



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 02:07 AM UTC

PDB ID : 8ASN / pdb_00008asn
Title : Crystal structure of the apo human TTL in complex with tubulin-stathmin
Authors : Vuillard, L.; Miallau, L.
Deposited on : 2022-08-19
Resolution : 2.57 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

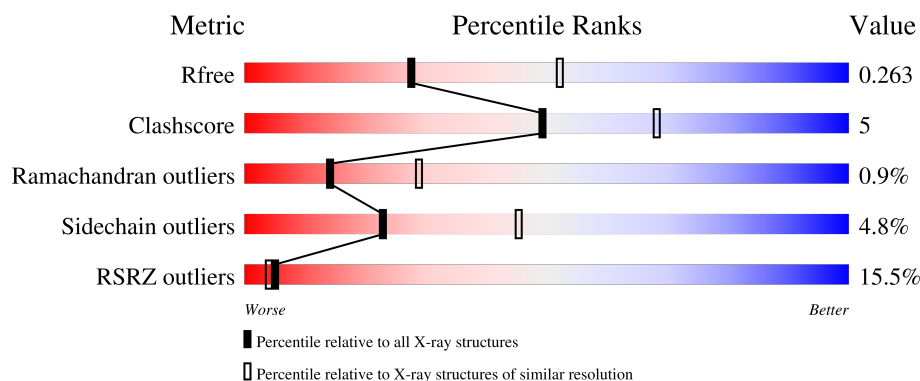
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	8% 78% 15% • 6%
1	C	451	17% 82% 12% • 5%
2	B	445	4% 81% 14% • •
2	D	445	16% 77% 16% • 5%
3	E	143	18% 77% 8% • 14%

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Mol	Chain	Length	Quality of chain
4	F	383	27% 65% 16% 17%
4	G	383	9% 77% 13% 10%
4	H	383	16% 76% 13% 10%
4	I	383	16% 74% 15% 10%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3353	2127	570	632	24			
1	C	430	Total	C	N	O	S	3	5	0
			3408	2156	578	649	25			

- 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	0	0	0
			3337	2097	569	645	26			
2	D	421	Total	C	N	O	S	0	0	0
			3305	2074	563	641	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	1	0
			1025	631	187	203	4			

There are 3 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
E	20	TRP	PHE	conflict	UNP P63043

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	18	0	0
			2588	1671	438	471	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	346	Total	C	N	O	S	0	0	0
			2826	1819	478	519	10			
4	H	345	Total	C	N	O	S	2	0	0
			2830	1827	477	516	10			
4	I	345	Total	C	N	O	S	0	0	0
			2828	1824	477	517	10			

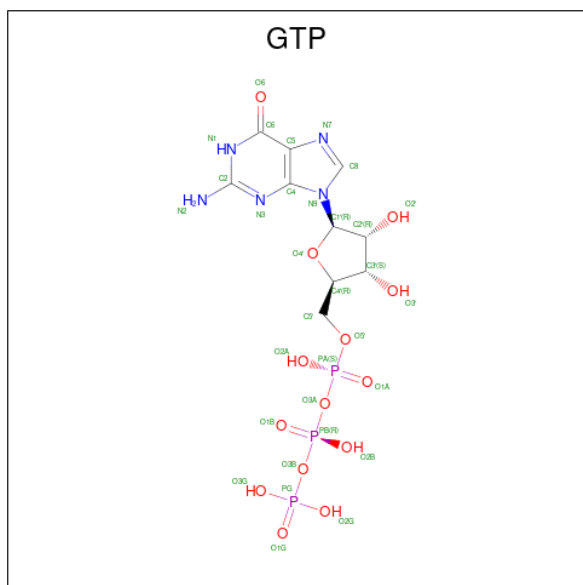
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	GLY	-	expression tag	UNP Q8NG68
F	380	GLU	-	expression tag	UNP Q8NG68
F	381	ASN	-	expression tag	UNP Q8NG68
F	382	LEU	-	expression tag	UNP Q8NG68
F	383	TYR	-	expression tag	UNP Q8NG68
F	384	PHE	-	expression tag	UNP Q8NG68
F	385	GLN	-	expression tag	UNP Q8NG68
G	2	GLY	-	expression tag	UNP Q8NG68
G	380	GLU	-	expression tag	UNP Q8NG68
G	381	ASN	-	expression tag	UNP Q8NG68
G	382	LEU	-	expression tag	UNP Q8NG68
G	383	TYR	-	expression tag	UNP Q8NG68
G	384	PHE	-	expression tag	UNP Q8NG68
G	385	GLN	-	expression tag	UNP Q8NG68
H	2	GLY	-	expression tag	UNP Q8NG68
H	380	GLU	-	expression tag	UNP Q8NG68
H	381	ASN	-	expression tag	UNP Q8NG68
H	382	LEU	-	expression tag	UNP Q8NG68
H	383	TYR	-	expression tag	UNP Q8NG68
H	384	PHE	-	expression tag	UNP Q8NG68
H	385	GLN	-	expression tag	UNP Q8NG68
I	2	GLY	-	expression tag	UNP Q8NG68
I	380	GLU	-	expression tag	UNP Q8NG68
I	381	ASN	-	expression tag	UNP Q8NG68
I	382	LEU	-	expression tag	UNP Q8NG68
I	383	TYR	-	expression tag	UNP Q8NG68
I	384	PHE	-	expression tag	UNP Q8NG68
I	385	GLN	-	expression tag	UNP Q8NG68

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

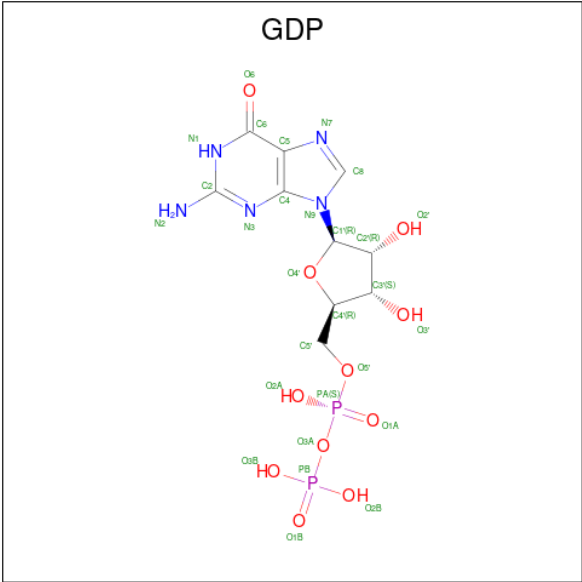
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	2	Total	Mg	0	0
			2	2		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



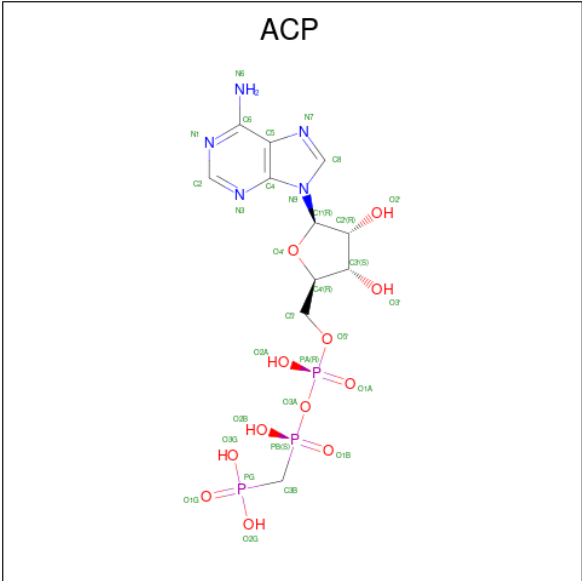
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
6	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	F	1	Total	C	N	O	P	4	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	G	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
8	H	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
8	I	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

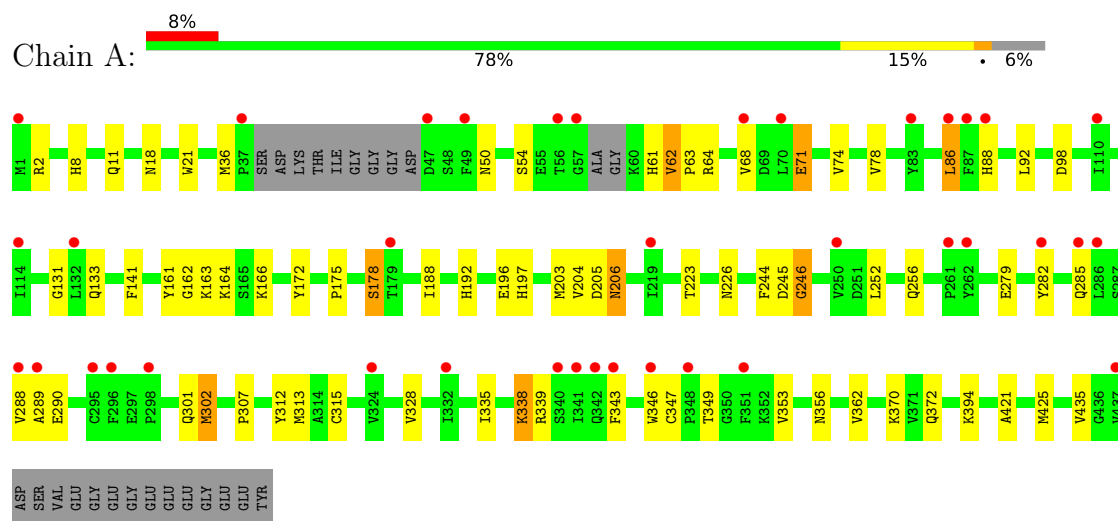
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	56	Total	O	0	0
			56	56		
9	B	64	Total	O	0	0
			64	64		
9	C	91	Total	O	0	0
			91	91		
9	D	55	Total	O	0	0
			55	55		
9	E	26	Total	O	0	0
			26	26		
9	F	49	Total	O	0	0
			49	49		
9	G	38	Total	O	0	0
			38	38		
9	H	39	Total	O	0	0
			39	39		
9	I	40	Total	O	0	0
			40	40		

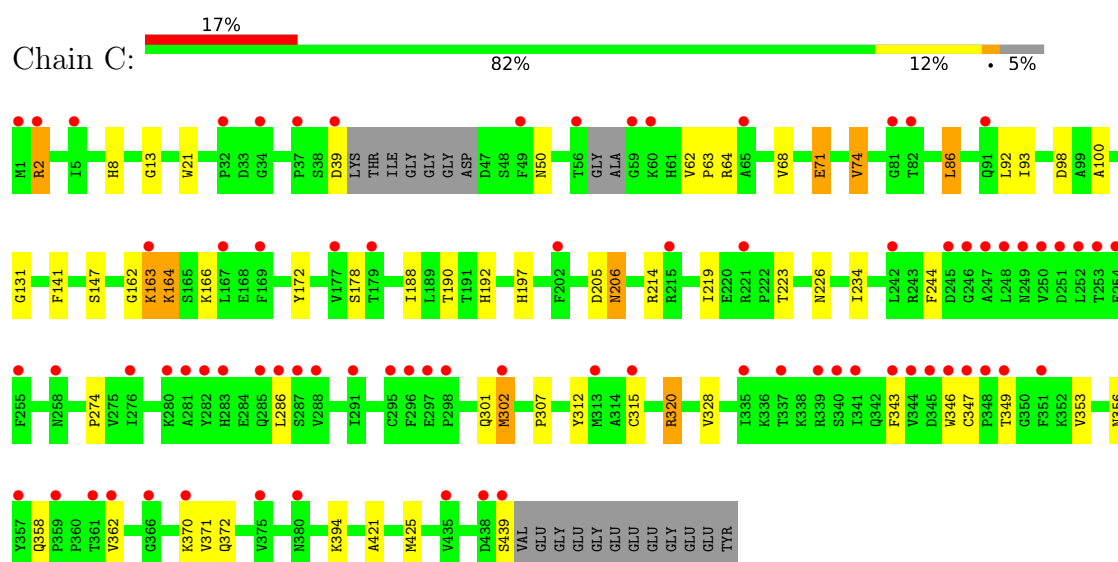
3 Residue-property plots [i](#)

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.

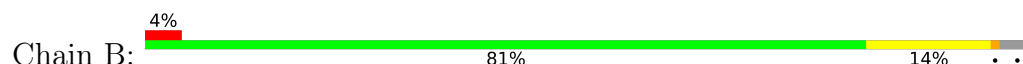
- Molecule 1: Tubulin alpha-1B chain

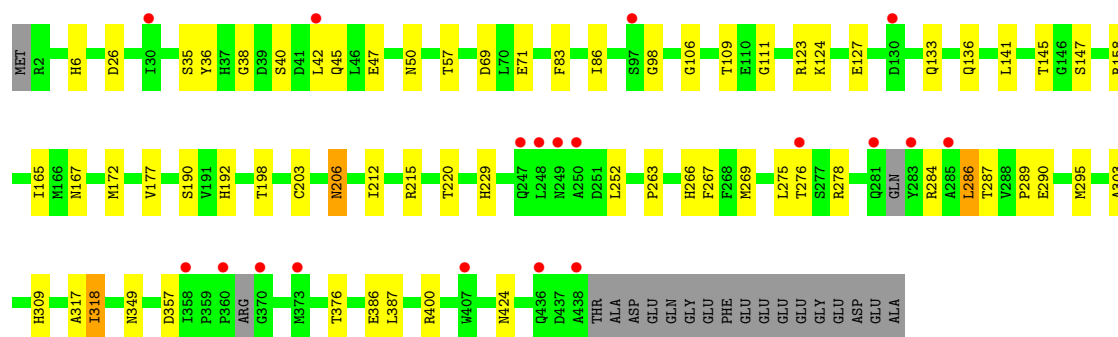


- Molecule 1: Tubulin alpha-1B chain

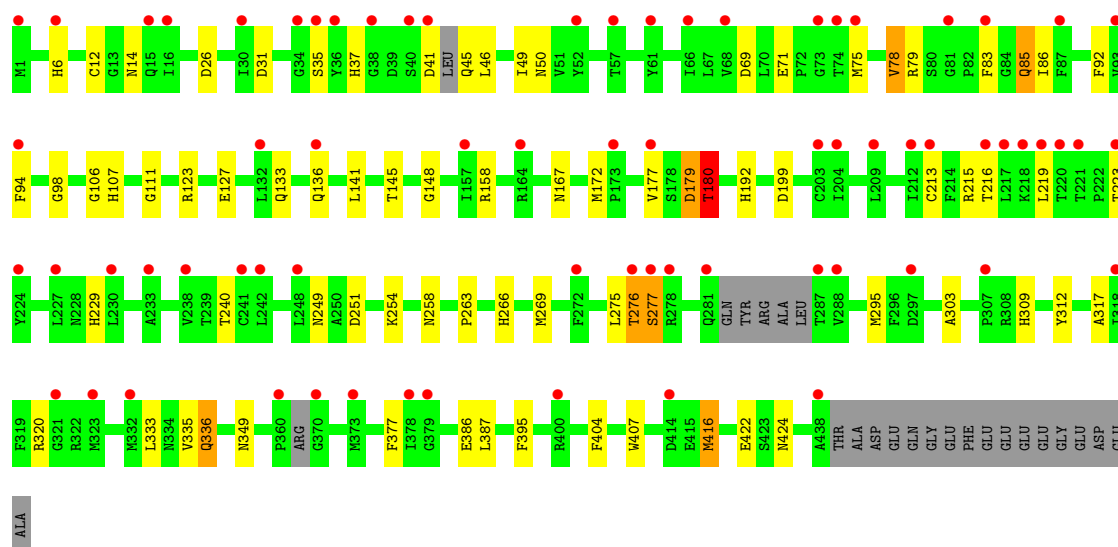
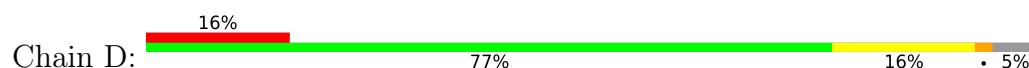


