



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:36 AM UTC

PDB ID : 5FNV / pdb_00005fnv
Title : a new complex structure of tubulin with an alpha-beta unsaturated lactone
Authors : Wang, Y.; Naismith, J.; Zhu, X.
Deposited on : 2015-11-16
Resolution : 2.61 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

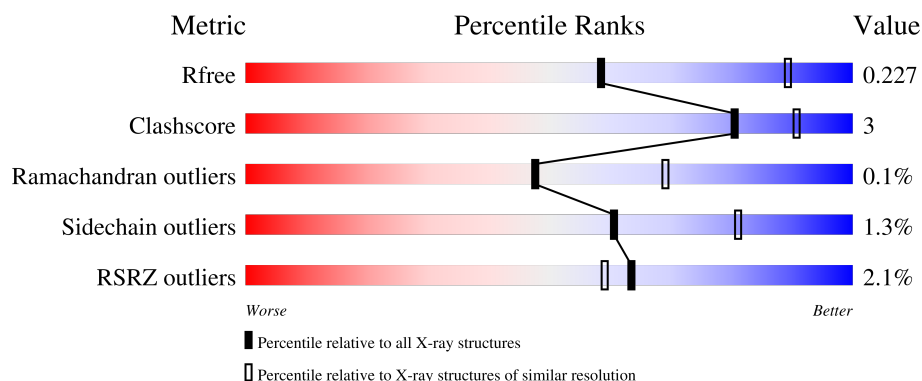
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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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 long green segment labeled '73%', a small yellow segment labeled '7%', and a grey segment at the end labeled '20%'. The segments are separated by small dots.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called TUBULIN ALPHA-1B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	3	0
			3373	2133	577	640	23			
1	C	439	Total	C	N	O	S	0	5	0
			3454	2184	585	662	23			

- Molecule 2 is a protein called TUBULIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	1	0
			3315	2086	567	637	25			
2	D	419	Total	C	N	O	S	0	1	0
			3288	2069	560	634	25			

- Molecule 3 is a protein called STATHMIN-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	119	Total	C	N	O	S	0	4	0
			1018	628	186	199	5			

There are 2 discrepancies between the modelled and reference sequences:

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

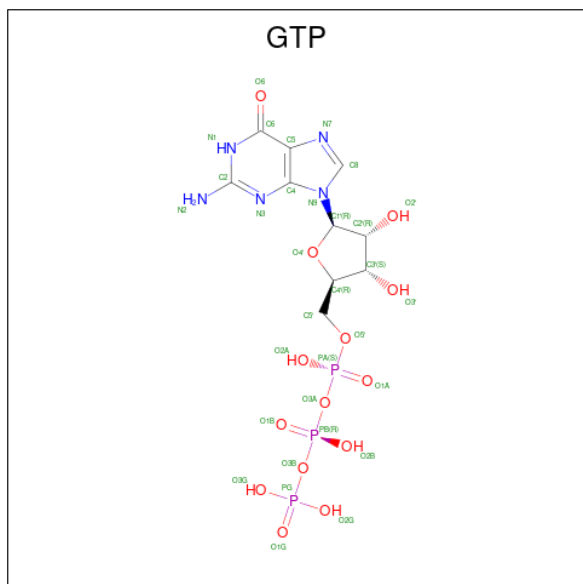
- Molecule 4 is a protein called TUBULIN TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	308	Total	C	N	O	S	0	2	0
			2551	1644	442	451	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

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

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

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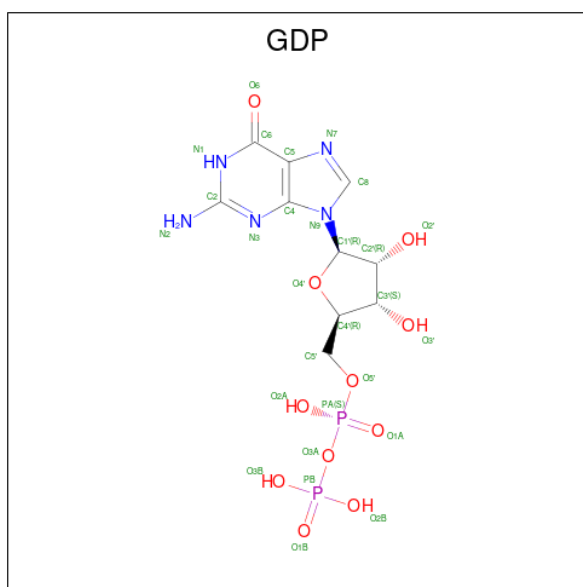
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

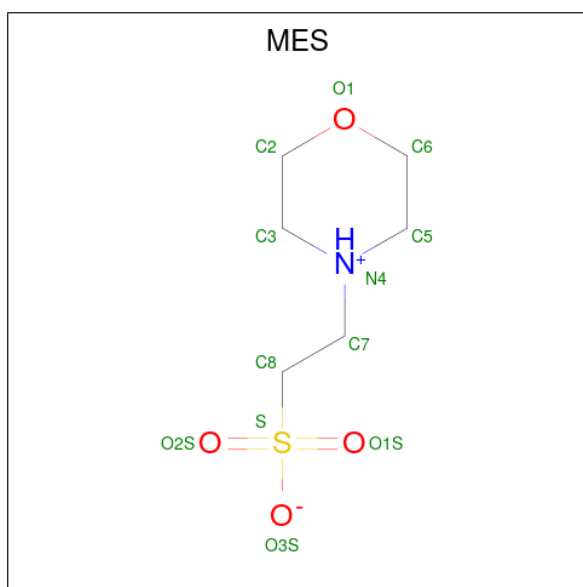
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



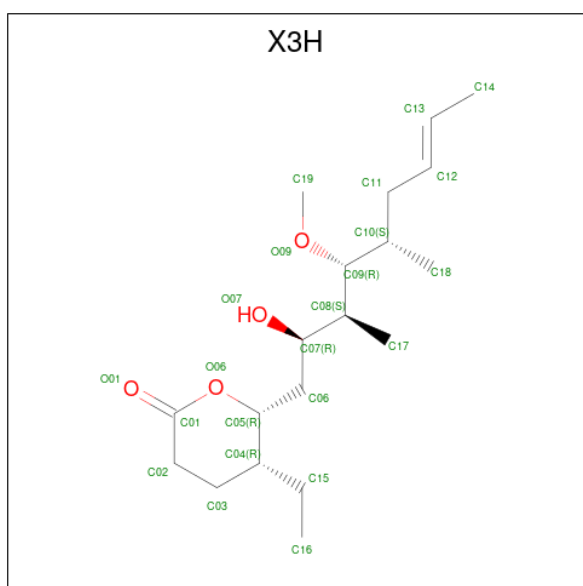
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	
			28	10	5	11	2	0

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



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

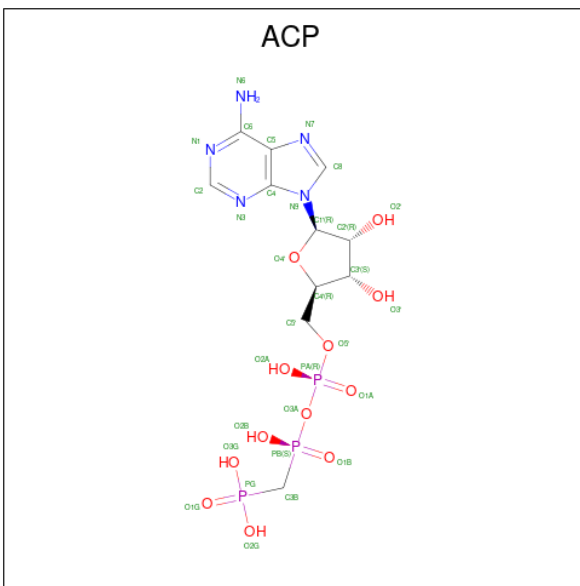
- Molecule 10 is PIRONETIN (CCD ID: X3H) (formula: $C_{19}H_{34}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			23	19	4		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

