP	1	0

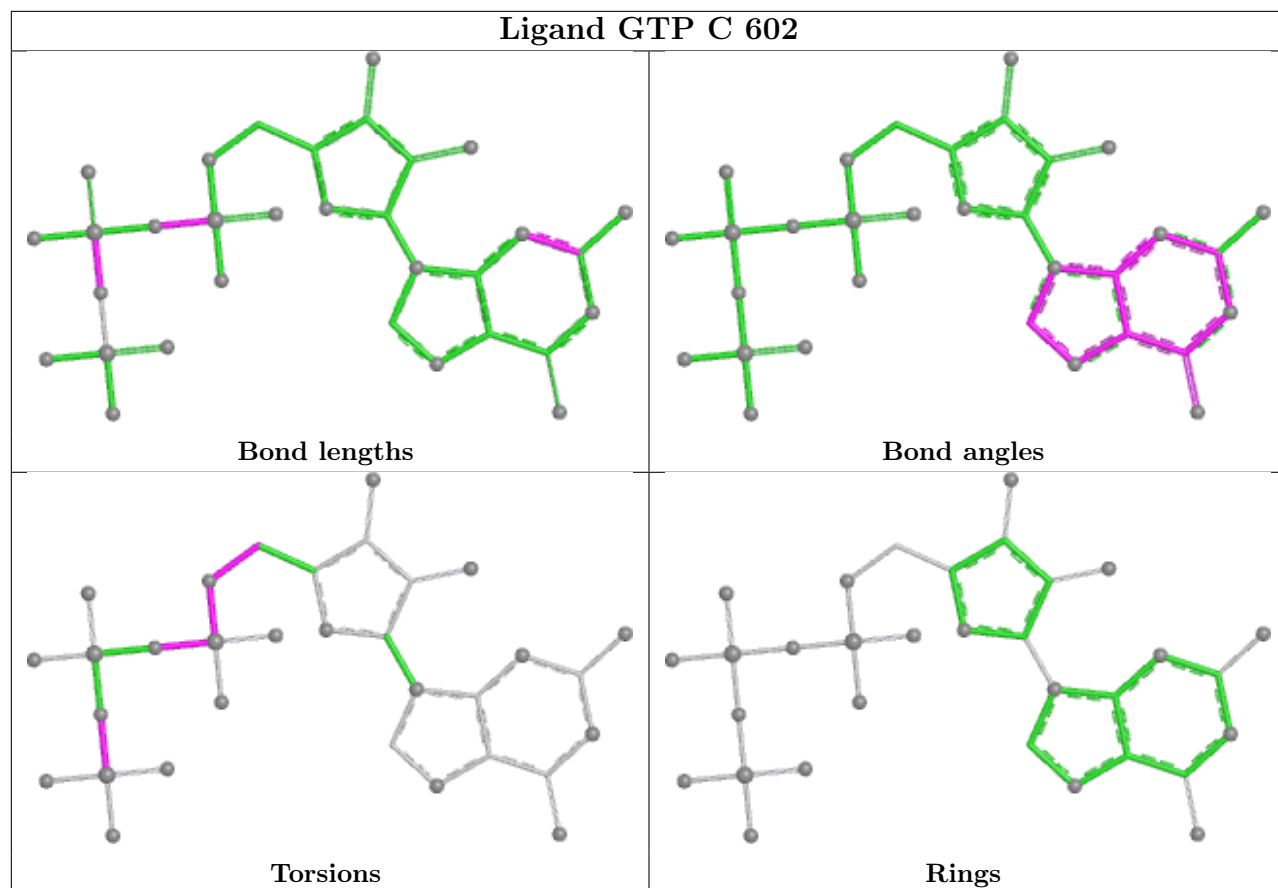
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

