



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:36 am BST

PDB ID : 5JCB
Title : Microtubule depolymerizing agent podophyllotoxin derivative YJTSF1
Authors : Guan, Z.; Zhao, W.; Yin, P.
Deposited on : 2016-04-14
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

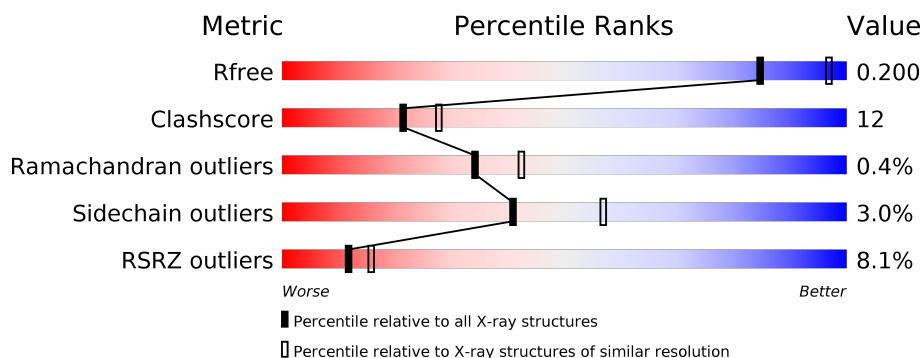
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>10%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• 6%</div> </div> </div>
3	E	152	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>13%</div> <div>• 20%</div> </div> </div>
4	F	388	<div> <div>19%</div> <div> <div></div> <div>56%</div> <div>21%</div> <div>• 20%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	NV4	D	507	-	-	X	-
7	GOL	C	501	-	-	X	X
7	GOL	C	504	-	-	X	-
8	IMD	A	505	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 18127 atoms, of which 13 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	439	Total	C	N	O	S	0	12	0
			3482	2213	585	659	25			
1	C	440	Total	C	N	O	S	0	9	0
			3481	2204	587	667	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	11	0
			3382	2129	570	657	26			
2	D	418	Total	C	N	O	S	0	5	0
			3316	2089	561	638	28			

- Molecule 3 is a protein called Stathmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1010	624	182	198	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP F2Z508
E	146	LEU	-	expression tag	UNP F2Z508
E	147	GLU	-	expression tag	UNP F2Z508
E	148	HIS	-	expression tag	UNP F2Z508
E	149	HIS	-	expression tag	UNP F2Z508
E	150	HIS	-	expression tag	UNP F2Z508
E	151	HIS	-	expression tag	UNP F2Z508
E	152	HIS	-	expression tag	UNP F2Z508
E	153	HIS	-	expression tag	UNP F2Z508
E	154	HIS	-	expression tag	UNP F2Z508

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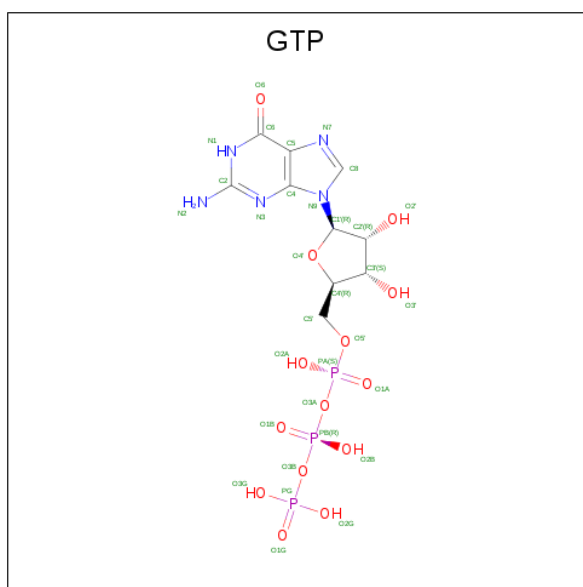
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Chain	Residue	Modelled	Actual	Comment	Reference
E	155	HIS	-	expression tag	UNP F2Z508

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	312	Total	C	N	O	S	0	4	0
			2577	1673	428	462	14			

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	2	Total	Mg	0	0
			2	2		
6	D	2	Total	Mg	0	0
			2	2		

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			6	3	3			
7	A	1	Total	C	O		0	0
			6	3	3			
7	C	1	Total	C	O		0	0
			6	3	3			
7	C	1	Total	C	O		0	0
			6	3	3			
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	D	1	Total	C	O		0	0
			6	3	3			
7	D	1	Total	C	O		0	0
			6	3	3			
7	D	1	Total	C	O		0	0
			6	3	3			

- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

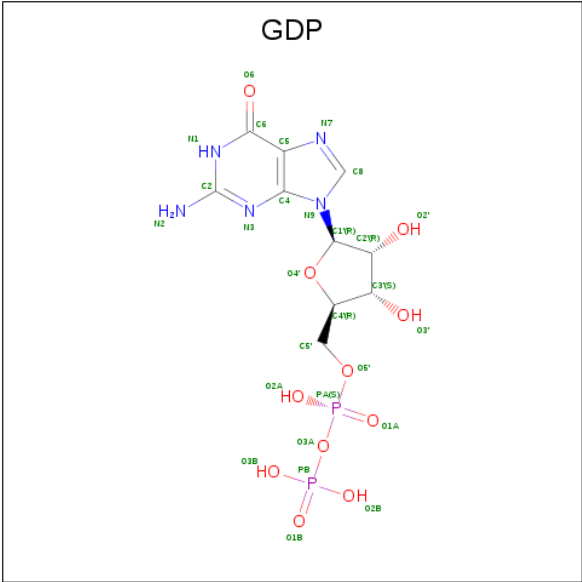


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	N	0	0
			10	3	5	2		
8	C	1	Total	C	N		0	0
			5	3	2			

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

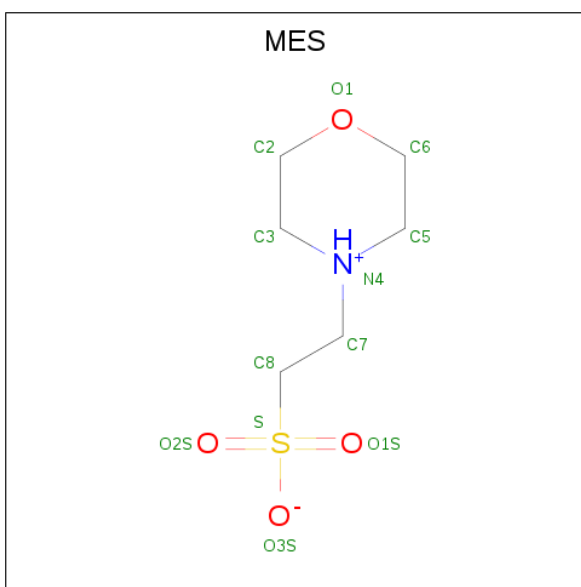


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
10	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

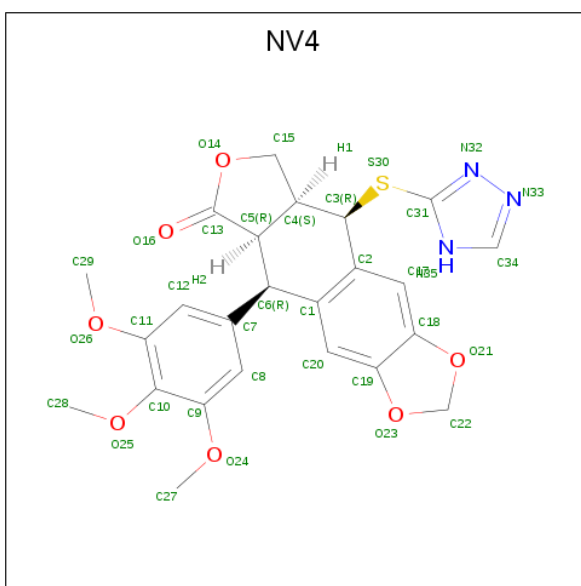
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Na	0	0
			1	1		
11	C	1	Total	Na	0	0
			1	1		

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



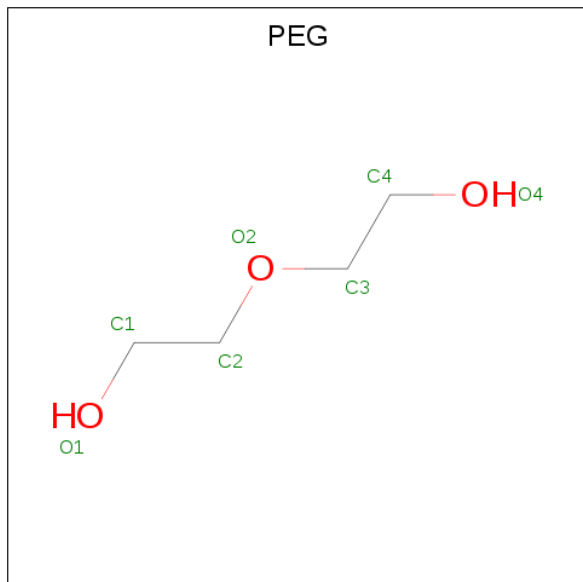
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 13 is (5R,5aR,8aS,9R)-9-[(4H-1,2,4-triazol-3-yl)sulfanyl]-5-(3,4,5-trimethoxyphenyl)-5,8,8a,9-tetrahydro-2H-furo[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one (three-letter code: NV4) (formula: C₂₄H₂₃N₃O₇S).



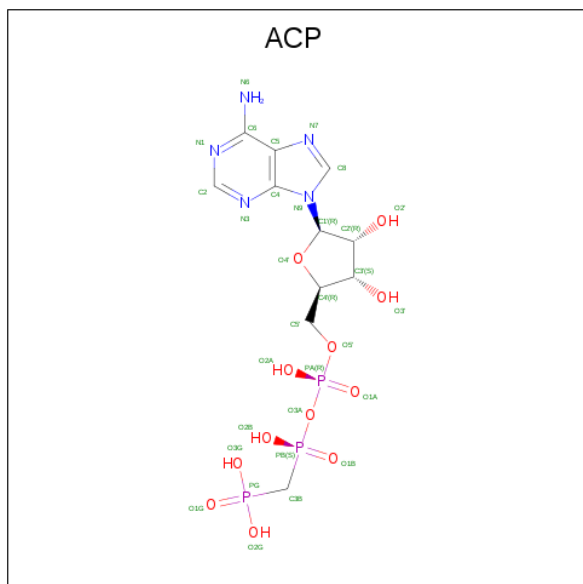
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 35	C 24	N 3	O 7	S 1	0	0
13	D	1	Total 35	C 24	N 3	O 7	S 1	0	0

- Molecule 14 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 15 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

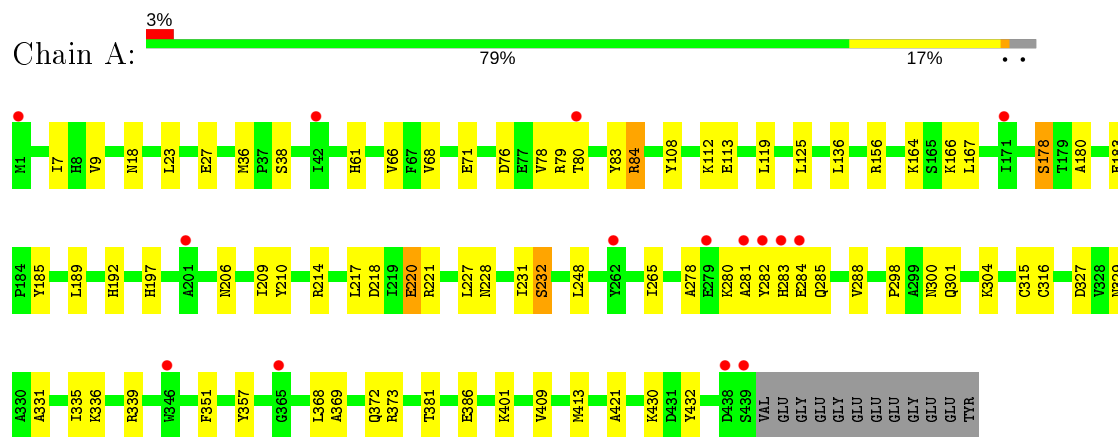
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	115	Total 115	O 115	0	0
16	B	84	Total 84	O 84	0	0
16	C	199	Total 199	O 199	0	0
16	D	66	Total 66	O 66	0	0
16	E	28	Total 28	O 28	0	0
16	F	65	Total 65	O 65	0	0

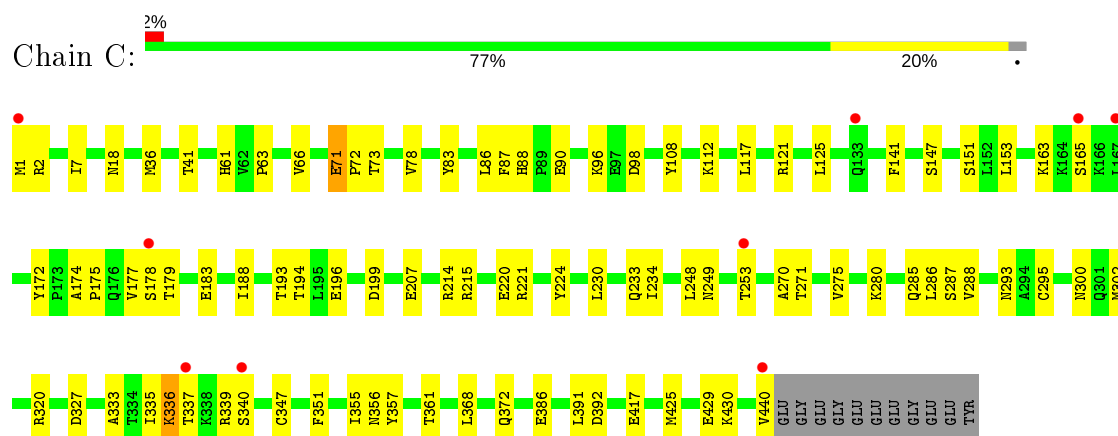
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