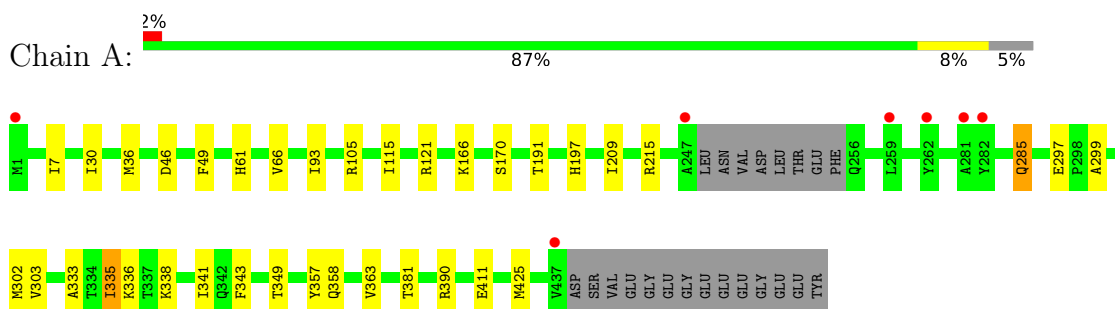
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	16	Total O 16 16	0	0
12	B	16	Total O 16 16	0	0
12	C	31	Total O 31 31	0	0
12	D	3	Total O 3 3	0	0
12	F	2	Total O 2 2	0	0

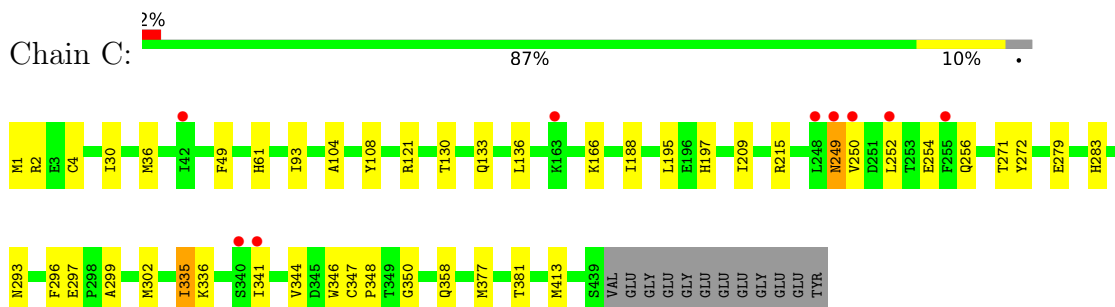
3 Residue-property plots [i](#)

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.

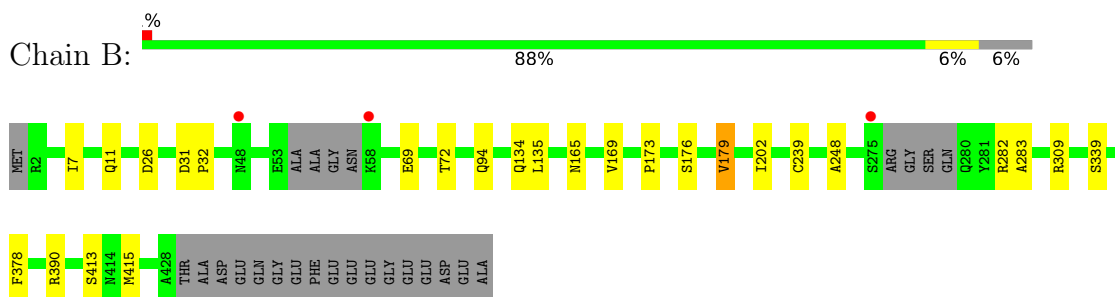
• Molecule 1: TUBULIN ALPHA-1B CHAIN



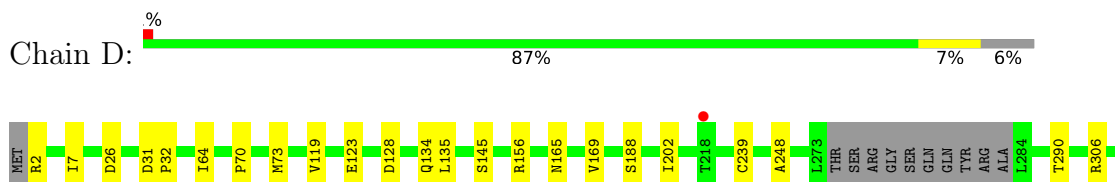
• Molecule 1: TUBULIN ALPHA-1B CHAIN

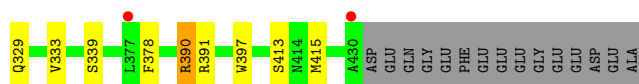


• Molecule 2: TUBULIN BETA CHAIN

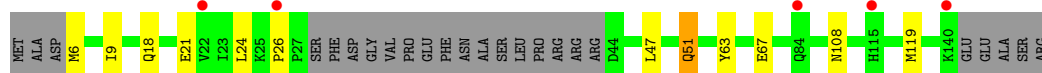
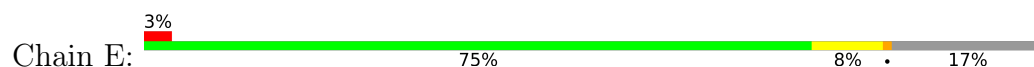


• Molecule 2: TUBULIN BETA CHAIN

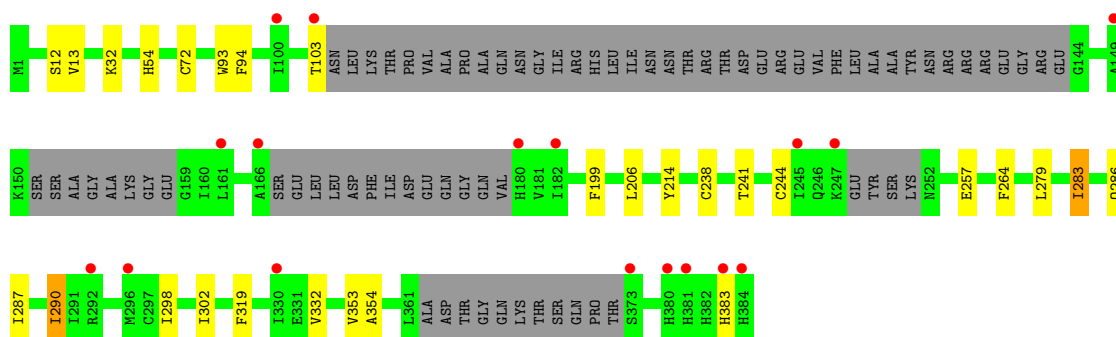




● Molecule 3: STATHMIN-4



● 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	106.16Å 157.20Å 181.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.88 – 2.61 118.88 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.6 (118.88-2.61) 94.7 (118.88-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.186 , 0.226 0.194 , 0.227	Depositor DCC
R_{free} test set	4397 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17276	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, CA, GTP, GDP, MES, X3H, MG