- Molecule 2: Tubulin beta-2B chain

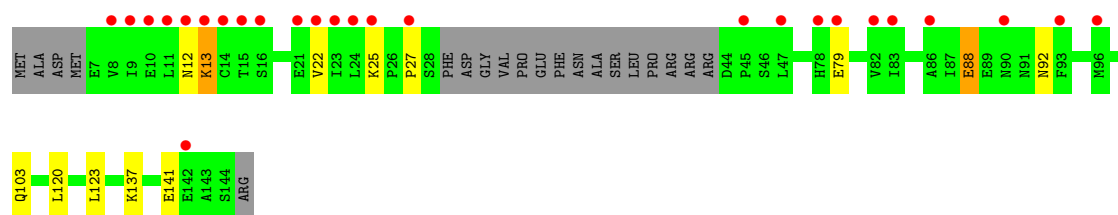




• Molecule 2: Tubulin beta-2B chain

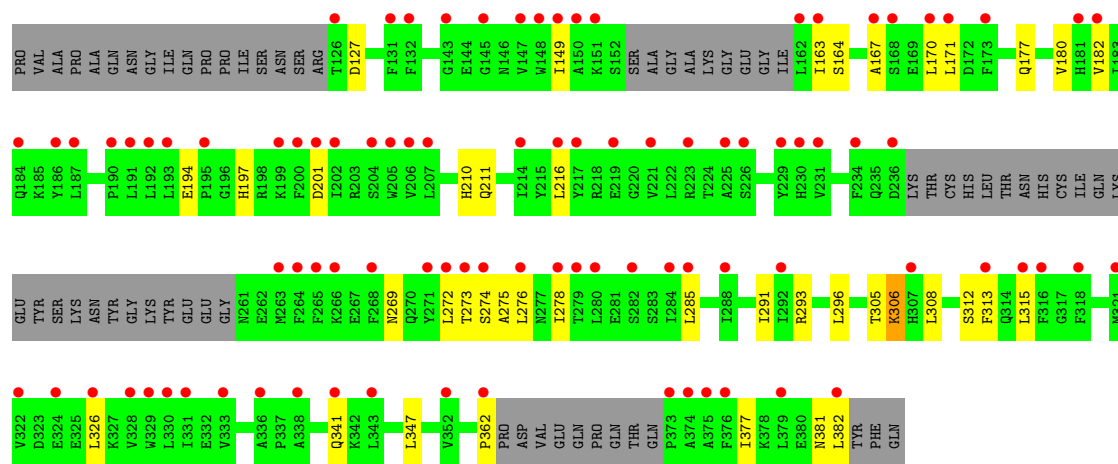


• Molecule 3: Stathmin-4

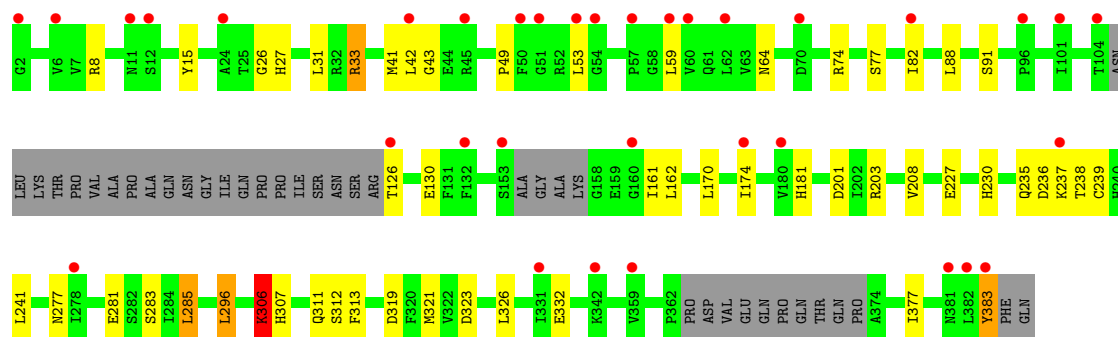
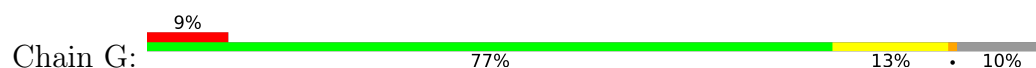


• Molecule 4: Tubulin-tyrosine ligase

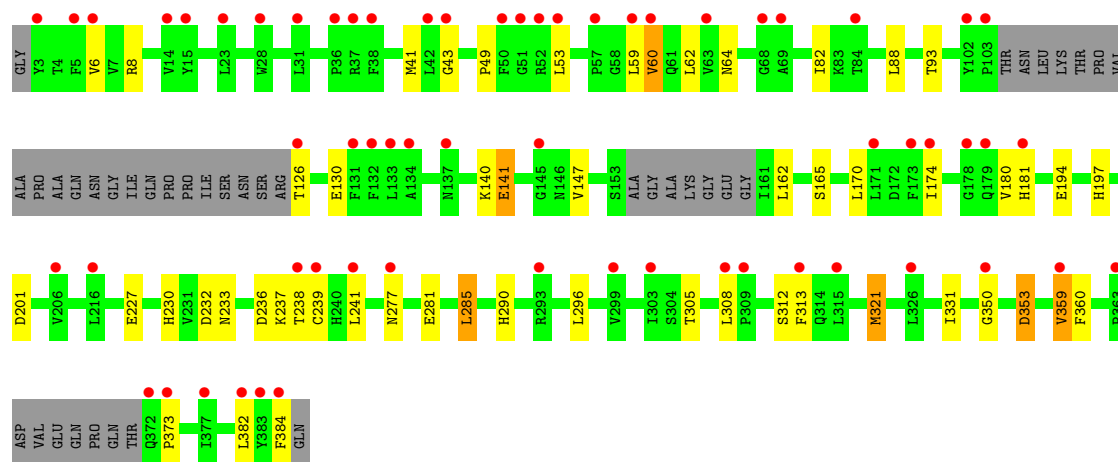
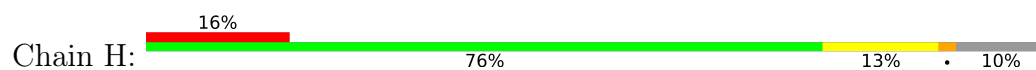