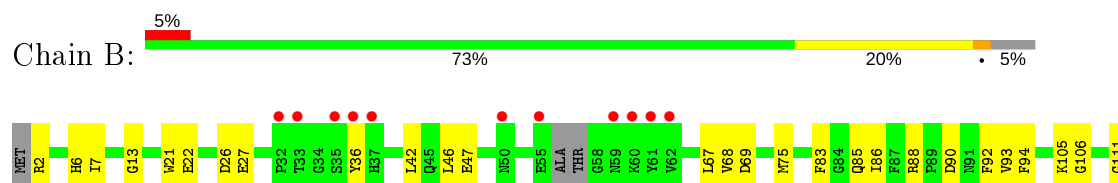
• Molecule 1: Tubulin alpha-1B chain

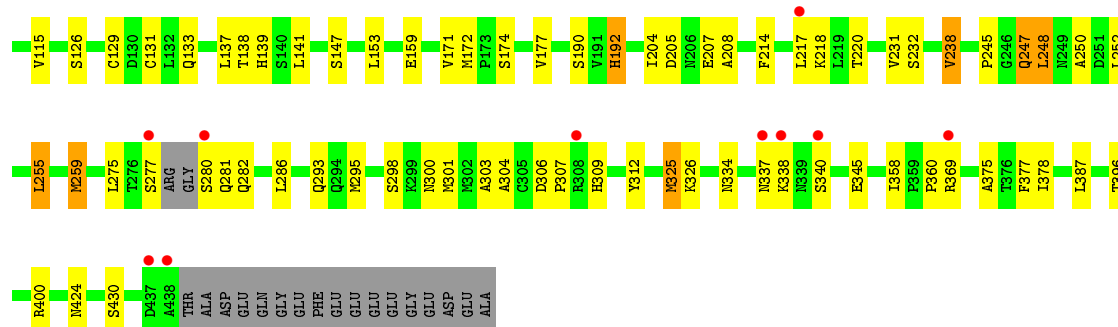


• Molecule 1: Tubulin alpha-1B chain

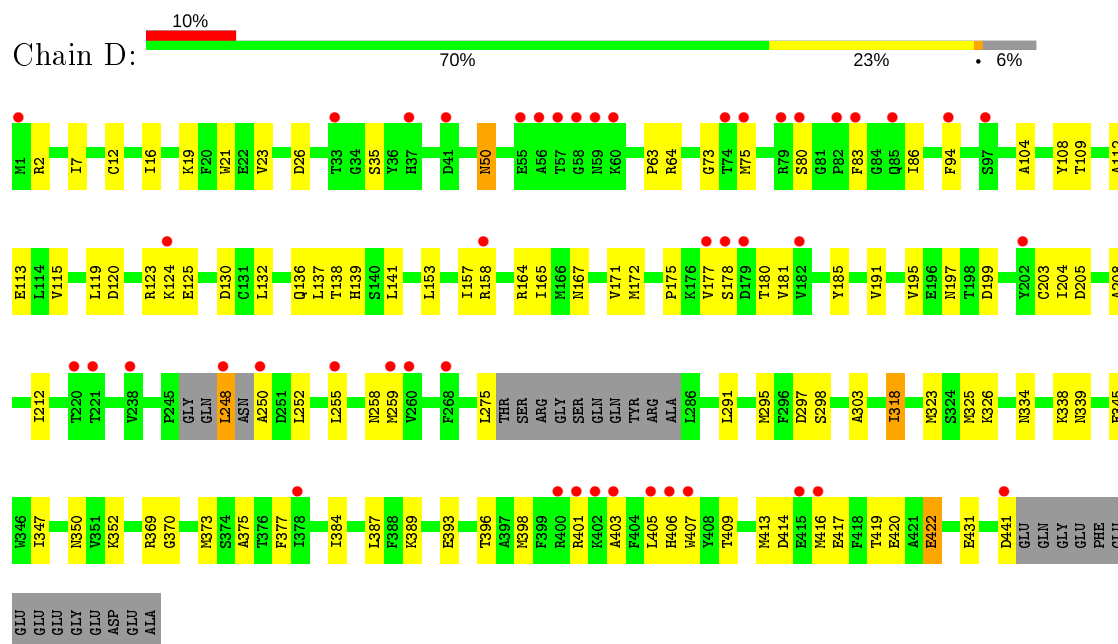


• Molecule 2: Tubulin beta chain

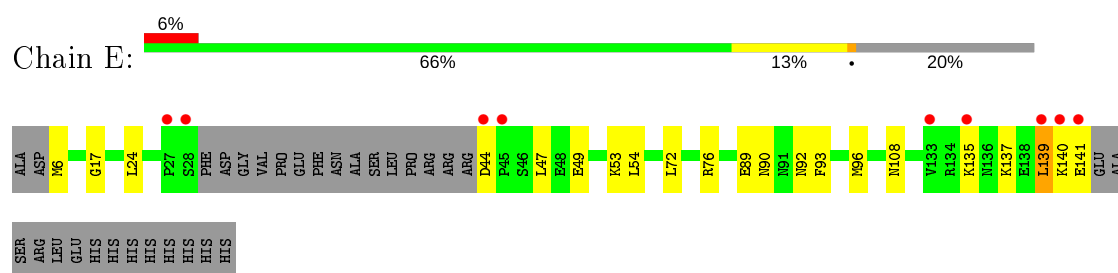




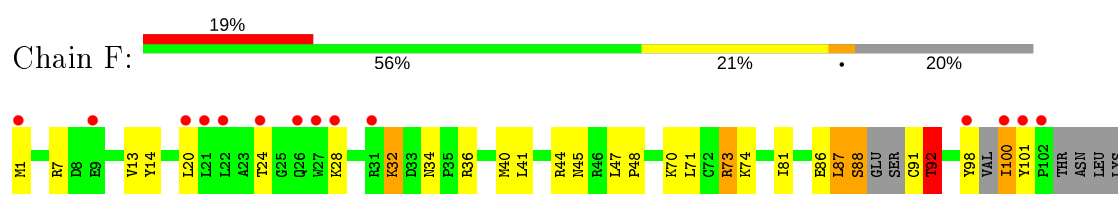
• Molecule 2: Tubulin beta chain

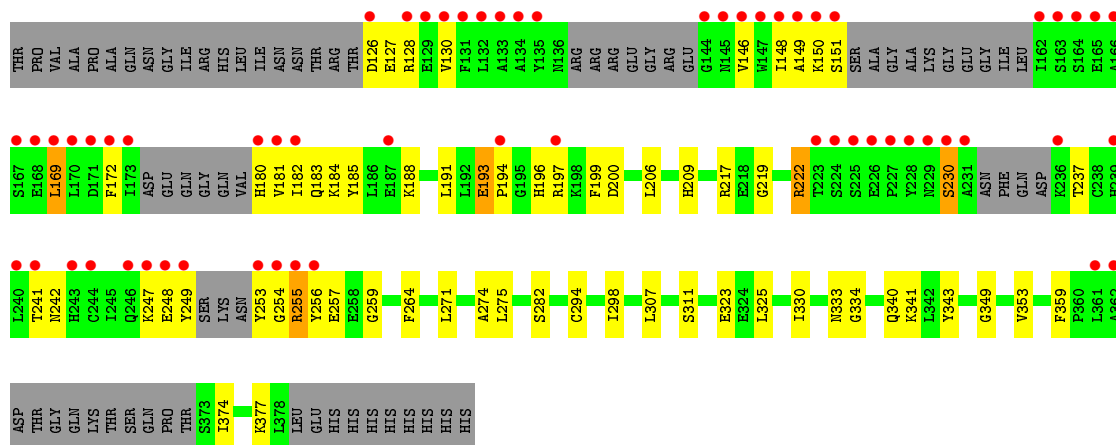


• Molecule 3: Stathmin



• 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	104.36Å 157.25Å 179.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.30 47.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.64-2.30) 99.8 (47.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.181 , 0.200 0.181 , 0.200	Depositor DCC
R_{free} test set	6500 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	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	0.95	EDS
Total number of atoms	18127	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: GDP, GOL, MG, NV4, IMD, NA, CA, GTP, ACP, MES, PEG

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	0.41	0/3596	0.56	0/4883
1	C	0.51	1/3583 (0.0%)	0.60	0/4866
2	B	0.42	0/3485	0.57	0/4718
2	D	0.37	0/3399	0.53	0/4602
3	E	0.38	0/1024	0.51	0/1358
4	F	0.42	0/2644	0.53	0/3566
All	All	0.43	1/17731 (0.0%)	0.56	0/23993

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-6.82	1.70	1.82

There are no bond angle outliers.