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	0.88	1/3452 (0.0%)	0.98	5/4682 (0.1%)
1	C	0.95	0/3538	1.02	6/4803 (0.1%)
2	B	0.84	0/3388	0.97	1/4588 (0.0%)
2	D	0.80	0/3361	0.98	3/4555 (0.1%)
3	E	0.96	1/1030 (0.1%)	1.07	0/1367
4	F	0.82	1/2614 (0.0%)	0.97	10/3531 (0.3%)
All	All	0.87	3/17383 (0.0%)	0.99	25/23526 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	103	THR	C-O	6.02	1.35	1.23
1	A	303	VAL	C-O	-6.01	1.18	1.24
3	E	26	PRO	CA-C	5.05	1.56	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	283	ILE	CB-CA-C	-8.01	103.92	111.05
1	C	358	GLN	CA-C-N	-7.00	114.55	119.66
1	C	358	GLN	C-N-CA	-7.00	114.55	119.66
1	C	350	GLY	N-CA-C	6.63	121.03	112.54
4	F	283	ILE	N-CA-C	6.31	116.60	111.62
2	D	306	ARG	CB-CG-CD	6.01	125.12	111.30
1	C	249	ASN	N-CA-C	5.95	118.68	110.35
4	F	72	CYS	N-CA-C	5.94	119.49	112.72
4	F	290	ILE	N-CA-CB	5.76	116.90	110.51
2	B	179	VAL	CB-CA-C	-5.76	102.94	112.26
1	A	358	GLN	CA-C-N	-5.74	115.47	119.66
1	A	358	GLN	C-N-CA	-5.74	115.47	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	SER	CB-CA-C	5.55	119.87	109.71
1	A	115	ILE	N-CA-C	5.44	115.65	110.42
1	A	363	VAL	CB-CA-C	-5.44	105.02	110.89
4	F	290	ILE	CB-CA-C	-5.35	105.04	111.88
4	F	94	PHE	CA-C-N	-5.24	114.56	119.85
4	F	94	PHE	C-N-CA	-5.24	114.56	119.85
1	C	283	HIS	N-CA-C	5.23	118.95	112.47
4	F	264	PHE	N-CA-C	5.09	116.91	111.36
2	D	397	TRP	CA-CB-CG	5.08	123.25	113.60
4	F	13	VAL	N-CA-C	5.03	115.25	110.42
2	D	390	ARG	N-CA-C	-5.03	102.20	109.59
1	C	188	ILE	CB-CA-C	-5.02	105.29	112.22
4	F	383	HIS	N-CA-C	5.00	116.88	108.73

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	3373	0	3288	19	0
1	C	3454	0	3357	29	0
2	B	3315	0	3196	14	0
2	D	3288	0	3169	17	0
3	E	1018	0	1031	8	0
4	F	2551	0	2524	9	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	28	0	12	0	0
9	B	24	0	26	0	0
10	C	23	0	0	0	0
11	F	31	0	14	0	0
12	A	16	0	0	0	0
12	B	16	0	0	0	0
12	C	31	0	0	0	0
12	D	3	0	0	0	0
12	F	2	0	0	0	0
All	All	17276	0	16653	87	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 3.

All (87) 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:D:64:ILE:HD12	2:D:119:VAL:HG12	1.63	0.80
2:B:309:ARG:NH1	2:B:339:SER:O	2.24	0.70
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.38	0.64
1:A:191:THR:HG22	1:A:425:MET:HE1	1.83	0.59
2:B:69:GLU:OE2	1:C:250:VAL:N	2.37	0.57
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.86	0.57
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.40	0.57
1:C:133:GLN:CB	1:C:252:LEU:HD12	2.35	0.57
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.22	0.55
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.43	0.54
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.43	0.54
1:C:104:ALA:HB2	1:C:413:MET:SD	2.48	0.54
1:A:333:ALA:HA	3:E:6:MET:HE1	1.91	0.53
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.88	0.53
1:C:346:TRP:CZ3	1:C:347:CYS:SG	3.02	0.53
2:D:329:GLN:O	2:D:333:VAL:HG23	2.09	0.52
1:C:36:MET:HE1	1:C:49:PHE:CD1	2.44	0.52
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.91	0.52
4:F:199:PHE:HA	4:F:241:THR:HG21	1.91	0.51
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.92	0.51
1:C:293:ASN:OD1	1:C:335:ILE:HD11	2.11	0.51
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.42	0.50
1:A:336:LYS:NZ	1:A:341:ILE:O	2.44	0.50
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD11	1:A:302:MET:SD	2.52	0.49
2:D:70:PRO:O	2:D:73:MET:HB3	2.12	0.49
1:A:36:MET:HE3	1:A:61:HIS:CD2	2.46	0.49
1:C:209:ILE:HD11	1:C:302:MET:SD	2.52	0.49
1:C:30:ILE:CG1	1:C:36:MET:HE2	2.42	0.49
1:A:390:ARG:HD3	4:F:54:HIS:CD2	2.48	0.48
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.48	0.48
1:A:36:MET:HE1	1:A:49:PHE:CD1	2.49	0.48
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.94	0.48
1:C:133:GLN:HB3	1:C:252:LEU:HD12	1.96	0.48
3:E:63:TYR:CZ	3:E:67:GLU:OE1	2.67	0.48
1:C:336:LYS:HA	1:C:341:ILE:HD11	1.95	0.47
1:A:30:ILE:CG1	1:A:36:MET:HE2	2.43	0.47
4:F:286:GLN:O	4:F:290:ILE:HG12	2.15	0.46
2:D:2:ARG:HB3	2:D:2:ARG:CZ	2.45	0.46
2:D:145[A]:SER:HG	2:D:188:SER:HG	1.61	0.46
4:F:287:ILE:HD12	4:F:319:PHE:CD2	2.51	0.46
2:B:173:PRO:HA	2:B:176:SER:HB2	1.98	0.46
2:D:390:ARG:O	2:D:391:ARG:HG2	2.16	0.46
1:A:7:ILE:HG23	1:A:66:VAL:HG23	1.98	0.45
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.81	0.45
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.99	0.45
1:C:2:ARG:HA	1:C:133:GLN:HG2	1.99	0.44
2:D:64:ILE:HD12	2:D:119:VAL:CG1	2.42	0.44
2:B:282:ARG:NH1	2:B:283:ALA:O	2.51	0.44
2:D:2:ARG:HE	2:D:128:ASP:HB3	1.83	0.44
1:A:215:ARG:NH2	1:A:299:ALA:O	2.51	0.44
1:C:133:GLN:HB2	1:C:252:LEU:HD12	1.99	0.43
2:B:94:GLN:O	1:C:250:VAL:HG11	2.17	0.43
1:C:215:ARG:NH2	1:C:299:ALA:O	2.51	0.43
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.43
2:D:134:GLN:HA	2:D:165:ASN:O	2.18	0.43
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.43
1:C:108:TYR:CD1	3:E:108:ASN:CG	2.97	0.43
2:D:378:PHE:HD1	2:D:415:MET:HE2	1.84	0.43
1:A:166:LYS:HE2	1:A:197:HIS:O	2.19	0.42
2:D:156:ARG:HG2	3:E:119:MET:HE3	2.01	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42
2:B:11:GLN:HA	2:B:72:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271[B]:THR:OG1	1:C:272:TYR:N	2.51	0.42
2:B:69:GLU:OE2	1:C:249:ASN:HA	2.18	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.50	0.42
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.42
1:C:30:ILE:HD11	1:C:36:MET:HE2	2.02	0.41
1:C:296:PHE:CE1	1:C:377:MET:HE1	2.55	0.41
2:B:239:CYS:O	2:B:248:ALA:HA	2.21	0.41
1:C:1:MET:HB3	1:C:130:THR:OG1	2.20	0.41
1:C:279:GLU:OE1	1:C:279:GLU:N	2.48	0.41
4:F:93:TRP:CG	4:F:290:ILE:HD12	2.55	0.41
1:A:30:ILE:HD11	1:A:36:MET:HE2	2.03	0.41
2:D:239:CYS:O	2:D:248:ALA:HA	2.20	0.41
3:E:6:MET:HE2	3:E:24:LEU:CD1	2.50	0.41
3:E:9:ILE:HD11	3:E:21:GLU:OE1	2.20	0.41
4:F:214:TYR:CE2	4:F:353:VAL:CG1	3.04	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.19	0.41
2:B:378:PHE:HD1	2:B:415:MET:HE2	1.86	0.41
1:A:105:ARG:HG3	1:A:411:GLU:CD	2.46	0.41
2:D:7:ILE:O	2:D:135:LEU:HA	2.21	0.41
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.91	0.41
1:C:336:LYS:HA	1:C:341:ILE:CD1	2.52	0.40
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.04	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	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	43	64
1	C	441/451 (98%)	425 (96%)	15 (3%)	1 (0%)	43	64
2	B	414/445 (93%)	403 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	415/445 (93%)	403 (97%)	12 (3%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	298/384 (78%)	280 (94%)	18 (6%)	0	100	100
All	All	2115/2319 (91%)	2044 (97%)	69 (3%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	LYS
1	C	254	GLU