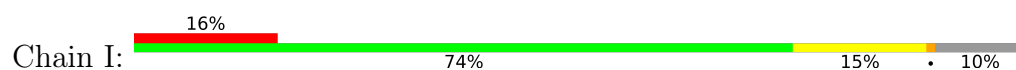
• Molecule 4: Tubulin–tyrosine ligase

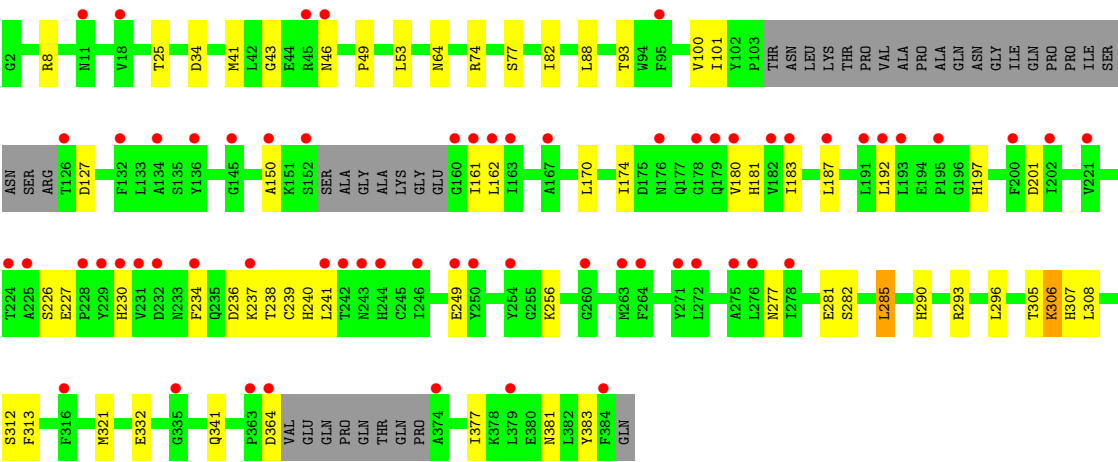


• Molecule 4: Tubulin–tyrosine ligase



• Molecule 4: Tubulin–tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.55Å 199.64Å 134.67Å 90.00° 97.02° 90.00°	Depositor
Resolution (Å)	133.66 – 2.57 133.66 – 2.57	Depositor EDS
% Data completeness (in resolution range)	65.1 (133.66-2.57) 65.1 (133.66-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.243 , 0.273 0.233 , 0.263	Depositor DCC
R_{free} test set	4463 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26206	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/3429	0.98	2/4655 (0.0%)
1	C	0.59	0/3484	0.95	3/4729 (0.1%)
2	B	0.61	0/3409	0.96	4/4614 (0.1%)
2	D	0.61	0/3376	1.00	9/4568 (0.2%)
3	E	0.60	0/1035	1.04	0/1376
4	F	0.56	0/2649	1.01	3/3584 (0.1%)
4	G	0.55	0/2894	1.00	4/3914 (0.1%)
4	H	0.55	0/2901	0.96	2/3927 (0.1%)
4	I	0.56	0/2898	0.99	4/3921 (0.1%)
All	All	0.58	0/26075	0.98	31/35288 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	353	ASP	N-CA-C	-7.33	101.07	110.53
1	A	141	PHE	CA-CB-CG	6.89	120.69	113.80
4	F	68	GLY	N-CA-C	-6.86	103.02	111.45
1	C	141	PHE	CA-CB-CG	6.73	120.53	113.80
4	F	103	PRO	N-CA-CB	6.35	109.92	103.25
2	D	78	VAL	N-CA-C	-6.27	103.22	110.05
2	D	336	GLN	N-CA-C	-5.99	102.81	110.53
1	C	74	VAL	N-CA-CB	5.91	120.98	111.23
4	G	306	LYS	CA-C-N	5.73	132.49	121.54
4	G	306	LYS	C-N-CA	5.73	132.49	121.54
2	D	179	ASP	CA-C-N	5.37	131.79	121.54
2	D	179	ASP	C-N-CA	5.37	131.79	121.54
2	D	215	ARG	CA-C-O	-5.36	115.48	121.81
2	D	179	ASP	CA-CB-CG	5.33	117.92	112.60
2	D	277	SER	N-CA-C	-5.31	99.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	276	THR	CA-C-N	5.26	131.58	121.54
2	D	276	THR	C-N-CA	5.26	131.58	121.54
4	I	43	GLY	N-CA-C	5.22	119.24	112.25
4	H	43	GLY	N-CA-C	5.21	119.23	112.25
2	B	220	THR	CB-CA-C	5.18	118.78	110.29
4	F	43	GLY	N-CA-C	5.18	119.19	112.25
2	B	158	ARG	CB-CG-CD	-5.17	99.41	111.30
2	B	215	ARG	CA-C-O	-5.13	115.42	120.70
4	G	43	GLY	N-CA-C	5.13	119.12	112.25
4	I	306	LYS	N-CA-C	-5.12	100.17	108.41
1	A	290	GLU	N-CA-C	-5.11	105.62	111.14
1	C	320	ARG	N-CA-C	5.11	119.86	113.43
4	I	306	LYS	CA-C-N	5.10	131.29	121.54
4	I	306	LYS	C-N-CA	5.10	131.29	121.54
2	B	42	LEU	N-CA-C	5.04	119.52	113.17
4	G	323	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3353	0	3261	46	0
1	C	3408	0	3311	37	0
2	B	3337	0	3208	31	0
2	D	3305	0	3177	48	0
3	E	1025	0	1032	4	0
4	F	2588	0	2551	36	0
4	G	2826	0	2775	27	0
4	H	2830	0	2783	27	0
4	I	2828	0	2779	34	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
6	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	32	0	12	2	0
7	B	28	0	12	1	0
7	D	28	0	12	1	0
8	F	31	0	14	1	0
8	G	31	0	14	3	0
8	H	31	0	14	0	0
8	I	31	0	14	4	0
9	A	56	0	0	0	0
9	B	64	0	0	0	0
9	C	91	0	0	0	0
9	D	55	0	0	0	0
9	E	26	0	0	0	0
9	F	49	0	0	0	0
9	G	38	0	0	0	0
9	H	39	0	0	0	0
9	I	40	0	0	0	0
All	All	26206	0	24981	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:HD21	6:C:502:GTP:HN22	1.05	0.99
4:I:174:ILE:HG23	4:I:181:HIS:HD2	1.29	0.98
4:H:174:ILE:HG23	4:H:181:HIS:HD2	1.28	0.98
4:G:174:ILE:HG23	4:G:181:HIS:HD2	1.31	0.95
1:A:206:ASN:HD21	6:A:502:GTP:HN22	0.96	0.93
1:C:223:THR:H	1:C:226:ASN:HD22	1.20	0.89
4:I:174:ILE:HG23	4:I:181:HIS:CD2	2.09	0.88
4:H:174:ILE:HG23	4:H:181:HIS:CD2	2.09	0.87
2:B:192:HIS:HD2	2:B:424:ASN:HD22	1.23	0.85
2:D:192:HIS:HD2	2:D:424:ASN:HD22	1.24	0.84
1:A:223:THR:H	1:A:226:ASN:HD22	1.21	0.84
4:G:174:ILE:HG23	4:G:181:HIS:CD2	2.11	0.84
4:F:22:LEU:HD22	4:F:28:TRP:CG	2.15	0.81
1:A:206:ASN:HD21	6:A:502:GTP:N2	1.79	0.78
1:A:394:LYS:NZ	2:B:349:ASN:HD21	1.82	0.77
4:F:22:LEU:HD22	4:F:28:TRP:CD1	2.24	0.72
1:A:394:LYS:HZ3	2:B:349:ASN:HD21	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:62:LEU:HD22	4:H:359:VAL:HG11	1.72	0.70
2:B:206:ASN:HD21	7:B:501:GDP:HN22	1.39	0.70
4:I:174:ILE:HD12	4:I:181:HIS:CG	2.26	0.70
2:B:318:ILE:HG23	2:B:376:THR:HB	1.74	0.69
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.73	0.69
2:D:192:HIS:CD2	2:D:424:ASN:HD22	2.09	0.69
2:D:158:ARG:NH1	2:D:199:ASP:OD2	2.26	0.67
1:A:63:PRO:HD3	1:A:86:LEU:HD22	1.76	0.67
2:B:192:HIS:CD2	2:B:424:ASN:HD22	2.08	0.67
1:C:63:PRO:HD3	1:C:86:LEU:HD22	1.76	0.66
4:F:94:TRP:CG	4:F:291:ILE:HD12	2.30	0.66
2:D:75:MET:SD	2:D:94:PHE:CE1	2.89	0.66
4:I:174:ILE:HD12	4:I:181:HIS:CD2	2.31	0.66
2:D:240:THR:HG21	2:D:320:ARG:HD2	1.78	0.65
4:F:94:TRP:CD2	4:F:291:ILE:HD12	2.33	0.64
1:A:335:ILE:HA	1:A:338:LYS:HD2	1.79	0.64
4:F:22:LEU:HD22	4:F:28:TRP:CD2	2.33	0.63
4:H:8:ARG:HD3	4:H:41:MET:HE3	1.79	0.63
1:C:206:ASN:HD21	6:C:502:GTP:N2	1.88	0.62
2:B:229:HIS:NE2	2:B:276:THR:HG23	2.14	0.62
4:G:8:ARG:HG2	4:G:33:ARG:HD2	1.80	0.62
2:D:192:HIS:HD2	2:D:424:ASN:ND2	1.95	0.62
1:A:206:ASN:ND2	6:A:502:GTP:HN22	1.82	0.62
2:B:192:HIS:HD2	2:B:424:ASN:ND2	1.95	0.60
4:H:140:LYS:O	4:H:141:GLU:HB3	2.02	0.59
4:G:15:TYR:HB3	4:G:42:LEU:HD13	1.84	0.58
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.58
4:F:15:TYR:HB3	4:F:42:LEU:HD13	1.83	0.58
1:A:335:ILE:HA	1:A:338:LYS:CD	2.33	0.58
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.22	0.58
1:C:394:LYS:NZ	2:D:349:ASN:HD21	2.02	0.58
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.69	0.58
4:H:93:THR:HG23	4:I:290:HIS:CE1	2.39	0.58
4:I:150:ALA:HB1	4:I:174:ILE:HD11	1.86	0.57
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.85	0.57
4:H:350:GLY:O	4:H:353:ASP:O	2.21	0.57
4:I:174:ILE:HD12	4:I:181:HIS:CB	2.35	0.57
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.86	0.57
4:I:174:ILE:CG2	4:I:181:HIS:HD2	2.12	0.57
2:D:85:GLN:H	2:D:85:GLN:NE2	2.02	0.57
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:MET:HE1	2:D:317:ALA:HB1	1.87	0.56
4:G:230:HIS:HE1	4:G:236:ASP:OD2	1.89	0.56
4:H:162:LEU:HD23	4:H:170:LEU:HD23	1.87	0.56
4:H:194:GLU:OE2	4:H:197:HIS:HD2	1.88	0.56
2:D:263:PRO:O	2:D:266:HIS:HD2	1.87	0.56
1:C:343:PHE:HB2	1:C:349:THR:HG22	1.88	0.56
4:F:94:TRP:CD1	4:F:291:ILE:HD12	2.41	0.56
2:D:14:ASN:ND2	2:D:75:MET:HE1	2.20	0.56
4:H:60:VAL:HG13	4:H:360:PHE:HE1	1.71	0.56
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.87	0.55
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.55	0.55
1:C:320:ARG:O	1:C:358:GLN:O	2.25	0.55
2:B:36:TYR:OH	2:B:40:SER:O	2.23	0.55
1:C:301:GLN:NE2	1:C:307:PRO:HG3	2.22	0.55
4:G:283:SER:HB2	4:G:326:LEU:HD13	1.88	0.55
2:B:309:HIS:HD2	2:B:386:GLU:OE2	1.90	0.55
2:D:309:HIS:HD2	2:D:386:GLU:OE2	1.89	0.55
4:I:162:LEU:HD23	4:I:170:LEU:HD23	1.87	0.55
2:B:6:HIS:HD2	2:B:136:GLN:HE21	1.55	0.55
2:D:6:HIS:HD2	2:D:136:GLN:HE21	1.56	0.54
2:D:14:ASN:CG	2:D:75:MET:HE1	2.33	0.54
4:G:162:LEU:HD23	4:G:170:LEU:HD23	1.88	0.54
1:C:320:ARG:O	1:C:356:ASN:O	2.25	0.54
2:D:251:ASP:OD1	2:D:254:LYS:HB2	2.08	0.54
4:F:2:GLY:O	4:F:27:HIS:O	2.26	0.54
4:F:194:GLU:OE2	4:F:197:HIS:HD2	1.91	0.54
4:H:62:LEU:HD22	4:H:359:VAL:CG1	2.37	0.54
2:D:85:GLN:H	2:D:85:GLN:HE21	1.55	0.53
1:A:245:ASP:O	1:A:246:GLY:O	2.27	0.53
2:B:295:MET:HE1	2:B:317:ALA:HB1	1.91	0.53
2:D:75:MET:O	2:D:78:VAL:O	2.27	0.53
4:H:230:HIS:HE1	4:H:236:ASP:OD2	1.91	0.53
4:I:161:ILE:HG21	4:I:241:LEU:HD21	1.89	0.53
4:G:321:MET:HE1	8:G:401:ACP:H2'	1.92	0.52
1:A:301:GLN:NE2	1:A:307:PRO:HG3	2.24	0.52
1:C:301:GLN:HE22	1:C:307:PRO:HG3	1.75	0.52
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.90	0.52
4:H:174:ILE:CG2	4:H:181:HIS:HD2	2.12	0.52
1:A:166:LYS:HE2	1:A:197:HIS:O	2.10	0.52
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.90	0.52
4:F:97:GLU:HG3	4:G:383:TYR:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:27:HIS:CE1	4:F:362:PRO:HA	2.44	0.52
4:H:290:HIS:CE1	4:I:93:THR:HG23	2.45	0.52
2:D:46:LEU:HA	2:D:49:ILE:HB	1.91	0.51
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.92	0.51
1:A:223:THR:H	1:A:226:ASN:ND2	2.00	0.51
4:F:94:TRP:CG	4:F:291:ILE:CD1	2.94	0.51
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.92	0.51
4:G:227:GLU:HG3	4:G:238:THR:HB	1.92	0.51
4:I:381:ASN:HD22	4:I:383:TYR:H	1.60	0.50
1:A:362:VAL:HG22	1:A:370:LYS:HE3	1.94	0.50
4:G:41:MET:HE1	4:G:49:PRO:HD2	1.94	0.50
4:H:321:MET:HG3	4:H:331:ILE:HG13	1.94	0.50
1:C:166:LYS:HE2	1:C:197:HIS:O	2.10	0.50
4:I:192:LEU:HD12	4:I:197:HIS:CE1	2.47	0.50
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.94	0.50
4:G:174:ILE:CG2	4:G:181:HIS:HD2	2.14	0.50
4:G:203:ARG:NH1	4:G:319:ASP:OD1	2.45	0.50
2:D:69:ASP:OD2	2:D:75:MET:HE3	2.12	0.50
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.05	0.49
4:F:164:SER:HB3	4:F:170:LEU:HG	1.93	0.49
4:F:82:ILE:HD13	4:F:88:LEU:HD13	1.95	0.49
1:A:335:ILE:HA	1:A:338:LYS:HZ2	1.77	0.49
3:E:137:LYS:O	3:E:141:GLU:HG2	2.12	0.49
1:C:223:THR:H	1:C:226:ASN:ND2	2.01	0.49
4:H:41:MET:HE1	4:H:49:PRO:HD2	1.95	0.49
4:I:41:MET:HE1	4:I:49:PRO:HD2	1.94	0.49
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.05	0.49
4:G:208:VAL:HG21	4:G:296:LEU:HD22	1.93	0.49
4:F:94:TRP:CE2	4:F:291:ILE:HD12	2.48	0.49
4:H:237:LYS:HD2	4:H:241:LEU:HD13	1.94	0.49
1:C:312:TYR:CD2	1:C:315[B]:CYS:SG	3.06	0.49
1:C:362:VAL:HG22	1:C:370:LYS:HE3	1.93	0.49
4:F:41:MET:HE1	4:F:49:PRO:HD2	1.94	0.49
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.31	0.49
1:C:163:LYS:NZ	1:C:163:LYS:HA	2.28	0.48
4:F:8:ARG:HD3	4:F:41:MET:HE3	1.95	0.48
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.77	0.48
4:I:321:MET:HE1	8:I:401:ACP:H2'	1.94	0.48
2:B:263:PRO:O	2:B:266:HIS:HD2	1.96	0.48
2:D:179:ASP:O	2:D:180:THR:OG1	2.29	0.48
4:F:94:TRP:CD2	4:F:291:ILE:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:161:ILE:HD11	8:I:401:ACP:O3G	2.14	0.48
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.06	0.48
4:I:281:GLU:HA	4:I:285:LEU:HB2	1.96	0.48
4:G:306:LYS:NZ	4:G:311:GLN:HE22	2.12	0.48
4:G:82:ILE:HD13	4:G:88:LEU:HD13	1.95	0.48
4:I:227:GLU:HG3	4:I:238:THR:HB	1.96	0.48
1:A:301:GLN:HE22	1:A:307:PRO:CD	2.27	0.48
1:C:234:ILE:HD12	1:C:302:MET:HE3	1.95	0.48
4:G:74:ARG:HB2	4:G:77:SER:OG	2.14	0.48
4:G:237:LYS:HD2	4:G:241:LEU:HD13	1.96	0.48
1:A:288:VAL:O	1:A:289:ALA:HB3	2.14	0.47
3:E:88:GLU:O	3:E:92:ASN:HB2	2.13	0.47
4:F:22:LEU:HD22	4:F:28:TRP:CE2	2.49	0.47
4:H:227:GLU:HG3	4:H:238:THR:HB	1.96	0.47
4:I:82:ILE:HD13	4:I:88:LEU:HD13	1.97	0.47
1:A:301:GLN:HE22	1:A:307:PRO:HG3	1.78	0.47
1:A:346:TRP:CE3	1:A:347:CYS:SG	3.06	0.47
4:G:174:ILE:HA	4:G:181:HIS:CD2	2.50	0.47
1:C:50:ASN:O	1:C:64:ARG:NH1	2.47	0.47
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.95	0.47
2:D:229:HIS:CE1	2:D:277:SER:HB2	2.49	0.47
4:I:74:ARG:HB2	4:I:77:SER:OG	2.15	0.47
4:F:17:GLU:O	4:F:21:LEU:HD22	2.16	0.46
4:H:230:HIS:CE1	4:H:239:CYS:SG	3.08	0.46
4:I:230:HIS:CE1	4:I:239:CYS:SG	3.09	0.46
1:A:394:LYS:HZ2	2:B:349:ASN:HD21	1.61	0.46
4:F:269:ASN:O	4:F:272:LEU:O	2.34	0.46
1:A:335:ILE:CG1	1:A:338:LYS:HZ2	2.28	0.46
2:D:41:ASP:HA	2:D:45:GLN:O	2.16	0.46
2:D:92:PHE:HB3	2:D:94:PHE:CE2	2.50	0.46
4:H:82:ILE:HD13	4:H:88:LEU:HD13	1.97	0.46
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.34	0.46
4:F:91:SER:HB2	4:G:91:SER:HB2	1.97	0.46
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.98	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
4:G:332:GLU:HG3	8:G:401:ACP:O2B	2.16	0.46
4:G:161:ILE:HD11	8:G:401:ACP:O3G	2.16	0.45
2:D:192:HIS:CD2	2:D:424:ASN:ND2	2.78	0.45
4:F:22:LEU:CD2	4:F:28:TRP:CD1	2.98	0.45
4:F:273:THR:HA	4:F:274:SER:HA	1.72	0.45
1:C:301:GLN:HE22	1:C:307:PRO:CD	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD12	2:B:172:MET:SD	2.56	0.45
2:B:147:SER:OG	2:B:190:SER:OG	2.28	0.45
4:G:8:ARG:HD3	4:G:41:MET:HE3	1.98	0.45
1:A:349:THR:HB	3:E:25:LYS:HG2	1.99	0.45
1:C:301:GLN:HE22	1:C:307:PRO:CG	2.29	0.45
2:B:136:GLN:HA	2:B:167:ASN:O	2.17	0.45
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.99	0.45
4:H:174:ILE:HA	4:H:181:HIS:CD2	2.51	0.45
4:F:276:LEU:HD13	4:F:326:LEU:HD21	1.99	0.45
4:I:174:ILE:HA	4:I:181:HIS:CD2	2.52	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
2:D:123:ARG:O	2:D:127:GLU:HG2	2.16	0.44
4:F:167:ALA:HA	4:F:170:LEU:HB2	1.97	0.44
4:F:210:HIS:O	4:F:211:GLN:HB2	2.17	0.44
4:H:93:THR:CG2	4:I:290:HIS:CE1	3.00	0.44
1:C:71:GLU:HB3	1:C:98:ASP:HB3	2.00	0.44
1:A:2:ARG:HA	1:A:131:GLY:O	2.17	0.44
1:C:394:LYS:HZ3	2:D:349:ASN:HD21	1.64	0.44
2:D:416:MET:HE2	2:D:416:MET:HB3	1.87	0.44
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.99	0.44
2:D:395:PHE:CE1	2:D:422:GLU:HB2	2.52	0.44
4:I:174:ILE:CD1	4:I:181:HIS:CD2	3.00	0.44
4:G:230:HIS:CE1	4:G:239:CYS:SG	3.11	0.44
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.44
2:B:123:ARG:O	2:B:127:GLU:HG2	2.18	0.44
4:I:332:GLU:HG3	8:I:401:ACP:O2B	2.17	0.44
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.00	0.43
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.18	0.43
2:D:78:VAL:O	2:D:79:ARG:CB	2.65	0.43
4:I:8:ARG:HD3	4:I:41:MET:HE3	1.99	0.43
2:D:141:LEU:HD12	2:D:172:MET:SD	2.57	0.43
4:F:216:LEU:HB3	4:F:377:ILE:HG13	2.00	0.43
4:F:305:THR:HG22	4:F:308:LEU:HD12	2.00	0.43
4:G:281:GLU:HA	4:G:285:LEU:HB2	2.01	0.43
4:I:101:ILE:HG13	4:I:183:ILE:HG13	1.99	0.43
2:D:92:PHE:HD2	2:D:94:PHE:CZ	2.36	0.43
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.99	0.43
1:A:50:ASN:O	1:A:64:ARG:NH1	2.51	0.43
4:I:230:HIS:HE1	4:I:236:ASP:OD2	2.01	0.43
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.83	0.43
2:D:107:HIS:HD2	2:D:148:GLY:O	2.02	0.43
4:G:208:VAL:HG21	4:G:296:LEU:CD2	2.49	0.43
4:H:281:GLU:HA	4:H:285:LEU:HB2	2.00	0.43
2:D:229:HIS:NE2	2:D:277:SER:HB2	2.34	0.43
4:I:234:PHE:HA	4:I:240:HIS:CD2	2.54	0.43
1:A:175:PRO:HA	1:A:178:SER:HB2	2.01	0.42
4:F:272:LEU:O	4:F:273:THR:HG22	2.19	0.42
4:I:187:LEU:HD23	8:I:401:ACP:N1	2.34	0.42
4:F:149:ILE:HD13	8:F:401:ACP:N7	2.35	0.42
1:A:244:PHE:HB2	1:A:356:ASN:HD21	1.84	0.42
4:I:237:LYS:HD2	4:I:241:LEU:HD12	2.01	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.42
1:A:204:VAL:HG22	1:A:302:MET:HE3	2.02	0.42
2:B:198:THR:OG1	2:B:266:HIS:CE1	2.72	0.42
2:D:31:ASP:HB3	2:D:37:HIS:CE1	2.54	0.42
2:D:12:CYS:HB2	7:D:501:GDP:C8	2.54	0.42
2:B:69:ASP:HA	2:B:145:THR:HG21	2.02	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
4:F:68:GLY:C	4:F:70:ASP:H	2.28	0.42
1:A:54:SER:OG	1:A:62:VAL:HG13	2.20	0.42
1:A:301:GLN:HE22	1:A:307:PRO:CG	2.32	0.42
1:C:68[B]:VAL:HG12	1:C:93:ILE:HB	2.01	0.42
4:F:72:LEU:HD12	4:F:78:LEU:HD13	2.02	0.42
4:F:315:LEU:HD21	4:F:347:LEU:HD21	2.02	0.42
1:A:313:MET:SD	1:A:435:VAL:HG11	2.60	0.41
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.02	0.41
1:C:8:HIS:HB3	1:C:13:GLY:O	2.20	0.41
2:D:404:PHE:HD1	2:D:407:TRP:HE1	1.67	0.41
4:F:64:ASN:C	4:F:313:PHE:O	2.64	0.41
4:I:305:THR:HG22	4:I:308:LEU:HD12	2.02	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.21	0.41
1:C:2:ARG:HA	1:C:131:GLY:O	2.19	0.41
2:D:249:ASN:HD21	2:D:258:ASN:HD22	1.68	0.41
4:G:64:ASN:C	4:G:313:PHE:O	2.63	0.41
4:H:290:HIS:CE1	4:I:93:THR:CG2	3.03	0.41
4:I:64:ASN:C	4:I:313:PHE:O	2.64	0.41
4:H:305:THR:HG22	4:H:308:LEU:HD12	2.02	0.41
4:F:211:GLN:HA	4:F:306:LYS:HE2	2.02	0.41
2:B:400:ARG:HD3	1:C:439:SER:HB3	2.03	0.41
1:C:147:SER:HB2	1:C:190:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:LEU:O	2:D:336:GLN:O	2.38	0.41
4:H:64:ASN:C	4:H:313:PHE:O	2.64	0.41
4:H:147:VAL:HG22	4:H:165:SER:HB3	2.03	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.62	0.40
2:D:69:ASP:HA	2:D:145:THR:HG21	2.03	0.40
1:A:203:MET:O	1:A:302:MET:HE3	2.21	0.40
1:C:214:ARG:HG2	1:C:219:ILE:O	2.21	0.40
2:D:213:CYS:O	2:D:219:LEU:HB2	2.21	0.40
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.40
2:B:286:LEU:HD22	2:B:290:GLU:HB3	2.03	0.40
2:B:212:ILE:HG23	2:B:275:LEU:HD13	2.03	0.40
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	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	422/451 (94%)	409 (97%)	10 (2%)	3 (1%)	18	36
1	C	429/451 (95%)	415 (97%)	10 (2%)	4 (1%)	14	29
2	B	417/445 (94%)	399 (96%)	14 (3%)	4 (1%)	12	26
2	D	413/445 (93%)	391 (95%)	19 (5%)	3 (1%)	18	36
3	E	120/143 (84%)	115 (96%)	3 (2%)	2 (2%)	7	14
4	F	307/383 (80%)	286 (93%)	16 (5%)	5 (2%)	7	15
4	G	338/383 (88%)	321 (95%)	14 (4%)	3 (1%)	14	29
4	H	337/383 (88%)	320 (95%)	15 (4%)	2 (1%)	21	39
4	I	337/383 (88%)	319 (95%)	15 (4%)	3 (1%)	14	29
All	All	3120/3467 (90%)	2975 (95%)	116 (4%)	29 (1%)	14	29

