



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:48 AM UTC

PDB ID : 9FYD / pdb_00009fyd
Title : tubulin - cryptophycin-uD[Dab] complex
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Deposited on : 2024-07-03
Resolution : 2.30 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

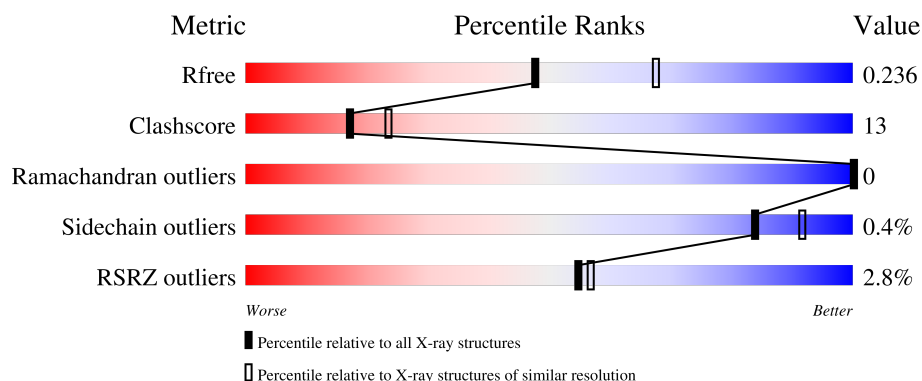
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	2% 71% 25% .
1	C	451	2% 77% 21% .
2	B	445	0% 70% 26% .
2	D	445	3% 65% 31% .
3	E	143	4% 64% 20% 16%

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '4%', followed by a large green segment labeled '64%', a yellow segment labeled '22%', and a small grey segment at the end labeled '14%'.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18038 atoms, of which 84 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	437	Total	C	N	O	S	0	10	0
			3465	2200	584	656	25			
1	C	440	Total	C	N	O	S	0	2	0
			3450	2184	586	658	22			

- 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	1	0
			3355	2108	574	646	27			
2	D	426	Total	C	N	O	S	0	0	0
			3343	2098	570	648	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			996	614	180	197	5			

There are 2 discrepancies between the modelled and reference sequences:

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

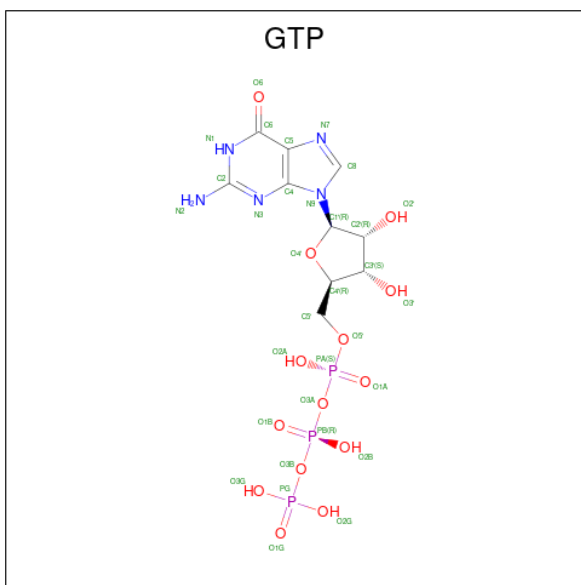
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	0	0
			2725	1752	465	494	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

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



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

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

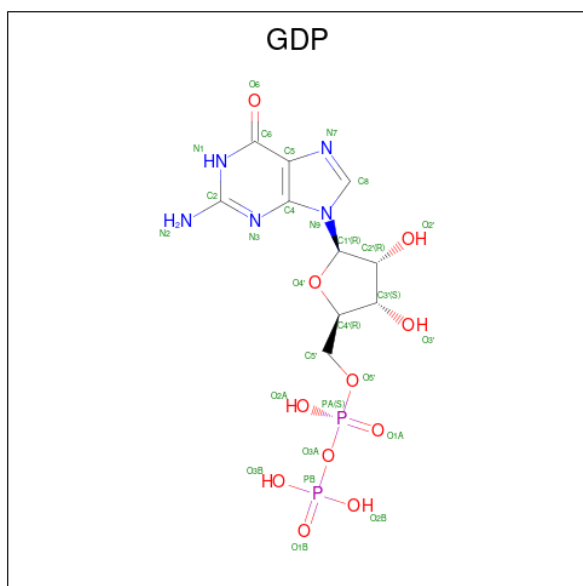
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	1	Total Ca 1 1	0	0

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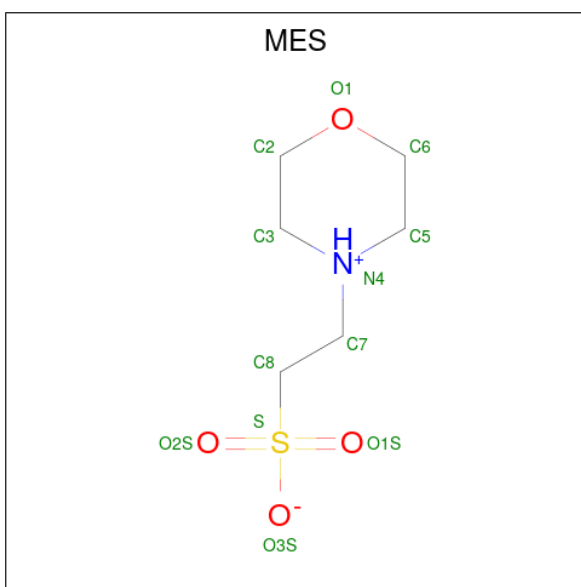
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



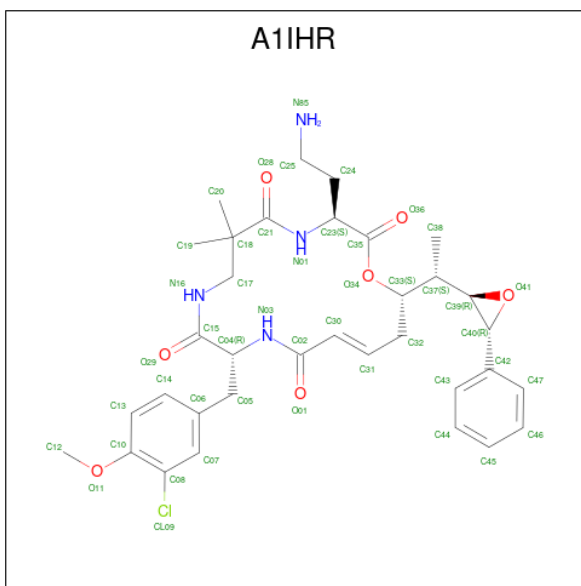
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



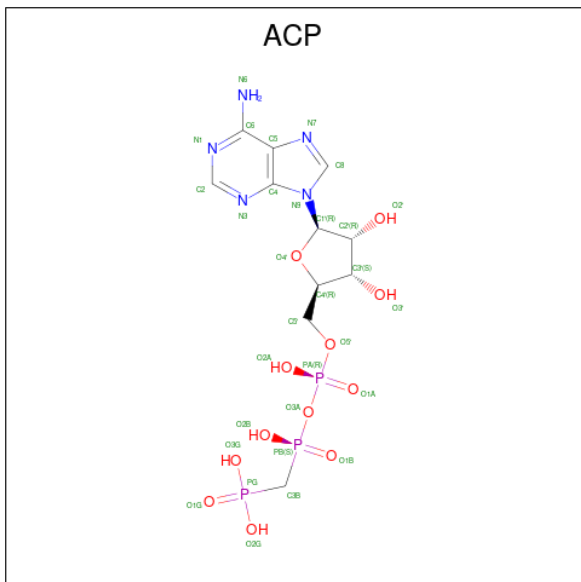
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is cryptophycin-uD[Dab] (CCD ID: A1IHR) (formula: $C_{34}H_{43}ClN_4O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	D	1	Total 88	C 34	Cl 1	H 42	N 4	O 7	0	0
10	D	1	Total 88	C 34	Cl 1	H 42	N 4	O 7	0	0

- 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

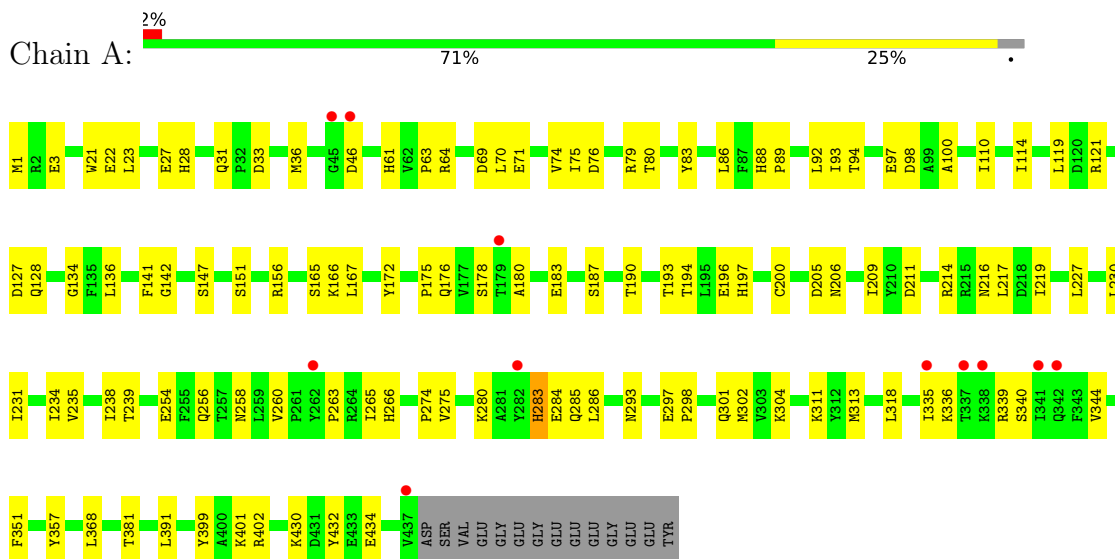
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	55	Total O 55 55	0	0
12	B	68	Total O 68 68	0	0
12	C	157	Total O 157 157	0	0
12	D	41	Total O 41 41	0	0
12	E	21	Total O 21 21	0	0
12	F	14	Total O 14 14	0	0

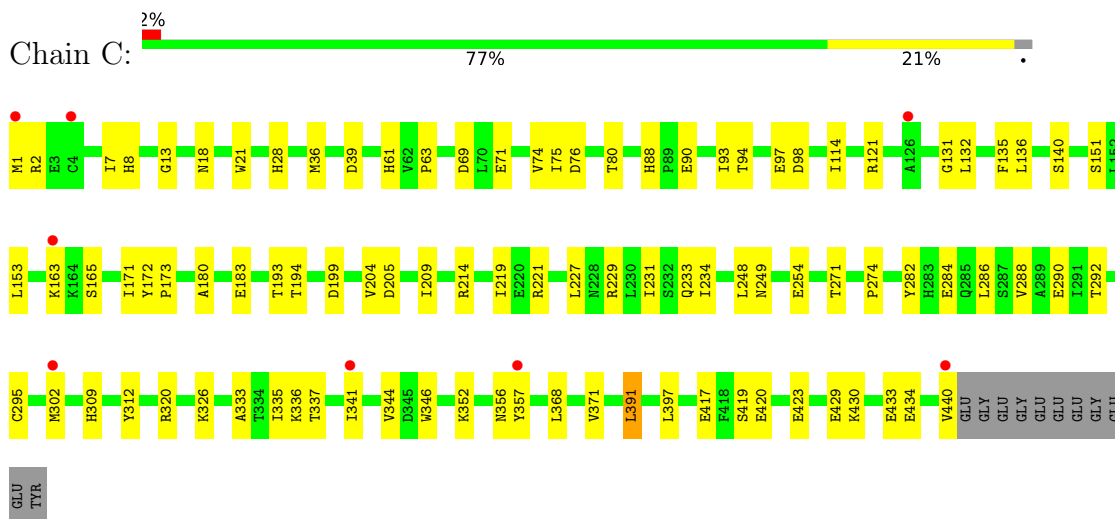
3 Residue-property plots [i](#)