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	363/379 (96%)	358 (99%)	5 (1%)	59	80
1	C	374/379 (99%)	369 (99%)	5 (1%)	61	81
2	B	364/381 (96%)	361 (99%)	3 (1%)	73	87
2	D	360/381 (94%)	357 (99%)	3 (1%)	73	87
3	E	111/127 (87%)	110 (99%)	1 (1%)	70	86
4	F	281/342 (82%)	275 (98%)	6 (2%)	47	72
All	All	1853/1989 (93%)	1830 (99%)	23 (1%)	61	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	285	GLN
1	A	297	GLU
1	A	335	ILE
1	A	381	THR
2	B	26	ASP

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Mol	Chain	Res	Type
2	B	390	ARG
2	B	413	SER
1	C	195	LEU
1	C	256	GLN
1	C	297	GLU
1	C	335	ILE
1	C	381	THR
2	D	26	ASP
2	D	339	SER
2	D	413	SER
3	E	51	GLN
4	F	12	SER
4	F	32	LYS
4	F	238	CYS
4	F	244	CYS
4	F	257	GLU
4	F	332	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	285	GLN
1	A	309	HIS
1	A	372	GLN
1	A	393	HIS
2	B	48	ASN
2	B	329	GLN
2	B	426	GLN
1	C	31	GLN
1	C	258	ASN
1	C	283	HIS
1	C	309	HIS
1	C	393	HIS
2	D	8	GLN
2	D	14	ASN
2	D	48	ASN
2	D	99	ASN
2	D	134	GLN
2	D	195	ASN
2	D	329	GLN
2	D	332	ASN

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Mol	Chain	Res	Type
2	D	396	HIS
2	D	426	GLN
3	E	51	GLN
4	F	26	GLN
4	F	196	HIS
4	F	229	ASN
4	F	333	ASN

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 15 ligands modelled in this entry, 7 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	1440	6	33,34,34	1.35	6 (18%)	50,54,54	1.53	7 (14%)
9	MES	B	1433	-	12,12,12	2.36	1 (8%)	15,16,16	1.13	1 (6%)
5	GTP	A	1438	6	33,34,34	1.37	6 (18%)	50,54,54	1.62	8 (16%)
11	ACP	F	1385	-	31,33,33	1.96	9 (29%)	47,52,52	1.80	11 (23%)
10	X3H	C	1443	1	23,23,23	1.41	2 (8%)	25,30,30	2.19	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	B	1429	6	29,30,30	1.50	5 (17%)	45,47,47	1.61	7 (15%)
5	GTP	D	1431	6	33,34,34	1.36	7 (21%)	50,54,54	1.67	8 (16%)
9	MES	B	1432	-	12,12,12	2.34	1 (8%)	15,16,16	1.32	1 (6%)

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	1440	6	-	6/22/38/38	0/3/3/3
9	MES	B	1433	-	-	2/6/14/14	0/1/1/1
5	GTP	A	1438	6	-	4/22/38/38	0/3/3/3
11	ACP	F	1385	-	-	3/19/38/38	0/3/3/3
10	X3H	C	1443	1	-	0/24/37/37	0/1/1/1
8	GDP	B	1429	6	-	3/16/32/32	0/3/3/3
5	GTP	D	1431	6	-	8/22/38/38	0/3/3/3
9	MES	B	1432	-	-	0/6/14/14	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1433	MES	C8-S	-7.91	1.66	1.77
9	B	1432	MES	C8-S	-7.75	1.66	1.77
11	F	1385	ACP	PG-O1G	5.78	1.61	1.50
10	C	1443	X3H	O06-C01	4.82	1.42	1.34
11	F	1385	ACP	C5-C4	4.75	1.47	1.39
8	B	1429	GDP	PA-O3A	4.62	1.64	1.59
10	C	1443	X3H	O06-C05	-3.65	1.41	1.46
5	A	1438	GTP	PB-O3A	3.36	1.63	1.59
5	D	1431	GTP	C5-C4	3.20	1.47	1.38
8	B	1429	GDP	C5-C4	3.20	1.47	1.38
5	C	1440	GTP	PB-O3A	3.18	1.62	1.59
5	C	1440	GTP	C5-C4	3.17	1.47	1.38
5	A	1438	GTP	C5-C4	3.00	1.47	1.38
5	A	1438	GTP	PA-O3A	2.99	1.62	1.59
11	F	1385	ACP	PG-O2G	2.99	1.61	1.55
11	F	1385	ACP	C5-N7	-2.95	1.33	1.39
5	D	1431	GTP	C5-N7	-2.81	1.33	1.39
5	C	1440	GTP	C5-N7	-2.69	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	1385	ACP	PG-O3G	-2.67	1.49	1.55
5	C	1440	GTP	PA-O3A	2.57	1.62	1.59
5	C	1440	GTP	C6-N1	-2.57	1.34	1.38
8	B	1429	GDP	C5-N7	-2.40	1.34	1.39
11	F	1385	ACP	C5-C6	2.40	1.47	1.41
5	D	1431	GTP	C6-N1	-2.38	1.34	1.38
5	D	1431	GTP	PA-O3A	2.37	1.62	1.59
11	F	1385	ACP	C8-N7	2.36	1.36	1.31
11	F	1385	ACP	PB-O2B	2.34	1.62	1.56
5	A	1438	GTP	PB-O3B	2.31	1.62	1.59
5	D	1431	GTP	PB-O3B	2.28	1.62	1.59
5	D	1431	GTP	PB-O3A	2.26	1.61	1.59
8	B	1429	GDP	C6-N1	-2.25	1.34	1.38
8	B	1429	GDP	C4-N9	-2.17	1.32	1.38
11	F	1385	ACP	PB-O3A	2.13	1.60	1.58
5	A	1438	GTP	C4-N9	-2.10	1.32	1.38
5	A	1438	GTP	C5-N7	-2.09	1.34	1.39
5	D	1431	GTP	C4-N9	-2.03	1.32	1.38
5	C	1440	GTP	C4-N9	-2.00	1.33	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1443	X3H	C03-C02-C01	-5.89	104.45	116.24
11	F	1385	ACP	C5-C4-N3	-5.75	118.80	126.72
5	D	1431	GTP	C5-C4-N3	-5.54	119.57	128.39
5	C	1440	GTP	C5-C4-N3	-4.99	120.45	128.39
5	A	1438	GTP	C5-C4-N3	-4.82	120.71	128.39
8	B	1429	GDP	C5-C4-N3	-4.80	120.76	128.39
11	F	1385	ACP	N3-C4-N9	4.61	135.01	127.17
5	D	1431	GTP	C2-N3-C4	4.37	119.83	112.30
5	A	1438	GTP	C2-N3-C4	4.33	119.76	112.30
10	C	1443	X3H	C02-C03-C04	4.31	120.23	111.43
5	D	1431	GTP	N9-C4-N3	4.21	134.38	125.95
10	C	1443	X3H	O06-C01-C02	4.18	127.55	118.89
10	C	1443	X3H	C03-C04-C05	-4.00	102.19	109.29
5	C	1440	GTP	N9-C4-N3	4.00	133.95	125.95
5	C	1440	GTP	C2-N3-C4	3.94	119.08	112.30
8	B	1429	GDP	C2-N3-C4	3.91	119.03	112.30
5	A	1438	GTP	N9-C4-N3	3.79	133.53	125.95
8	B	1429	GDP	N9-C4-N3	3.66	133.28	125.95
8	B	1429	GDP	C6-C5-N7	3.56	136.77	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1438	GTP	C6-C5-N7	3.51	136.68	130.29
11	F	1385	ACP	N3-C2-N1	-3.44	123.37	128.58
11	F	1385	ACP	C2-N3-C4	3.44	120.23	111.83
11	F	1385	ACP	C4-C5-N7	-3.30	106.81	110.58
5	D	1431	GTP	C6-C5-N7	3.06	135.87	130.29
5	D	1431	GTP	O3G-PG-O2G	3.04	119.19	107.80
9	B	1432	MES	O1S-S-C8	2.80	110.95	106.73
5	C	1440	GTP	C6-C5-N7	2.73	135.25	130.29
11	F	1385	ACP	C5-N7-C8	2.60	107.54	103.45
5	D	1431	GTP	O2G-PG-O3B	-2.55	96.08	104.64
11	F	1385	ACP	C4-N9-C8	2.52	108.39	105.74
5	A	1438	GTP	O3B-PB-O1B	-2.49	103.22	110.70
9	B	1433	MES	O3S-S-C8	2.46	110.83	106.00
5	D	1431	GTP	C4-C5-N7	-2.44	106.81	110.67
5	A	1438	GTP	C4-C5-N7	-2.37	106.91	110.67
8	B	1429	GDP	C4-C5-N7	-2.36	106.93	110.67
10	C	1443	X3H	O06-C05-C06	2.33	110.43	106.41
5	A	1438	GTP	O6-C6-C5	-2.31	120.43	126.53
5	C	1440	GTP	O3G-PG-O2G	2.23	116.17	107.80
11	F	1385	ACP	C2-N1-C6	2.21	122.36	118.73
10	C	1443	X3H	O09-C09-C08	2.18	111.19	107.97
5	A	1438	GTP	O2B-PB-O3B	2.18	113.16	107.27
11	F	1385	ACP	O2A-PA-O3A	2.16	113.11	107.27
11	F	1385	ACP	PB-O3A-PA	-2.15	125.36	132.37
5	C	1440	GTP	O3'-C3'-C4'	-2.15	104.92	111.08
8	B	1429	GDP	O3B-PB-O2B	2.13	115.80	107.80
5	C	1440	GTP	C4-C5-N7	-2.07	107.38	110.67
8	B	1429	GDP	C2'-C1'-N9	2.04	118.94	113.25
11	F	1385	ACP	N9-C8-N7	-2.02	111.06	113.94
5	D	1431	GTP	O4'-C1'-N9	-2.02	103.78	108.36