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
1	A	246	GLY
1	A	285	GLN
2	B	286	LEU
1	C	74	VAL
1	C	162	GLY
2	D	180	THR
3	E	13	LYS
4	G	26	GLY
4	G	27	HIS
4	G	307	HIS
4	H	373	PRO
4	I	307	HIS
1	C	164	LYS
3	E	27	PRO
4	I	127	ASP
4	I	282	SER
2	B	57	THR
4	F	3	TYR
4	F	275	ALA
4	F	381	ASN
2	B	278	ARG
2	D	216	THR
4	F	127	ASP
4	H	233	ASN
1	C	286	LEU
4	F	103	PRO
2	B	98	GLY
2	D	98	GLY

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	361/379 (95%)	343 (95%)	18 (5%)	22 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	371/379 (98%)	359 (97%)	12 (3%)	34	59
2	B	366/383 (96%)	353 (96%)	13 (4%)	31	56
2	D	364/383 (95%)	351 (96%)	13 (4%)	31	56
3	E	111/127 (87%)	104 (94%)	7 (6%)	16	34
4	F	282/340 (83%)	263 (93%)	19 (7%)	15	31
4	G	308/340 (91%)	293 (95%)	15 (5%)	22	44
4	H	310/340 (91%)	292 (94%)	18 (6%)	18	37
4	I	309/340 (91%)	290 (94%)	19 (6%)	17	35
All	All	2782/3011 (92%)	2648 (95%)	134 (5%)	23	45

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	68	VAL
1	A	71	GLU
1	A	86	LEU
1	A	88	HIS
1	A	92	LEU
1	A	133	GLN
1	A	163	LYS
1	A	178	SER
1	A	196	GLU
1	A	206	ASN
1	A	252	LEU
1	A	256	GLN
1	A	279	GLU
1	A	282	TYR
1	A	302	MET
1	A	338	LYS
1	A	372	GLN
2	B	26	ASP
2	B	35	SER
2	B	47	GLU
2	B	50	ASN
2	B	71	GLU
2	B	109	THR
2	B	124	LYS
2	B	133	GLN

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Mol	Chain	Res	Type
2	B	177	VAL
2	B	206	ASN
2	B	284	ARG
2	B	318	ILE
2	B	357	ASP
1	C	2	ARG
1	C	39	ASP
1	C	62	VAL
1	C	71	GLU
1	C	86	LEU
1	C	92	LEU
1	C	163	LYS
1	C	164	LYS
1	C	178	SER
1	C	206	ASN
1	C	302	MET
1	C	372	GLN
2	D	26	ASP
2	D	35	SER
2	D	50	ASN
2	D	71	GLU
2	D	85	GLN
2	D	133	GLN
2	D	177	VAL
2	D	180	THR
2	D	223	THR
2	D	275	LEU
2	D	276	THR
2	D	335	VAL
2	D	416	MET
3	E	12	ASN
3	E	13	LYS
3	E	22	VAL
3	E	79	GLU
3	E	88	GLU
3	E	103	GLN
3	E	120	LEU
4	F	21	LEU
4	F	27	HIS
4	F	34	ASP
4	F	53	LEU
4	F	59	LEU

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Mol	Chain	Res	Type
4	F	163	ILE
4	F	171	LEU
4	F	177	GLN
4	F	180	VAL
4	F	182	VAL
4	F	201	ASP
4	F	278	ILE
4	F	285	LEU
4	F	293	ARG
4	F	296	LEU
4	F	306	LYS
4	F	312	SER
4	F	341	GLN
4	F	382	LEU
4	G	31	LEU
4	G	33	ARG
4	G	53	LEU
4	G	59	LEU
4	G	126	THR
4	G	130	GLU
4	G	201	ASP
4	G	235	GLN
4	G	277	ASN
4	G	285	LEU
4	G	296	LEU
4	G	306	LYS
4	G	312	SER
4	G	377	ILE
4	G	383	TYR
4	H	6	VAL
4	H	53	LEU
4	H	59	LEU
4	H	60	VAL
4	H	126	THR
4	H	130	GLU
4	H	141	GLU
4	H	180	VAL
4	H	201	ASP
4	H	232	ASP
4	H	277	ASN
4	H	285	LEU
4	H	296	LEU

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Mol	Chain	Res	Type
4	H	312	SER
4	H	321	MET
4	H	359	VAL
4	H	382	LEU
4	H	384	PHE
4	I	25	THR
4	I	34	ASP
4	I	46	ASN
4	I	53	LEU
4	I	100	VAL
4	I	180	VAL
4	I	201	ASP
4	I	226	SER
4	I	249	GLU
4	I	256	LYS
4	I	277	ASN
4	I	285	LEU
4	I	293	ARG
4	I	296	LEU
4	I	306	LYS
4	I	312	SER
4	I	341	GLN
4	I	364	ASP
4	I	377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	ASN
1	A	88	HIS
1	A	101	ASN
1	A	206	ASN
1	A	226	ASN
1	A	256	GLN
1	A	301	GLN
1	A	356	ASN
1	A	393	HIS
2	B	6	HIS
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN

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Mol	Chain	Res	Type
2	B	15	GLN
2	B	50	ASN
2	B	59	ASN
2	B	107	HIS
2	B	136	GLN
2	B	192	HIS
2	B	193	GLN
2	B	206	ASN
2	B	266	HIS
2	B	309	HIS
2	B	331	GLN
2	B	337	ASN
2	B	339	ASN
2	B	349	ASN
1	C	8	HIS
1	C	11	GLN
1	C	61	HIS
1	C	206	ASN
1	C	226	ASN
1	C	283	HIS
1	C	301	GLN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	15	GLN
2	D	50	ASN
2	D	59	ASN
2	D	85	GLN
2	D	136	GLN
2	D	167	ASN
2	D	186	ASN
2	D	192	HIS
2	D	197	ASN
2	D	249	ASN
2	D	266	HIS
2	D	309	HIS
2	D	336	GLN
2	D	337	ASN
2	D	349	ASN

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Mol	Chain	Res	Type
3	E	91	ASN
4	F	27	HIS
4	F	39	ASN
4	F	197	HIS
4	F	261	ASN
4	F	311	GLN
4	G	39	ASN
4	G	177	GLN
4	G	181	HIS
4	G	230	HIS
4	G	233	ASN
4	G	235	GLN
4	G	311	GLN
4	H	39	ASN
4	H	137	ASN
4	H	177	GLN
4	H	181	HIS
4	H	197	HIS
4	H	230	HIS
4	H	235	GLN
4	H	307	HIS
4	H	311	GLN
4	H	349	GLN
4	I	39	ASN
4	I	177	GLN
4	I	181	HIS
4	I	210	HIS
4	I	230	HIS
4	I	270	GLN
4	I	294	ASN
4	I	311	GLN
4	I	381	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	ACP	F	401	-	31,33,33	1.02	2 (6%)	47,52,52	0.70	2 (4%)
6	GTP	A	502	5	33,34,34	0.51	0	50,54,54	0.49	0
6	GTP	C	502	5	33,34,34	0.52	0	50,54,54	0.50	0
8	ACP	G	401	-	31,33,33	1.24	2 (6%)	47,52,52	0.74	3 (6%)
7	GDP	D	501	-	29,30,30	0.45	0	45,47,47	0.48	0
8	ACP	I	401	-	31,33,33	1.35	2 (6%)	47,52,52	0.72	3 (6%)
7	GDP	B	501	5	29,30,30	0.42	0	45,47,47	0.45	0
8	ACP	H	401	-	31,33,33	1.51	2 (6%)	47,52,52	0.68	2 (4%)