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

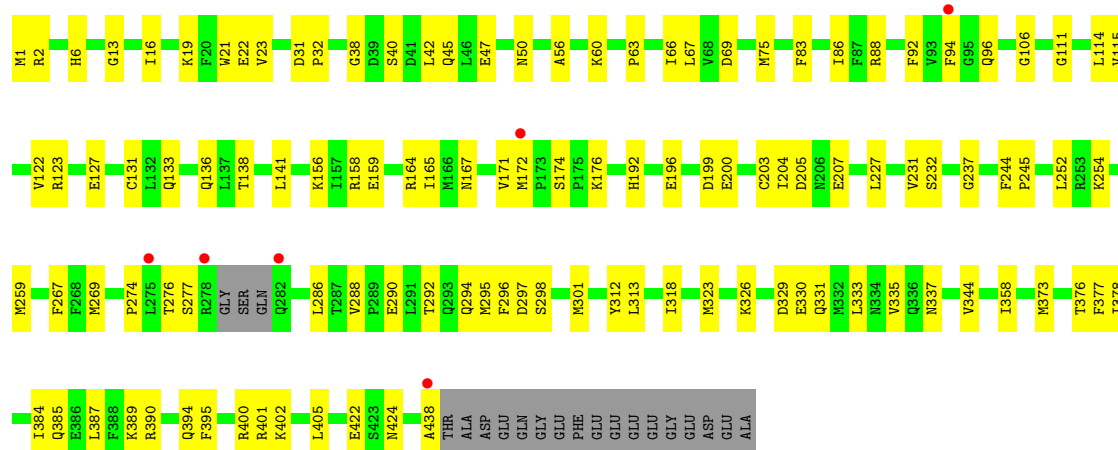


- Molecule 1: Tubulin alpha-1B chain

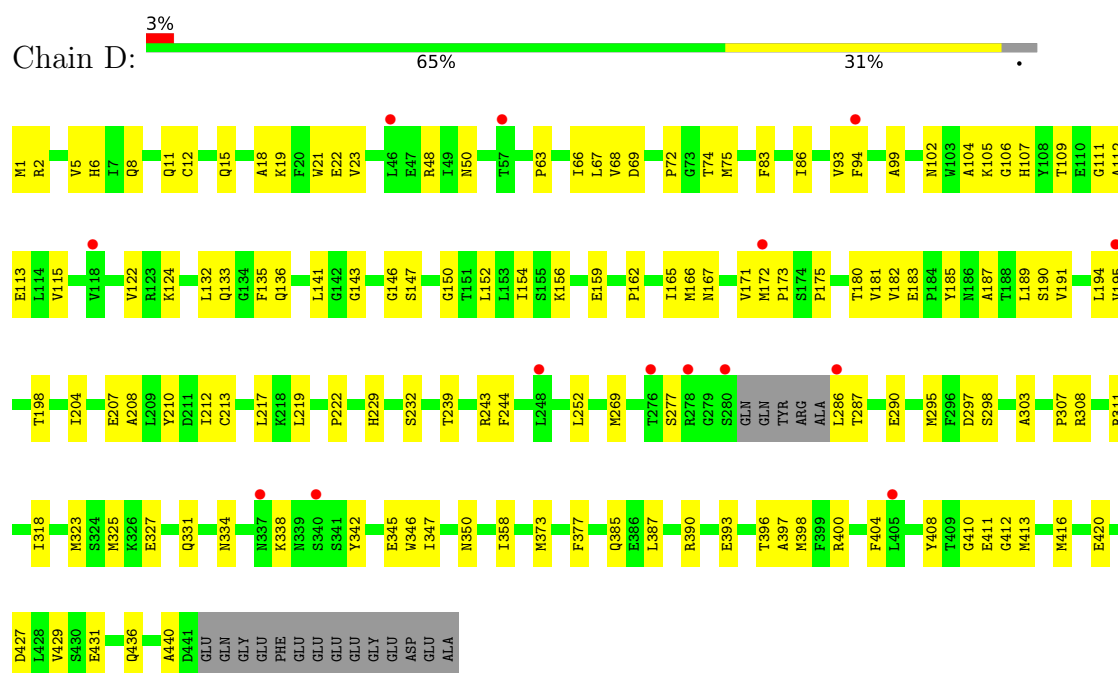


- Molecule 2: Tubulin beta-2B chain

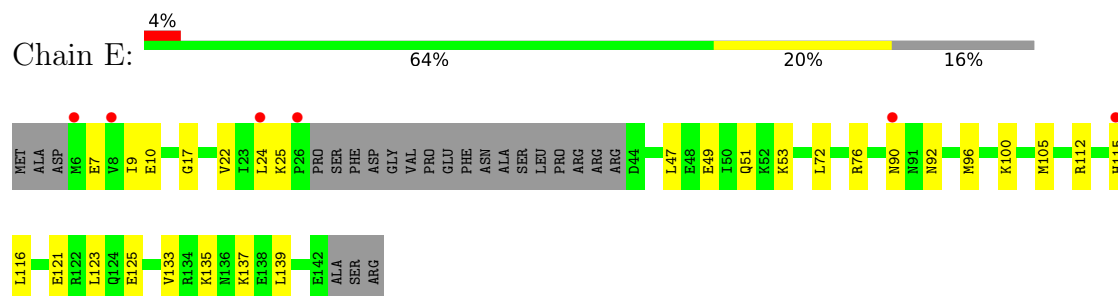




• Molecule 2: Tubulin beta-2B chain

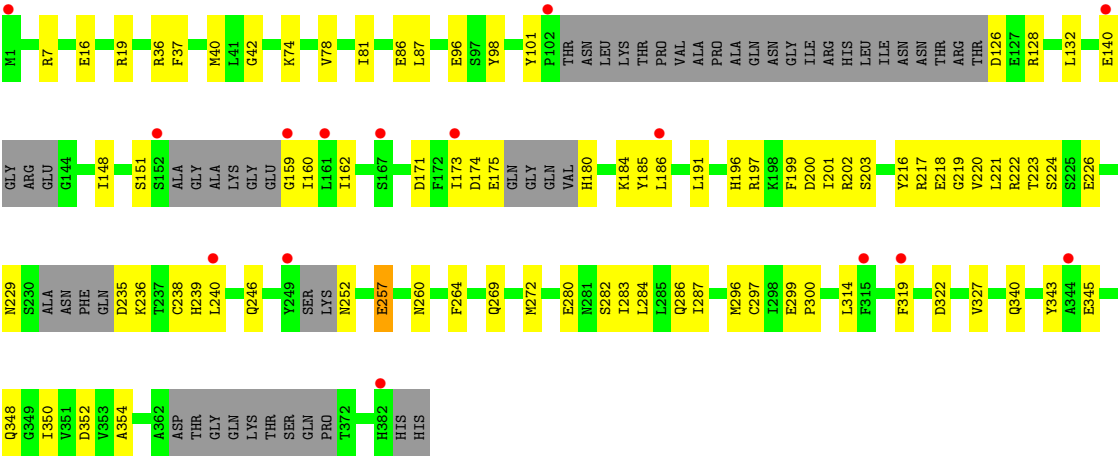


• Molecule 3: Stathmin-4



• 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	104.14Å 157.67Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.30 49.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.37-2.30) 99.5 (49.37-2.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.200 , 0.236 0.201 , 0.236	Depositor DCC
R_{free} test set	6569 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18038	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, A1IHR, GDP, MES, MG, GTP, CA

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	0.10	0/3570	0.25	0/4846
1	C	0.13	0/3535	0.30	0/4800
2	B	0.11	0/3432	0.27	0/4647
2	D	0.10	0/3416	0.25	0/4626
3	E	0.10	0/1003	0.19	0/1329
4	F	0.08	0/2786	0.23	0/3759
All	All	0.11	0/17742	0.26	0/24007