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1438	GTP	C5'-O5'-PA-O3A
5	A	1438	GTP	C5'-O5'-PA-O1A
5	A	1438	GTP	C5'-O5'-PA-O2A
5	C	1440	GTP	C5'-O5'-PA-O3A
5	C	1440	GTP	C5'-O5'-PA-O1A
5	C	1440	GTP	C5'-O5'-PA-O2A
5	D	1431	GTP	PB-O3B-PG-O3G

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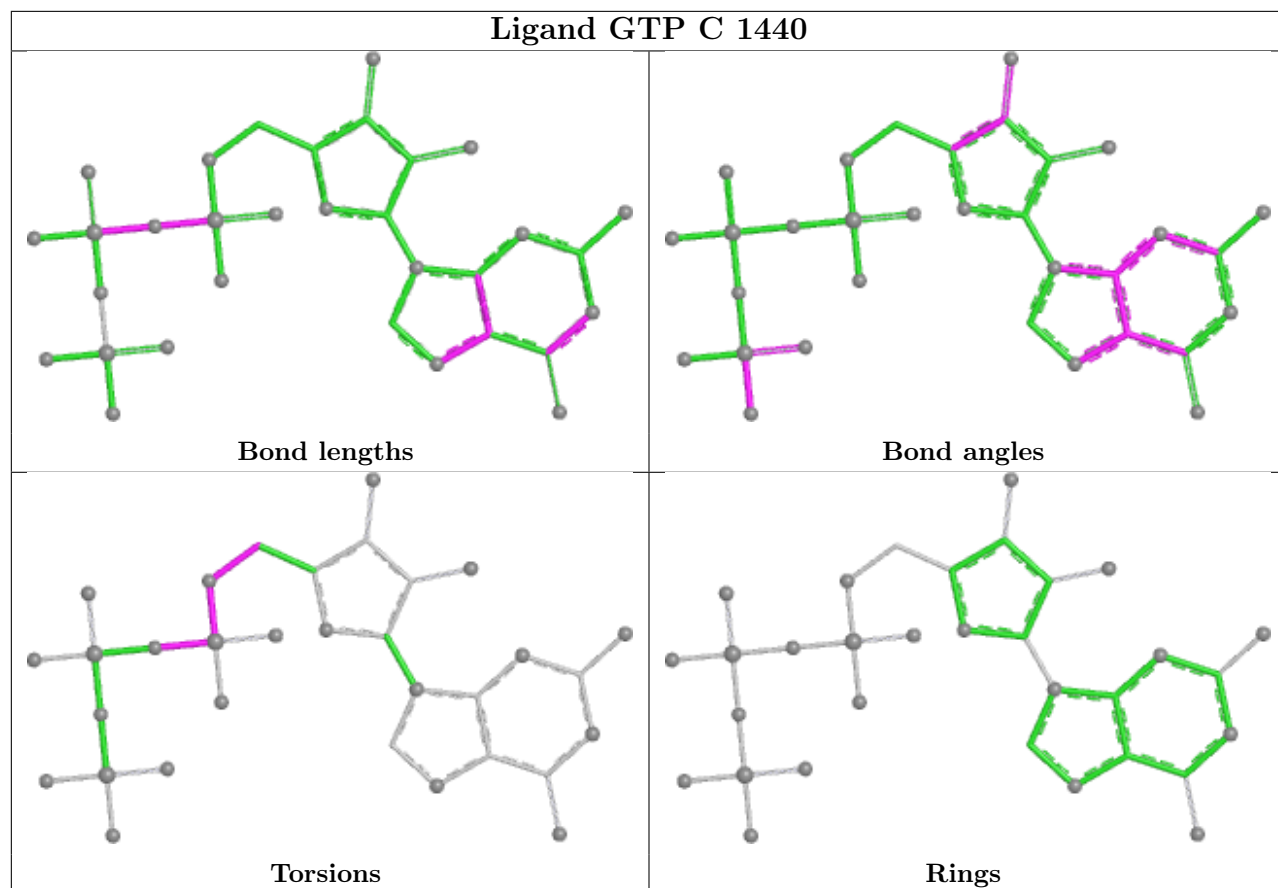
Mol	Chain	Res	Type	Atoms
5	D	1431	GTP	C5'-O5'-PA-O3A
5	D	1431	GTP	C5'-O5'-PA-O1A
5	D	1431	GTP	C5'-O5'-PA-O2A
8	B	1429	GDP	C5'-O5'-PA-O3A
8	B	1429	GDP	C5'-O5'-PA-O1A
11	F	1385	ACP	O4'-C4'-C5'-O5'
5	D	1431	GTP	PB-O3B-PG-O2G
8	B	1429	GDP	C5'-O5'-PA-O2A
9	B	1433	MES	C8-C7-N4-C3
5	D	1431	GTP	PB-O3A-PA-O1A
11	F	1385	ACP	PB-O3A-PA-O2A
5	C	1440	GTP	C4'-C5'-O5'-PA
5	D	1431	GTP	C4'-C5'-O5'-PA
9	B	1433	MES	C8-C7-N4-C5
5	A	1438	GTP	PB-O3B-PG-O3G
11	F	1385	ACP	C3'-C4'-C5'-O5'
5	C	1440	GTP	PB-O3A-PA-O1A
5	C	1440	GTP	PB-O3A-PA-O2A
5	D	1431	GTP	PB-O3A-PA-O2A

There are no ring outliers.