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	ACP	F	401	-	-	7/19/38/38	0/3/3/3
6	GTP	A	502	5	-	5/22/38/38	0/3/3/3
6	GTP	C	502	5	-	5/22/38/38	0/3/3/3
8	ACP	G	401	-	-	6/19/38/38	0/3/3/3
7	GDP	D	501	-	-	6/16/32/32	0/3/3/3
8	ACP	I	401	-	-	6/19/38/38	0/3/3/3
7	GDP	B	501	5	-	6/16/32/32	0/3/3/3
8	ACP	H	401	-	-	6/19/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	401	ACP	PB-O3A	7.72	1.67	1.58
8	I	401	ACP	PB-O3A	6.73	1.65	1.58
8	G	401	ACP	PB-O3A	5.96	1.65	1.58
8	F	401	ACP	PB-O3A	4.46	1.63	1.58
8	F	401	ACP	PB-O2B	-2.44	1.50	1.56
8	G	401	ACP	PB-O2B	-2.26	1.50	1.56
8	H	401	ACP	PB-O2B	-2.16	1.51	1.56
8	I	401	ACP	PB-O2B	-2.11	1.51	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	401	ACP	O2B-PB-O1B	3.05	119.89	109.95
8	G	401	ACP	O2B-PB-O1B	2.71	118.78	109.95
8	I	401	ACP	O2B-PB-O1B	2.71	118.77	109.95
8	H	401	ACP	O2B-PB-O1B	2.56	118.30	109.95
8	G	401	ACP	O1G-PG-C3B	-2.47	105.99	111.37
8	F	401	ACP	O1G-PG-C3B	-2.45	106.03	111.37
8	I	401	ACP	O1G-PG-C3B	-2.30	106.37	111.37
8	H	401	ACP	O1G-PG-C3B	-2.24	106.49	111.37
8	G	401	ACP	PB-O3A-PA	2.23	139.63	132.37
8	I	401	ACP	PB-O3A-PA	2.13	139.32	132.37

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	GTP	C5'-O5'-PA-O3A
6	A	502	GTP	C5'-O5'-PA-O1A
6	A	502	GTP	C5'-O5'-PA-O2A
6	C	502	GTP	PB-O3B-PG-O2G
6	C	502	GTP	C5'-O5'-PA-O3A
6	C	502	GTP	C5'-O5'-PA-O1A
6	C	502	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
7	D	501	GDP	PA-O3A-PB-O2B
7	D	501	GDP	C5'-O5'-PA-O3A
7	D	501	GDP	C5'-O5'-PA-O1A
7	D	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
8	F	401	ACP	PB-C3B-PG-O1G
8	F	401	ACP	PB-C3B-PG-O2G
8	F	401	ACP	PB-C3B-PG-O3G
8	F	401	ACP	PG-C3B-PB-O1B
8	F	401	ACP	PG-C3B-PB-O3A
8	F	401	ACP	PB-O3A-PA-O5'
8	G	401	ACP	PB-C3B-PG-O1G
8	G	401	ACP	PB-C3B-PG-O2G
8	G	401	ACP	PB-C3B-PG-O3G
8	G	401	ACP	PG-C3B-PB-O1B
8	G	401	ACP	PG-C3B-PB-O2B
8	G	401	ACP	PG-C3B-PB-O3A
8	H	401	ACP	PB-C3B-PG-O1G
8	H	401	ACP	PB-C3B-PG-O2G
8	H	401	ACP	PG-C3B-PB-O1B
8	H	401	ACP	PG-C3B-PB-O2B
8	H	401	ACP	PG-C3B-PB-O3A
8	I	401	ACP	PB-C3B-PG-O1G
8	I	401	ACP	PB-C3B-PG-O2G
8	I	401	ACP	PB-C3B-PG-O3G
8	I	401	ACP	PG-C3B-PB-O1B
8	I	401	ACP	PG-C3B-PB-O2B
8	I	401	ACP	PG-C3B-PB-O3A
6	C	502	GTP	PB-O3B-PG-O1G
8	F	401	ACP	O4'-C4'-C5'-O5'
8	H	401	ACP	PB-C3B-PG-O3G
7	B	501	GDP	PB-O3A-PA-O1A
7	B	501	GDP	PB-O3A-PA-O2A
7	B	501	GDP	PA-O3A-PB-O1B
6	A	502	GTP	C4'-C5'-O5'-PA
7	D	501	GDP	C4'-C5'-O5'-PA
7	D	501	GDP	PA-O3A-PB-O1B
6	A	502	GTP	PG-O3B-PB-O2B

There are no ring outliers.

7 monomers are involved in 15 short contacts:

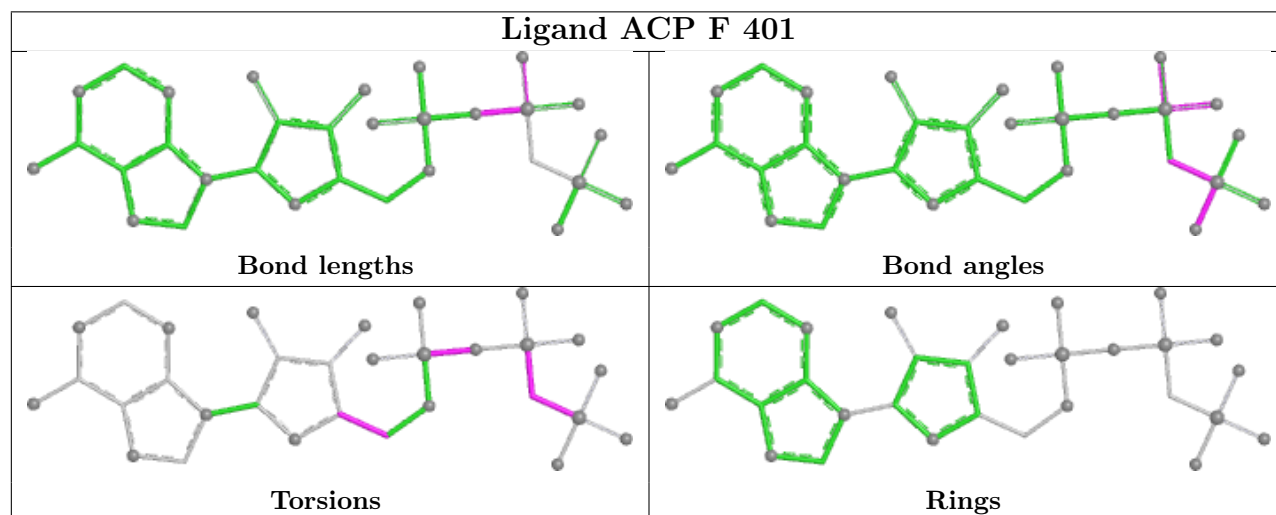
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	401	ACP	1	0
6	A	502	GTP	3	0
6	C	502	GTP	2	0
8	G	401	ACP	3	0

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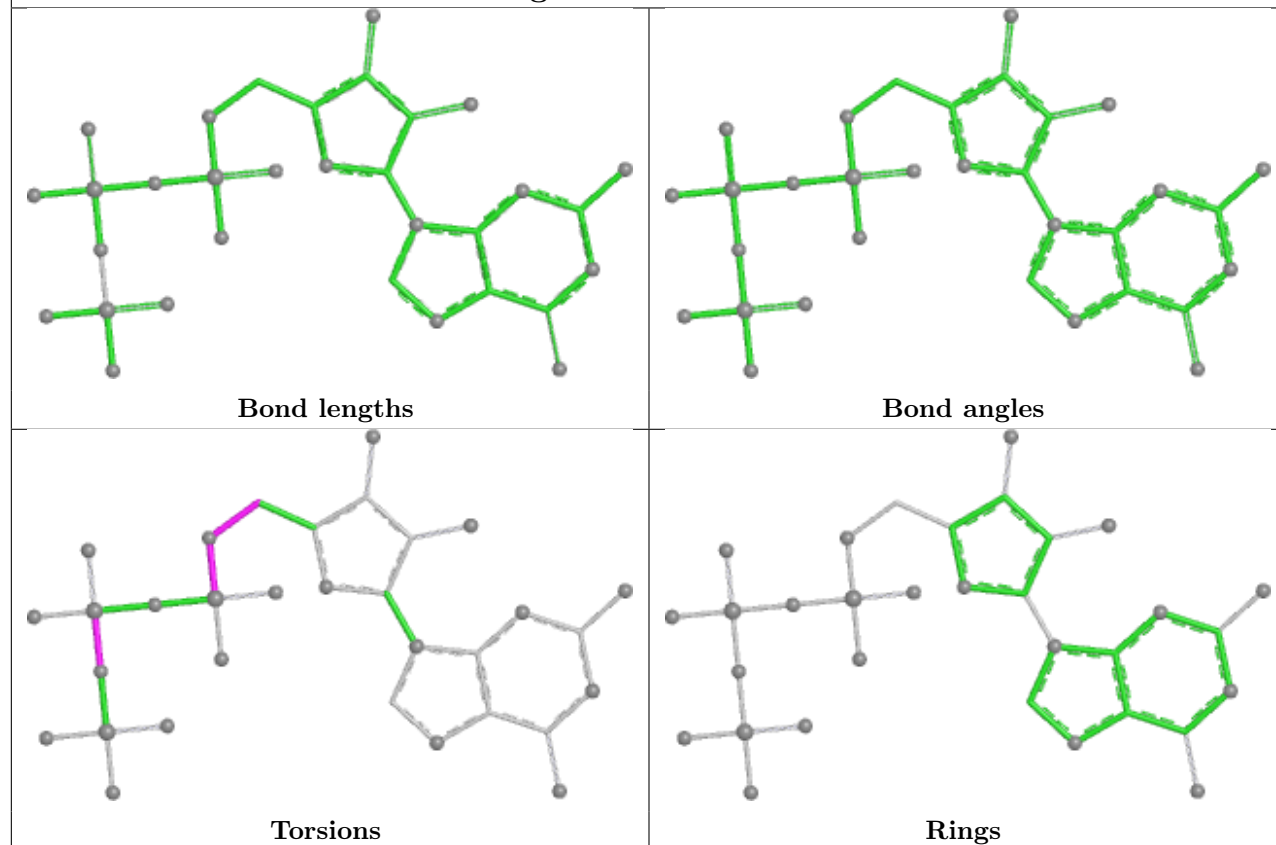
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	501	GDP	1	0
8	I	401	ACP	4	0
7	B	501	GDP	1	0

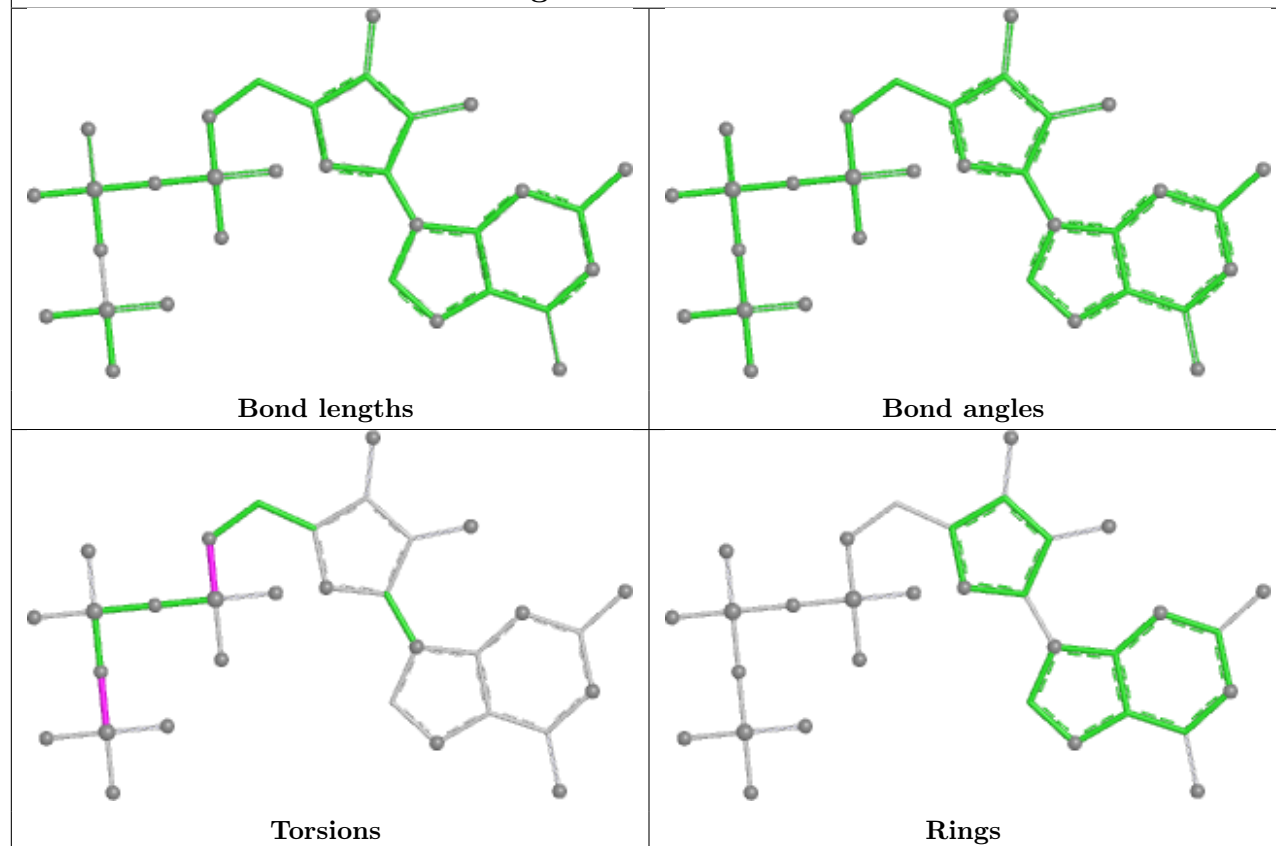
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