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	3465	0	3406	99	0
1	C	3450	0	3361	80	0
2	B	3355	0	3239	89	0
2	D	3343	0	3222	101	0
3	E	996	0	1012	32	0
4	F	2725	0	2687	65	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	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	2	0
9	B	12	0	12	1	0
10	D	92	84	0	2	0
11	F	31	0	14	1	0
12	A	55	0	0	7	0
12	B	68	0	0	7	0
12	C	157	0	0	10	0
12	D	41	0	0	3	0
12	E	21	0	0	4	0
12	F	14	0	0	2	0
All	All	17954	84	17001	437	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.33	1.10
1:C:234:ILE:HG21	1:C:302:MET:HE1	1.50	0.93
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.50	0.92
1:A:234:ILE:HG12	1:A:302[B]:MET:HE2	1.53	0.91
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.58	0.85
4:F:296:MET:HG2	12:F:502:HOH:O	1.78	0.83
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.62	0.81
2:B:424:ASN:HB3	12:B:648:HOH:O	1.80	0.81
3:E:9:ILE:HG22	3:E:10:GLU:HG3	1.63	0.80
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.64	0.80
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.64	0.80
1:C:234:ILE:HG21	1:C:302:MET:CE	2.12	0.79
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:O	2:B:86:ILE:HG22	1.85	0.77
4:F:151:SER:HB3	4:F:180:HIS:HA	1.65	0.77
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.68	0.75
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.68	0.75
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.17	0.75
1:C:204:VAL:HG22	1:C:302:MET:SD	2.29	0.73
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.87	0.73
2:D:136:GLN:HA	2:D:167:ASN:O	1.88	0.73
1:A:280:LYS:HB2	1:A:283:HIS:CD2	2.24	0.72
1:A:336:LYS:HD3	3:E:24:LEU:HD22	1.71	0.72
1:A:336:LYS:CD	3:E:24:LEU:HD13	2.20	0.71
2:B:13:GLY:HA2	2:B:138:THR:HG22	1.73	0.71
1:C:221:ARG:HG3	2:D:325:MET:HG3	1.71	0.71
1:C:76:ASP:O	1:C:80:THR:HG22	1.91	0.70
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.19	0.69
2:D:11:GLN:O	2:D:15:GLN:HG2	1.93	0.69
1:C:302:MET:HB2	12:C:717:HOH:O	1.93	0.69
2:B:136:GLN:HA	2:B:167:ASN:O	1.93	0.69
2:D:286:LEU:HA	12:D:624:HOH:O	1.93	0.69
1:A:142:GLY:HA3	1:A:183:GLU:OE1	1.93	0.68
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.58	0.68
2:D:323:MET:HE2	2:D:373:MET:HE3	1.76	0.67
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.28	0.66
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.76	0.66
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.78	0.66
4:F:229:ASN:O	4:F:239:HIS:NE2	2.29	0.66
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.78	0.66
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.12	0.65
1:C:2:ARG:HD3	12:C:670:HOH:O	1.96	0.64
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.64
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.78	0.64
2:D:290:GLU:HA	12:D:623:HOH:O	1.96	0.64
1:A:28:HIS:O	1:A:36:MET:HE3	1.96	0.64
1:C:229:ARG:HD2	12:C:652:HOH:O	1.96	0.64
2:D:393:GLU:O	2:D:396:THR:HG22	1.98	0.64
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.97	0.64
1:C:312:TYR:CD2	1:C:341:ILE:HG23	2.33	0.64
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.98	0.64
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.32	0.63
2:B:274:PRO:HB3	2:B:286:LEU:HD21	1.79	0.63
1:C:163:LYS:HG3	3:E:90:ASN:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:CB	1:A:391:LEU:HD21	2.28	0.63
1:C:320:ARG:HA	1:C:356:ASN:O	1.98	0.63
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.81	0.63
2:D:152:LEU:O	2:D:156:LYS:HG2	1.99	0.63
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.81	0.62
2:D:5:VAL:HG23	2:D:132:LEU:HD11	1.80	0.62
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.39	0.62
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.17	0.62
2:D:102:ASN:HB3	2:D:105:LYS:HD3	1.81	0.62
2:D:1:MET:SD	2:D:50:ASN:HB2	2.40	0.61
2:D:19:LYS:O	2:D:23:VAL:HG23	2.00	0.61
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.30	0.61
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.00	0.61
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.82	0.61
4:F:173:ILE:HG23	4:F:180:HIS:HB2	1.82	0.61
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.00	0.61
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.36	0.61
2:B:176:LYS:HG3	12:B:642:HOH:O	2.00	0.61
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.83	0.60
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.37	0.60
2:D:109:THR:O	2:D:113:GLU:HG2	2.02	0.60
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.83	0.60
2:D:104:ALA:HB2	2:D:413:MET:SD	2.42	0.60
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.83	0.60
2:D:208:ALA:O	2:D:212:ILE:HG13	2.01	0.60
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.01	0.59
3:E:121:GLU:O	3:E:125:GLU:HG2	2.03	0.59
1:A:234:ILE:HG12	1:A:302[B]:MET:CE	2.30	0.59
2:B:96:GLN:CB	1:C:1:MET:HE2	2.33	0.59
1:C:88[A]:HIS:CE1	1:C:90:GLU:HG3	2.38	0.59
1:C:420:GLU:HB2	12:C:709:HOH:O	2.03	0.59
1:A:76:ASP:O	1:A:80:THR:HG22	2.03	0.58
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.33	0.58
4:F:159:GLY:C	4:F:160:ILE:HD12	2.28	0.58
2:D:191:VAL:O	2:D:195:VAL:HG23	2.02	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.58
1:C:271:THR:HG21	1:C:295:CYS:O	2.04	0.58
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.85	0.58
2:D:1:MET:HE1	2:D:48:ARG:HA	1.85	0.58
1:C:417:GLU:OE1	12:C:601:HOH:O	2.17	0.57
2:D:217:LEU:HA	2:D:277:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:NH1	2:B:196:GLU:O	2.37	0.57
2:B:326:LYS:O	2:B:330:GLU:HG3	2.04	0.57
1:C:234:ILE:CG2	1:C:302:MET:HE1	2.31	0.57
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.33	0.57
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.87	0.57
1:C:88[A]:HIS:HE1	1:C:90:GLU:HG3	1.70	0.57
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.40	0.57
2:D:141:LEU:HD12	2:D:172:MET:SD	2.45	0.56
2:B:141:LEU:HD12	2:B:172:MET:SD	2.45	0.56
4:F:151:SER:HB3	4:F:180:HIS:CG	2.41	0.56
1:A:180:ALA:O	1:A:183:GLU:HG3	2.05	0.56
2:B:276:THR:HG22	2:B:277:SER:O	2.06	0.56
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.87	0.56
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.86	0.56
1:C:282:TYR:O	1:C:284:GLU:HG2	2.06	0.56
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.36	0.56
1:A:336:LYS:HD2	3:E:24:LEU:HB3	1.88	0.56
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.87	0.56
2:D:180:THR:HA	10:D:502:A1IHR:O01	2.06	0.56
1:A:23:LEU:O	1:A:27:GLU:HG3	2.05	0.55
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.41	0.55
3:E:53:LYS:HD3	12:E:209:HOH:O	2.07	0.55
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.06	0.55
3:E:92:ASN:O	3:E:96:MET:HG2	2.06	0.55
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.89	0.55
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.71	0.55
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.47	0.55
1:A:63:PRO:CD	1:A:86:LEU:HG	2.35	0.55
3:E:115:HIS:HB2	12:E:219:HOH:O	2.06	0.55
2:D:175:PRO:HB2	10:D:503:A1IHR:O28	2.08	0.54
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.42	0.54
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.43	0.54
2:B:164:ARG:HD2	12:B:650:HOH:O	2.07	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.90	0.54
1:A:318:LEU:HD13	12:A:603:HOH:O	2.07	0.54
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.32	0.54
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.90	0.54
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.89	0.54
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.87	0.54
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.43	0.54
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.90	0.54
4:F:257:GLU:HG2	4:F:260:ASN:HA	1.89	0.54
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.38	0.54
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.54
4:F:101:TYR:HD1	4:F:126:ASP:HA	1.73	0.54
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.90	0.53
4:F:171:ASP:O	4:F:175:GLU:HG3	2.07	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.43	0.53
2:D:63:PRO:HG2	2:D:86:ILE:HG23	1.91	0.53
3:E:49:GLU:O	3:E:53:LYS:HG2	2.08	0.53
1:A:297:GLU:CD	1:A:339:ARG:HH22	2.17	0.53
1:C:214:ARG:HG2	1:C:219:ILE:O	2.08	0.53
2:B:69:ASP:O	2:B:94:PHE:HA	2.08	0.53
1:C:18:ASN:OD1	12:C:602:HOH:O	2.19	0.53
4:F:86:GLU:HB2	12:F:512:HOH:O	2.09	0.53
2:B:295:MET:CG	2:B:377:PHE:HB2	2.39	0.53
2:B:192:HIS:HD2	12:B:648:HOH:O	1.93	0.52
2:B:323:MET:HB3	2:B:373:MET:CE	2.39	0.52
2:B:19:LYS:HB3	2:B:232:SER:OG	2.10	0.52
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.45	0.52
2:D:147:SER:HB3	2:D:190:SER:OG	2.09	0.52
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.90	0.52
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.45	0.52
1:A:285:GLN:HB2	12:A:647:HOH:O	2.10	0.52
2:B:42:LEU:H	2:B:42:LEU:HD12	1.74	0.52
1:A:340:SER:HA	12:A:636:HOH:O	2.10	0.52
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.09	0.52
2:B:1:MET:HB3	2:B:50[B]:ASN:ND2	2.25	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.10	0.52
2:D:323:MET:HB3	2:D:373:MET:HE3	1.90	0.52
1:C:165:SER:HA	1:C:199:ASP:OD2	2.09	0.52
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.42	0.52
1:A:206:ASN:HA	1:A:209[B]:ILE:HG12	1.92	0.52
2:D:311:ARG:NH1	2:D:436:GLN:O	2.42	0.52
2:D:67:LEU:N	2:D:67:LEU:HD12	2.25	0.51
1:C:151:SER:HB2	1:C:193:THR:CG2	2.41	0.51
2:B:205:ASP:OD1	2:B:207:GLU:N	2.42	0.51
2:B:295:MET:HE3	2:B:296:PHE:CE2	2.45	0.51
4:F:162:ILE:HD13	4:F:185:TYR:CE2	2.45	0.51
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:HE2	2:B:438:ALA:HB1	1.93	0.51
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.92	0.51
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.93	0.51
4:F:197:ARG:HB2	4:F:224:SER:O	2.11	0.51
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.46	0.51
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.46	0.51
1:C:440:VAL:HG12	1:C:440:VAL:O	2.10	0.51
2:D:182:VAL:HB	2:D:408:TYR:OH	2.10	0.51
2:D:229:HIS:HB3	12:D:634:HOH:O	2.11	0.51
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.93	0.50
1:A:235:VAL:O	1:A:239:THR:HG23	2.11	0.50
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.92	0.50
3:E:7:GLU:O	3:E:22:VAL:HA	2.11	0.50
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.28	0.50
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.37	0.50
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.46	0.50
1:A:71:GLU:OE2	12:A:601:HOH:O	2.19	0.50
1:C:234:ILE:HD13	1:C:302:MET:CE	2.42	0.50
1:C:227:LEU:O	1:C:231:ILE:HG13	2.11	0.50
1:C:419:SER:O	1:C:423:GLU:HG3	2.11	0.50
2:D:75:MET:SD	2:D:94:PHE:HB3	2.51	0.50
2:B:199:ASP:OD1	9:B:504:MES:H62	2.11	0.50
1:C:309:HIS:ND1	12:C:606:HOH:O	2.34	0.50
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.46	0.50
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.93	0.50
2:D:19:LYS:NZ	2:D:22:GLU:OE1	2.34	0.50
3:E:96:MET:HB3	3:E:100:LYS:HE3	1.93	0.50
1:A:176:GLN:HB2	12:A:632:HOH:O	2.11	0.49
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.47	0.49
1:C:336:LYS:HE3	12:C:748:HOH:O	2.11	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.49
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.93	0.49
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.77	0.49
1:A:175:PRO:HA	1:A:178:SER:HB3	1.94	0.49
2:B:323:MET:HE2	2:B:373:MET:HE2	1.94	0.49
2:D:15:GLN:NE2	2:D:74:THR:HG23	2.27	0.49
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.45	0.49
1:A:256:GLN:NE2	1:A:260:VAL:O	2.45	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.49
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.48	0.49