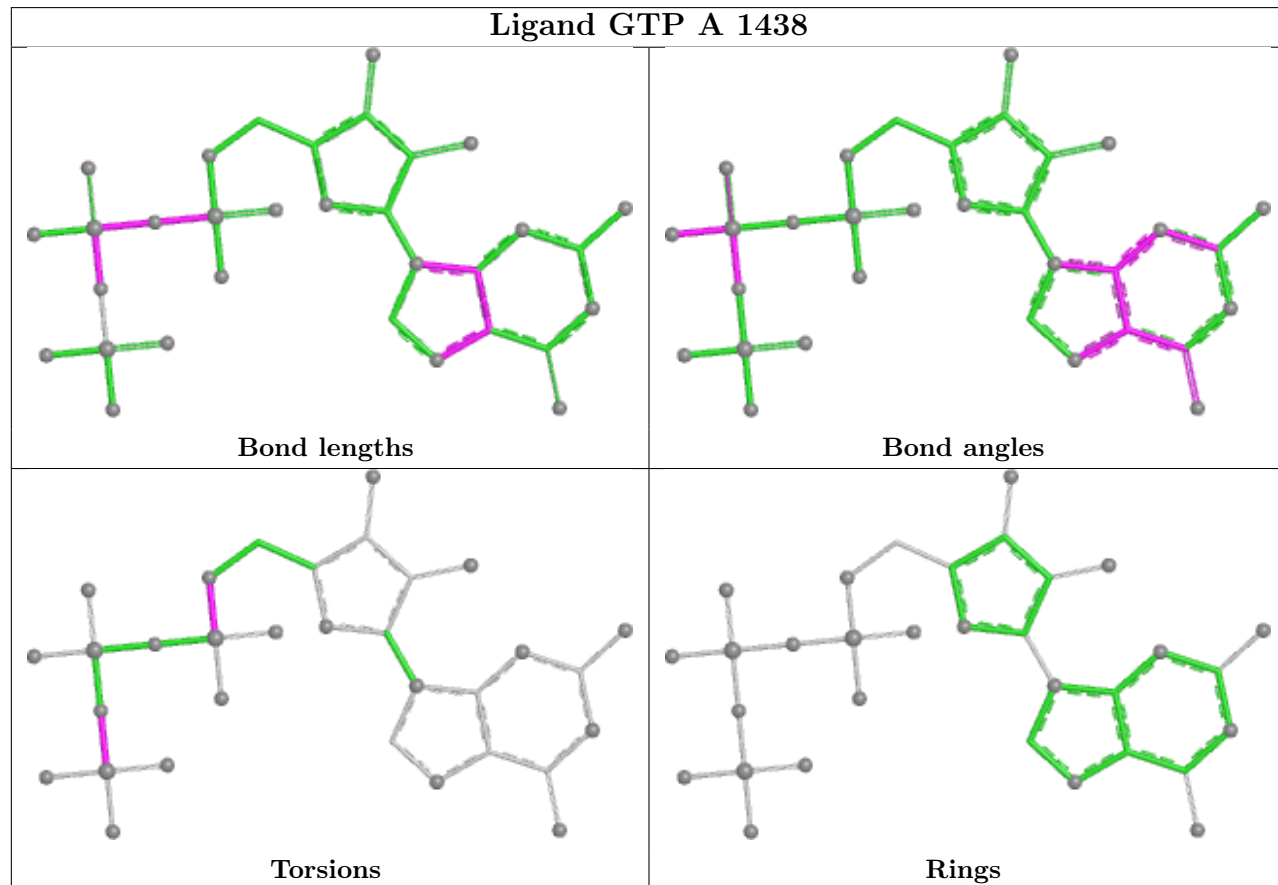
No monomer is involved in short contacts.

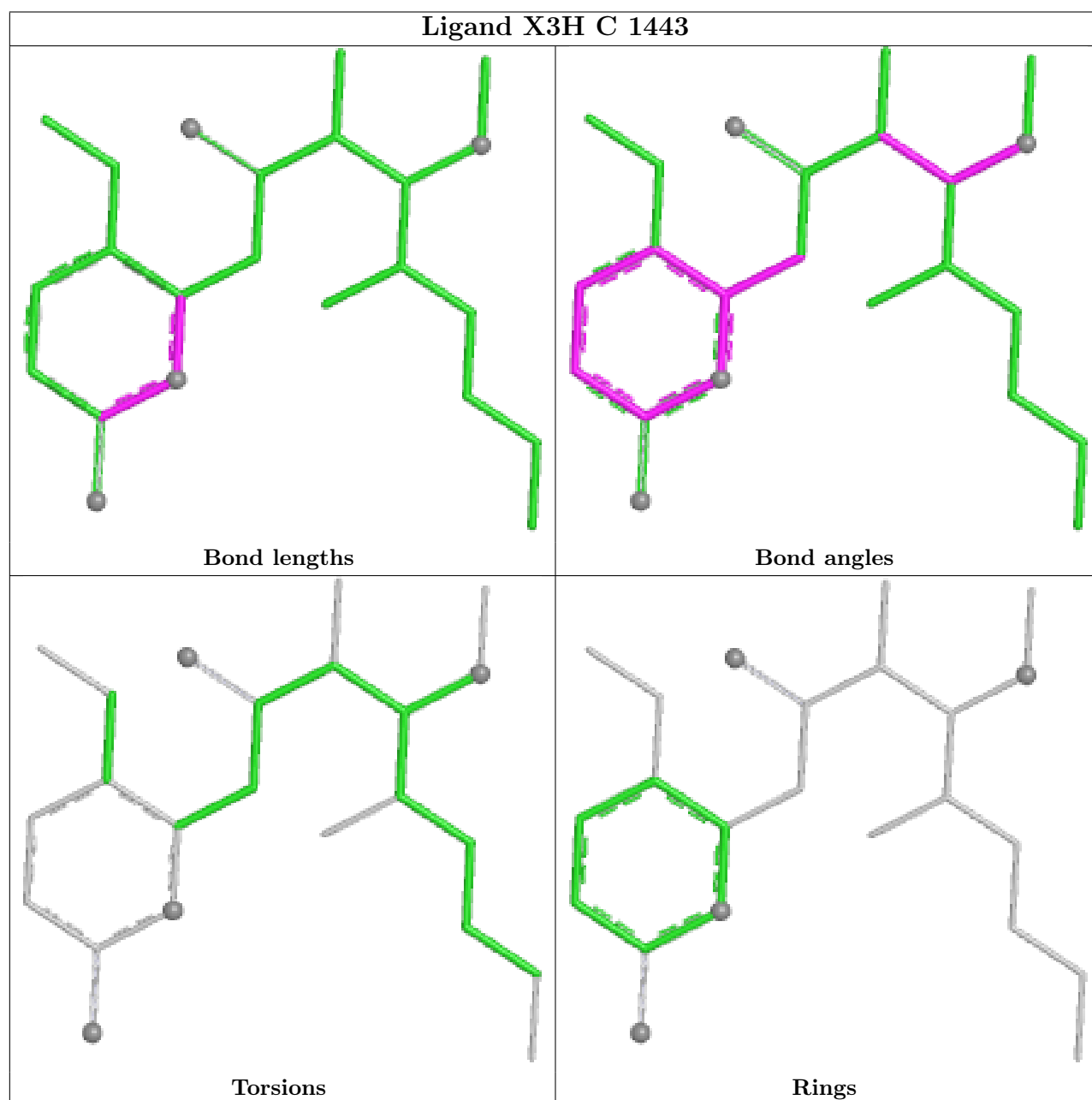
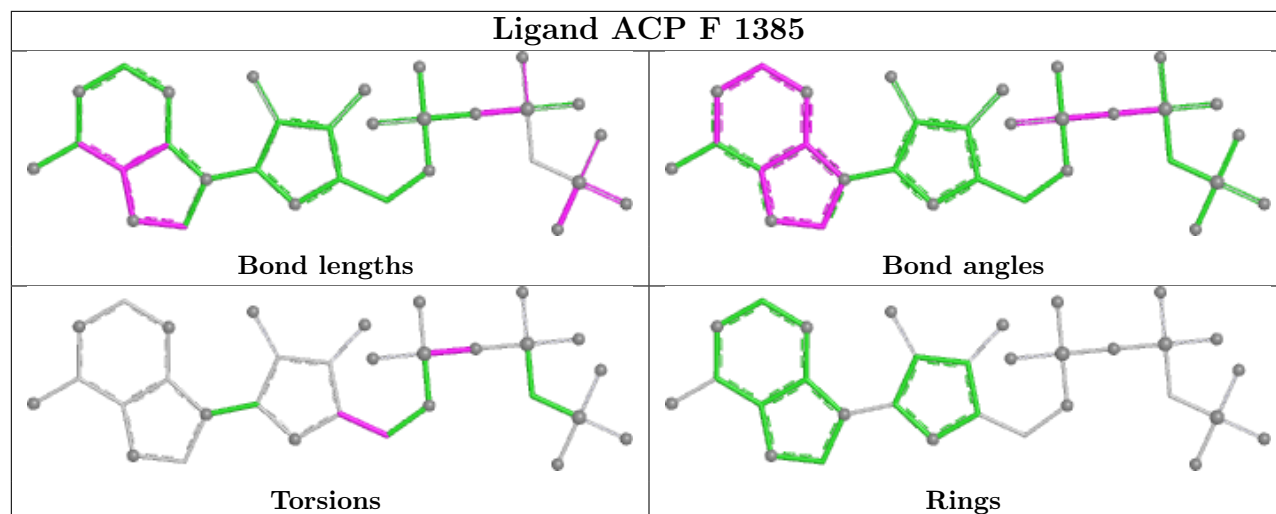
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