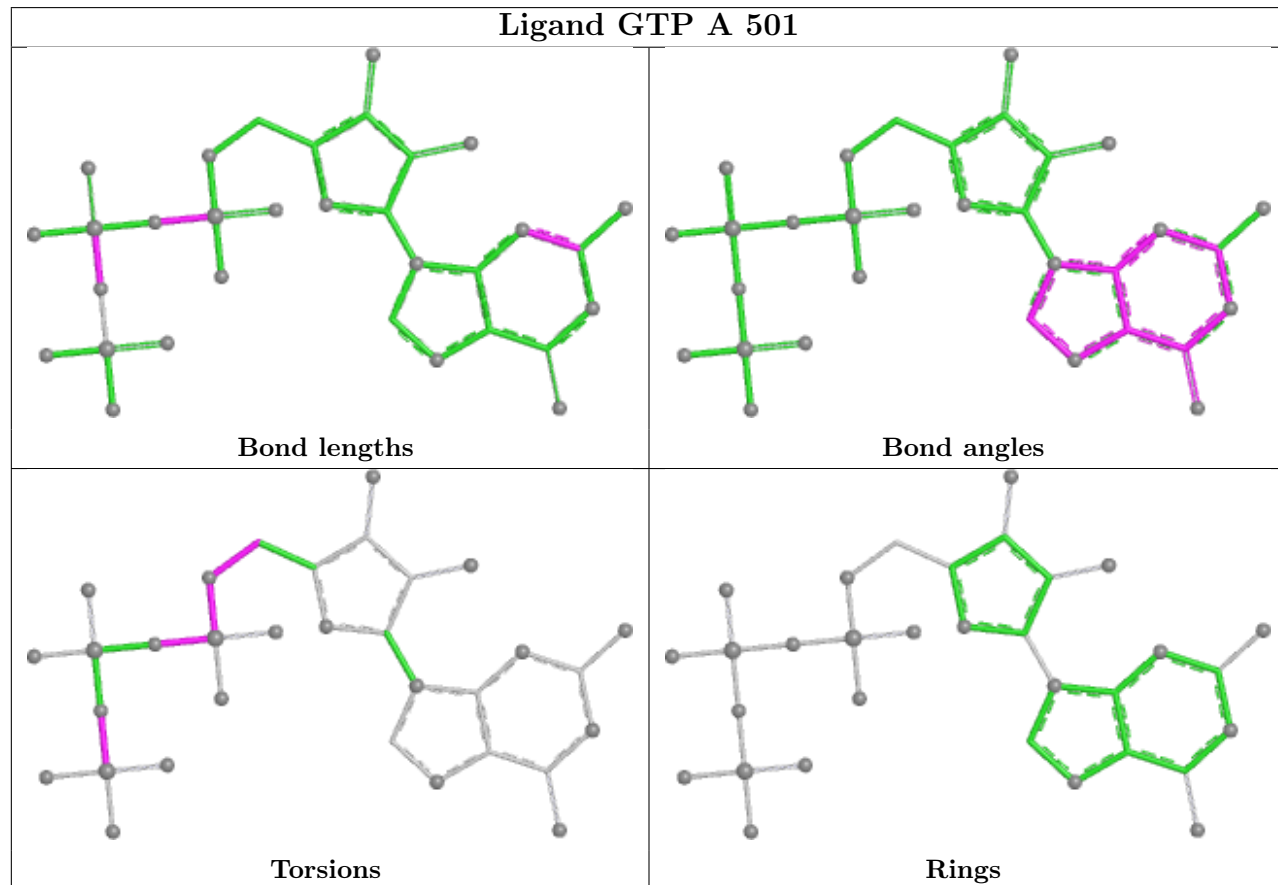




Ligand GTP C 602



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%)	0.45	19 (4%)	40	39	49, 67, 105, 165	0
1	C	440/451 (97%)	0.14	18 (4%)	41	41	26, 54, 79, 113	1 (0%)
2	B	425/445 (95%)	0.44	21 (4%)	35	34	41, 63, 104, 140	4 (0%)
2	D	428/445 (96%)	0.55	25 (5%)	29	27	48, 73, 108, 138	4 (0%)
3	E	123/143 (86%)	0.97	13 (10%)	11	11	53, 84, 127, 166	0
4	F	349/384 (90%)	0.76	32 (9%)	14	13	60, 94, 162, 196	0
All	All	2203/2319 (94%)	0.48	128 (5%)	29	27	26, 69, 125, 196	9 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	249	ASN	6.2
2	B	248	LEU	5.7
2	D	285	ALA	4.9
3	E	143	ALA	4.8
2	B	241	CYS	4.5
4	F	159	GLY	4.4
2	D	281	GLN	4.4
4	F	371	PRO	4.2
1	C	440	VAL	4.2
2	B	247	GLN	3.7
2	B	250	ALA	3.6
4	F	249	TYR	3.5
1	C	284	GLU	3.5
3	E	26	PRO	3.4
4	F	125	THR	3.3
2	B	1	MET	3.2
2	D	57	THR	3.2
3	E	6	MET	3.2
2	B	333	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	248	LEU	3.1
4	F	152	SER	3.1
4	F	167	SER	3.1
1	C	128	GLN	3.1
1	C	245	ASP	3.1
2	D	247	GLN	3.1
2	D	56	ALA	3.1
2	D	407	TRP	3.0
1	A	281	ALA	3.0
1	A	282	TYR	3.0
4	F	173	ILE	3.0
2	D	2	ARG	2.9
2	B	285	ALA	2.9
1	A	337	THR	2.9
1	A	362	VAL	2.9
2	B	57	THR	2.9
2	B	284	ARG	2.8
4	F	381	HIS	2.8
1	C	340	SER	2.8
1	A	316	CYS	2.8
2	D	1	MET	2.8
1	A	88	HIS	2.7
4	F	243	HIS	2.7
1	A	340	SER	2.7
2	B	286	LEU	2.7
4	F	186	LEU	2.7
1	C	2	ARG	2.7
4	F	362	ALA	2.6
3	E	139	LEU	2.6