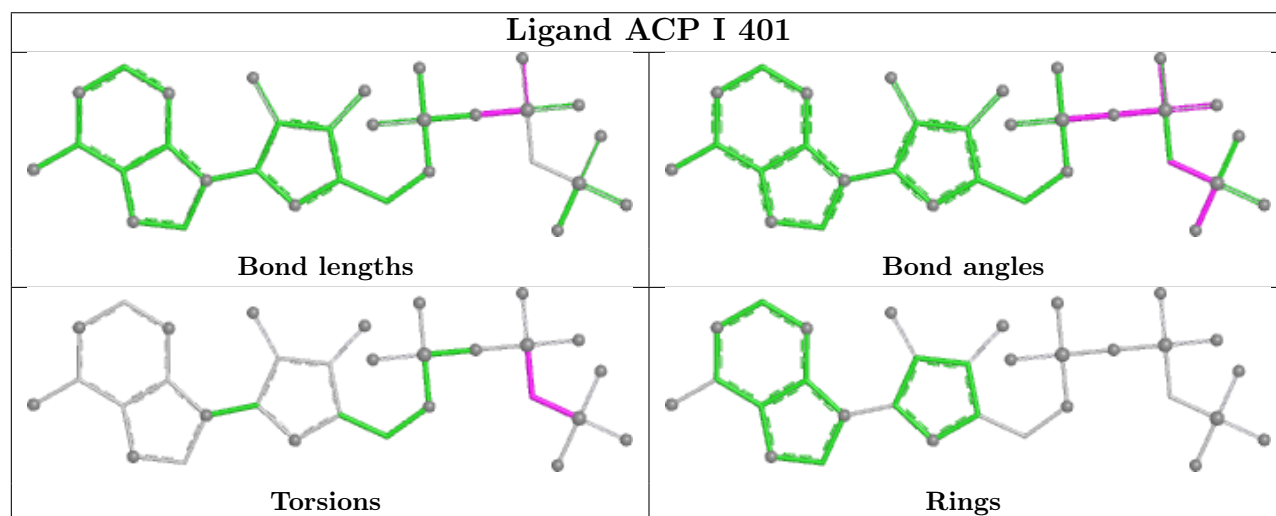
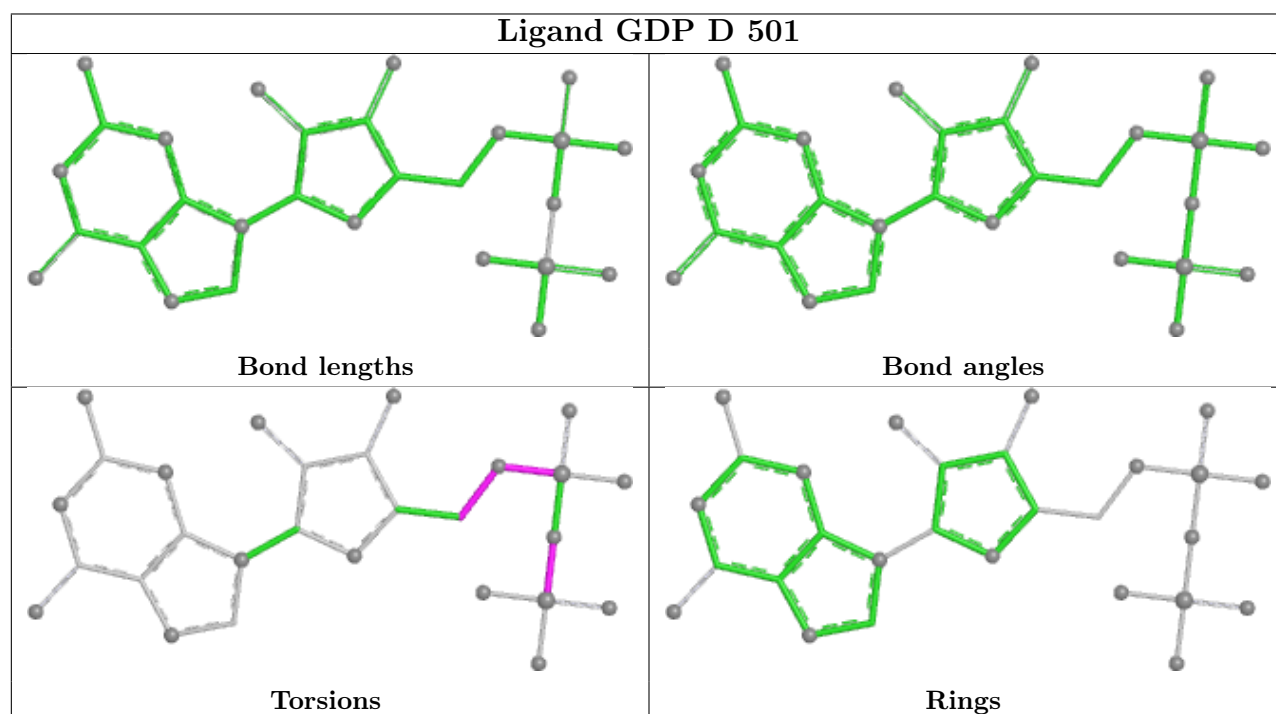
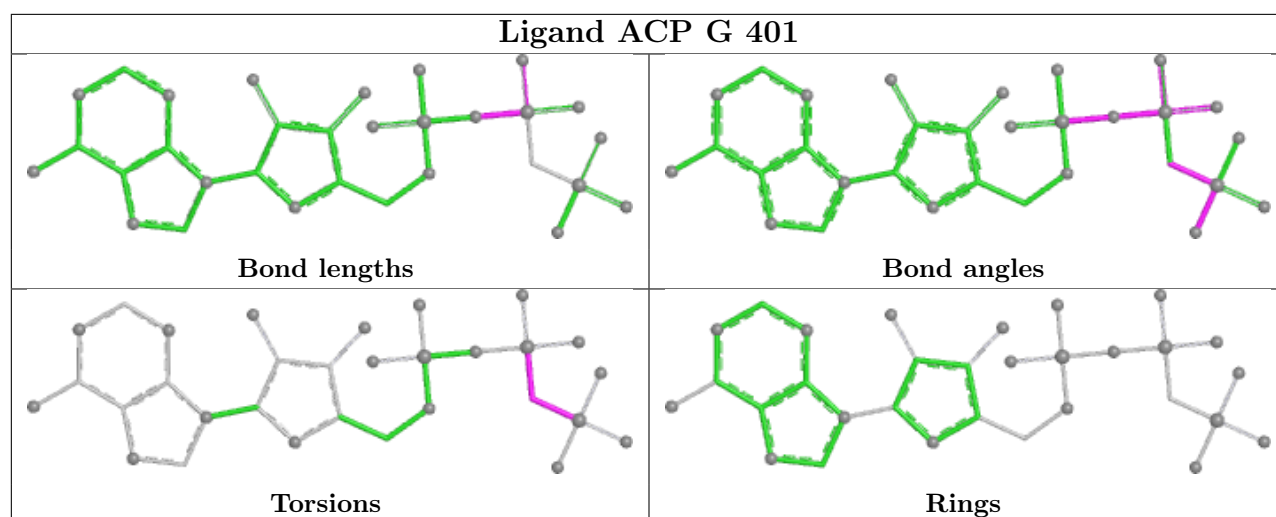


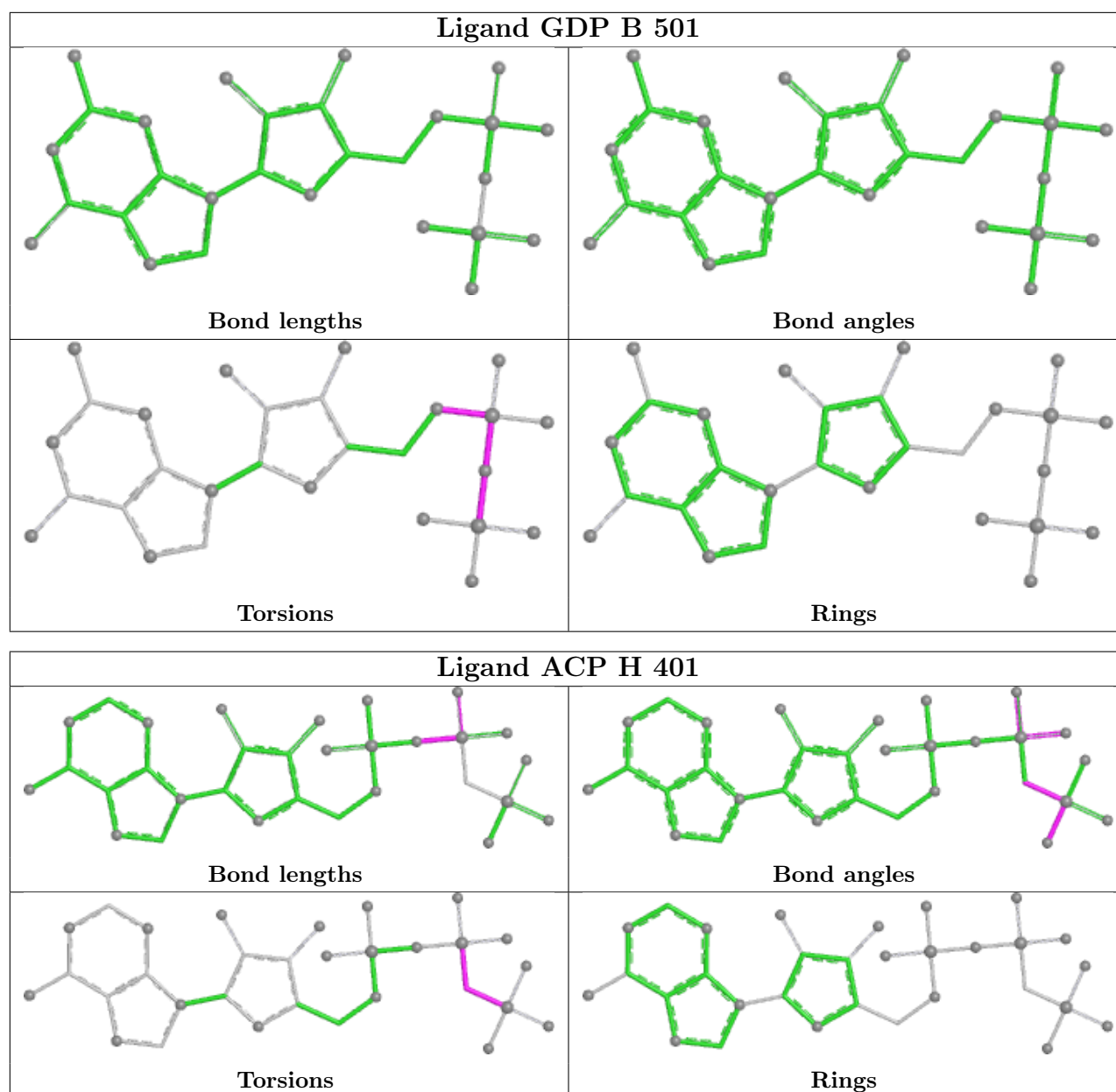
Ligand GTP A 502



Ligand GTP C 502







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	42:LEU	C	45:GLN	N	2.99

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	426/451 (94%)	0.79	38 (8%) 15 12	27, 55, 91, 108	2 (0%)
1	C	430/451 (95%)	0.99	77 (17%) 3 3	24, 55, 92, 112	6 (1%)
2	B	425/445 (95%)	0.47	19 (4%) 38 34	28, 48, 73, 102	1 (0%)
2	D	421/445 (94%)	1.09	71 (16%) 4 3	30, 62, 97, 113	1 (0%)
3	E	123/143 (86%)	1.24	26 (21%) 2 2	19, 67, 92, 101	1 (0%)
4	F	317/383 (82%)	1.64	103 (32%) 1 1	43, 87, 127, 145	5 (1%)
4	G	346/383 (90%)	0.95	34 (9%) 13 10	41, 68, 98, 110	0
4	H	345/383 (90%)	1.20	62 (17%) 3 3	42, 78, 116, 125	1 (0%)
4	I	345/383 (90%)	1.24	63 (18%) 3 3	47, 76, 104, 110	0
All	All	3178/3467 (91%)	1.03	493 (15%) 5 4	19, 65, 107, 145	17 (0%)