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	3482	0	3434	66	0
1	C	3481	0	3401	82	0
2	B	3382	0	3270	82	0
2	D	3316	0	3213	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1010	0	1033	25	0
4	F	2577	0	2576	100	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	1	0	0	0	0
7	A	12	0	16	2	0
7	C	18	8	24	10	0
7	D	18	0	23	2	0
8	A	5	5	5	4	0
8	C	5	0	5	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
12	B	12	0	12	0	0
13	B	35	0	0	3	0
13	D	35	0	0	9	0
14	C	7	0	10	0	0
15	F	31	0	13	3	0
16	A	115	0	0	10	1
16	B	84	0	0	4	0
16	C	199	0	0	17	1
16	D	66	0	0	7	0
16	E	28	0	0	6	0
16	F	65	0	0	9	0
All	All	18114	13	17083	416	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (416) 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:221:ARG:HD2	2:D:325:MET:HB3	1.29	1.09
4:F:100:ILE:HD11	4:F:127:GLU:H	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:HB3	2:D:326:LYS:HE3	1.46	0.98
2:B:27:GLU:HA	2:B:369:ARG:HH22	1.27	0.98
4:F:32:LYS:HD2	4:F:32:LYS:H	1.24	0.98
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.45	0.98
4:F:254:GLY:O	16:F:501:HOH:O	1.82	0.97
1:C:417:GLU:OE1	16:C:601:HOH:O	1.84	0.94
4:F:91:CYS:O	4:F:92:THR:HB	1.67	0.92
2:B:220:THR:O	16:B:601:HOH:O	1.85	0.92
2:D:175:PRO:HA	2:D:178:SER:HB2	1.51	0.92
2:D:370:GLY:O	16:D:602:HOH:O	1.86	0.91
4:F:100:ILE:HD11	4:F:127:GLU:N	1.84	0.91
1:C:98:ASP:OD1	16:C:602:HOH:O	1.87	0.90
2:D:180:THR:HG22	2:D:181:VAL:H	1.37	0.90
2:D:431:GLU:OE2	16:D:603:HOH:O	1.88	0.89
4:F:73:ARG:HD2	4:F:74:LYS:H	1.35	0.89
1:C:386:GLU:OE2	16:C:603:HOH:O	1.92	0.87
2:B:27:GLU:HA	2:B:369:ARG:NH2	1.88	0.87
3:E:53:LYS:O	16:E:201:HOH:O	1.92	0.87
4:F:247:LYS:HZ1	4:F:259:GLY:HA2	1.39	0.87
4:F:100:ILE:CD1	4:F:127:GLU:H	1.90	0.83
4:F:169:LEU:HD13	4:F:172:PHE:HB3	1.59	0.83
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.59	0.82
1:A:218:ASP:HB3	16:A:610:HOH:O	1.79	0.82
2:B:159:GLU:OE2	16:B:602:HOH:O	1.97	0.82
1:C:221:ARG:CD	2:D:325:MET:HB3	2.09	0.81
1:C:214:ARG:NH1	16:C:607:HOH:O	2.10	0.80
4:F:1:MET:SD	4:F:28:LYS:HD3	2.21	0.80
2:B:247:GLN:HG3	2:B:248:LEU:H	1.45	0.80
4:F:151:SER:OG	4:F:180:HIS:HA	1.82	0.79
1:C:41:THR:OG1	16:C:604:HOH:O	2.01	0.79
4:F:247:LYS:NZ	4:F:259:GLY:HA2	1.97	0.79
4:F:359:PHE:O	16:F:504:HOH:O	2.01	0.79
4:F:237:THR:HG21	4:F:249:TYR:HD1	1.48	0.78
2:D:389:LYS:NZ	16:D:604:HOH:O	2.16	0.77
2:B:42:LEU:HD12	2:B:42:LEU:H	1.50	0.76
2:B:247:GLN:O	16:B:603:HOH:O	2.02	0.76
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.19	0.76
1:C:288:VAL:HG23	7:C:504:GOL:H2	1.67	0.76
4:F:150:LYS:HD2	4:F:151:SER:H	1.51	0.75
4:F:100:ILE:N	4:F:180:HIS:O	2.19	0.75
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:200:ASP:OD1	4:F:222:ARG:NH2	2.18	0.75
7:A:507:GOL:O1	16:A:601:HOH:O	1.95	0.75
1:C:215:ARG:NH1	16:C:605:HOH:O	2.03	0.74
2:B:281:GLN:HG2	2:B:281:GLN:O	1.88	0.74
3:E:108[B]:ASN:OD1	16:E:202:HOH:O	2.06	0.73
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.54	0.73
4:F:169:LEU:CD1	4:F:172:PHE:HB3	2.19	0.73
1:C:287:SER:HB2	7:C:504:GOL:H12	1.71	0.73
1:C:96:LYS:HE3	2:D:130:ASP:OD1	1.90	0.72
2:B:26:ASP:OD2	2:B:369:ARG:NE	2.21	0.72
4:F:237:THR:HG21	4:F:249:TYR:CD1	2.24	0.72
1:C:214:ARG:NE	16:C:607:HOH:O	2.12	0.71
4:F:73:ARG:HD2	4:F:74:LYS:N	2.05	0.71
4:F:334:GLY:O	16:F:505:HOH:O	2.08	0.70
1:C:18:ASN:OD1	16:C:606:HOH:O	2.09	0.70
1:C:163:LYS:HE2	3:E:93:PHE:CD2	2.27	0.69
2:D:441:ASP:N	16:D:601:HOH:O	1.86	0.69
1:A:288:VAL:H	8:A:505:IMD:HN1	1.41	0.69
4:F:32:LYS:HD2	4:F:32:LYS:N	2.04	0.68
4:F:87:LEU:O	4:F:88:SER:HB3	1.93	0.68
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.93	0.68
1:A:228:ASN:O	1:A:232:SER:OG	2.10	0.68
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.57	0.68
1:C:215:ARG:HD2	16:C:605:HOH:O	1.95	0.67
1:A:221:ARG:HG2	2:B:325:MET:HG2	1.76	0.67
1:C:327:ASP:OD2	16:C:608:HOH:O	2.13	0.67
4:F:254:GLY:CA	16:F:501:HOH:O	2.42	0.67
2:D:370:GLY:C	16:D:602:HOH:O	2.26	0.67
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.77	0.67
1:C:221:ARG:HG2	1:C:221:ARG:O	1.93	0.66
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.21	0.66
4:F:146:VAL:O	4:F:184:LYS:NZ	2.28	0.66
1:A:386:GLU:OE2	16:A:602:HOH:O	2.14	0.66
1:C:280:LYS:HD3	16:C:640:HOH:O	1.95	0.66
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.77	0.66
2:B:340:SER:CB	4:F:34:ASN:HD21	2.08	0.65
2:D:416:MET:O	2:D:420:GLU:HG3	1.96	0.65
2:D:136:GLN:HA	2:D:167:ASN:O	1.97	0.65
4:F:127:GLU:HB2	4:F:130:VAL:CG2	2.27	0.64
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.33	0.64
2:B:280:SER:O	2:B:281:GLN:HB3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:333:ASN:ND2	15:F:402:ACP:O2G	2.27	0.63
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.79	0.63
4:F:193:GLU:HG3	4:F:196:HIS:H	1.65	0.62
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.82	0.62
1:A:373:ARG:CZ	8:A:505:IMD:H5	2.29	0.62
3:E:92:ASN:O	3:E:96:MET:HG2	2.00	0.62
4:F:169:LEU:O	4:F:169:LEU:HD12	1.98	0.62
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.35	0.62
2:B:105[B]:LYS:NZ	7:C:501:GOL:H31	2.14	0.61
4:F:100:ILE:HG23	4:F:126:ASP:OD2	2.00	0.61
2:B:247:GLN:HG3	2:B:248:LEU:N	2.15	0.61
2:B:250:ALA:HB1	13:B:505:NV4:O16	2.00	0.61
4:F:100:ILE:HD11	4:F:127:GLU:C	2.21	0.61
1:A:283:HIS:HD2	1:A:284:GLU:O	1.84	0.61
4:F:341:LYS:CB	16:F:502:HOH:O	2.49	0.61
4:F:100:ILE:HD11	4:F:127:GLU:CA	2.32	0.60
2:B:248:LEU:HD11	13:B:505:NV4:S30	2.41	0.60
2:D:323:MET:HB3	2:D:373:MET:CE	2.32	0.60
1:C:1:MET:O	1:C:2:ARG:HB2	2.02	0.60
2:D:352:LYS:HG3	13:D:507:NV4:C17	2.32	0.60
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.42	0.60
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.83	0.60
4:F:100:ILE:HG22	4:F:101:TYR:N	2.16	0.60
2:B:2:ARG:NE	2:B:133:GLN:HG3	2.17	0.60
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.22	0.60
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.20	0.59
2:D:258:ASN:HB3	13:D:507:NV4:C18	2.32	0.59
1:C:339:ARG:O	16:C:609:HOH:O	2.17	0.59
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.84	0.59
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.67	0.59
1:A:304:LYS:HB2	16:A:614:HOH:O	2.03	0.59
1:C:271:THR:HG23	1:C:300:ASN:C	2.23	0.59
4:F:188:LYS:HD2	4:F:323:GLU:CD	2.23	0.59
2:B:42:LEU:HD12	2:B:42:LEU:N	2.17	0.58
4:F:184:LYS:HD2	4:F:185:TYR:N	2.18	0.58
2:B:345:GLU:CD	2:B:345:GLU:H	2.06	0.58
2:B:47:GLU:HB3	2:B:245:PRO:HG3	1.84	0.58
2:D:2:ARG:NH2	16:D:605:HOH:O	2.26	0.58
1:C:163:LYS:HE2	3:E:93:PHE:CG	2.38	0.58
1:C:214:ARG:CZ	16:C:607:HOH:O	2.41	0.57
2:D:401:ARG:HE	2:D:403:ALA:HB2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.85	0.57
1:C:253:THR:HB	7:C:501:GOL:H11	1.84	0.57
2:D:50:ASN:ND2	2:D:50:ASN:H	2.02	0.57
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.40	0.57
4:F:148:ILE:HG22	4:F:183:GLN:O	2.04	0.57
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.04	0.57
2:D:295:MET:CG	2:D:377:PHE:HB2	2.34	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.56
2:D:255:LEU:HD13	13:D:507:NV4:C8	2.35	0.56
2:D:180:THR:HG22	2:D:181:VAL:N	2.16	0.56
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.87	0.56
4:F:150:LYS:O	4:F:151:SER:OG	2.12	0.56
2:B:42:LEU:H	2:B:42:LEU:CD1	2.17	0.56
1:C:287:SER:HA	7:C:504:GOL:O2	2.06	0.56
4:F:100:ILE:CG2	4:F:101:TYR:N	2.69	0.56
4:F:74:LYS:NZ	4:F:150:LYS:HE3	2.20	0.56
1:A:288:VAL:HG23	8:A:505:IMD:HN1	1.71	0.55
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.88	0.55
1:C:71:GLU:HG2	1:C:72:PRO:N	2.21	0.55
2:D:203:CYS:SG	2:D:384[B]:ILE:HD11	2.46	0.55
2:D:153:LEU:O	2:D:157:ILE:HG13	2.07	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.06	0.55
4:F:149:ALA:HB2	4:F:182:ILE:CD1	2.36	0.55
4:F:255:ARG:HB2	4:F:256:TYR:CD2	2.42	0.55
4:F:40:MET:HE2	4:F:47:LEU:HG	1.88	0.55
3:E:135:LYS:NZ	3:E:139:LEU:HD21	2.20	0.55
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.40	0.55
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.42	0.55
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.72	0.55
2:B:105[A]:LYS:NZ	7:C:501:GOL:H31	2.22	0.54
1:C:293:ASN:HA	1:C:335:ILE:HD11	1.89	0.54
3:E:89:GLU:OE2	16:E:203:HOH:O	2.18	0.54
4:F:151:SER:CB	4:F:180:HIS:HA	2.38	0.54
4:F:70:LYS:CE	4:F:298:ILE:HD11	2.37	0.54
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.89	0.54
4:F:341:LYS:HB3	16:F:502:HOH:O	2.08	0.54
1:A:23:LEU:O	1:A:27:GLU:HG3	2.07	0.54
1:A:206:ASN:HA	1:A:209[B]:ILE:HG12	1.89	0.54
1:A:304:LYS:CB	16:A:614:HOH:O	2.55	0.54
3:E:108[A]:ASN:OD1	16:E:204:HOH:O	2.19	0.54
2:D:112:ALA:O	2:D:115:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:HH22	4:F:151:SER:C	2.10	0.54
1:C:271:THR:HG23	1:C:300:ASN:O	2.07	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.54
2:B:396:THR:O	2:B:400:ARG:HG2	2.09	0.53
2:D:323:MET:HB3	2:D:373:MET:HE1	1.91	0.53
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.39	0.53
2:B:301:MET:HE1	2:B:307:PRO:HG2	1.90	0.53
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.44	0.53
2:D:393:GLU:HA	2:D:396:THR:HG22	1.90	0.53
2:B:238:VAL:HG22	2:B:378:ILE:HG12	1.90	0.53
2:B:105[B]:LYS:HZ2	7:C:501:GOL:H31	1.73	0.53
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.91	0.53
1:C:288:VAL:H	7:C:504:GOL:H12	1.73	0.52
2:D:258:ASN:HB3	13:D:507:NV4:C17	2.38	0.52
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.90	0.52
2:D:248:LEU:O	2:D:248:LEU:HG	2.09	0.52
4:F:247:LYS:HD3	4:F:253:TYR:CE2	2.44	0.52
1:A:220:GLU:CG	2:B:326:LYS:HD2	2.40	0.52
2:D:16:ILE:HD11	2:D:138:THR:HB	1.91	0.52
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.10	0.52
2:D:191:VAL:O	2:D:195:VAL:HG23	2.08	0.52
3:E:44:ASP:N	16:E:206:HOH:O	2.42	0.52
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.45	0.52
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.52
4:F:100:ILE:HD13	4:F:126:ASP:CG	2.30	0.52
4:F:98:TYR:O	4:F:181:VAL:HA	2.10	0.52
3:E:135:LYS:HZ1	3:E:139:LEU:HD21	1.75	0.52
1:C:440:VAL:HG12	1:C:440:VAL:O	2.09	0.51
2:B:2:ARG:HA	2:B:131:CYS:O	2.10	0.51
1:C:2:ARG:HA	1:C:2:ARG:NE	2.25	0.51
1:C:221:ARG:CG	1:C:221:ARG:O	2.57	0.51
2:D:208:ALA:O	2:D:212:ILE:HG13	2.11	0.51
2:B:42:LEU:HB2	2:B:358:ILE:HD11	1.92	0.51
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.11	0.51
2:B:27:GLU:CA	2:B:369:ARG:NH2	2.68	0.51
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.44	0.51
2:D:409:THR:O	3:E:140:LYS:HE2	2.10	0.51
4:F:100:ILE:CG2	4:F:101:TYR:H	2.25	0.50
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.26	0.50
1:A:79:ARG:O	1:A:84:ARG:HB3	2.11	0.50
2:B:255:LEU:HD22	2:B:259:MET:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158[A]:ARG:NH2	2:D:197:ASN:OD1	2.44	0.50
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	0.50
4:F:44:ARG:NH1	16:F:511:HOH:O	2.45	0.50
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.93	0.50
2:D:250:ALA:HB1	13:D:507:NV4:O16	2.11	0.50
4:F:217:ARG:HG3	4:F:374:ILE:O	2.12	0.49
1:A:221:ARG:NH1	2:B:325:MET:O	2.45	0.49
4:F:199:PHE:HA	4:F:241:THR:HG21	1.93	0.49
4:F:249:TYR:O	4:F:249:TYR:CD1	2.65	0.49
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.93	0.49
2:D:419:THR:O	2:D:422:GLU:OE1	2.31	0.49
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	1.95	0.49
2:B:217:LEU:HD13	2:B:277:SER:HB3	1.93	0.49
2:D:119:LEU:O	2:D:123:ARG:HG3	2.12	0.49
2:D:323:MET:HB3	2:D:373:MET:HE2	1.95	0.48
4:F:70:LYS:HE3	4:F:298:ILE:HD11	1.95	0.48
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.13	0.48
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.78	0.48
2:D:7:ILE:O	2:D:137:LEU:HD12	2.14	0.48
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.13	0.48
2:B:2:ARG:HE	2:B:133:GLN:HG3	1.77	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.54	0.48
2:D:158[A]:ARG:NH2	16:D:609:HOH:O	2.47	0.48
2:B:295:MET:SD	2:B:375:ALA:HB1	2.53	0.48
1:C:340:SER:HA	16:C:609:HOH:O	2.13	0.48
4:F:151:SER:HB2	4:F:180:HIS:ND1	2.29	0.48
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.96	0.48
1:A:401:LYS:NZ	16:A:609:HOH:O	2.40	0.48
1:A:178:SER:OG	13:B:505:NV4:N32	2.46	0.48
2:D:132:LEU:HD23	2:D:164:ARG:HH11	1.78	0.48
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.48
2:B:2:ARG:CZ	2:B:133:GLN:HG3	2.43	0.48
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.96	0.48
2:D:177:VAL:HG12	2:D:177:VAL:O	2.14	0.48
3:E:44:ASP:OD1	3:E:44:ASP:N	2.46	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.12	0.48
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.95	0.48
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.49	0.48
4:F:169:LEU:HD11	4:F:172:PHE:CD2	2.49	0.48
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.95	0.47
2:D:7:ILE:O	2:D:137:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:CB	2:D:326:LYS:HE3	2.31	0.47
4:F:127:GLU:HB2	4:F:130:VAL:HG22	1.96	0.47
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.95	0.47
1:A:285:GLN:OE1	1:A:372[B]:GLN:HG3	2.14	0.47
1:C:179:THR:HA	1:C:183:GLU:OE1	2.14	0.47
2:B:83:PHE:O	2:B:86:ILE:HG22	2.14	0.47
1:A:192:HIS:CG	1:A:421:ALA:HA	2.49	0.47
2:D:318:ILE:HG12	13:D:507:NV4:C28	2.44	0.47
4:F:150:LYS:HD2	4:F:151:SER:N	2.25	0.47
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.49	0.47
1:C:196[B]:GLU:HG2	16:C:666:HOH:O	2.15	0.47
1:C:230:LEU:O	1:C:234:ILE:HD12	2.14	0.47
2:D:339:ASN:CB	7:D:506:GOL:H32	2.45	0.47
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.50	0.47
1:C:287:SER:HB2	7:C:504:GOL:C1	2.43	0.47
2:D:75:MET:CE	2:D:94:PHE:HD2	2.28	0.47
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.28	0.47
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.47
4:F:341:LYS:N	16:F:502:HOH:O	1.86	0.46
1:A:83:TYR:O	1:A:84:ARG:C	2.54	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.46
2:B:286:LEU:N	2:B:286:LEU:HD12	2.31	0.46
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.50	0.46
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.80	0.46
3:E:137:LYS:HG3	3:E:140:LYS:NZ	2.30	0.46
1:A:221:ARG:HG2	2:B:325:MET:CE	2.45	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.46
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.46	0.46
2:D:109:THR:O	2:D:113:GLU:OE1	2.34	0.46
2:D:248:LEU:HD23	2:D:250:ALA:HB2	1.96	0.46
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	1.98	0.46
1:C:270:ALA:HB3	1:C:302:MET:HG2	1.98	0.46
1:A:304:LYS:CG	16:A:614:HOH:O	2.63	0.46
2:B:298:SER:HA	2:B:301:MET:HE2	1.98	0.46
1:C:336:LYS:HE2	16:C:785:HOH:O	2.14	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.16	0.45
2:D:158[B]:ARG:NH2	2:D:199:ASP:OD2	2.49	0.45
2:B:298:SER:HA	2:B:301:MET:CE	2.46	0.45
2:B:301:MET:HE1	2:B:307:PRO:CG	2.46	0.45
4:F:247:LYS:HA	4:F:253:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.82	0.45
1:C:2:ARG:NH2	16:C:619:HOH:O	2.49	0.45
1:A:185:TYR:O	1:A:189:LEU:HG	2.17	0.45
1:C:392:ASP:OD2	1:C:429:GLU:OE1	2.35	0.45
4:F:100:ILE:HD13	4:F:126:ASP:HB3	1.99	0.45
3:E:49:GLU:OE2	3:E:53:LYS:HE2	2.17	0.45
1:A:112:LYS:HG3	3:E:54:LEU:HB3	1.99	0.45
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.47	0.44
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.17	0.44
1:C:288:VAL:CG2	7:C:504:GOL:H2	2.43	0.44
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.35	0.44
2:B:2:ARG:NH2	2:B:133:GLN:HG3	2.31	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.52	0.44
1:A:327:ASP:OD2	16:A:603:HOH:O	2.21	0.44
2:D:318:ILE:CG1	13:D:507:NV4:C28	2.96	0.44
13:D:507:NV4:C28	13:D:507:NV4:O24	2.65	0.44
4:F:169:LEU:HA	4:F:169:LEU:HD13	1.77	0.44
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.50	0.44
1:A:209[B]:ILE:HG13	1:A:210:TYR:N	2.32	0.44
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.49	0.44
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.89	0.44
2:B:208:ALA:HB2	2:B:304:ALA:N	2.33	0.44
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.00	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.48	0.44
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.18	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.18	0.44
2:D:352:LYS:HD3	2:D:352:LYS:HA	1.78	0.44
4:F:193:GLU:HA	4:F:194:PRO:C	2.37	0.44
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.17	0.44
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.99	0.43
4:F:127:GLU:HB2	4:F:130:VAL:HG21	1.99	0.43
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.18	0.43
1:C:177:VAL:CG1	1:C:224:TYR:CE1	3.01	0.43
2:D:318:ILE:HD11	13:D:507:NV4:C28	2.48	0.43
2:B:68:VAL:HA	2:B:93:VAL:O	2.18	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.43
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.48	0.43
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:CD2	1:C:86:LEU:HD22	2.53	0.43
1:A:288:VAL:N	8:A:505:IMD:HN1	2.12	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.01	0.43
2:D:185:TYR:CE2	2:D:398:MET:HE2	2.53	0.43
4:F:230:SER:OG	4:F:230:SER:O	2.33	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.39	0.43
2:D:387:LEU:C	2:D:387:LEU:HD23	2.39	0.43
1:A:66[A]:VAL:HG23	1:A:125:LEU:HD12	2.01	0.43
1:A:280:LYS:HE2	1:A:283:HIS:ND1	2.34	0.43
2:B:334:ASN:O	2:B:338:LYS:HG2	2.18	0.43
1:C:175:PRO:HA	1:C:179:THR:HG21	2.01	0.43
1:C:177:VAL:HG11	1:C:224:TYR:HE1	1.83	0.42
1:A:331:ALA:O	1:A:335:ILE:HG13	2.19	0.42
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.54	0.42
4:F:100:ILE:HD13	4:F:126:ASP:CB	2.49	0.42
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.54	0.42
2:B:115:VAL:HG23	2:B:153:LEU:HD23	2.01	0.42
2:B:301:MET:HE2	2:B:301:MET:HB2	1.65	0.42
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.77	0.42
1:A:218:ASP:CB	16:A:610:HOH:O	2.55	0.42
1:A:300:ASN:OD1	7:A:504:GOL:H12	2.20	0.42
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.65	0.42
2:D:297:ASP:OD1	2:D:298:SER:N	2.53	0.42
3:E:90:ASN:ND2	16:E:205:HOH:O	2.29	0.42
4:F:247:LYS:CE	4:F:259:GLY:HA2	2.49	0.42
1:A:304:LYS:HG3	16:A:614:HOH:O	2.19	0.42
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.42
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.84	0.42
1:A:329:ASN:HB3	3:E:6:MET:HE1	2.02	0.42
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.85	0.42
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.54	0.42
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.35	0.42
2:D:19:LYS:O	2:D:23:VAL:HG23	2.20	0.42
4:F:241:THR:OG1	15:F:402:ACP:O3'	2.38	0.42
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.41
4:F:81:ILE:O	4:F:87:LEU:O	2.38	0.41
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.84	0.41
4:F:242:ASN:OD1	15:F:402:ACP:H5'1	2.20	0.41
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	2.02	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.41
2:B:218:LYS:HA	2:B:218:LYS:HD3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ALA:O	1:C:337:THR:HG23	2.19	0.41
2:B:214:PHE:CD1	2:B:220:THR:HA	2.56	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.41
1:C:248:LEU:HD12	1:C:357:TYR:CZ	2.55	0.41
4:F:74:LYS:HZ3	4:F:150:LYS:HE3	1.84	0.41
4:F:247:LYS:HZ1	4:F:259:GLY:CA	2.23	0.41
4:F:271:LEU:HD23	4:F:275[B]:LEU:HD12	2.01	0.41
2:B:22[B]:GLU:HG3	2:B:83:PHE:CE1	2.56	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.41
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	0.41
4:F:209:HIS:HA	4:F:311:SER:O	2.20	0.41
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.41
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.56	0.41
4:F:13:VAL:HG23	16:F:524:HOH:O	2.21	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.74	0.41
1:C:141:PHE:O	1:C:147:SER:HB3	2.19	0.41
1:C:1:MET:O	1:C:2:ARG:CB	2.69	0.41
2:D:291:LEU:HG	2:D:375:ALA:HB2	2.02	0.41
3:E:47:LEU:HD12	3:E:47:LEU:O	2.21	0.41
2:B:75:MET:N	16:B:614:HOH:O	2.41	0.41
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	2.02	0.41
4:F:188:LYS:HD3	4:F:188:LYS:HA	1.94	0.41
4:F:14:TYR:CD1	4:F:41:LEU:HD22	2.56	0.41
4:F:47:LEU:HD23	4:F:48:PRO:HD2	2.03	0.41
2:D:414:ASP:N	2:D:414:ASP:OD1	2.54	0.41
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.51	0.41
1:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.62	0.40
2:B:192:HIS:ND1	2:B:424[B]:ASN:ND2	2.67	0.40
1:C:177:VAL:HG11	1:C:224:TYR:CE1	2.55	0.40
2:D:339:ASN:CG	7:D:506:GOL:H32	2.41	0.40
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.40
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.24	0.40
2:D:83:PHE:O	2:D:86:ILE:HG22	2.20	0.40
2:B:126:SER:O	2:B:129:CYS:HB2	2.21	0.40
2:B:36:TYR:CD2	2:B:46:LEU:HD11	2.56	0.40
1:C:248:LEU:HD13	1:C:355:ILE:HD12	2.03	0.40
4:F:188:LYS:HD2	4:F:323:GLU:OE2	2.21	0.40
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	2.03	0.40
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.22	0.40
4:F:191:LEU:HD23	4:F:191:LEU:HA	1.86	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.34	0.40
1:C:351:PHE:N	1:C:351:PHE:CD1	2.89	0.40
4:F:274:ALA:C	4:F:275[A]:LEU:HD22	2.42	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:665:HOH:O	16:C:677:HOH:O[3_554]	1.70	0.50