2:D:68:VAL:HA	2:D:93:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:350:ILE:O	4:F:354:ALA:HB3	2.13	0.49
4:F:280:GLU:HA	4:F:284:LEU:CB	2.42	0.49
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.93	0.49
1:A:147:SER:HB2	1:A:190:THR:HB	1.95	0.49
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.95	0.49
3:E:92:ASN:OD1	3:E:96:MET:HE2	2.13	0.49
4:F:140:GLU:O	4:F:140:GLU:HG2	2.12	0.49
1:A:298:PRO:HA	1:A:301:GLN:CD	2.38	0.48
2:D:239:THR:O	2:D:243:ARG:HG3	2.14	0.48
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.94	0.48
2:D:412:GLY:C	3:E:133:VAL:HG13	2.38	0.48
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.78	0.48
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.13	0.48
4:F:128:ARG:O	4:F:132:LEU:HG	2.12	0.48
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.96	0.48
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.12	0.48
1:A:214:ARG:HA	1:A:219:ILE:O	2.14	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.48
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.95	0.48
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.94	0.48
1:A:1:MET:CB	1:A:46:ASP:HB2	2.43	0.48
2:B:390:ARG:O	2:B:394:GLN:HG3	2.14	0.48
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.96	0.48
4:F:224:SER:OG	4:F:238:CYS:HA	2.14	0.48
2:B:2:ARG:HA	2:B:131:CYS:O	2.13	0.48
4:F:280:GLU:HA	4:F:284:LEU:HB3	1.96	0.48
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.94	0.48
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.96	0.48
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.43	0.48
1:C:28:HIS:O	1:C:36:MET:HE3	2.14	0.48
1:A:128:GLN:O	1:A:128:GLN:HG2	2.13	0.47
2:D:410:GLY:O	3:E:137:LYS:HG3	2.14	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.80	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
2:B:2:ARG:HH12	2:B:164:ARG:HH12	1.62	0.47
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.97	0.47
2:D:124:LYS:C	2:D:124:LYS:HD3	2.39	0.47
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.15	0.47
2:D:411:GLU:HA	3:E:137:LYS:HD2	1.97	0.47
4:F:74:LYS:O	4:F:78:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.15	0.46
1:C:163:LYS:HE2	3:E:90:ASN:HA	1.96	0.46
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.50	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.46
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.27	0.46
1:A:311:LYS:HD3	1:A:344:VAL:HG12	1.98	0.46
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.46
1:C:97:GLU:HG3	2:D:2:ARG:CZ	2.45	0.46
1:C:221:ARG:HG3	2:D:325:MET:CG	2.41	0.46
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.14	0.46
2:B:115:VAL:HG21	2:B:156:LYS:HD2	1.98	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.46
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.50	0.46
4:F:223:THR:O	4:F:260:ASN:HB3	2.16	0.46
2:B:290:GLU:O	2:B:294:GLN:HG3	2.16	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
1:A:293:ASN:HA	1:A:335:ILE:CD1	2.46	0.46
2:B:88:ARG:HD2	12:B:652:HOH:O	2.15	0.46
2:B:387:LEU:C	2:B:387:LEU:HD23	2.40	0.46
2:D:1:MET:HG3	2:D:50:ASN:HD22	1.81	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.97	0.45
2:D:297:ASP:OD1	2:D:298:SER:N	2.48	0.45
1:A:209[A]:ILE:CG2	1:A:227:LEU:HD22	2.39	0.45
2:B:42:LEU:HD12	2:B:42:LEU:N	2.30	0.45
2:B:227:LEU:O	2:B:231:VAL:HG23	2.17	0.45
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.16	0.45
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.49	0.45
4:F:202:ARG:HB3	4:F:220:VAL:HG23	1.98	0.45
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.97	0.45
3:E:25:LYS:HE3	3:E:25:LYS:HB3	1.82	0.45
1:A:127:ASP:HB2	12:A:648:HOH:O	2.16	0.45
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.99	0.45
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.98	0.45
2:D:2:ARG:O	2:D:133:GLN:NE2	2.44	0.45
4:F:235:ASP:OD1	4:F:236:LYS:N	2.50	0.45
2:D:6:HIS:HE2	2:D:8:GLN:CG	2.30	0.45
2:D:327:GLU:O	2:D:331:GLN:HG2	2.16	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.52	0.45
4:F:299:GLU:N	4:F:300:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:GLU:CG	3:E:123:LEU:HD13	2.47	0.45
3:E:135:LYS:NZ	3:E:139:LEU:HD11	2.32	0.45
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.32	0.45
4:F:202:ARG:HB3	4:F:220:VAL:CG2	2.47	0.45
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.99	0.45
2:B:2:ARG:O	2:B:133:GLN:NE2	2.45	0.44
1:C:302:MET:HB2	1:C:302:MET:HE3	1.84	0.44
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.32	0.44
1:C:131:GLY:O	1:C:132:LEU:C	2.59	0.44
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.98	0.44
4:F:226:GLU:OE2	4:F:252:ASN:HB2	2.17	0.44
4:F:269:GLN:HA	4:F:272:MET:CE	2.47	0.44
4:F:283:ILE:HG23	4:F:327:VAL:HG21	1.98	0.44
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.49	0.44
1:C:151:SER:HB2	1:C:193:THR:HG22	2.00	0.44
2:B:313:LEU:HD23	2:B:344:VAL:HG11	2.00	0.44
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.44
1:C:173:PRO:HB3	1:C:183:GLU:OE1	2.17	0.44
1:A:234:ILE:CG1	1:A:302[B]:MET:HE2	2.35	0.44
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.17	0.44
2:D:6:HIS:HE2	2:D:8:GLN:HE21	1.65	0.44
2:D:298:SER:HB3	2:D:307:PRO:HD2	2.00	0.44
2:D:427:ASP:O	2:D:431:GLU:HG3	2.17	0.44
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.00	0.44
2:B:329:ASP:O	2:B:333:LEU:HG	2.17	0.44
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.99	0.44
4:F:202:ARG:HD3	4:F:203:SER:N	2.33	0.44
1:A:97:GLU:OE1	2:B:2:ARG:NH1	2.51	0.44
2:B:88:ARG:HG2	12:B:606:HOH:O	2.17	0.44
1:C:204:VAL:HA	1:C:302:MET:CG	2.48	0.44
2:D:72:PRO:HB3	2:D:94:PHE:CE2	2.53	0.44
2:D:112:ALA:O	2:D:115:VAL:HG12	2.17	0.44
1:A:134:GLY:HA3	1:A:165:SER:O	2.17	0.44
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.38	0.44
1:A:401:LYS:CE	2:B:438:ALA:HB1	2.48	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.44
1:C:234:ILE:HD13	1:C:302:MET:HE2	2.00	0.44
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.51	0.44
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.99	0.44
2:B:288:VAL:HG12	2:B:331:GLN:CG	2.44	0.44
2:B:114:LEU:O	2:B:114:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.48	0.43
1:A:351:PHE:CE1	3:E:24:LEU:HD11	2.53	0.43
2:D:23:VAL:HG21	2:D:232:SER:HB2	2.01	0.43
4:F:86:GLU:OE1	4:F:297:CYS:HB2	2.18	0.43
2:B:22:GLU:HB2	12:B:601:HOH:O	2.19	0.43
2:B:301:MET:HE1	2:B:312:TYR:OH	2.17	0.43
2:B:318:ILE:N	2:B:318:ILE:HD12	2.33	0.43
1:C:8:HIS:HB3	1:C:13:GLY:O	2.18	0.43
2:D:99:ALA:O	2:D:105:LYS:HD3	2.18	0.43
4:F:246:GLN:HB3	4:F:260:ASN:ND2	2.34	0.43
2:B:323:MET:HB3	2:B:373:MET:HE1	2.01	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.19	0.43
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.49	0.43
1:C:288:VAL:HG23	12:C:671:HOH:O	2.19	0.43
2:D:181:VAL:HG22	2:D:398:MET:SD	2.58	0.43
3:E:47:LEU:HD11	3:E:51:GLN:HE21	1.84	0.43
2:B:40:SER:OG	2:B:42:LEU:HD13	2.19	0.43
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.48	0.43
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.01	0.43
1:C:397:LEU:HB3	2:D:346:TRP:HA	2.01	0.42
2:D:287:THR:OG1	2:D:290:GLU:HG3	2.19	0.42
3:E:72:LEU:O	3:E:76:ARG:HG2	2.19	0.42
1:A:293:ASN:HA	1:A:335:ILE:HD11	2.00	0.42
1:A:263:PRO:O	1:A:266:HIS:HD2	2.02	0.42
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.54	0.42
3:E:112:ARG:NH2	12:E:202:HOH:O	2.45	0.42
4:F:269:GLN:HA	4:F:272:MET:HE2	2.00	0.42
2:D:162:PRO:HB2	3:E:116:LEU:HD22	2.01	0.42
4:F:184:LYS:O	11:F:401:ACP:N6	2.49	0.42
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.02	0.42
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.42
4:F:151:SER:HB3	4:F:180:HIS:CA	2.44	0.42
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.55	0.42
2:B:269:MET:HG2	2:B:384:ILE:HD13	2.02	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.54	0.42
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.55	0.42
1:A:100:ALA:HA	2:B:254:LYS:HG3	2.02	0.42
1:C:204:VAL:HG13	1:C:302:MET:HG3	2.00	0.42
1:C:341:ILE:HD12	1:C:341:ILE:N	2.34	0.42
4:F:186:LEU:HD21	4:F:322:ASP:HB3	2.02	0.42
1:A:234:ILE:O	1:A:238:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASN:CA	1:A:335:ILE:HD11	2.49	0.42
1:C:74:VAL:HB	12:C:613:HOH:O	2.19	0.42
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.60	0.42
2:D:69:ASP:O	2:D:94:PHE:HA	2.20	0.42
2:D:181:VAL:HG11	2:D:404:PHE:CZ	2.55	0.42
2:D:323:MET:CE	2:D:373:MET:HE3	2.47	0.42
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.01	0.41
1:C:75:ILE:HB	1:C:94:THR:CG2	2.50	0.41
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.50	0.41
2:D:180:THR:HB	2:D:183:GLU:HG3	2.00	0.41
2:B:159:GLU:HB2	3:E:72:LEU:HD13	2.01	0.41
2:B:174:SER:CB	2:B:207:GLU:HB2	2.50	0.41
1:A:114:ILE:O	1:A:114:ILE:HG12	2.20	0.41
2:D:207:GLU:HB3	2:D:390:ARG:HH12	1.86	0.41
4:F:19:ARG:HD2	4:F:19:ARG:C	2.44	0.41
1:A:74:VAL:HB	12:A:604:HOH:O	2.20	0.41
1:A:336:LYS:CD	3:E:24:LEU:HB3	2.50	0.41
1:C:204:VAL:HA	1:C:302:MET:HG2	2.02	0.41
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.41
2:D:185:TYR:O	2:D:189:LEU:HG	2.19	0.41
2:D:194:LEU:CD2	2:D:198:THR:HG21	2.50	0.41
4:F:282:SER:O	4:F:286:GLN:NE2	2.53	0.41
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.28	0.41
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.03	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.36	0.41
1:C:333:ALA:O	1:C:337:THR:HG23	2.21	0.41
1:C:429:GLU:O	1:C:433:GLU:HG3	2.21	0.41
2:D:66:ILE:HD12	2:D:122:VAL:HG22	2.03	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.41
1:A:399:TYR:O	1:A:402:ARG:NH1	2.50	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.20	0.41
1:C:135:PHE:O	1:C:136:LEU:HD23	2.21	0.41
2:D:146:GLY:O	2:D:150:GLY:HA3	2.19	0.41
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.56	0.41
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.56	0.41
2:D:416:MET:O	2:D:420:GLU:HG3	2.20	0.41
1:A:75:ILE:HB	1:A:94:THR:CG2	2.51	0.41
1:A:284:GLU:O	1:A:284:GLU:HG3	2.21	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
1:C:180:ALA:O	1:C:183:GLU:HG3	2.20	0.41
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.03	0.41
1:A:1:MET:HB2	1:A:46:ASP:HB2	2.02	0.40
1:C:194:THR:O	1:C:194:THR:HG22	2.21	0.40
2:D:18:ALA:O	2:D:22:GLU:HG3	2.21	0.40
3:E:53:LYS:HE2	12:E:215:HOH:O	2.20	0.40
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.40
2:B:199:ASP:C	2:B:200:GLU:HG3	2.45	0.40
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.02	0.40
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.40
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.87	0.40
1:A:151:SER:HB2	1:A:193[A]:THR:OG1	2.21	0.40
1:A:1:MET:HB3	1:A:46:ASP:HB2	2.04	0.40
1:A:265:ILE:HD12	1:A:432:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/451 (99%)	438 (98%)	7 (2%)	0	100	100
1	C	440/451 (98%)	432 (98%)	8 (2%)	0	100	100
2	B	422/445 (95%)	415 (98%)	7 (2%)	0	100	100
2	D	422/445 (95%)	416 (99%)	6 (1%)	0	100	100
3	E	116/143 (81%)	116 (100%)	0	0	100	100
4	F	315/384 (82%)	308 (98%)	7 (2%)	0	100	100
All	All	2160/2319 (93%)	2125 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/379 (100%)	375 (99%)	3 (1%)	73	86
1	C	373/379 (98%)	371 (100%)	2 (0%)	81	90
2	B	369/383 (96%)	369 (100%)	0	100	100
2	D	368/383 (96%)	368 (100%)	0	100	100
3	E	108/127 (85%)	107 (99%)	1 (1%)	70	84
4	F	300/342 (88%)	299 (100%)	1 (0%)	86	93
All	All	1896/1993 (95%)	1889 (100%)	7 (0%)	84	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	283	HIS
1	A	381	THR
1	C	326	LYS
1	C	391	LEU
3	E	105	MET
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	293	ASN
1	A	300	ASN
1	A	393	HIS
2	B	167	ASN
2	B	193	GLN
2	B	282	GLN
2	B	349	ASN
1	C	11	GLN
1	C	256	GLN