1	C	357	TYR	2.6
2	D	82	PRO	2.6
4	F	240	LEU	2.6
4	F	142	ARG	2.6
4	F	160	ILE	2.6
4	F	306	HIS	2.6
2	B	255	LEU	2.6
4	F	169	LEU	2.6
2	D	167	ASN	2.6
1	A	437	VAL	2.6
2	B	133	GLN	2.5
2	D	42	LEU	2.5
4	F	231	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	2.5
2	D	195	VAL	2.5
2	D	280	SER	2.5
4	F	179	VAL	2.5
2	D	323	MET	2.5
3	E	28	SER	2.5
3	E	122	ARG	2.4
1	C	341	ILE	2.4
2	D	325	MET	2.4
4	F	161	LEU	2.4
2	B	400	ARG	2.4
3	E	76	ARG	2.4
2	D	246	GLY	2.4
4	F	130	VAL	2.4
4	F	330	ILE	2.4
4	F	105	LEU	2.4
4	F	382	HIS	2.4
2	B	281	GLN	2.4
1	A	284	GLU	2.4
2	D	39	ASP	2.4
4	F	90	SER	2.4
1	A	250	VAL	2.4
2	B	246	GLY	2.3
2	B	325	MET	2.3
2	D	124	LYS	2.3
1	A	285	GLN	2.3
1	A	180	ALA	2.3
2	D	117	SER	2.3
2	B	251	ASP	2.3
4	F	245	ILE	2.3
2	D	181	VAL	2.3
2	B	229	HIS	2.2
1	C	133	GLN	2.2
4	F	373	SER	2.2
1	A	346	TRP	2.2
1	A	381	THR	2.2
1	C	337	THR	2.2
1	A	262	TYR	2.2
1	C	163	LYS	2.2
1	C	4[A]	CYS	2.2
1	A	179	THR	2.2
1	C	308	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	2.1
3	E	59	GLU	2.1
1	C	339	ARG	2.1
1	C	179	THR	2.1
2	D	278	ARG	2.1
4	F	251	LYS	2.1
2	D	371	LEU	2.1
3	E	47	LEU	2.1
4	F	242	ASN	2.1
3	E	8	VAL	2.1
1	C	350	GLY	2.1
2	D	241	CYS	2.1
4	F	372	THR	2.1
3	E	27	PRO	2.1
3	E	45	PRO	2.1
2	D	83	PHE	2.1
4	F	92	THR	2.0
2	D	37	HIS	2.0
2	B	283	TYR	2.0
4	F	315	PHE	2.0
1	C	80	THR	2.0
3	E	125	GLU	2.0
1	A	58	ALA	2.0
4	F	344	ALA	2.0
2	B	59	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