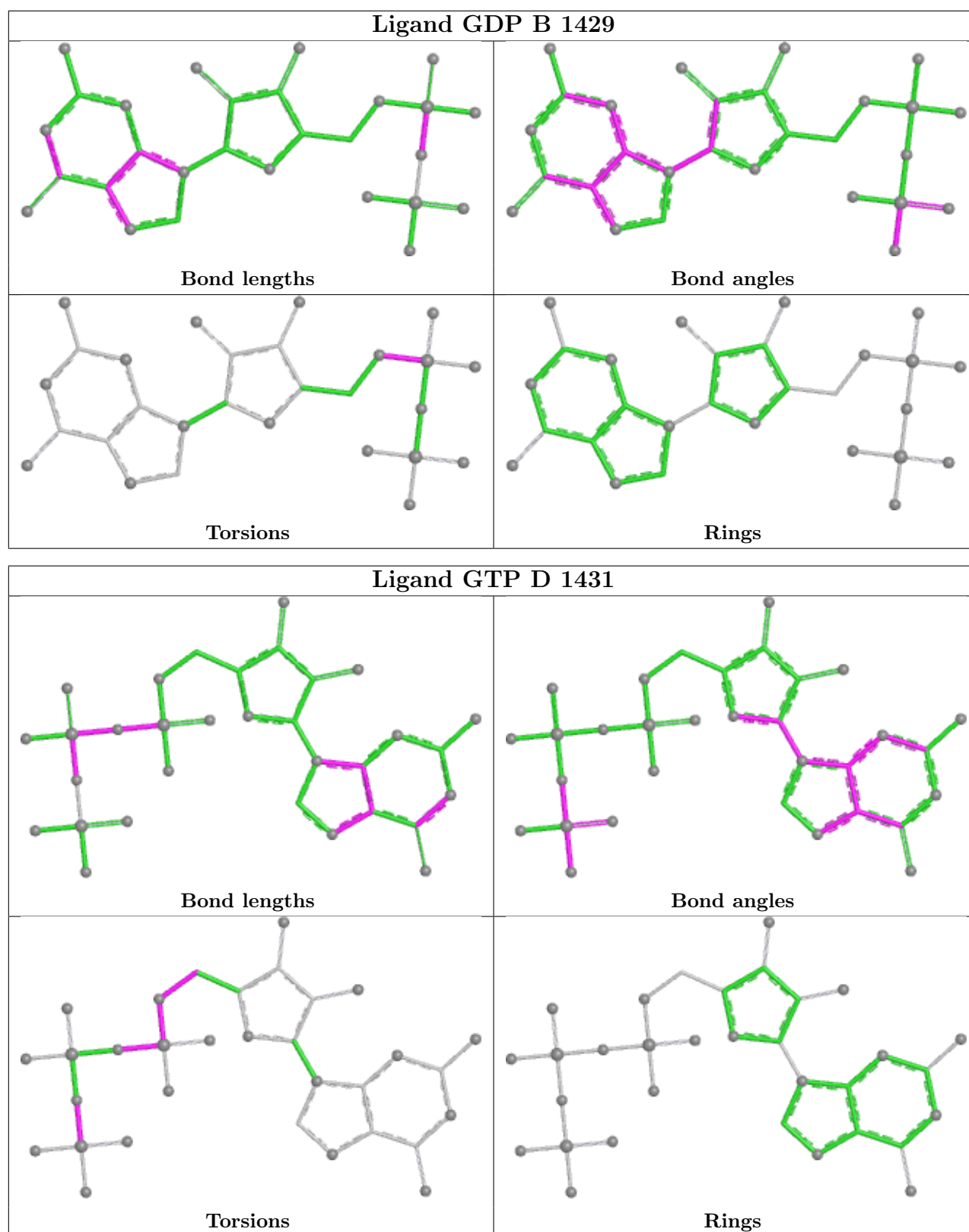
Ligand GTP C 1440



Ligand GTP A 1438







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	429/451 (95%)	-0.06	7 (1%)	70	67	37, 76, 119, 147	3 (0%)
1	C	439/451 (97%)	-0.25	9 (2%)	63	59	23, 61, 101, 128	4 (0%)
2	B	419/445 (94%)	-0.13	3 (0%)	84	82	31, 69, 103, 126	2 (0%)
2	D	419/445 (94%)	0.03	3 (0%)	84	82	56, 88, 125, 149	4 (0%)
3	E	119/143 (83%)	0.21	5 (4%)	40	35	28, 87, 125, 132	4 (3%)
4	F	308/384 (80%)	0.15	17 (5%)	30	25	32, 91, 132, 162	2 (0%)
All	All	2133/2319 (91%)	-0.05	44 (2%)	63	59	23, 77, 120, 162	19 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	ALA	8.3
4	F	381[A]	HIS	7.7
4	F	166	ALA	4.8
1	C	250	VAL	3.9
1	C	255	PHE	3.4
1	C	341	ILE	3.4
3	E	26	PRO	3.3
4	F	330	ILE	3.2
3	E	140	LYS	3.2
1	A	437	VAL	3.2
4	F	383	HIS	3.1
4	F	384	HIS	3.1
4	F	161	LEU	3.1
2	B	48	ASN	2.9
4	F	182	ILE	2.8
2	D	218	THR	2.8
4	F	245	ILE	2.7
4	F	100	ILE	2.7
1	A	259	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	247	LYS	2.6
4	F	373	SER	2.6
2	D	430	ALA	2.5
1	A	1	MET	2.5
1	A	282	TYR	2.4
2	B	275	SER	2.4
1	A	262	TYR	2.4
1	C	249	ASN	2.4
1	C	340	SER	2.3
2	B	58	LYS	2.3
1	C	163	LYS	2.2
1	C	42	ILE	2.2
3	E	115[A]	HIS	2.2
4	F	180	HIS	2.2
4	F	149	ALA	2.1
4	F	292[A]	ARG	2.1
3	E	84[A]	GLN	2.1
1	C	248	LEU	2.1
4	F	380	HIS	2.1
4	F	103	THR	2.1
1	A	281	ALA	2.1
4	F	296	MET	2.1
1	C	252	LEU	2.1
2	D	377	LEU	2.1
3	E	22	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