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Mol	Chain	Res	Type
1	C	309	HIS
2	D	50	ASN
2	D	96	GLN
2	D	133	GLN
2	D	136	GLN
2	D	197	ASN
3	E	12	ASN
3	E	18	GLN
3	E	103	GLN
4	F	269	GLN
4	F	306	HIS
4	F	380	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 17 ligands modelled in this entry, 9 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	$\# Z > 2$
5	GTP	C	501	6	33,34,34	0.96	2 (6%)	50,54,54	1.52	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	A1IHR	D	502	-	48,49,49	0.99	2 (4%)	60,69,69	1.33	6 (10%)
10	A1IHR	D	503	-	48,49,49	0.93	2 (4%)	60,69,69	1.39	7 (11%)
9	MES	B	504	-	12,12,12	2.27	1 (8%)	15,16,16	1.84	2 (13%)
5	GTP	A	501	6	33,34,34	0.97	2 (6%)	50,54,54	1.52	8 (16%)
8	GDP	D	501	6	29,30,30	1.28	4 (13%)	45,47,47	1.95	9 (20%)
8	GDP	B	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.71	6 (13%)
11	ACP	F	401	6	31,33,33	0.58	1 (3%)	47,52,52	1.08	1 (2%)

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
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	A1IHR	D	502	-	-	7/59/64/64	0/3/4/4
10	A1IHR	D	503	-	-	4/59/64/64	0/3/4/4
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
8	GDP	D	501	6	-	3/16/32/32	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
11	ACP	F	401	6	-	4/19/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.58	1.67	1.77
8	D	501	GDP	C5-C4	3.33	1.47	1.38
8	B	501	GDP	C5-C4	3.06	1.47	1.38
8	D	501	GDP	PA-O3A	2.94	1.62	1.59
11	F	401	ACP	PB-O3A	2.94	1.61	1.58
10	D	502	A1IHR	C02-N03	2.49	1.39	1.34
10	D	503	A1IHR	C21-N01	2.48	1.38	1.34
10	D	502	A1IHR	C21-N01	2.46	1.38	1.34
8	B	501	GDP	C6-N1	-2.45	1.34	1.38
5	C	501	GTP	PB-O3B	2.31	1.62	1.59
8	D	501	GDP	C6-N1	-2.21	1.34	1.38
10	D	503	A1IHR	C15-N16	2.19	1.38	1.33
5	A	501	GTP	C2-N3	2.18	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	PB-O3B	2.03	1.61	1.59
5	C	501	GTP	PA-O3A	2.03	1.61	1.59
8	D	501	GDP	C5-N7	-2.02	1.35	1.39
8	B	501	GDP	PA-O3A	2.00	1.61	1.59

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-7.23	108.77	132.37
8	B	501	GDP	C5-C4-N3	-5.97	118.88	128.39
8	D	501	GDP	C2-N3-C4	5.93	122.51	112.30
8	D	501	GDP	C5-C4-N3	-5.86	119.06	128.39
9	B	504	MES	C5-N4-C3	5.03	119.67	108.84
8	B	501	GDP	C2-N3-C4	5.01	120.92	112.30
10	D	503	A1IHR	C33-O34-C35	4.98	125.37	117.85
5	A	501	GTP	C5-C4-N3	-4.92	120.56	128.39
8	D	501	GDP	N9-C4-N3	4.73	135.42	125.95
5	C	501	GTP	C5-C4-N3	-4.70	120.92	128.39
5	A	501	GTP	C2-N3-C4	4.52	120.08	112.30
5	C	501	GTP	C2-N3-C4	4.51	120.06	112.30
8	B	501	GDP	N9-C4-N3	4.34	134.64	125.95
8	D	501	GDP	C6-C5-N7	4.22	137.96	130.29
10	D	502	A1IHR	C39-O41-C40	4.11	63.69	60.82
10	D	503	A1IHR	C39-O41-C40	3.95	63.58	60.82
10	D	502	A1IHR	C18-C17-N16	-3.67	109.34	114.20
8	B	501	GDP	C6-C5-N7	3.41	136.50	130.29
10	D	503	A1IHR	C38-C37-C39	-3.40	105.42	111.40
10	D	502	A1IHR	O41-C39-C40	-3.26	57.98	60.08
5	A	501	GTP	N9-C4-N3	3.12	132.20	125.95
10	D	503	A1IHR	C18-C17-N16	-3.10	110.09	114.20
10	D	503	A1IHR	O41-C39-C40	-2.99	58.15	60.08
5	C	501	GTP	N9-C4-N3	2.90	131.75	125.95
10	D	502	A1IHR	O34-C33-C32	2.88	112.31	107.45
5	A	501	GTP	C2-N1-C6	-2.83	119.97	125.11
5	C	501	GTP	N9-C8-N7	-2.78	108.24	113.40
5	C	501	GTP	C2-N1-C6	-2.76	120.11	125.11
8	B	501	GDP	C4-C5-N7	-2.66	106.45	110.67
5	A	501	GTP	N9-C8-N7	-2.66	108.47	113.40
10	D	502	A1IHR	O34-C35-C23	2.61	117.36	111.41
8	D	501	GDP	C4-C5-N7	-2.59	106.57	110.67
5	C	501	GTP	C8-N7-C5	2.54	108.79	104.26
5	A	501	GTP	C8-N7-C5	2.54	108.78	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O2S-S-C8	2.51	110.52	106.73
5	A	501	GTP	C5-C6-N1	2.43	119.43	113.25
5	C	501	GTP	O6-C6-C5	-2.33	120.38	126.53
5	C	501	GTP	C5-C6-N1	2.32	119.17	113.25
8	D	501	GDP	C5-C6-N1	2.32	119.15	113.25
5	A	501	GTP	O6-C6-C5	-2.27	120.53	126.53
8	D	501	GDP	C6-C5-C4	-2.23	115.47	118.83
10	D	502	A1IHR	C33-O34-C35	2.17	121.14	117.85
8	D	501	GDP	O6-C6-C5	-2.13	120.90	126.53
8	D	501	GDP	C8-N9-C4	2.12	110.00	106.03
10	D	503	A1IHR	O34-C35-C23	2.11	116.23	111.41
8	B	501	GDP	O6-C6-C5	-2.09	121.02	126.53
10	D	503	A1IHR	O41-C40-C42	2.07	121.09	116.76

There are no chirality outliers.

All (37) 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	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
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
10	D	502	A1IHR	C23-C24-C25-N85
10	D	503	A1IHR	C35-C23-C24-C25
10	D	503	A1IHR	N01-C23-C24-C25
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	504	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
10	D	502	A1IHR	N03-C02-C30-C31
10	D	502	A1IHR	O34-C33-C37-C39
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A

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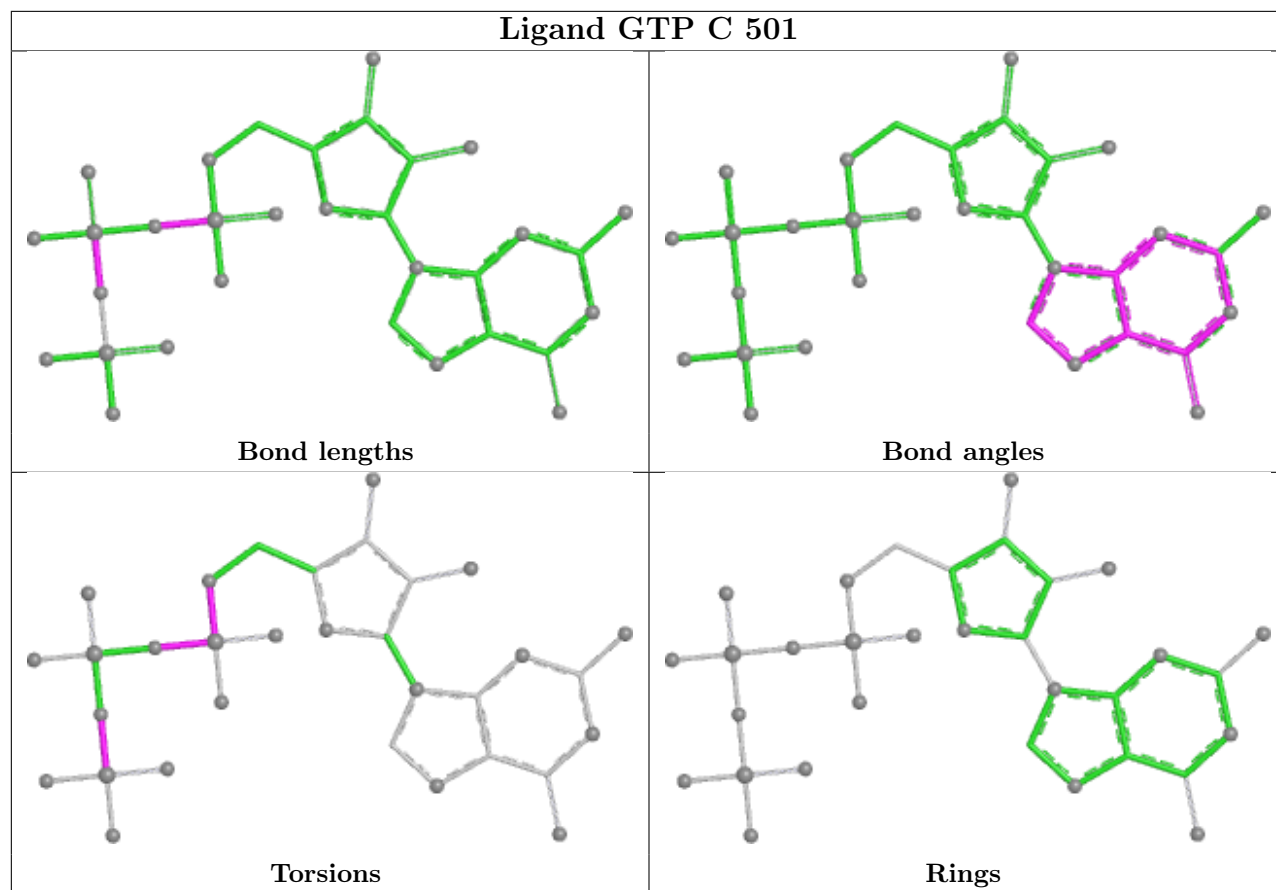
Mol	Chain	Res	Type	Atoms
10	D	502	A1IHR	O28-C21-N01-C23
9	B	504	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3A-PA-O2A
10	D	503	A1IHR	C17-C18-C21-O28
10	D	503	A1IHR	C17-C18-C21-N01
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
10	D	502	A1IHR	C19-C18-C21-O28
5	A	501	GTP	PB-O3A-PA-O2A
10	D	502	A1IHR	O01-C02-C30-C31
10	D	502	A1IHR	C19-C18-C21-N01
5	C	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