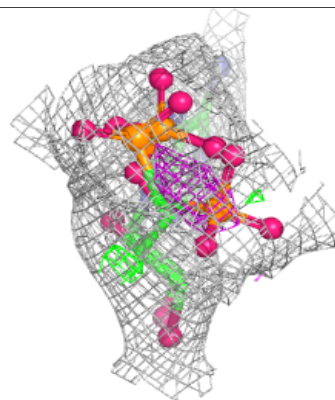
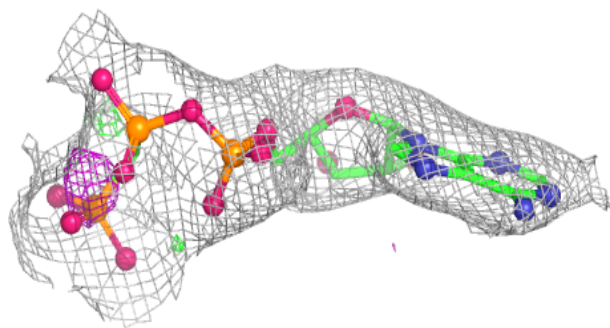
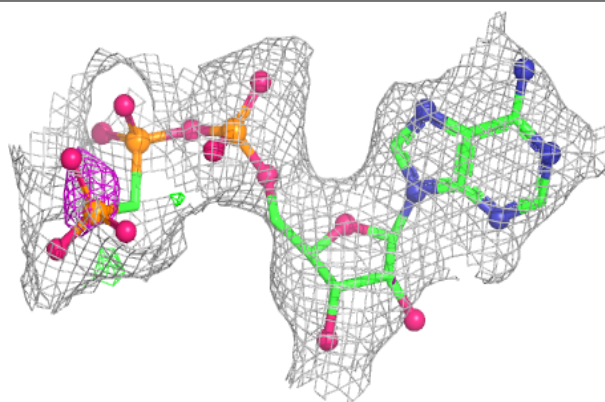
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	B	503	1/1	0.68	0.23	107,107,107,107	0
7	CA	A	504	1/1	0.81	0.14	99,99,99,99	0
9	MES	B	504	12/12	0.84	0.18	86,92,112,116	0
11	ACP	F	401	31/31	0.86	0.11	97,107,114,118	0
6	MG	F	402	1/1	0.87	0.13	97,97,97,97	0
6	MG	D	502	1/1	0.89	0.11	68,68,68,68	0
10	W0A	C	601	16/16	0.92	0.11	49,59,70,75	31
8	GDP	D	501	28/28	0.94	0.10	65,69,76,86	0
5	GTP	A	501	32/32	0.97	0.07	44,50,56,58	0
7	CA	A	503	1/1	0.98	0.04	84,84,84,84	0
8	GDP	B	501	28/28	0.98	0.05	39,46,50,54	0
5	GTP	C	602	32/32	0.98	0.06	40,45,48,50	0
7	CA	C	604	1/1	0.99	0.02	72,72,72,72	0
6	MG	B	502	1/1	0.99	0.04	36,36,36,36	0
6	MG	A	502	1/1	0.99	0.03	50,50,50,50	0
6	MG	C	603	1/1	1.00	0.02	46,46,46,46	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.

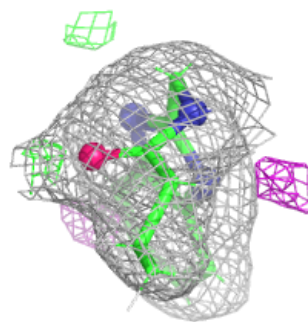
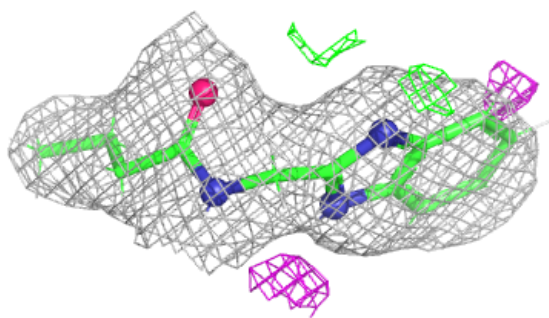
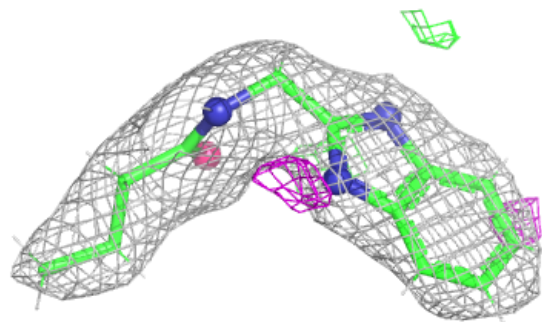
Electron density around ACP F 401:

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



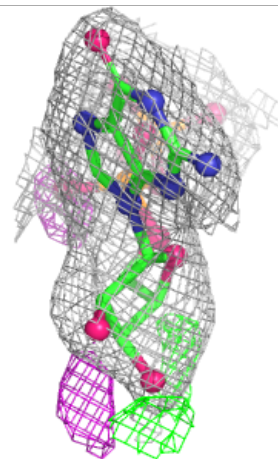
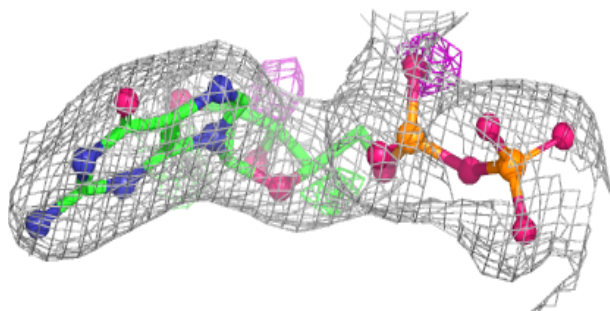
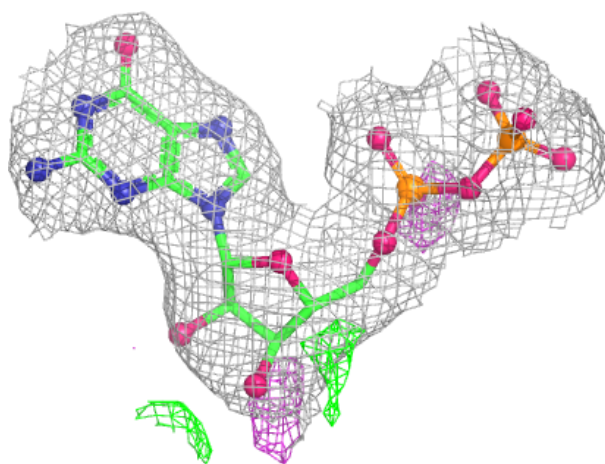
Electron density around W0A C 601:

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



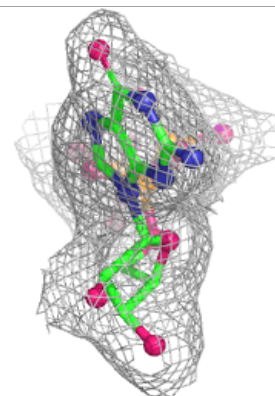
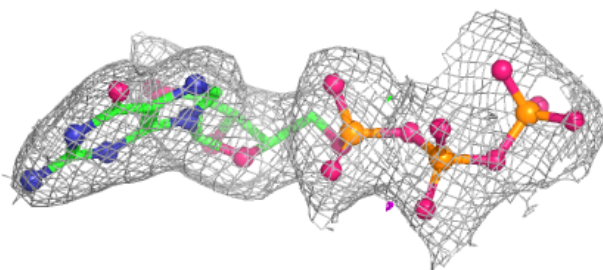
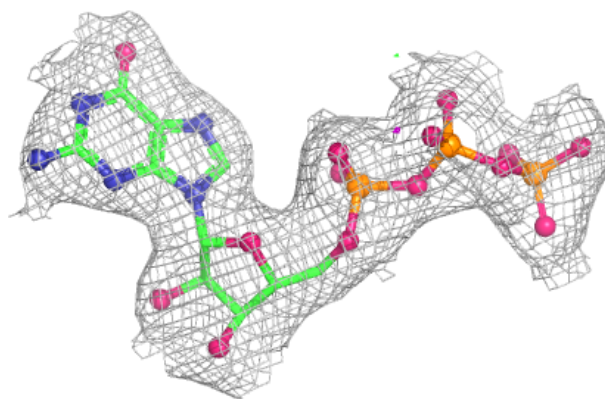
Electron density around GDP D 501:

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



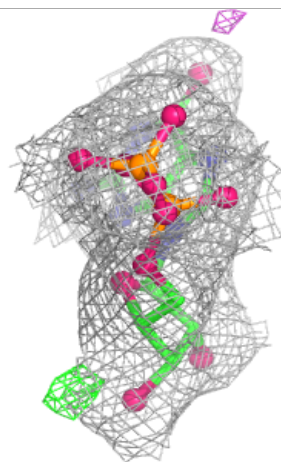
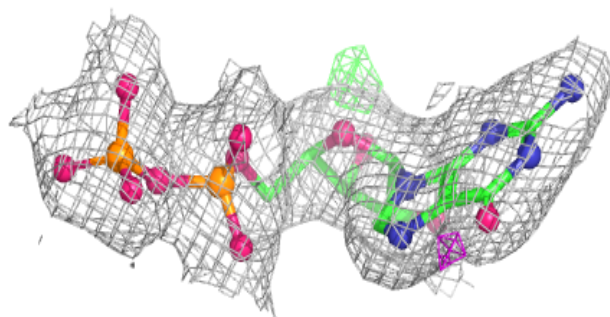
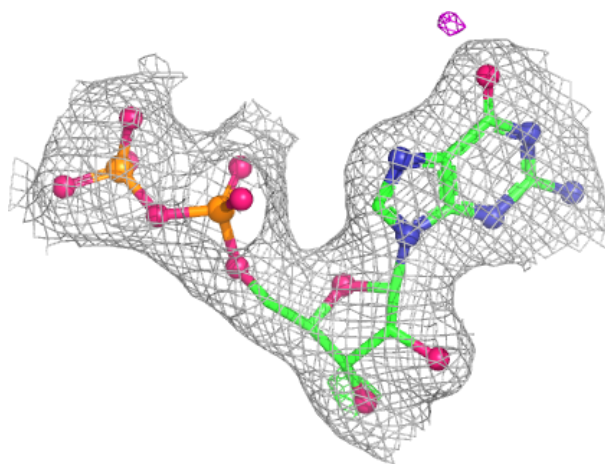
Electron density around GTP A 501:

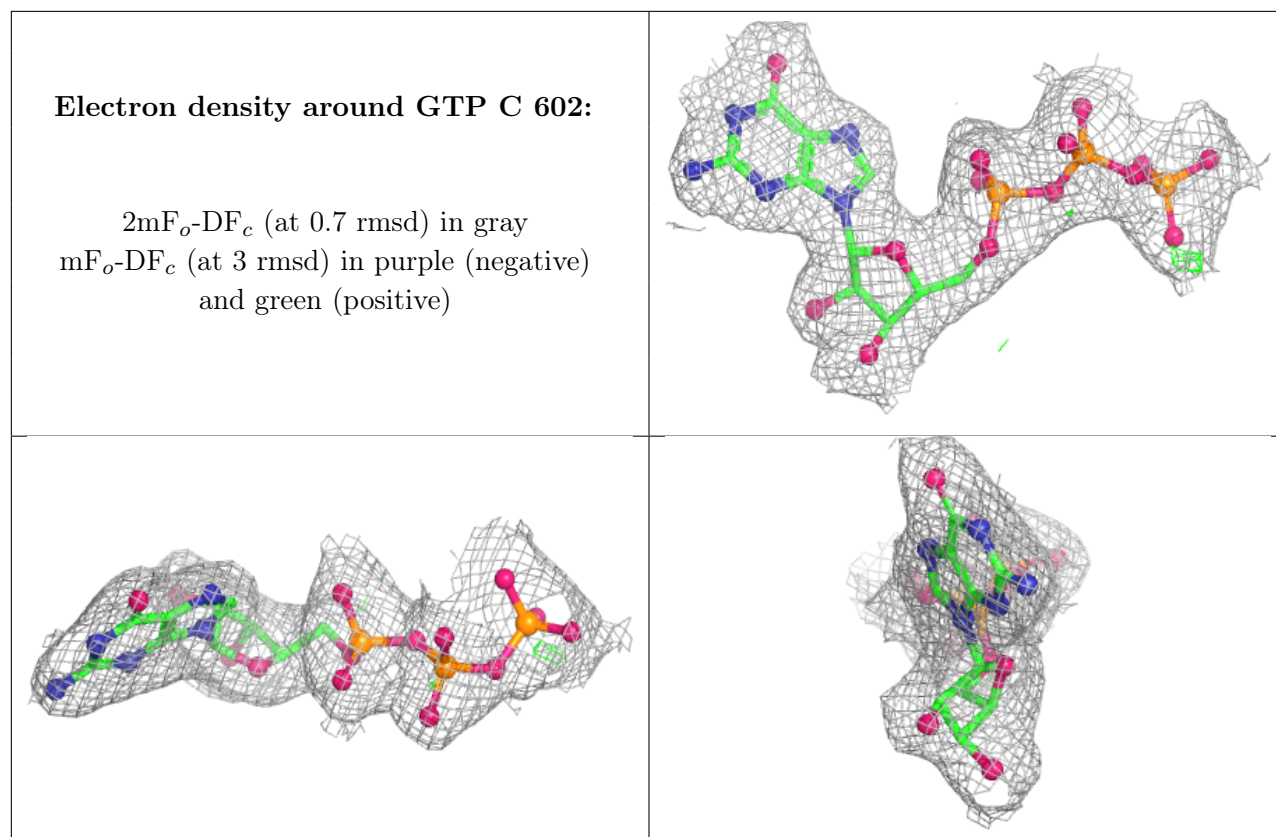
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.