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	255	PHE	6.0
4	F	322	VAL	5.8
1	C	252	LEU	5.6
2	B	248	LEU	5.4
1	C	340	SER	5.2
4	I	187	LEU	5.2
4	G	104	THR	5.0
4	F	151	LYS	4.7
1	C	250	VAL	4.7
4	F	162	LEU	4.6
1	A	57	GLY	4.6
4	F	265	PHE	4.6
2	D	220	THR	4.5
1	C	346	TRP	4.5
3	E	23	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	163	LYS	4.4
2	D	438	ALA	4.4
1	C	281	ALA	4.4
1	C	343	PHE	4.3
1	C	258	ASN	4.3
4	F	280	LEU	4.3
2	D	276	THR	4.2
4	G	59	LEU	4.2
4	I	221	VAL	4.2
3	E	24	LEU	4.2
4	G	11	ASN	4.2
4	F	205	TRP	4.2
1	C	351	PHE	4.1
4	F	187	LEU	4.1
4	F	278	ILE	4.1
2	B	42	LEU	4.1
4	F	382	LEU	4.0
4	F	191	LEU	4.0
4	I	234	PHE	3.9
1	C	349	THR	3.9
4	F	104	THR	3.9
1	C	344	VAL	3.9
1	A	282	TYR	3.9
4	F	373	PRO	3.9
1	C	341	ILE	3.9
1	A	351	PHE	3.8
1	C	59	GLY	3.8
4	I	278	ILE	3.8
2	D	277	SER	3.8
1	A	1	MET	3.7
2	D	41	ASP	3.7
4	F	236	ASP	3.7
1	C	339	ARG	3.7
2	B	250	ALA	3.6
4	F	374	ALA	3.6
4	F	149	ILE	3.6
4	H	372	GLN	3.6
3	E	8	VAL	3.6
4	F	182	VAL	3.6
4	I	276	LEU	3.6
4	F	200	PHE	3.6
4	F	284	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	6	HIS	3.5
1	A	346	TRP	3.5
4	H	179	GLN	3.5
4	I	152	SER	3.5
4	I	178	GLY	3.5
3	E	9	ILE	3.5
3	E	83	ILE	3.5
1	C	302	MET	3.5
4	I	182	VAL	3.5
4	I	231	VAL	3.5
2	D	370	GLY	3.5
4	F	225	ALA	3.5
4	I	225	ALA	3.5
4	H	60	VAL	3.5
1	C	439	SER	3.5
4	I	275	ALA	3.5
1	C	296	PHE	3.5
4	F	100	VAL	3.4
4	H	53	LEU	3.4
1	A	83	TYR	3.4
4	F	234	PHE	3.4
1	C	249	ASN	3.4
4	F	231	VAL	3.4
4	F	15	TYR	3.4
4	G	60	VAL	3.4
1	C	34	GLY	3.4
4	I	260	GLY	3.4
4	G	153	SER	3.4
4	F	376	PHE	3.3
4	G	126	THR	3.3
2	D	157	ILE	3.3
3	E	10	GLU	3.3
4	I	150	ALA	3.3
2	B	249	ASN	3.3
4	F	264	PHE	3.3
4	F	330	LEU	3.3
1	C	56	THR	3.3
4	H	5	PHE	3.2
4	I	162	LEU	3.2
2	B	276	THR	3.2
4	F	341	GLN	3.2
4	I	364	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
4	H	102	TYR	3.2
4	I	200	PHE	3.2
4	G	53	LEU	3.2
4	F	271	TYR	3.2
4	F	201	ASP	3.2
4	F	276	LEU	3.2
1	A	288	VAL	3.2
4	I	160	GLY	3.2
1	C	253	THR	3.2
1	A	262	TYR	3.1
1	C	288	VAL	3.1
4	H	6	VAL	3.1
1	A	110	ILE	3.1
1	C	291	ILE	3.1
1	C	251	ASP	3.1
4	F	195	PRO	3.1
2	D	216	THR	3.1
4	F	126	THR	3.1
1	C	295	CYS	3.1
4	F	331	ILE	3.1
4	I	363	PRO	3.1
2	B	130	ASP	3.1
4	H	59	LEU	3.1
4	G	2	GLY	3.1
4	F	202	ILE	3.1
4	F	328	VAL	3.1
3	E	21	GLU	3.0
2	D	241	CYS	3.0
4	G	382	LEU	3.0
3	E	90	ASN	3.0
1	C	335	ILE	3.0
1	C	348	PRO	3.0
1	C	167	LEU	3.0
1	A	342	GLN	3.0
1	C	361	THR	3.0
1	C	283	HIS	3.0
1	A	37	PRO	3.0
4	I	254	TYR	3.0
4	H	382	LEU	3.0
1	C	315[A]	CYS	3.0
1	C	380	ASN	3.0
4	I	11	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
4	H	134	ALA	2.9
4	H	309	PRO	2.9
4	F	193	LEU	2.9
4	F	272	LEU	2.9
4	H	132	PHE	2.9
4	H	51	GLY	2.9
4	F	288	ILE	2.9
3	E	15	THR	2.9
3	E	78	HIS	2.9
4	F	375	ALA	2.9
1	C	37	PRO	2.9
1	C	282	TYR	2.9
1	C	254	GLU	2.9
2	B	358	ILE	2.9
2	D	318	ILE	2.9
4	I	18	VAL	2.9
1	C	2	ARG	2.9
2	D	132	LEU	2.9
4	F	217	TYR	2.9
4	H	384	PHE	2.9
2	B	281	GLN	2.9
2	D	212	ILE	2.9
4	G	101	ILE	2.9
3	E	22	VAL	2.9
2	D	287	THR	2.9
4	I	241	LEU	2.9
4	F	266	LYS	2.8
4	G	82	ILE	2.8
1	C	1	MET	2.8
1	C	345	ASP	2.8
2	D	34	GLY	2.8
2	D	164	ARG	2.8
4	F	292	ILE	2.8
4	H	377	ILE	2.8
4	F	150	ALA	2.8
1	A	70	LEU	2.8
3	E	93	PHE	2.8
4	H	350	GLY	2.8
2	D	68	VAL	2.8
4	H	359	VAL	2.8
4	I	126	THR	2.8
4	G	42	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	I	191	LEU	2.8
1	C	347[A]	CYS	2.8
1	A	47	ASP	2.8
4	F	131	PHE	2.8
4	F	190	PRO	2.8
4	F	279	THR	2.8
4	F	285	LEU	2.8
4	H	313	PHE	2.8
4	F	163	ILE	2.7
4	G	331	ILE	2.7
2	D	227	LEU	2.7
4	F	326	LEU	2.7
1	A	343	PHE	2.7
1	C	435	VAL	2.7
2	B	283	TYR	2.7
3	E	11	LEU	2.7
4	H	133	LEU	2.7
4	F	147	VAL	2.7
2	D	217	LEU	2.7
4	F	199	LYS	2.7
4	G	237	LYS	2.7
1	C	221	ARG	2.7
4	H	68	GLY	2.7
4	I	176	ASN	2.7
4	G	45	ARG	2.7
2	D	360	PRO	2.6
3	E	14	CYS	2.6
4	H	50	PHE	2.6
4	G	180	VAL	2.6
4	I	249	GLU	2.6
2	D	36	TYR	2.6
4	H	28	TRP	2.6
2	D	379	GLY	2.6
4	I	335	GLY	2.6
1	A	179	THR	2.6
4	F	148	TRP	2.6
4	H	57	PRO	2.6
4	G	62	LEU	2.6
1	C	285	GLN	2.6
2	B	247	GLN	2.6
3	E	27	PRO	2.6
4	I	272	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	13	LYS	2.6
4	I	229	TYR	2.6
2	D	1	MET	2.5
4	H	178	GLY	2.5
4	H	363	PRO	2.5
1	A	341	ILE	2.5
2	D	83	PHE	2.5
4	G	132	PHE	2.5
1	C	375	VAL	2.5
4	F	230	HIS	2.5
2	D	35	SER	2.5
4	F	274	SER	2.5
1	C	32	PRO	2.5
1	C	39	ASP	2.5
4	F	192	LEU	2.5
4	F	315	LEU	2.5
4	H	42	LEU	2.5
4	I	179	GLN	2.5
1	A	437	VAL	2.5
1	C	177	VAL	2.5
2	D	177	VAL	2.5
4	H	43	GLY	2.5
4	G	174	ILE	2.5
2	D	219	LEU	2.5
4	G	50	PHE	2.5
2	D	218	LYS	2.5
3	E	82	VAL	2.5
4	H	126	THR	2.5
3	E	45	PRO	2.5
1	C	81	GLY	2.5
4	I	246	ILE	2.5
2	D	230	LEU	2.5
2	D	242	LEU	2.5
4	H	315	LEU	2.5
1	A	49	PHE	2.5
4	H	14	VAL	2.5
4	H	277	ASN	2.5
4	G	24	ALA	2.5
2	D	221	THR	2.5
4	G	160	GLY	2.4
1	C	438	ASP	2.4
3	E	25	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	174	ILE	2.4
4	I	136	TYR	2.4
3	E	47	LEU	2.4
4	H	31	LEU	2.4
1	C	91	GLN	2.4
2	D	87	PHE	2.4
4	F	173	PHE	2.4
4	I	316	PHE	2.4
4	I	384	PHE	2.4
4	I	242	THR	2.4
3	E	16	SER	2.4
3	E	142	GLU	2.4
4	F	143	GLY	2.4
1	A	86	LEU	2.4
1	A	285	GLN	2.4
2	D	209	LEU	2.4
4	F	216	LEU	2.4
4	H	171	LEU	2.4
4	F	181	HIS	2.4
1	A	324	VAL	2.4
4	H	63	VAL	2.4
2	D	323	MET	2.4
1	A	56	THR	2.4
2	B	360	PRO	2.4
1	C	366	GLY	2.4
4	F	145	GLY	2.4
1	A	295	CYS	2.4
2	D	414	ASP	2.4
4	F	336	ALA	2.4
1	C	370	LYS	2.4
4	G	57	PRO	2.4
2	D	40	SER	2.4
2	D	248	LEU	2.4
4	H	308	LEU	2.4
1	C	202	PHE	2.4
4	F	318	PHE	2.4
1	C	65	ALA	2.4
1	C	280	LYS	2.4
2	B	438	ALA	2.4
4	G	342	LYS	2.4
4	I	167	ALA	2.4
1	C	82	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	H	373	PRO	2.3
4	I	195	PRO	2.3
1	C	287	SER	2.3
1	C	246	GLY	2.3
4	G	278	ILE	2.3
4	I	183	ILE	2.3
4	I	230	HIS	2.3
4	I	379	LEU	2.3
3	E	96	MET	2.3
1	C	49	PHE	2.3
1	C	169	PHE	2.3
4	F	186	TYR	2.3
4	H	3	TYR	2.3
2	D	238	VAL	2.3
1	A	261	PRO	2.3
2	D	278	ARG	2.3
1	C	313	MET	2.3
4	H	239	CYS	2.3
2	D	61	TYR	2.3
4	F	221	VAL	2.3
4	F	324	GLU	2.3
1	C	298	PRO	2.3
2	D	307	PRO	2.3
4	I	228	PRO	2.3
1	C	337	THR	2.3
2	B	370	GLY	2.3
2	D	281	GLN	2.3
4	F	226	SER	2.3
1	C	242	LEU	2.3
1	C	248	LEU	2.3
1	C	276	ILE	2.3
4	I	193	LEU	2.3
4	F	132	PHE	2.3
4	H	38	PHE	2.3
4	I	95	PHE	2.3
4	I	132	PHE	2.3
1	A	88	HIS	2.3
2	B	97	SER	2.3
4	F	282	SER	2.3
4	H	181	HIS	2.3
1	A	114	ILE	2.3
1	A	132	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	332	ILE	2.3
2	D	30	ILE	2.3
4	F	23	LEU	2.3
4	F	379	LEU	2.3
2	D	75	MET	2.3
2	D	373	MET	2.3
1	A	87	PHE	2.3
1	A	296	PHE	2.3
1	A	68	VAL	2.3
4	F	206	VAL	2.3
1	C	247	ALA	2.2
2	D	52	TYR	2.3
3	E	12	ASN	2.2
1	A	340	SER	2.2
1	C	286	LEU	2.2
2	B	373	MET	2.2
4	F	168	SER	2.2
4	F	321	MET	2.2
4	I	163	ILE	2.2
2	D	272	PHE	2.2
4	H	173	PHE	2.2
1	A	250	VAL	2.2
4	I	45	ARG	2.2
4	F	338	ALA	2.2
4	H	137	ASN	2.2
1	C	357	TYR	2.2
4	F	229	TYR	2.2
4	F	184	GLN	2.2
4	I	145	GLY	2.2
4	F	170	LEU	2.2
4	I	232	ASP	2.2
1	C	297	GLU	2.2
2	D	400	ARG	2.2
4	I	264	PHE	2.2
4	G	381	ASN	2.2
4	I	237	LYS	2.2
4	I	271	TYR	2.2
2	D	81	GLY	2.2
4	F	343	LEU	2.2
4	H	326	LEU	2.2
2	D	16	ILE	2.2
4	F	214	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	297	ASP	2.2
1	C	362	VAL	2.2
2	D	93	VAL	2.2
3	E	86	ALA	2.2
4	H	69	ALA	2.2
2	B	436	GLN	2.2
2	D	136	GLN	2.2
4	F	3	TYR	2.2
4	F	21	LEU	2.2
4	G	54	GLY	2.2
1	C	5	ILE	2.2
4	G	70	ASP	2.2
1	C	215	ARG	2.2
4	F	362	PRO	2.2
4	H	131	PHE	2.2
2	B	285	ALA	2.1
1	A	286	LEU	2.1
1	C	179	THR	2.1
2	D	73	GLY	2.1
4	I	192	LEU	2.1
4	I	224	THR	2.1
2	D	224	TYR	2.1
4	F	102	TYR	2.1
4	I	202	ILE	2.1
4	I	250	TYR	2.1
4	F	204	SER	2.1
1	C	60	LYS	2.1
4	H	103	PRO	2.1
2	B	407	TRP	2.1
4	F	268	PHE	2.1
4	F	313	PHE	2.1
4	F	316	PHE	2.1
4	F	333	VAL	2.1
4	F	352	VAL	2.1
4	I	244	HIS	2.1
4	I	263	MET	2.1
2	D	233	ALA	2.1
4	F	167	ALA	2.1
4	I	374	ALA	2.1
2	D	223	THR	2.1
4	F	171	LEU	2.1
4	H	23	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	84	THR	2.1
1	A	219	ILE	2.1
2	D	378	ILE	2.1
1	C	359	PRO	2.1
2	D	173	PRO	2.1
4	F	7	VAL	2.1
4	G	6	VAL	2.1
4	H	299	VAL	2.1
4	I	180	VAL	2.1
4	F	28	TRP	2.1
4	I	134	ALA	2.1
2	D	321	GLY	2.1
4	F	207	LEU	2.1
4	H	293	ARG	2.1
4	F	219	GLU	2.1
4	G	383	TYR	2.1
1	A	298	PRO	2.1
2	D	94	PHE	2.1
4	H	206	VAL	2.1
1	A	289	ALA	2.1
4	F	223	ARG	2.1
4	G	51	GLY	2.1
4	H	52	ARG	2.1
4	H	145	GLY	2.1
2	D	74	THR	2.1
4	H	238	THR	2.1
2	D	204	ILE	2.1
2	D	213	CYS	2.1
4	G	96	PRO	2.1
4	H	36	PRO	2.1
4	F	22	LEU	2.0
4	H	216	LEU	2.0
4	I	46	ASN	2.0
3	E	79	GLU	2.0
2	D	57	THR	2.0
2	D	66	ILE	2.0
4	H	303	ILE	2.0
1	C	245	ASP	2.0
1	A	348	PRO	2.0
4	F	263	MET	2.0
4	G	12	SER	2.0
4	F	307	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	15	GLN	2.0
2	D	203	CYS	2.0
2	D	288	VAL	2.0
4	F	5	PHE	2.0
4	G	359	VAL	2.0
4	H	37	ARG	2.0
4	H	241	LEU	2.0
2	D	38	GLY	2.0
4	I	243	ASN	2.0
2	B	30	ILE	2.0
4	F	273	THR	2.0
4	I	161	ILE	2.0
4	F	329	TRP	2.0
2	D	332	MET	2.0
4	H	15	TYR	2.0
4	H	383	TYR	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
8	ACP	F	401	31/31	0.80	0.31	74,75,79,79	31
8	ACP	I	401	31/31	0.80	0.18	112,113,118,118	4
8	ACP	H	401	31/31	0.87	0.14	85,88,100,100	0
8	ACP	G	401	31/31	0.89	0.12	73,77,91,91	0
7	GDP	D	501	28/28	0.93	0.11	56,58,59,59	0
5	MG	A	501	1/1	0.94	0.25	42,42,42,42	0
5	MG	B	503	1/1	0.96	0.06	51,51,51,51	0

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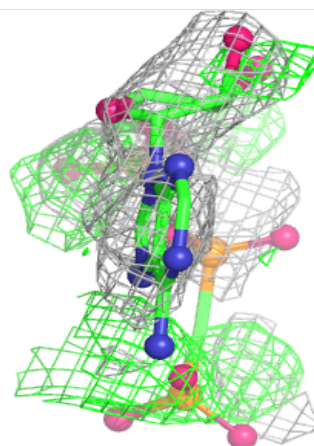
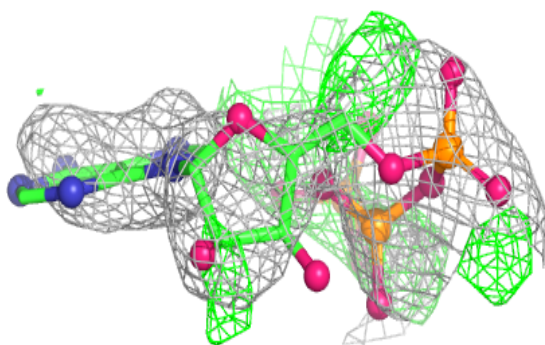
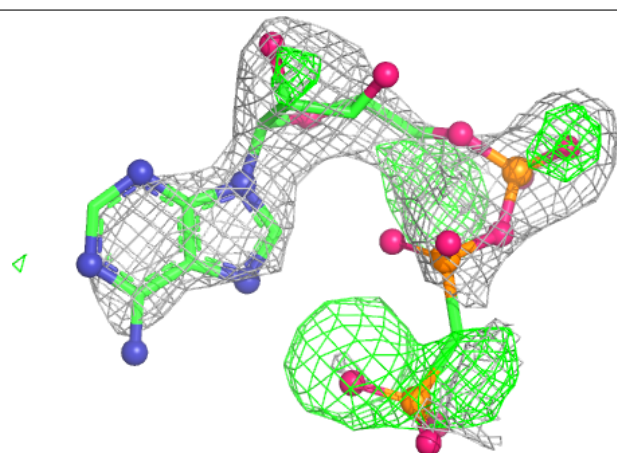
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	502	1/1	0.97	0.04	32,32,32,32	0
5	MG	C	501	1/1	0.97	0.10	33,33,33,33	0
6	GTP	A	502	32/32	0.97	0.06	36,38,39,39	0
6	GTP	C	502	32/32	0.97	0.07	37,43,43,43	0
7	GDP	B	501	28/28	0.97	0.06	34,37,38,39	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.