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	449/451 (100%)	437 (97%)	10 (2%)	2 (0%)	34	42
1	C	447/451 (99%)	434 (97%)	12 (3%)	1 (0%)	47	58
2	B	428/445 (96%)	414 (97%)	12 (3%)	2 (0%)	29	35
2	D	416/445 (94%)	407 (98%)	8 (2%)	1 (0%)	47	58
3	E	119/152 (78%)	118 (99%)	1 (1%)	0	100	100
4	F	296/388 (76%)	288 (97%)	6 (2%)	2 (1%)	22	26
All	All	2155/2332 (92%)	2098 (97%)	49 (2%)	8 (0%)	34	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
2	D	73	GLY
4	F	92	THR
4	F	255	ARG
1	A	178	SER

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Mol	Chain	Res	Type
2	B	177	VAL
1	C	178	SER
2	B	360	PRO

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	382/379 (101%)	372 (97%)	10 (3%)	46	63
1	C	380/379 (100%)	374 (98%)	6 (2%)	62	78
2	B	377/383 (98%)	364 (97%)	13 (3%)	37	51
2	D	367/383 (96%)	357 (97%)	10 (3%)	44	61
3	E	111/136 (82%)	110 (99%)	1 (1%)	78	89
4	F	285/346 (82%)	270 (95%)	15 (5%)	22	31
All	All	1902/2006 (95%)	1847 (97%)	55 (3%)	41	58

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	71	GLU
1	A	84	ARG
1	A	113	GLU
1	A	164	LYS
1	A	220	GLU
1	A	232	SER
1	A	282	TYR
1	A	381	THR
1	A	430	LYS
2	B	85	GLN
2	B	139	HIS
2	B	192	HIS
2	B	232	SER
2	B	238	VAL

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Mol	Chain	Res	Type
2	B	247	GLN
2	B	248	LEU
2	B	255	LEU
2	B	259	MET
2	B	282	GLN
2	B	293	GLN
2	B	325	MET
2	B	430	SER
1	C	71	GLU
1	C	286	LEU
1	C	336	LYS
1	C	347	CYS
1	C	361	THR
1	C	430	LYS
2	D	35	SER
2	D	50	ASN
2	D	80	SER
2	D	124	LYS
2	D	139	HIS
2	D	248	LEU
2	D	259	MET
2	D	318	ILE
2	D	345	GLU
2	D	422	GLU
3	E	139	LEU
4	F	32	LYS
4	F	45	ASN
4	F	73	ARG
4	F	86	GLU
4	F	87	LEU
4	F	88	SER
4	F	92	THR
4	F	100	ILE
4	F	128	ARG
4	F	169	LEU
4	F	193	GLU
4	F	222	ARG
4	F	230	SER
4	F	248	GLU
4	F	377	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
2	B	101	ASN
4	F	196	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 11 are monoatomic - leaving 19 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
13	NV4	D	507	-	34,40,40	2.06	7 (20%)	49,59,59	2.53	19 (38%)
7	GOL	C	504	-	5,5,5	0.40	0	5,5,5	0.22	0
7	GOL	D	506	-	5,5,5	0.40	0	5,5,5	0.73	0
7	GOL	A	504	-	5,5,5	0.43	0	5,5,5	0.48	0
7	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.25	0
5	GTP	C	502	6	26,34,34	1.12	1 (3%)	33,54,54	1.68	5 (15%)
13	NV4	B	505	-	34,40,40	2.11	8 (23%)	49,59,59	2.21	12 (24%)
14	PEG	C	505	-	6,6,6	0.50	0	5,5,5	0.40	0
15	ACP	F	402	6	27,33,33	4.93	9 (33%)	32,52,52	2.68	5 (15%)
10	GDP	D	501	6	24,30,30	1.30	3 (12%)	31,47,47	1.84	7 (22%)
7	GOL	D	504	-	5,5,5	0.34	0	5,5,5	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	IMD	C	508	-	3,5,5	0.48	0	4,5,5	0.37	0
7	GOL	C	509	-	5,5,5	0.40	0	5,5,5	0.50	0
5	GTP	A	501	6	26,34,34	1.04	1 (3%)	33,54,54	2.11	10 (30%)
10	GDP	B	501	6	24,30,30	1.36	3 (12%)	31,47,47	1.92	6 (19%)
8	IMD	A	505	-	3,5,5	0.32	0	4,5,5	0.75	0
12	MES	B	504	-	12,12,12	2.09	1 (8%)	14,16,16	2.23	5 (35%)
7	GOL	C	501	-	5,5,5	0.36	0	5,5,5	0.39	0
7	GOL	D	505	2	5,5,5	0.35	0	5,5,5	0.52	0