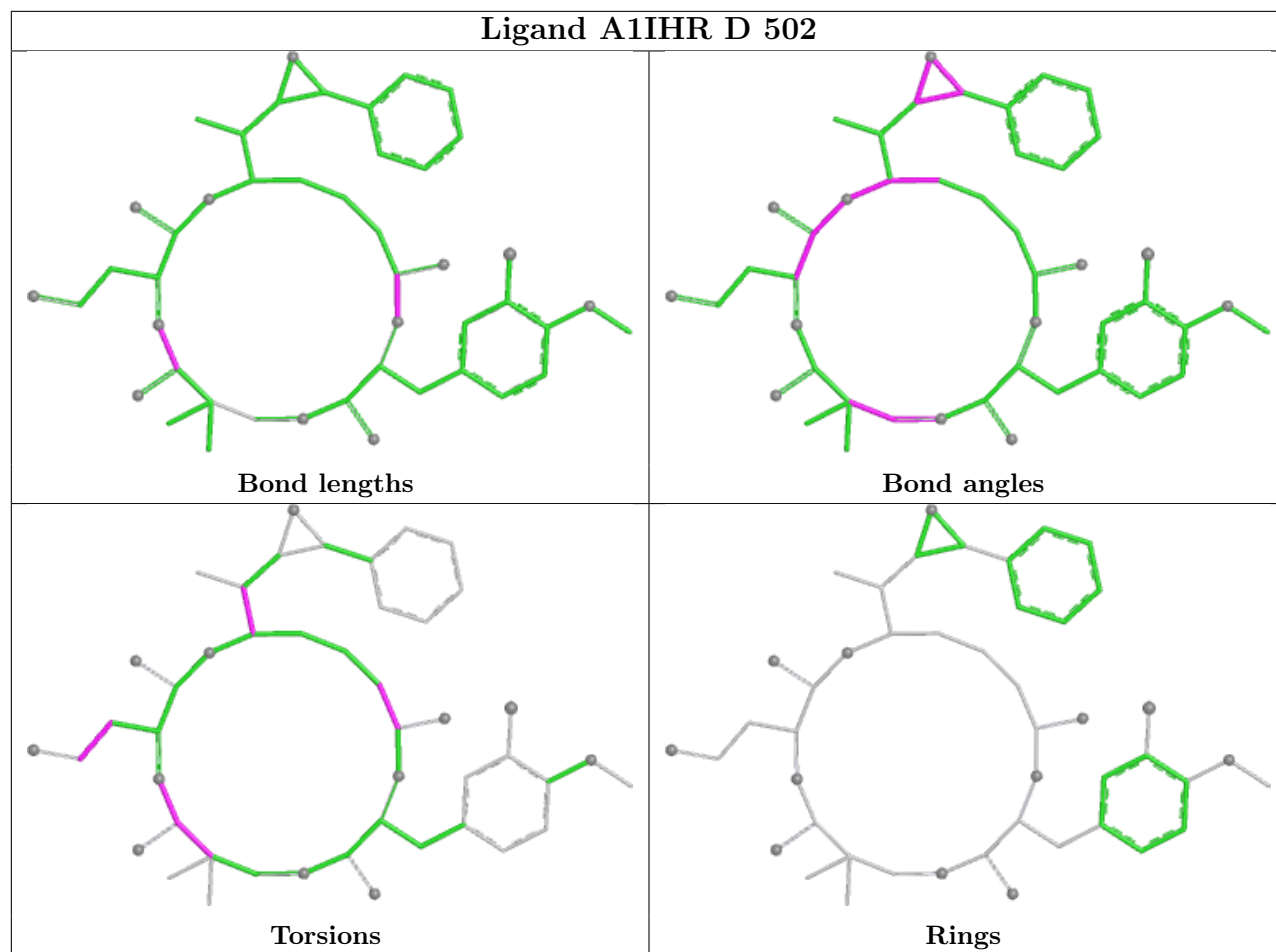
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	A1IHR	1	0
10	D	503	A1IHR	1	0
9	B	504	MES	1	0
5	A	501	GTP	1	0
8	D	501	GDP	2	0
11	F	401	ACP	1	0

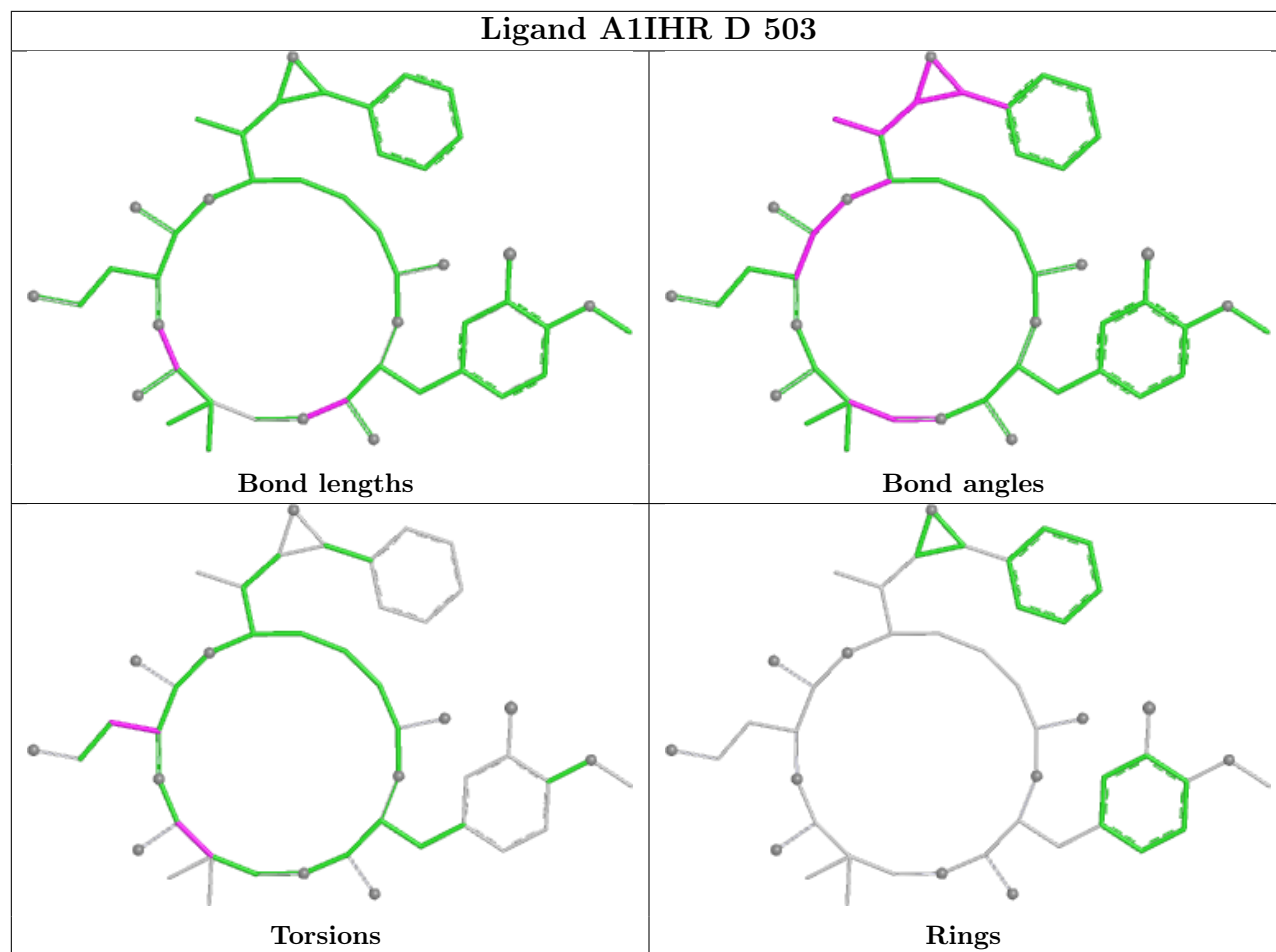
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

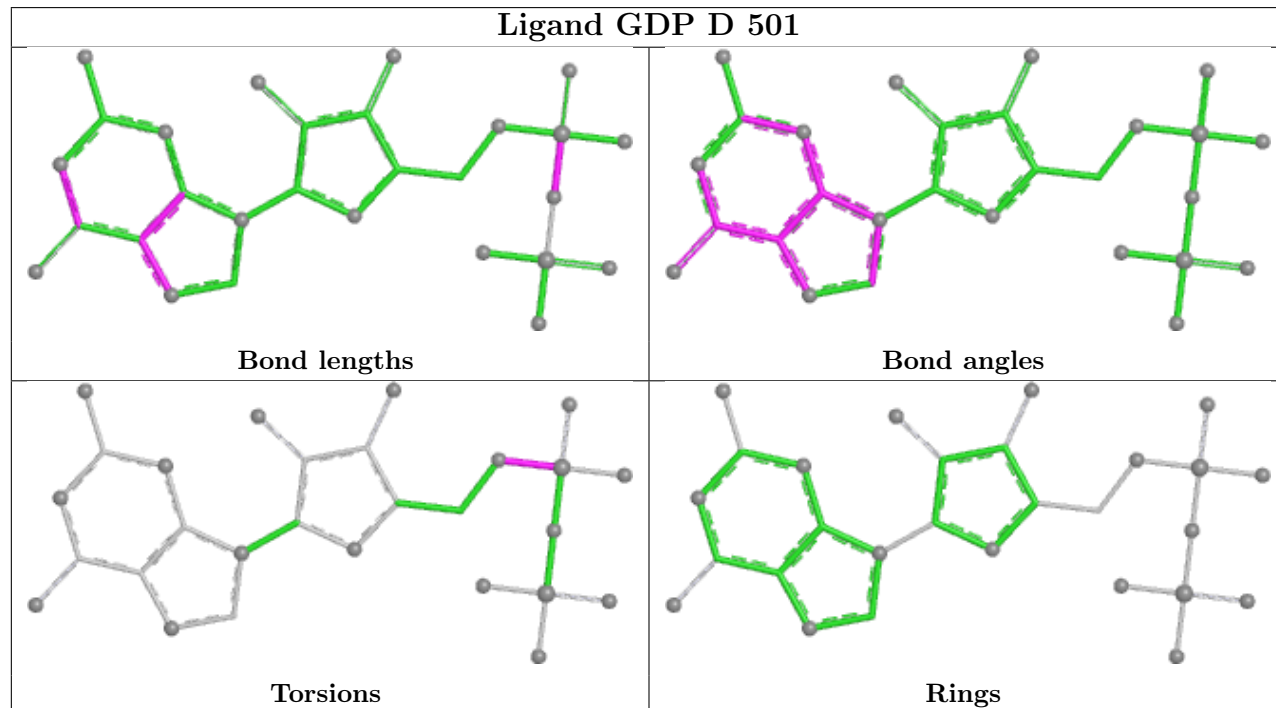
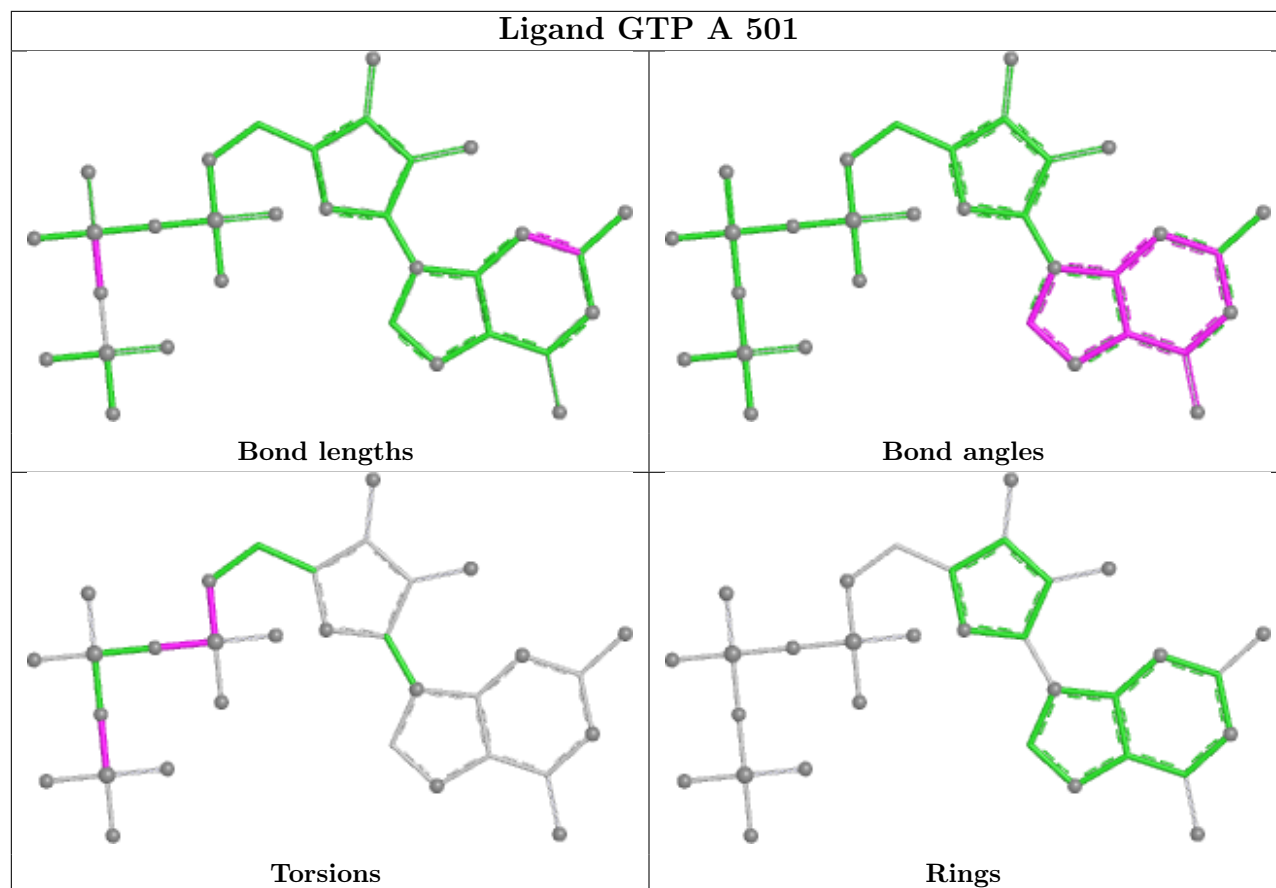