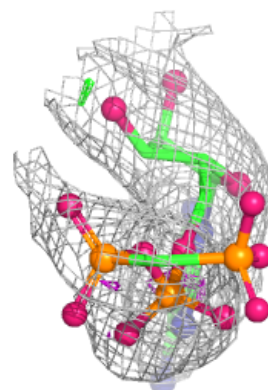
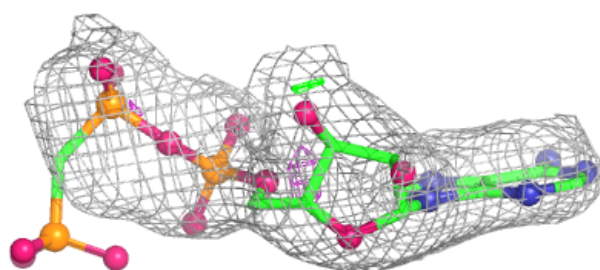
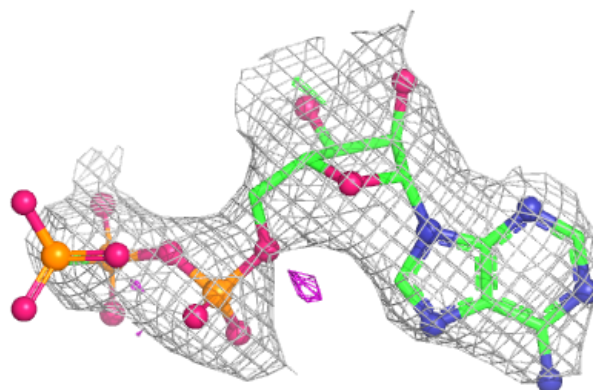
Electron density around ACP F 401:

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

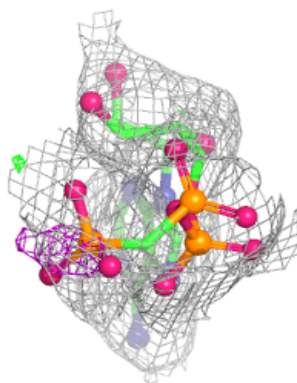
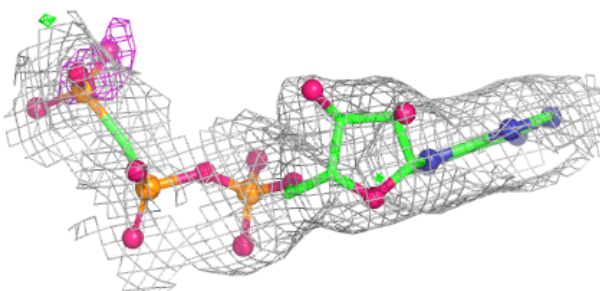
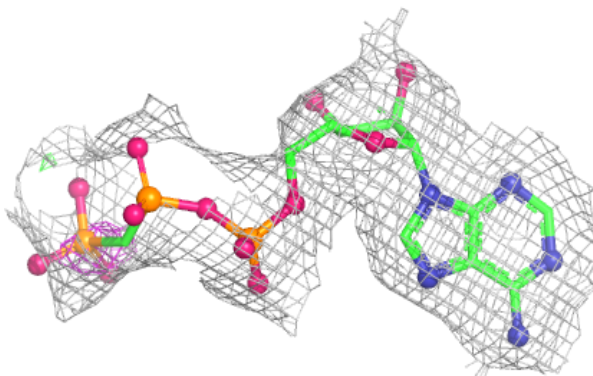


Electron density around ACP I 401:

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

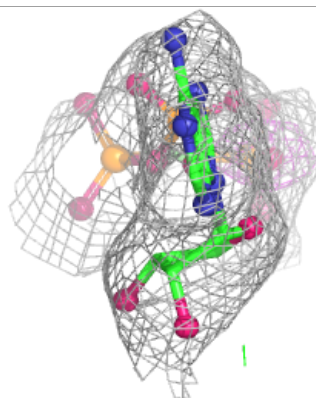
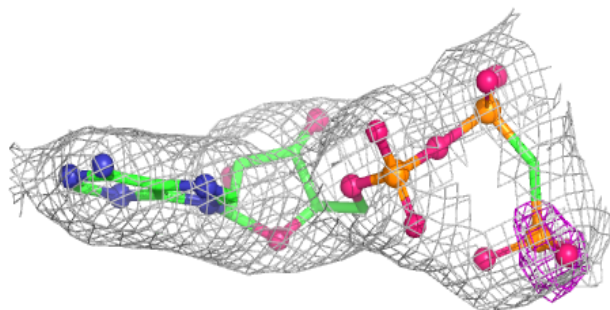
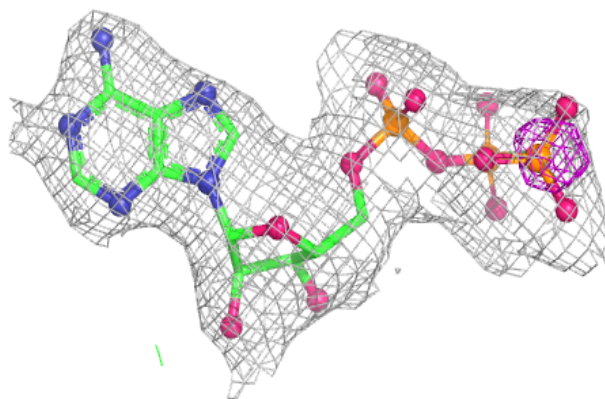
**Electron density around ACP H 401:**

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



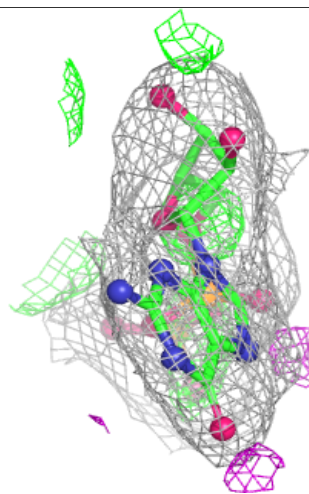
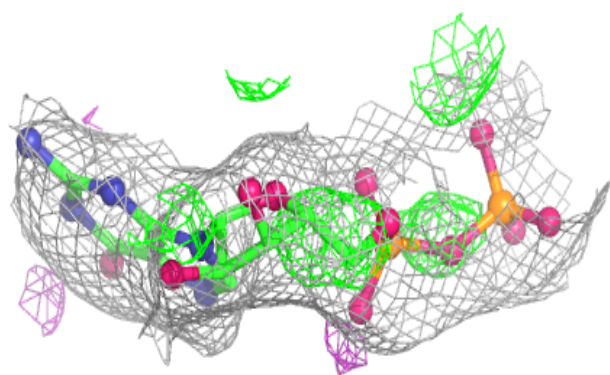
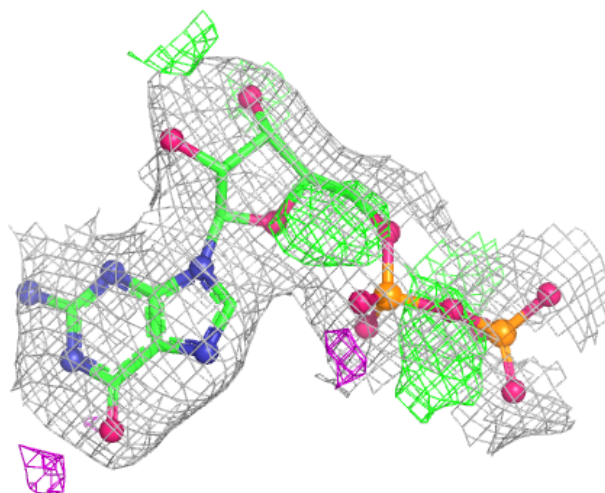
Electron density around ACP G 401:

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



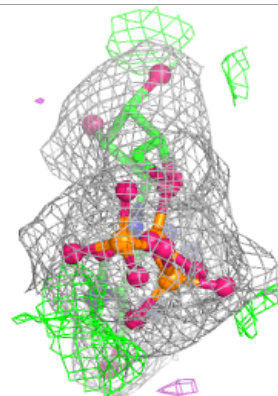
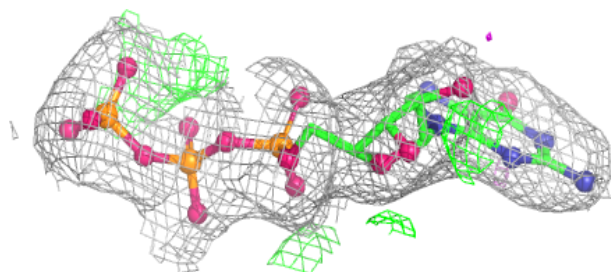
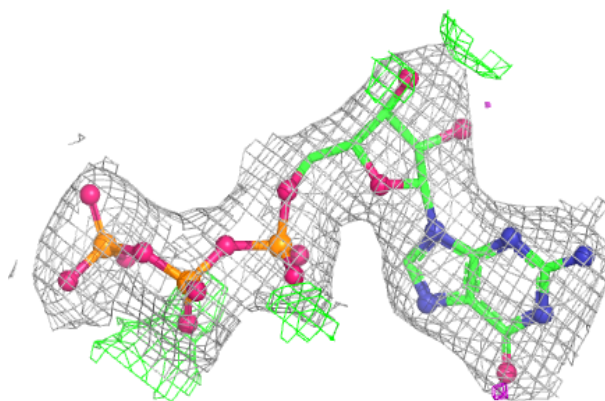
Electron density around GDP D 501:

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

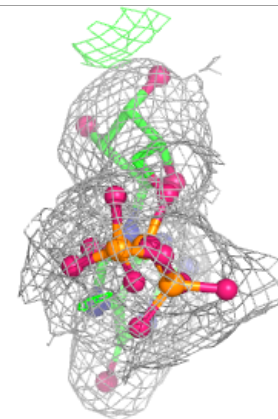
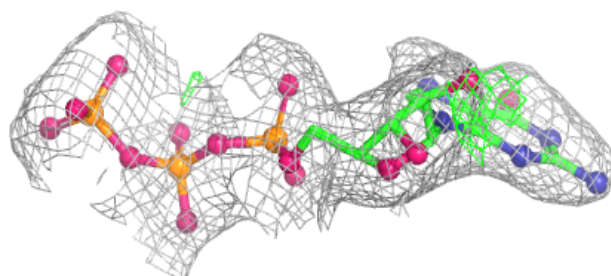
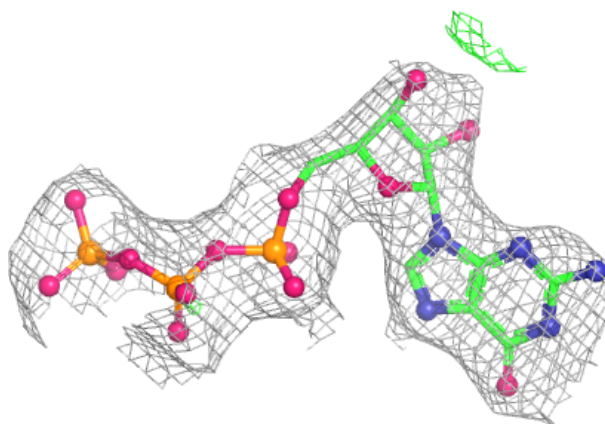


Electron density around GTP A 502:

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

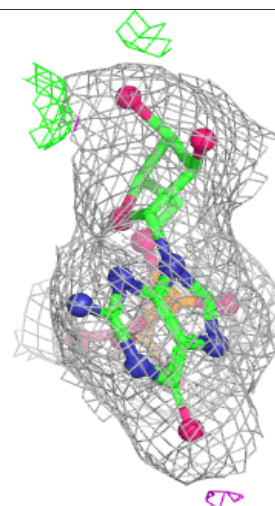
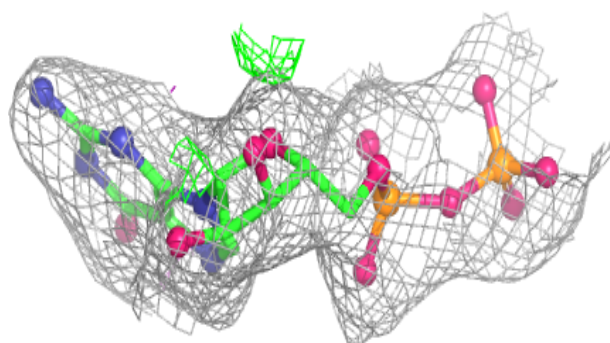
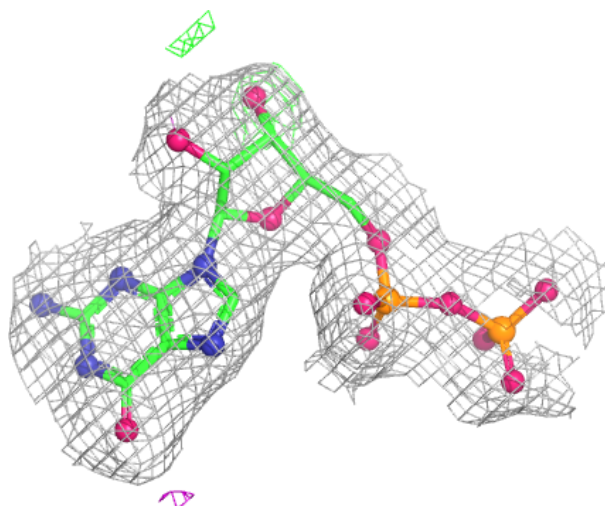
**Electron density around GTP C 502:**

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



Electron density around 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.