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
13	NV4	D	507	-	-	3/12/49/49	0/6/6/6
7	GOL	C	504	-	-	2/4/4/4	-
7	GOL	D	506	-	-	2/4/4/4	-
8	IMD	C	508	-	-	-	0/1/1/1
7	GOL	A	504	-	-	4/4/4/4	-
7	GOL	A	507	-	-	3/4/4/4	-
5	GTP	C	502	6	-	7/18/38/38	0/3/3/3
13	NV4	B	505	-	-	1/12/49/49	0/6/6/6
14	PEG	C	505	-	-	1/4/4/4	-
15	ACP	F	402	6	-	8/15/38/38	0/3/3/3
10	GDP	D	501	6	-	5/12/32/32	0/3/3/3
7	GOL	D	504	-	-	2/4/4/4	-
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
7	GOL	C	509	-	-	2/4/4/4	-
10	GDP	B	501	6	-	4/12/32/32	0/3/3/3
8	IMD	A	505	-	-	-	0/1/1/1
12	MES	B	504	-	-	1/6/14/14	0/1/1/1
7	GOL	C	501	-	-	2/4/4/4	-
7	GOL	D	505	2	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	402	ACP	O4'-C1'	15.05	1.62	1.41
15	F	402	ACP	C2'-C1'	-14.85	1.31	1.53
15	F	402	ACP	PB-O3A	7.87	1.67	1.58
12	B	504	MES	C8-S	-7.12	1.67	1.77
15	F	402	ACP	O4'-C4'	-7.12	1.29	1.45
13	B	505	NV4	C1-C2	6.18	1.50	1.40
13	D	507	NV4	C1-C2	6.01	1.50	1.40
15	F	402	ACP	C6-N6	5.30	1.53	1.34
13	B	505	NV4	O14-C13	4.94	1.46	1.35
13	B	505	NV4	C3-S30	-4.47	1.78	1.84
13	D	507	NV4	C3-S30	-4.32	1.78	1.84
13	D	507	NV4	O14-C13	4.24	1.44	1.35
10	D	501	GDP	C6-C5	4.21	1.48	1.41
13	D	507	NV4	C9-C10	4.07	1.49	1.41
13	D	507	NV4	C11-C10	3.95	1.49	1.41
10	B	501	GDP	C6-C5	3.88	1.48	1.41
13	B	505	NV4	C11-C10	3.86	1.49	1.41
15	F	402	ACP	O2'-C2'	3.69	1.51	1.43
13	B	505	NV4	C9-C10	3.48	1.48	1.41
15	F	402	ACP	C2-N3	3.36	1.37	1.32
15	F	402	ACP	PB-O2B	-3.25	1.48	1.56
5	C	502	GTP	C6-N1	3.25	1.38	1.33
5	A	501	GTP	C6-N1	3.16	1.38	1.33
13	B	505	NV4	O25-C10	2.98	1.43	1.38
13	D	507	NV4	O25-C10	2.87	1.43	1.38
15	F	402	ACP	O3'-C3'	-2.71	1.36	1.43
13	B	505	NV4	C19-C18	2.63	1.45	1.39
10	B	501	GDP	O4'-C1'	2.60	1.44	1.41
10	D	501	GDP	C5-C4	2.46	1.47	1.40
10	B	501	GDP	PB-O2B	-2.46	1.45	1.54
13	D	507	NV4	C19-C18	2.44	1.45	1.39
10	D	501	GDP	C2'-C1'	-2.33	1.50	1.53
13	B	505	NV4	C1-C6	-2.06	1.48	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	402	ACP	C5-C6-N6	10.51	136.33	120.35
15	F	402	ACP	N6-C6-N1	-7.01	104.03	118.57
13	D	507	NV4	C9-C10-C11	-6.65	112.76	119.57
13	D	507	NV4	O25-C10-C11	-6.63	110.58	120.12
5	A	501	GTP	N3-C2-N1	-6.39	118.70	127.22
13	B	505	NV4	C9-C10-C11	-6.11	113.31	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	504	MES	C5-N4-C3	5.82	121.92	108.83
5	C	502	GTP	N3-C2-N1	-5.46	119.94	127.22
13	B	505	NV4	C7-C6-C5	5.43	121.95	113.31
10	B	501	GDP	C2-N3-C4	5.41	121.54	115.36
15	F	402	ACP	N3-C2-N1	-5.13	120.66	128.68
13	D	507	NV4	C15-C4-C5	4.95	108.94	101.79
5	A	501	GTP	C2-N3-C4	4.81	120.85	115.36
13	D	507	NV4	O25-C10-C9	-4.72	113.33	120.12
13	B	505	NV4	C15-C4-C5	4.46	108.23	101.79
13	B	505	NV4	O25-C10-C9	-4.43	113.75	120.12
10	D	501	GDP	C6-C5-C4	-4.39	116.61	120.80
13	D	507	NV4	C5-C4-C3	4.36	119.87	111.50
10	D	501	GDP	C2-N3-C4	4.33	120.30	115.36
13	B	505	NV4	C4-C5-C6	4.10	120.94	113.21
13	D	507	NV4	C4-C5-C6	3.96	120.69	113.21
5	C	502	GTP	C2-N3-C4	3.94	119.86	115.36
5	A	501	GTP	C6-N1-C2	3.88	122.09	115.93
15	F	402	ACP	C3'-C2'-C1'	3.84	106.77	100.98
13	D	507	NV4	C27-O24-C9	3.83	123.31	117.53
10	D	501	GDP	C6-N1-C2	3.81	121.98	115.93
13	B	505	NV4	O16-C13-C5	-3.77	124.54	129.38
5	A	501	GTP	C5-C6-N1	-3.76	118.28	123.43
10	B	501	GDP	C6-C5-C4	-3.76	117.21	120.80
10	B	501	GDP	C6-N1-C2	3.75	121.89	115.93
12	B	504	MES	O1S-S-C8	3.73	111.40	106.92
10	B	501	GDP	N3-C2-N1	-3.68	122.31	127.22
10	D	501	GDP	C5-C6-N1	-3.61	118.49	123.43
10	B	501	GDP	C5-C6-N1	-3.59	118.53	123.43
13	B	505	NV4	C5-C4-C3	3.48	118.18	111.50
13	D	507	NV4	O16-C13-C5	-3.28	125.17	129.38
13	D	507	NV4	C22-O23-C19	3.27	109.59	105.34
13	D	507	NV4	C1-C6-C5	3.22	112.00	106.58
13	D	507	NV4	C2-C1-C6	3.11	122.62	114.40
13	B	505	NV4	C22-O23-C19	3.02	109.26	105.34
15	F	402	ACP	PA-O3A-PB	-2.99	123.09	132.56
5	A	501	GTP	PA-O3A-PB	-2.98	122.58	132.83
5	A	501	GTP	N2-C2-N1	2.96	121.86	117.25
10	D	501	GDP	N3-C2-N1	-2.90	123.36	127.22
13	B	505	NV4	C2-C1-C6	2.89	122.04	114.40
13	D	507	NV4	C12-C11-C10	2.85	123.45	120.22
13	B	505	NV4	C22-O21-C18	2.83	109.02	105.34
5	C	502	GTP	C6-N1-C2	2.80	120.38	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	507	NV4	C22-O21-C18	2.79	108.97	105.34
13	B	505	NV4	O14-C13-O16	2.72	124.24	121.42
10	D	501	GDP	PA-O3A-PB	-2.70	123.56	132.83
13	D	507	NV4	O24-C9-C10	2.63	119.78	115.16
5	C	502	GTP	C5-C6-N1	-2.60	119.87	123.43
5	A	501	GTP	C4-C5-N7	-2.56	106.74	109.40
13	B	505	NV4	O26-C11-C12	-2.54	119.74	124.12
10	D	501	GDP	C4-C5-N7	-2.53	106.76	109.40
12	B	504	MES	O3S-S-C8	2.52	109.85	105.77
13	D	507	NV4	C9-C8-C7	2.48	123.80	119.83
5	C	502	GTP	N2-C2-N3	2.44	121.77	117.79
13	D	507	NV4	O24-C9-C8	-2.44	119.92	124.12
10	B	501	GDP	C4-C5-N7	-2.41	106.89	109.40
5	A	501	GTP	C5'-C4'-C3'	-2.40	106.18	115.18
13	D	507	NV4	O26-C11-C12	-2.39	120.01	124.12
5	A	501	GTP	C6-C5-C4	-2.26	118.64	120.80
13	D	507	NV4	C29-O26-C11	2.25	120.93	117.53
5	A	501	GTP	PB-O3B-PG	-2.16	125.41	132.83
12	B	504	MES	O2S-S-O1S	-2.16	106.48	113.95
13	D	507	NV4	C7-C6-C5	2.05	116.58	113.31
12	B	504	MES	C2-C3-N4	2.04	113.19	110.10

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	507	GOL	O1-C1-C2-C3
15	F	402	ACP	PB-C3B-PG-O1G
15	F	402	ACP	PB-C3B-PG-O2G
15	F	402	ACP	PB-C3B-PG-O3G
15	F	402	ACP	PG-C3B-PB-O1B
15	F	402	ACP	PG-C3B-PB-O3A
15	F	402	ACP	O4'-C4'-C5'-O5'
7	D	504	GOL	O1-C1-C2-C3
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O1A
13	D	507	NV4	C10-C9-O24-C27

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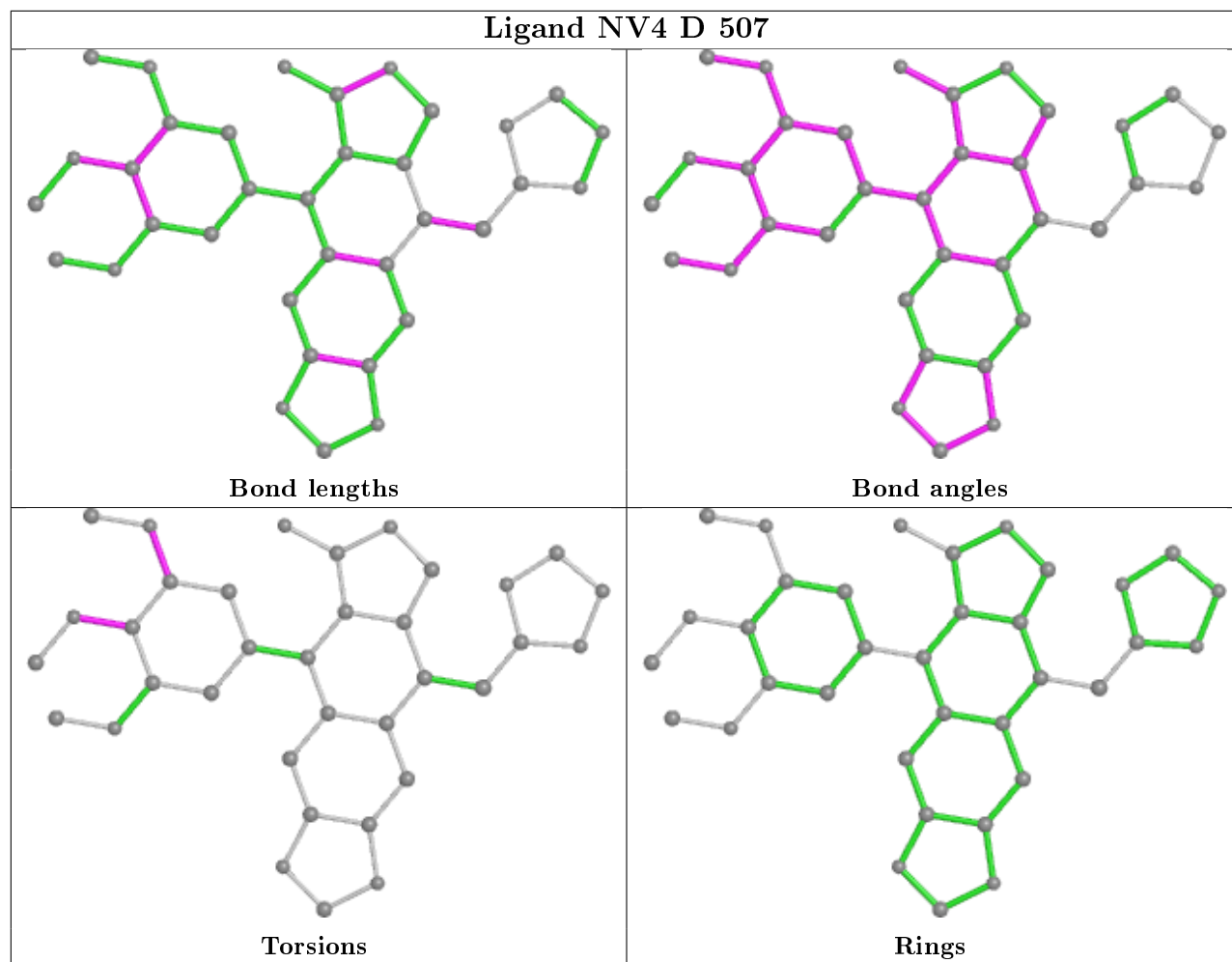
Mol	Chain	Res	Type	Atoms
13	D	507	NV4	C11-C10-O25-C28
15	F	402	ACP	C3'-C4'-C5'-O5'
13	D	507	NV4	C8-C9-O24-C27
7	A	504	GOL	O2-C2-C3-O3
7	C	509	GOL	C1-C2-C3-O3
7	C	501	GOL	O1-C1-C2-C3
7	A	504	GOL	O1-C1-C2-C3
7	A	504	GOL	C1-C2-C3-O3
7	D	506	GOL	C1-C2-C3-O3
7	D	505	GOL	C1-C2-C3-O3
7	A	507	GOL	O1-C1-C2-O2
7	D	504	GOL	O1-C1-C2-O2
7	C	509	GOL	O2-C2-C3-O3
7	A	504	GOL	O1-C1-C2-O2
12	B	504	MES	C8-C7-N4-C3
7	C	501	GOL	O1-C1-C2-O2
7	D	506	GOL	O2-C2-C3-O3
13	B	505	NV4	C11-C10-O25-C28
10	D	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O2A
15	F	402	ACP	PG-C3B-PB-O2B
5	A	501	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O2A
7	D	505	GOL	O1-C1-C2-C3
5	C	502	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
10	B	501	GDP	PB-O3A-PA-O2A
7	A	507	GOL	C1-C2-C3-O3
7	C	504	GOL	C1-C2-C3-O3
7	C	504	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O3A
14	C	505	PEG	O1-C1-C2-O2
5	C	502	GTP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A