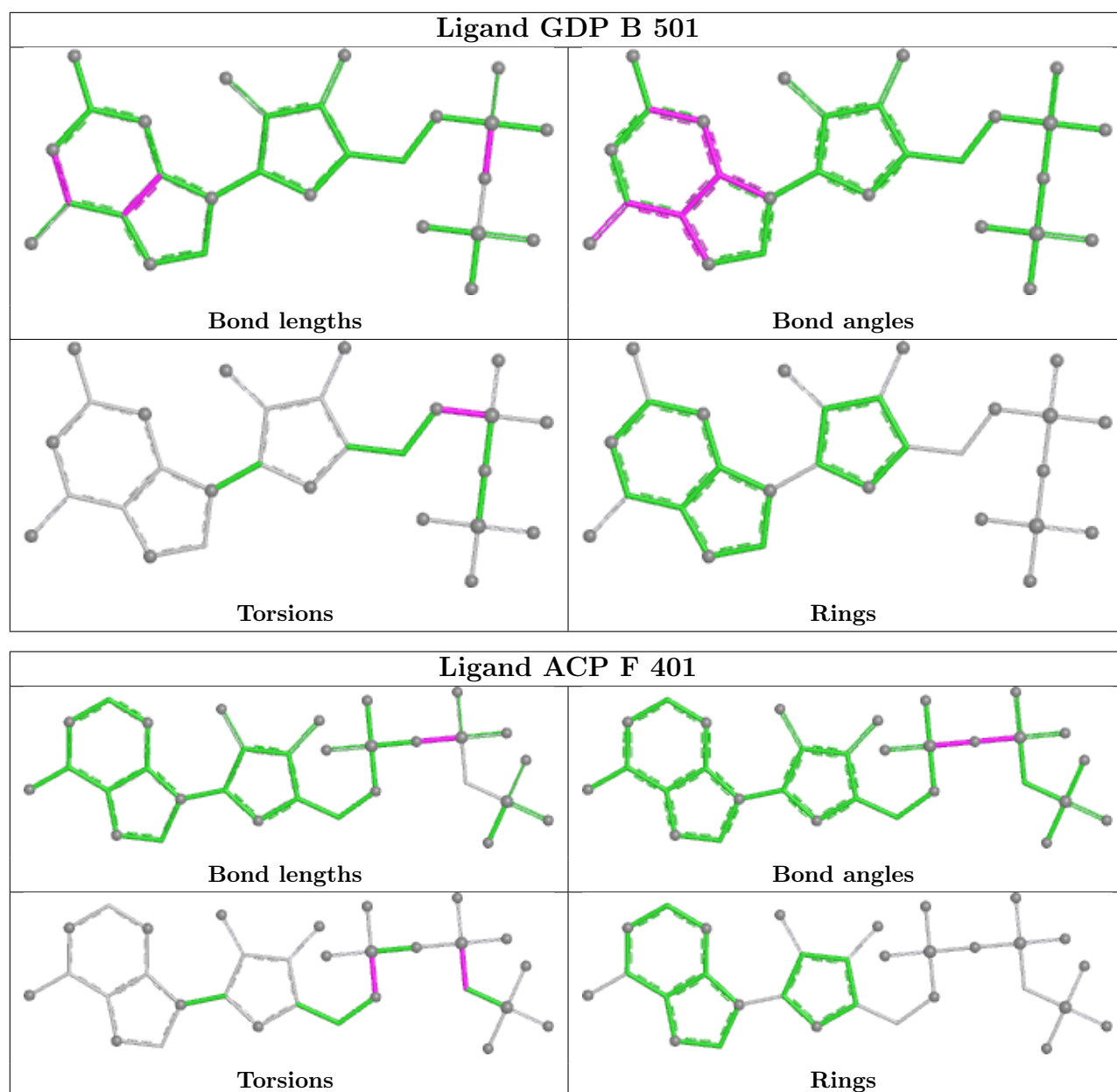
Ligand A1IHR D 502



Ligand A1IHR D 503







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	437/451 (96%)	0.21	11 (2%) 58 60	31, 65, 97, 152	10 (2%)
1	C	440/451 (97%)	-0.12	8 (1%) 67 69	31, 50, 72, 124	2 (0%)
2	B	425/445 (95%)	0.16	6 (1%) 73 75	37, 60, 94, 136	1 (0%)
2	D	426/445 (95%)	0.34	14 (3%) 49 51	48, 72, 100, 132	0
3	E	120/143 (83%)	0.34	6 (5%) 34 35	53, 75, 116, 140	0
4	F	331/384 (86%)	0.58	15 (4%) 38 40	61, 90, 133, 150	0
All	All	2179/2319 (93%)	0.22	60 (2%) 55 57	31, 67, 113, 152	13 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	286	LEU	4.4
1	C	440	VAL	4.0
4	F	186	LEU	4.0
2	D	276	THR	3.8
4	F	159	GLY	3.6
4	F	249	TYR	3.5
2	B	275	LEU	3.5
3	E	26	PRO	3.3
1	A	337	THR	3.3
1	A	437	VAL	3.3
4	F	173	ILE	3.1
4	F	319	PHE	3.0
1	C	302	MET	2.9
4	F	102	PRO	2.9
1	A	179	THR	2.8
2	D	118	VAL	2.8
4	F	382	HIS	2.7
2	D	172	MET	2.7
1	C	163	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	2.7
1	A	282	TYR	2.6
1	C	357	TYR	2.6
4	F	1	MET	2.5
4	F	315	PHE	2.4
1	A	335	ILE	2.4
1	A	46	ASP	2.4
2	D	340	SER	2.4
3	E	115	HIS	2.4
2	D	405	LEU	2.3
1	C	1	MET	2.3
2	D	278	ARG	2.3
2	D	94	PHE	2.3
4	F	140	GLU	2.3
2	D	57	THR	2.3
1	A	342	GLN	2.3
3	E	90	ASN	2.3
1	A	262	TYR	2.3
2	D	280	SER	2.3
4	F	152	SER	2.3
4	F	344	ALA	2.2
1	A	341	ILE	2.2
2	B	278	ARG	2.2
4	F	240	LEU	2.2
2	B	172	MET	2.2
2	D	337	ASN	2.2
2	D	248	LEU	2.1
3	E	24	LEU	2.1
3	E	8	VAL	2.1
2	B	282	GLN	2.1
1	C	341	ILE	2.1
2	B	94	PHE	2.1
2	D	195	VAL	2.1
1	C	4	CYS	2.1
1	C	126	ALA	2.1
4	F	161	LEU	2.1
1	A	45	GLY	2.1
3	E	6	MET	2.0
2	B	438	ALA	2.0
2	D	46	LEU	2.0
1	A	338	LYS	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](#)

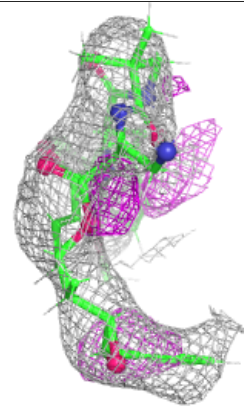
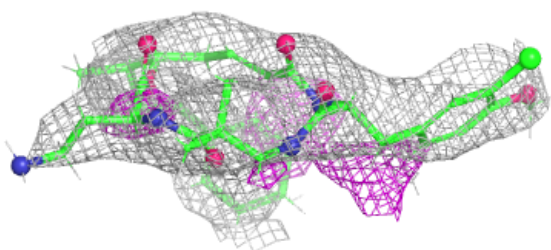
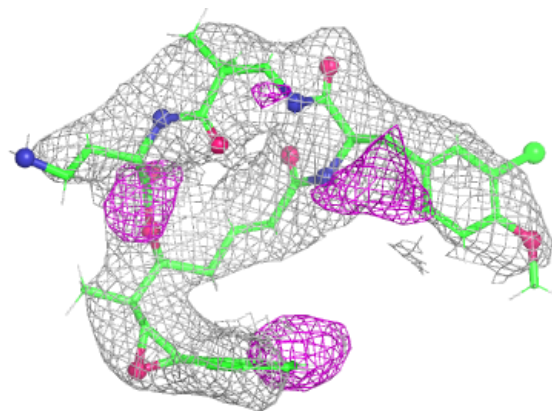
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	A1IHR	D	503	46/46	0.70	0.12	77,98,118,136	0
10	A1IHR	D	502	46/46	0.80	0.13	69,91,113,115	0
6	MG	F	402	1/1	0.90	0.09	88,88,88,88	0
8	GDP	D	501	28/28	0.92	0.10	64,69,79,88	0
9	MES	B	504	12/12	0.92	0.10	53,67,81,84	0
11	ACP	F	401	31/31	0.93	0.07	97,106,115,126	0
6	MG	D	504	1/1	0.94	0.05	73,73,73,73	0
7	CA	B	503	1/1	0.95	0.07	91,91,91,91	0
7	CA	A	503	1/1	0.96	0.07	89,89,89,89	0
7	CA	A	504	1/1	0.96	0.12	101,101,101,101	0
8	GDP	B	501	28/28	0.97	0.06	43,47,55,59	0
5	GTP	C	501	32/32	0.97	0.06	43,43,49,50	0
5	GTP	A	501	32/32	0.97	0.06	43,50,56,64	0
6	MG	B	502	1/1	0.98	0.06	44,44,44,44	0
6	MG	C	502	1/1	0.99	0.03	43,43,43,43	0
6	MG	A	502	1/1	0.99	0.03	46,46,46,46	0
7	CA	C	503	1/1	0.99	0.03	68,68,68,68	0