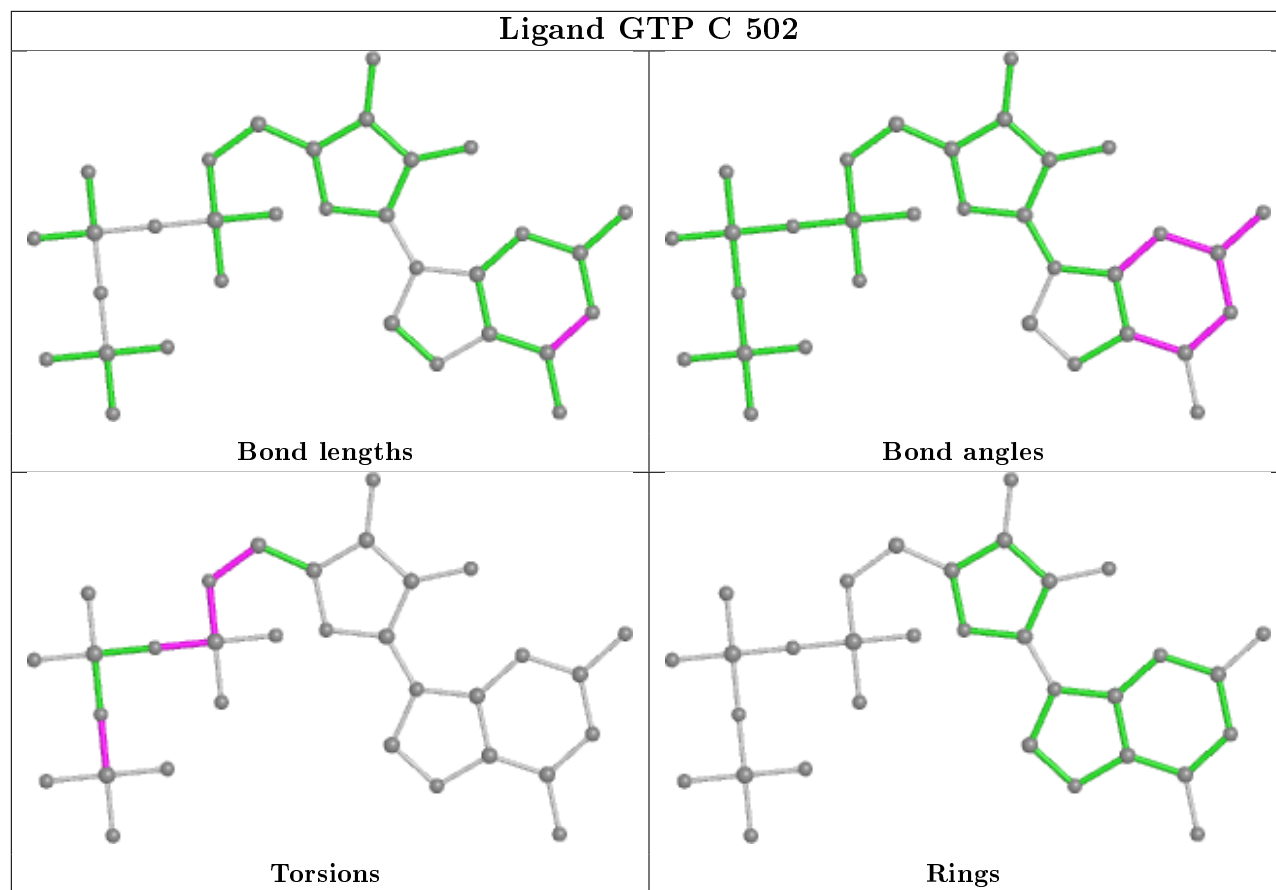
There are no ring outliers.

10 monomers are involved in 34 short contacts:

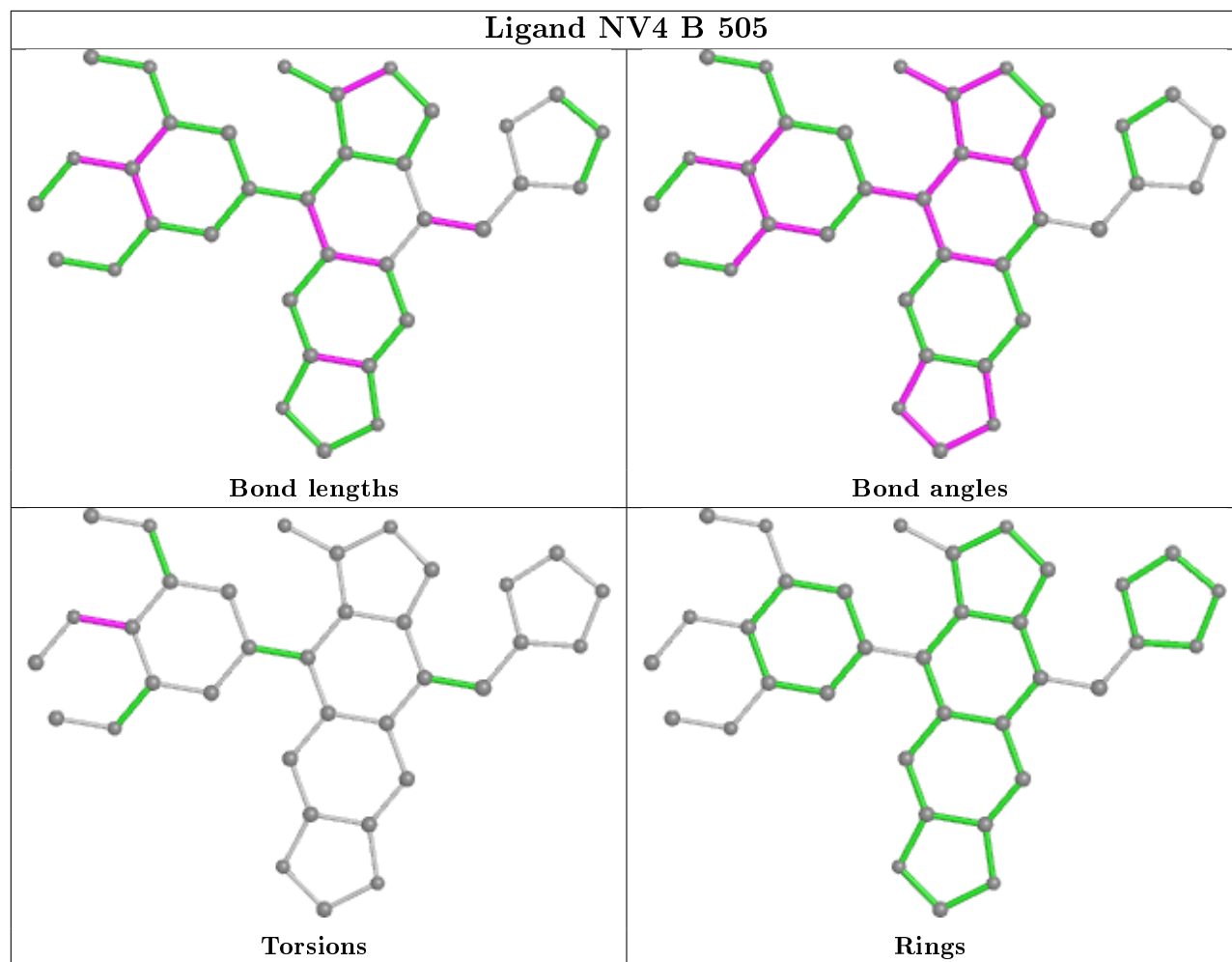
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	507	NV4	9	0
7	C	504	GOL	6	0
7	D	506	GOL	2	0
7	A	504	GOL	1	0
7	A	507	GOL	1	0
13	B	505	NV4	3	0
15	F	402	ACP	3	0
10	D	501	GDP	1	0
8	A	505	IMD	4	0
7	C	501	GOL	4	0

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.

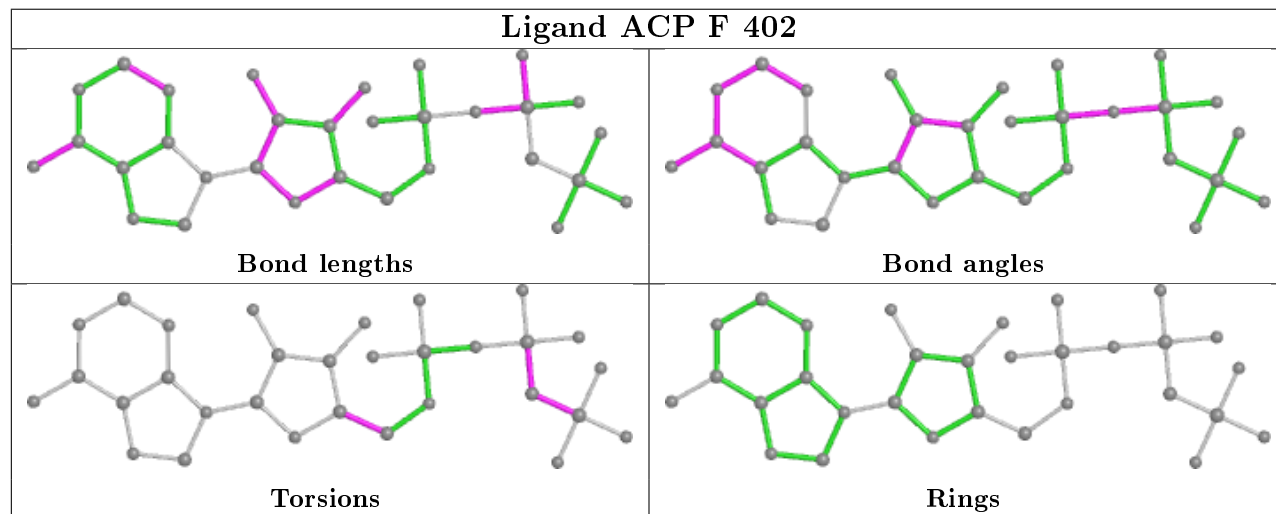


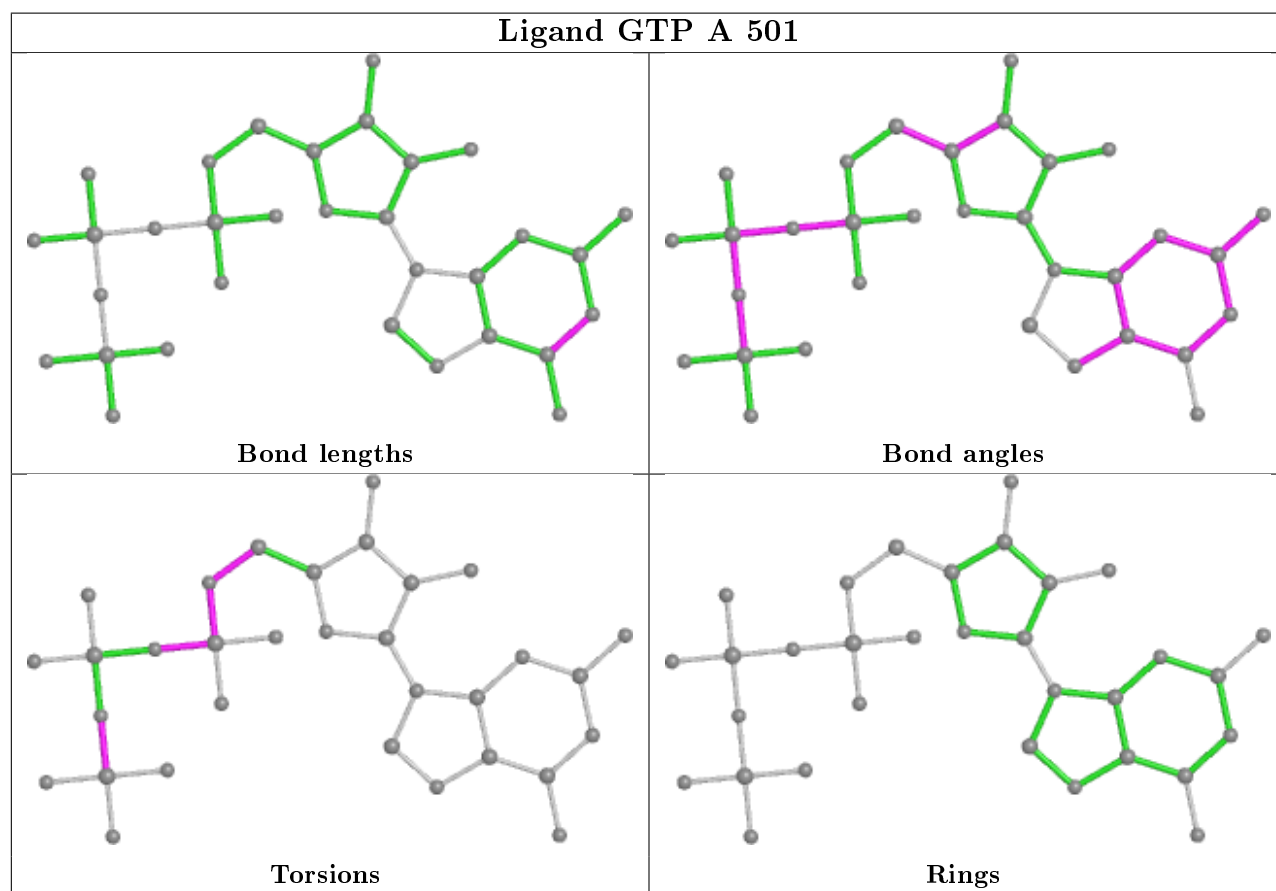
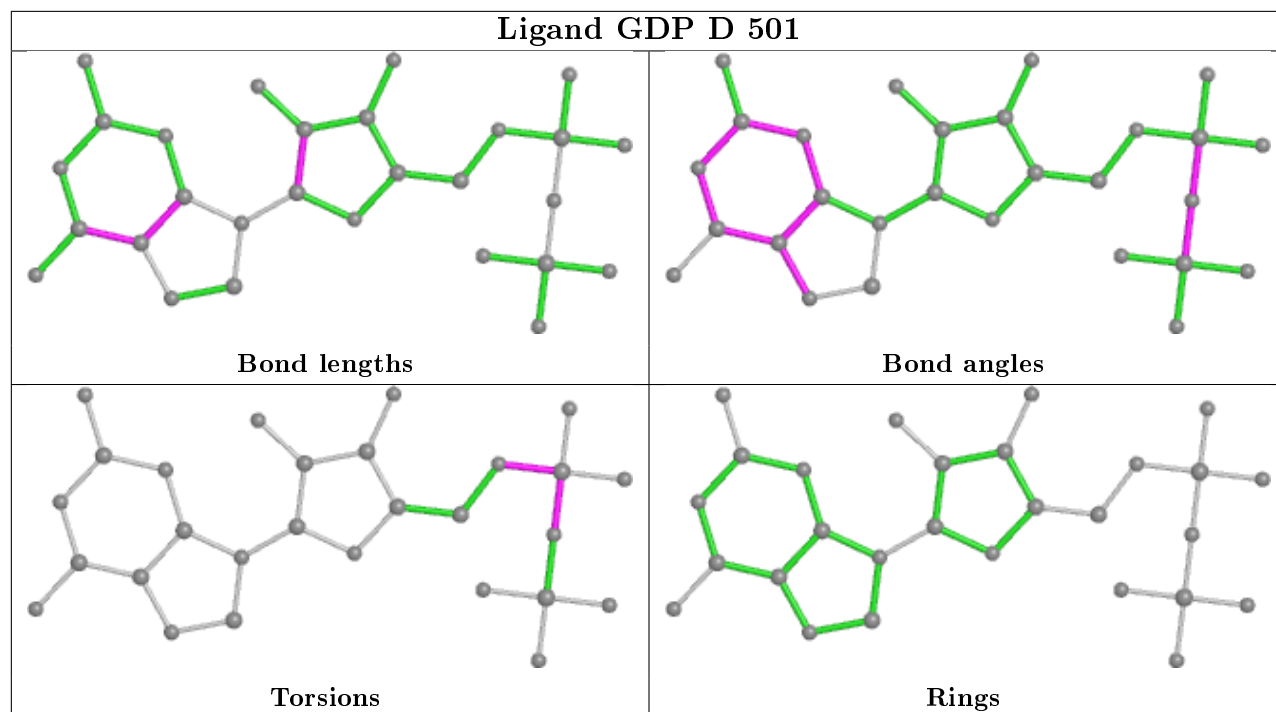