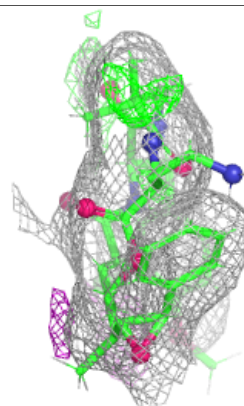
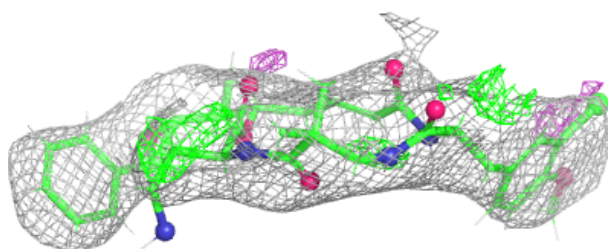
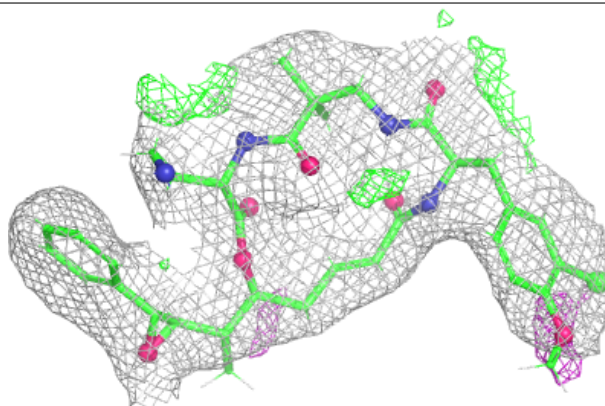
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IHR D 503:

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

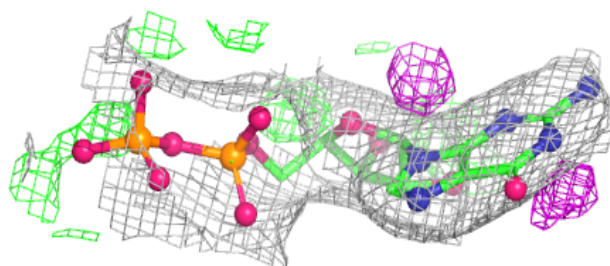
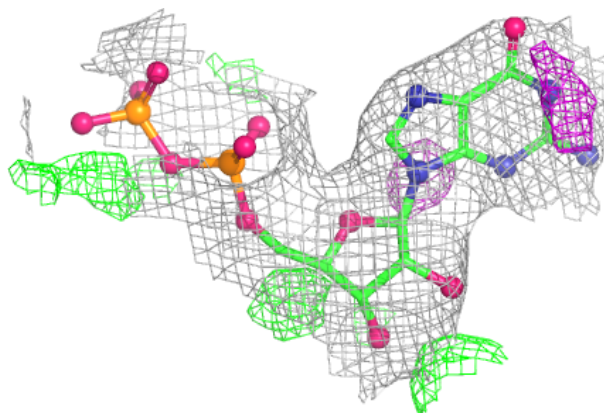
**Electron density around A1IHR D 502:**

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

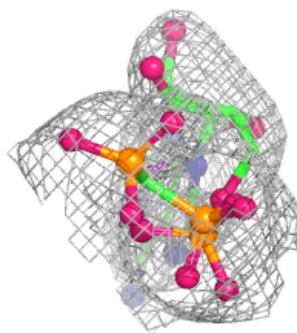
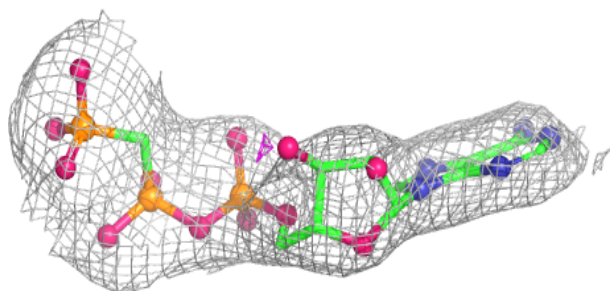
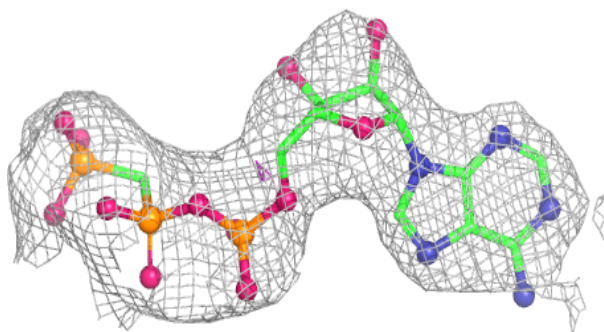


Electron density around GDP D 501:

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

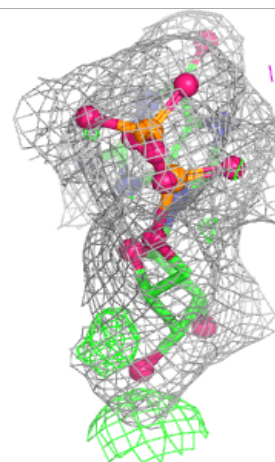
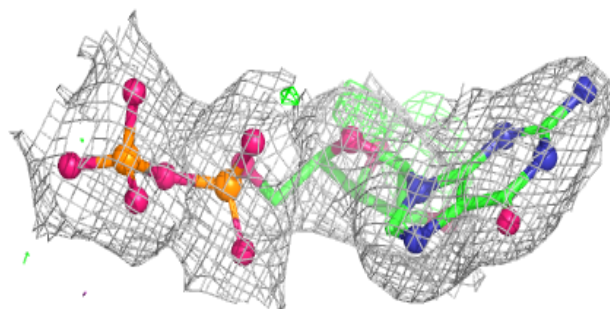
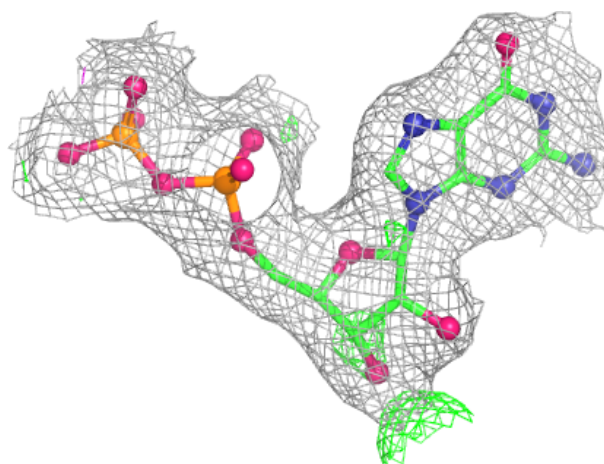
**Electron density around ACP F 401:**

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



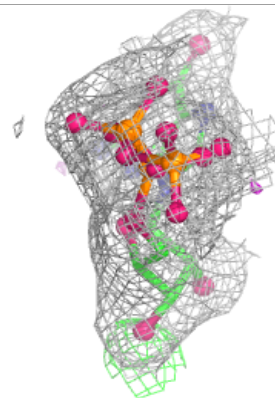
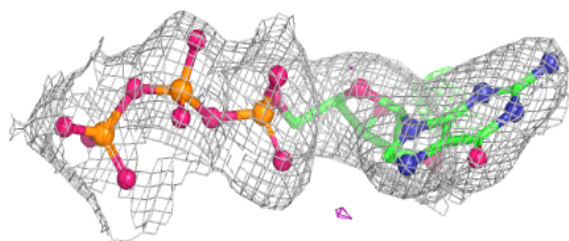
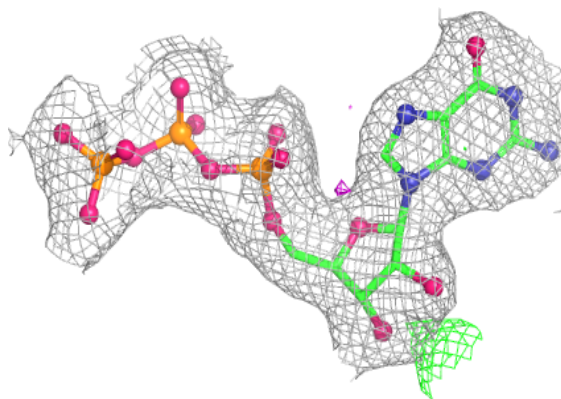
Electron density around GDP B 501:

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

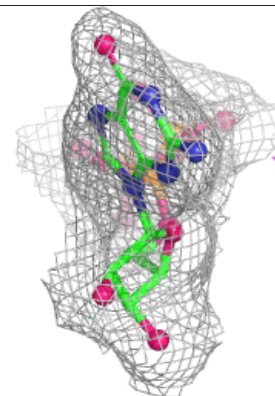
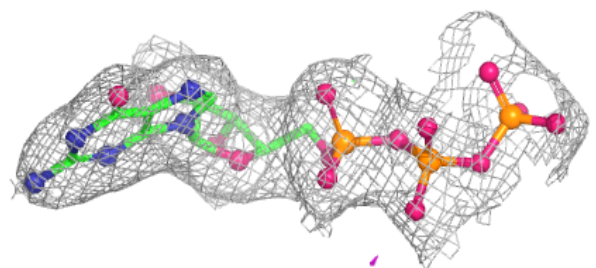
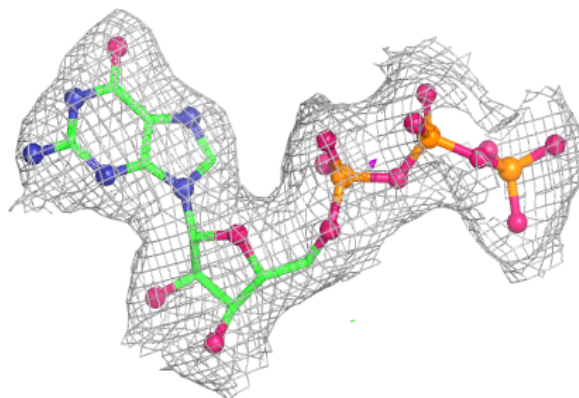


Electron density around GTP C 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.