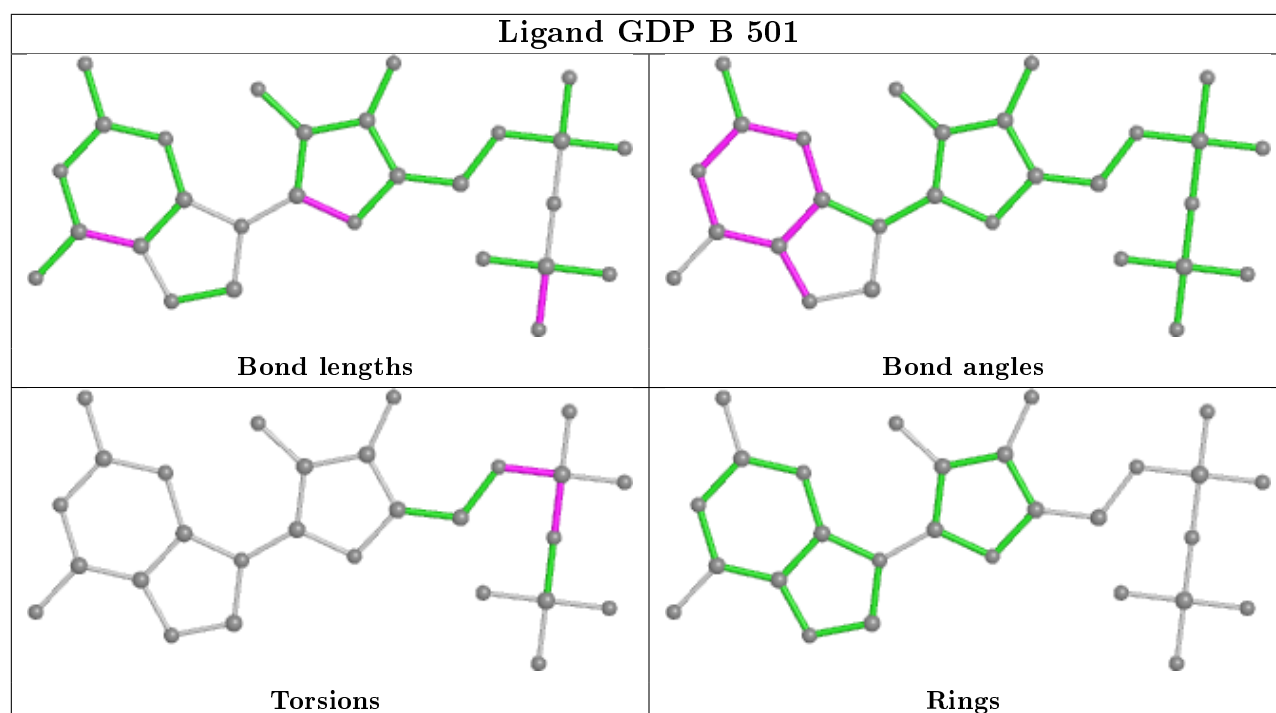
Ligand NV4 B 505



Ligand ACP F 402







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	439/451 (97%)	0.17	15 (3%) 45 52	25, 41, 76, 126	0
1	C	440/451 (97%)	-0.05	9 (2%) 65 71	20, 32, 61, 98	0
2	B	423/445 (95%)	0.16	21 (4%) 28 35	20, 40, 80, 114	1 (0%)
2	D	418/445 (93%)	0.45	46 (11%) 5 7	27, 49, 84, 126	2 (0%)
3	E	121/152 (79%)	0.35	9 (7%) 14 19	29, 53, 90, 106	0
4	F	312/388 (80%)	0.90	74 (23%) 0 0	30, 61, 113, 144	0
All	All	2153/2332 (92%)	0.29	174 (8%) 12 16	20, 44, 87, 144	3 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	THR	10.6
4	F	253	TYR	9.3
4	F	173	ILE	8.8
4	F	102	PRO	6.9
1	A	439	SER	6.5
1	A	282	TYR	6.4
4	F	170	LEU	6.2
4	F	244	CYS	5.9
4	F	182	ILE	5.6
4	F	172	PHE	5.4
4	F	130	VAL	5.4
4	F	249	TYR	5.4
4	F	101	TYR	5.3
4	F	134	ALA	5.2
2	B	59	ASN	5.1
4	F	167	SER	5.0
3	E	139	LEU	5.0
4	F	362	ALA	4.9
4	F	171	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	4.8
1	A	281	ALA	4.8
3	E	28	SER	4.7
4	F	133	ALA	4.7
4	F	132	LEU	4.7
4	F	129	GLU	4.7
2	D	182	VAL	4.7
4	F	166	ALA	4.6
4	F	126	ASP	4.5
4	F	162	ILE	4.5
4	F	169	LEU	4.4
1	C	340	SER	4.3
2	D	248	LEU	4.3
4	F	256	TYR	4.2
3	E	140	LYS	4.2
4	F	255	ARG	4.1
4	F	163	SER	4.1
4	F	231	ALA	4.0
2	D	60	LYS	4.0
2	B	438	ALA	3.9
2	D	179	ASP	3.9
4	F	131	PHE	3.9
4	F	100	ILE	3.9
2	D	1	MET	3.8
2	D	97	SER	3.8
4	F	227	PRO	3.7
2	D	58	GLY	3.7
4	F	361	LEU	3.6
2	B	37	HIS	3.6
4	F	168	GLU	3.6
4	F	20	LEU	3.6
4	F	149	ALA	3.5
4	F	165	GLU	3.5
4	F	194	PRO	3.5
1	C	440	VAL	3.5
2	D	405	LEU	3.5
2	D	74	THR	3.4
4	F	21	LEU	3.4
4	F	27	TRP	3.4
4	F	181	VAL	3.4
3	E	45	PRO	3.4
2	B	277	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	283	HIS	3.3
2	B	33	THR	3.3
3	E	27	PRO	3.3
2	D	56	ALA	3.3
4	F	240	LEU	3.3
2	D	82	PRO	3.3
4	F	164	SER	3.3
2	B	280	SER	3.2
2	D	415	GLU	3.2
4	F	230	SER	3.2
2	B	60	LYS	3.1
2	D	400	ARG	3.1
2	B	437	ASP	3.1
2	D	416	MET	3.1
2	D	250	ALA	3.1
2	D	441	ASP	3.0
3	E	135	LYS	3.0
4	F	225	SER	3.0
4	F	239	HIS	3.0
1	A	42	ILE	2.9
4	F	180	HIS	2.9
1	A	279	GLU	2.9
4	F	147	TRP	2.9
2	B	61	TYR	2.9
4	F	135	TYR	2.8
2	D	407	TRP	2.8
4	F	151	SER	2.8
2	D	221[A]	THR	2.8
4	F	26	GLN	2.8
2	D	85	GLN	2.7
4	F	228	TYR	2.7
2	D	83	PHE	2.7
2	D	94	PHE	2.7
1	C	178	SER	2.6
2	D	260	VAL	2.6
2	B	337	ASN	2.6
4	F	145	ASN	2.6
2	D	79	ARG	2.6
1	A	171	ILE	2.6
2	B	35	SER	2.5
2	B	338	LYS	2.5
2	D	59	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	178	SER	2.5
1	C	133	GLN	2.5
1	A	365	GLY	2.5
2	B	50[A]	ASN	2.5
4	F	1	MET	2.5
4	F	22	LEU	2.5
3	E	141	GLU	2.5
4	F	128	ARG	2.5
4	F	236	LYS	2.5
4	F	254	GLY	2.5
4	F	224	SER	2.4
2	D	403	ALA	2.4
1	C	337	THR	2.4
2	D	33	THR	2.4
2	D	220	THR	2.4
4	F	31	ARG	2.4
4	F	9	GLU	2.4
2	D	75	MET	2.4
2	B	62	VAL	2.4
2	B	369	ARG	2.4
3	E	44	ASP	2.4
1	A	262	TYR	2.4
4	F	28	LYS	2.3
2	D	255	LEU	2.3
2	D	259	MET	2.3
4	F	150	LYS	2.3
2	D	202	TYR	2.3
4	F	243	HIS	2.3
1	C	1	MET	2.3
4	F	241	THR	2.3
4	F	247	LYS	2.3
2	B	340	SER	2.3
4	F	98	TYR	2.3
2	D	238	VAL	2.3
2	D	406	HIS	2.2
2	D	37	HIS	2.2
4	F	246	GLN	2.2
2	B	36	TYR	2.2
2	D	401	ARG	2.2
2	D	402	LYS	2.2
4	F	146	VAL	2.2
1	A	284	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	55	GLU	2.2
4	F	226	GLU	2.2
1	A	346	TRP	2.2
4	F	248	GLU	2.2
2	D	158[A]	ARG	2.1
4	F	148	ILE	2.1
1	C	167	LEU	2.1
4	F	24	THR	2.1
4	F	223	THR	2.1
1	C	165	SER	2.1
3	E	133	VAL	2.1
2	D	55	GLU	2.1
1	A	1	MET	2.1
1	A	201	ALA	2.1
4	F	229	ASN	2.1
2	B	217	LEU	2.1
2	D	41	ASP	2.1
4	F	187	GLU	2.1
2	D	378	ILE	2.1
2	B	32	PRO	2.1
1	A	80[A]	THR	2.0
2	B	308	ARG	2.0
4	F	197	ARG	2.0
4	F	144	GLY	2.0
2	D	177	VAL	2.0
2	D	268	PHE	2.0
1	C	253	THR	2.0
2	D	80	SER	2.0
2	D	124	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

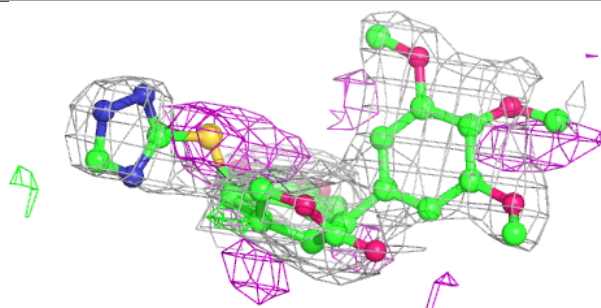
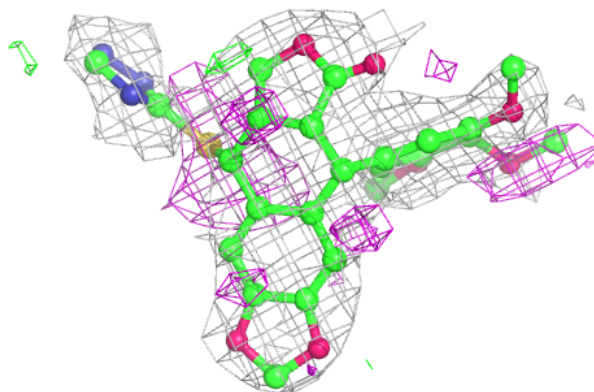
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	C	501	6/6	0.71	0.61	78,80,88,94	0
7	GOL	C	509	6/6	0.78	0.16	80,97,100,100	0
6	MG	D	502	1/1	0.80	0.09	52,52,52,52	0
9	CA	C	507	1/1	0.82	0.14	105,105,105,105	0
7	GOL	D	505	6/6	0.84	0.30	79,81,84,86	0
6	MG	A	502	1/1	0.85	0.22	40,40,40,40	0
14	PEG	C	505	7/7	0.85	0.17	42,77,82,82	0
7	GOL	A	507	6/6	0.85	0.13	75,82,90,90	0
7	GOL	D	504	6/6	0.86	0.29	90,103,104,104	0
7	GOL	A	504	6/6	0.86	0.19	47,68,71,76	0
13	NV4	D	507	35/35	0.86	0.25	41,64,88,100	0
7	GOL	C	504	6/6	0.89	0.58	67,70,83,84	0
8	IMD	A	505	5/5	0.90	0.34	68,82,95,98	0
7	GOL	D	506	6/6	0.92	0.20	54,62,67,68	0
6	MG	C	503	1/1	0.93	0.14	27,27,27,27	0
8	IMD	C	508	5/5	0.93	0.15	38,48,56,56	0
6	MG	F	401	1/1	0.93	0.09	75,75,75,75	0
15	ACP	F	402	31/31	0.93	0.12	51,78,113,122	0
6	MG	D	503	1/1	0.95	0.10	60,60,60,60	0
11	NA	B	503	1/1	0.96	0.33	78,78,78,78	0
6	MG	B	502	1/1	0.96	0.27	20,20,20,20	0
13	NV4	B	505	35/35	0.96	0.19	30,41,78,92	0
11	NA	C	506	1/1	0.97	0.17	27,27,27,27	0
12	MES	B	504	12/12	0.98	0.11	35,41,56,59	0
5	GTP	A	501	32/32	0.98	0.17	23,31,45,46	0
10	GDP	D	501	28/28	0.98	0.09	40,47,51,59	0
6	MG	A	503	1/1	0.98	0.39	74,74,74,74	0
10	GDP	B	501	28/28	0.99	0.16	17,28,33,35	0
9	CA	A	506	1/1	0.99	0.04	53,53,53,53	0
5	GTP	C	502	32/32	0.99	0.14	21,24,32,36	0

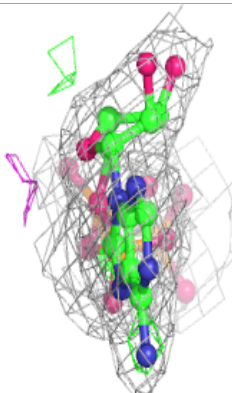
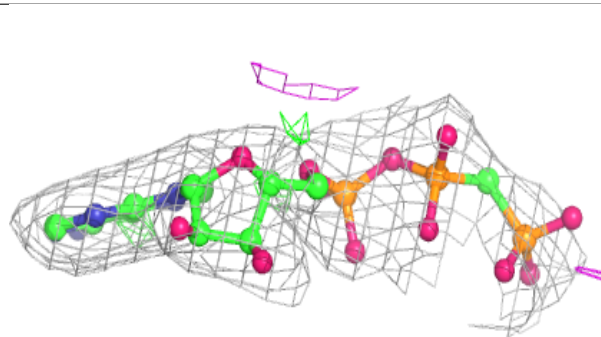
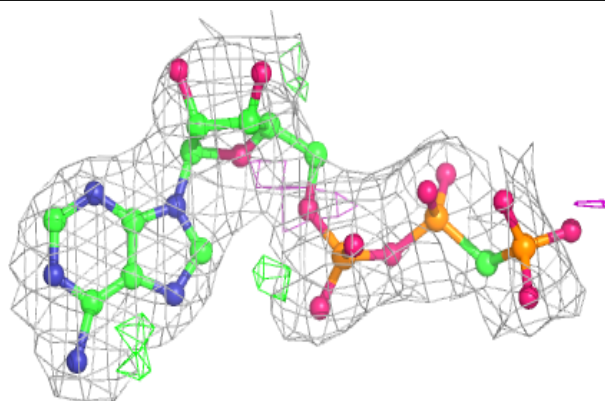
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NV4 D 507:

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

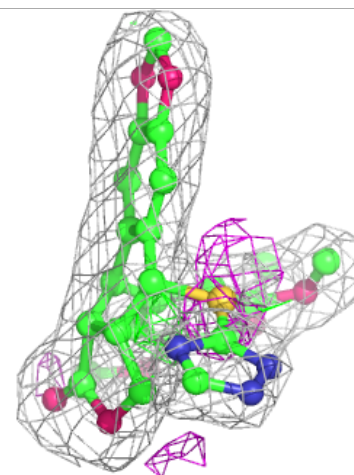
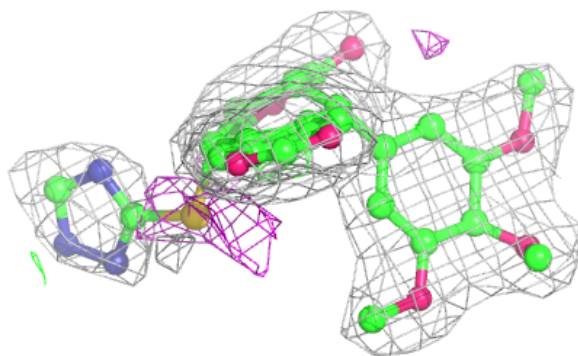
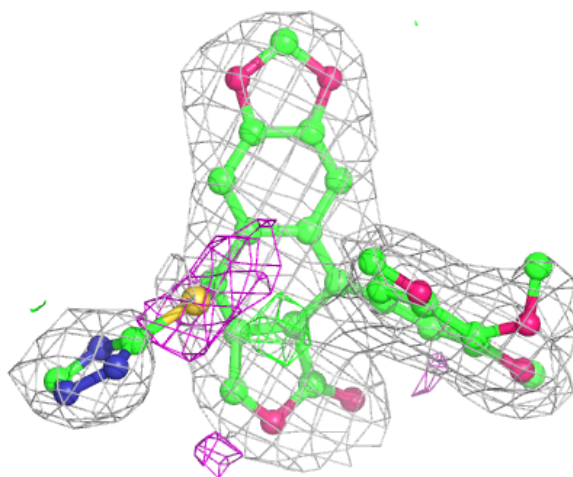
**Electron density around ACP F 402:**

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



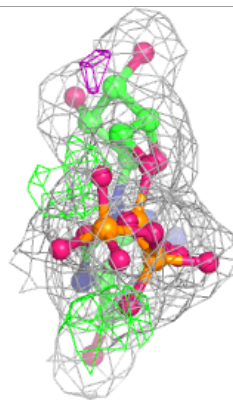
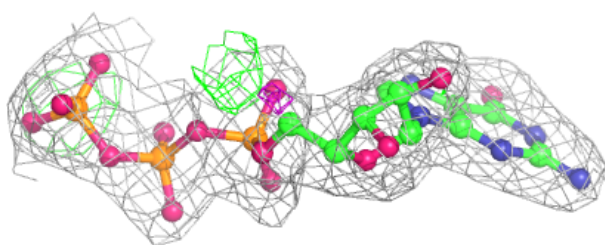
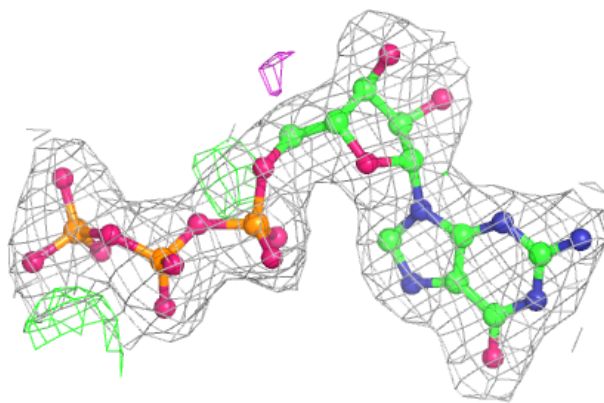
Electron density around NV4 B 505:

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

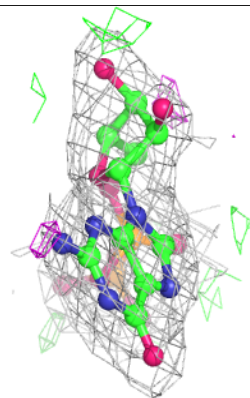
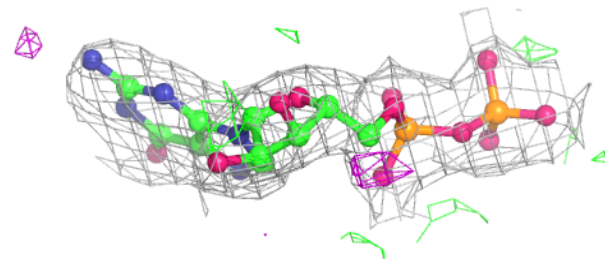
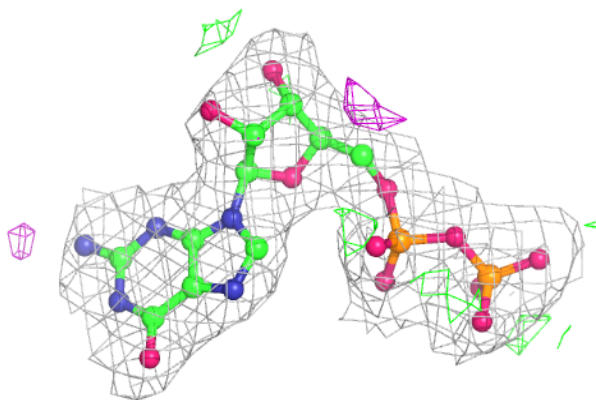


Electron density around GTP A 501:

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

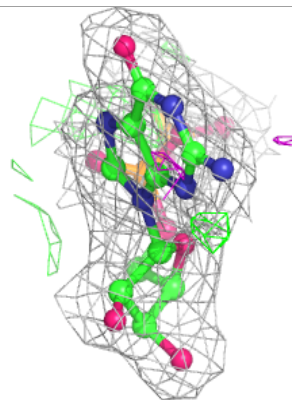
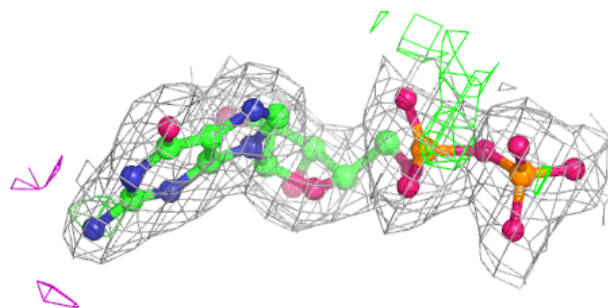
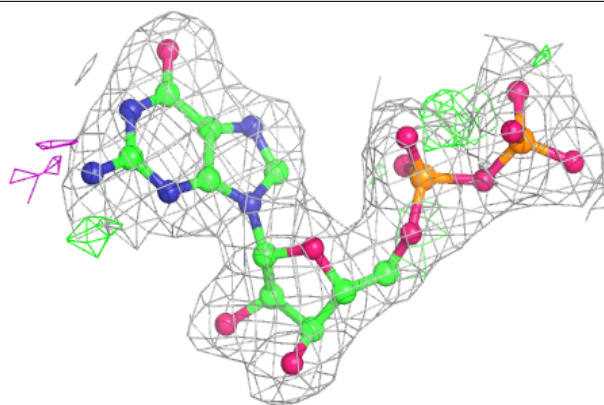
**Electron density around GDP D 501:**

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

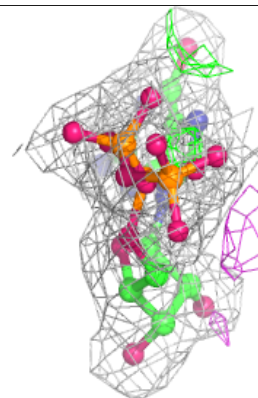
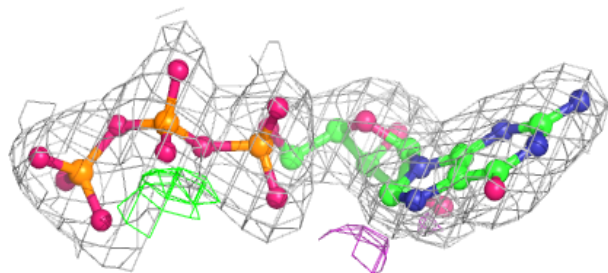
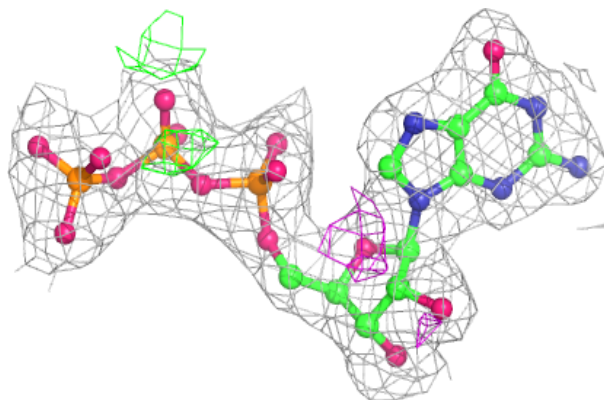


Electron density around GDP B 501:

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

**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)



6.5 Other polymers

There are no such residues in this entry.