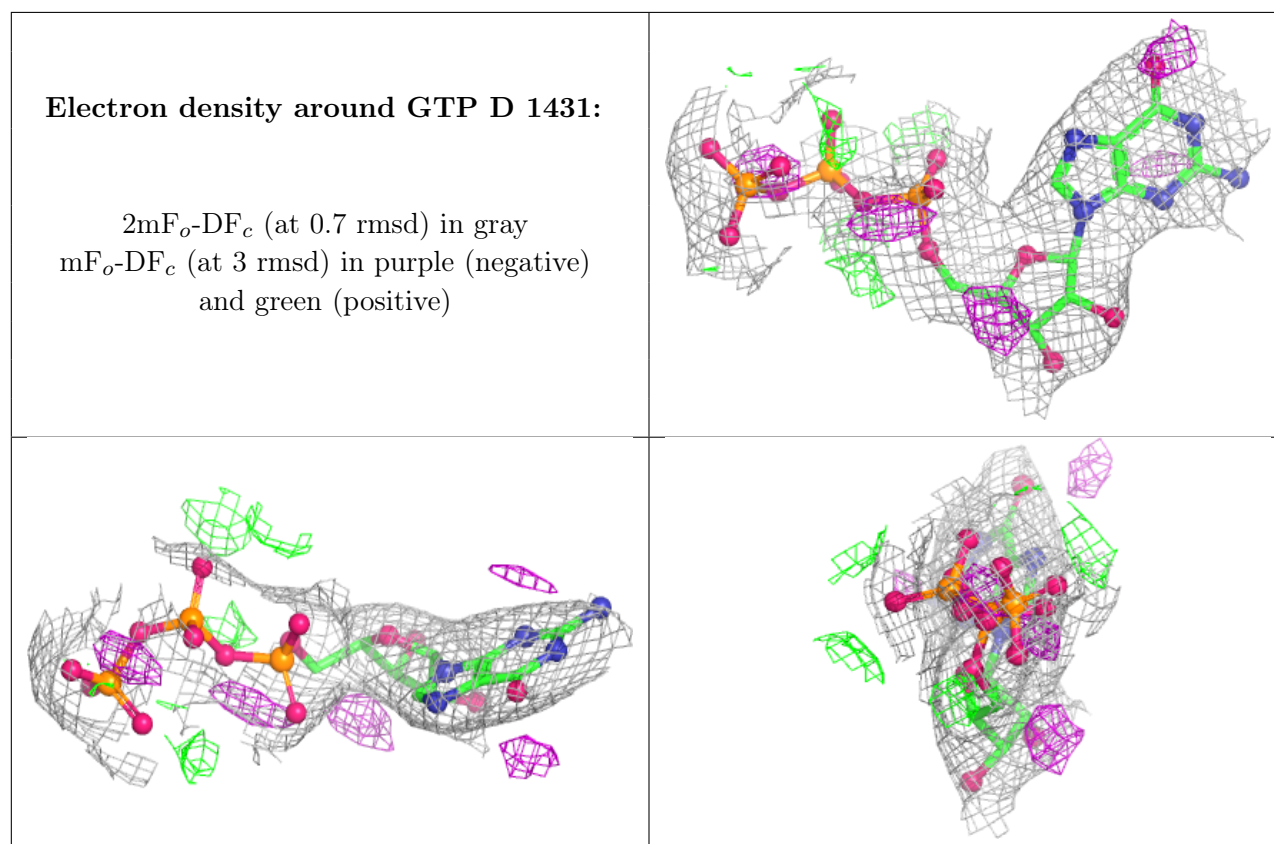
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

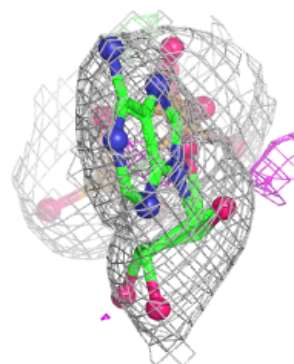
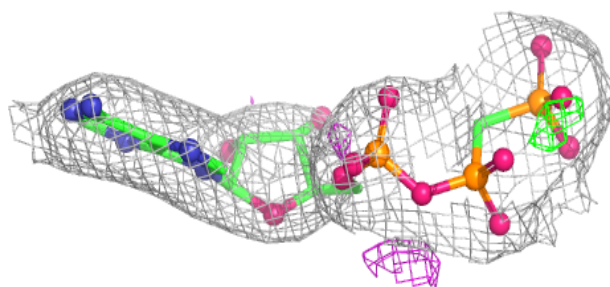
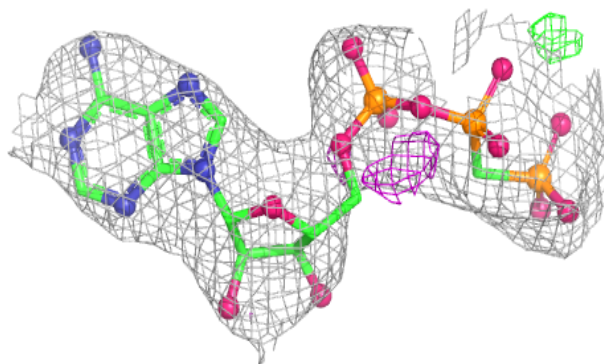
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	1430	1/1	0.71	0.17	75,75,75,75	0
6	MG	D	1432	1/1	0.71	0.22	85,85,85,85	0
7	CA	B	1431	1/1	0.91	0.08	97,97,97,97	0
5	GTP	D	1431	32/32	0.92	0.09	69,79,97,108	0
9	MES	B	1432	12/12	0.92	0.11	60,67,74,82	0
11	ACP	F	1385	31/31	0.92	0.08	86,94,121,132	0
9	MES	B	1433	12/12	0.93	0.10	93,103,107,111	0
10	X3H	C	1443	23/23	0.96	0.10	58,63,72,72	0
8	GDP	B	1429	28/28	0.97	0.06	47,55,58,66	0
7	CA	A	1440	1/1	0.98	0.05	97,97,97,97	0
5	GTP	C	1440	32/32	0.98	0.05	41,48,51,53	0
7	CA	C	1442	1/1	0.98	0.04	83,83,83,83	0
5	GTP	A	1438	32/32	0.98	0.04	44,52,55,57	0
6	MG	C	1441	1/1	1.00	0.02	50,50,50,50	0
6	MG	A	1439	1/1	1.00	0.03	51,51,51,51	0

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

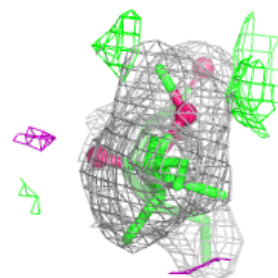
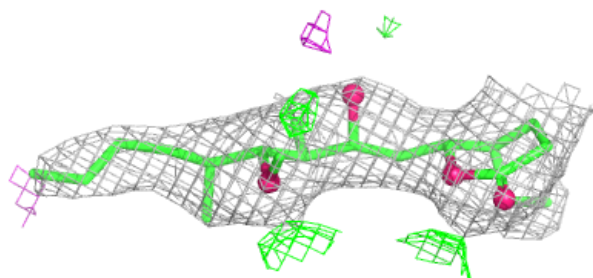
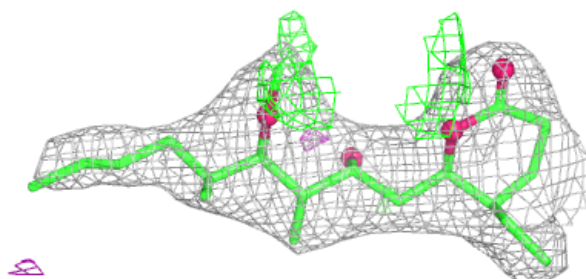


Electron density around ACP F 1385:

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

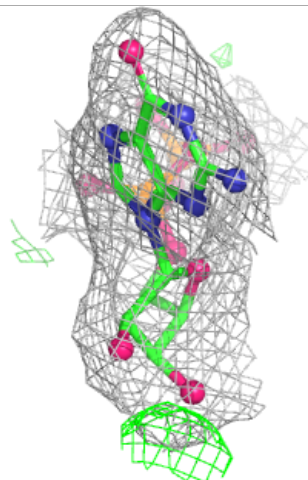
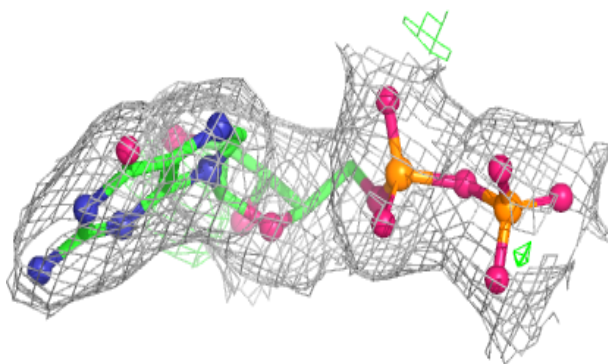
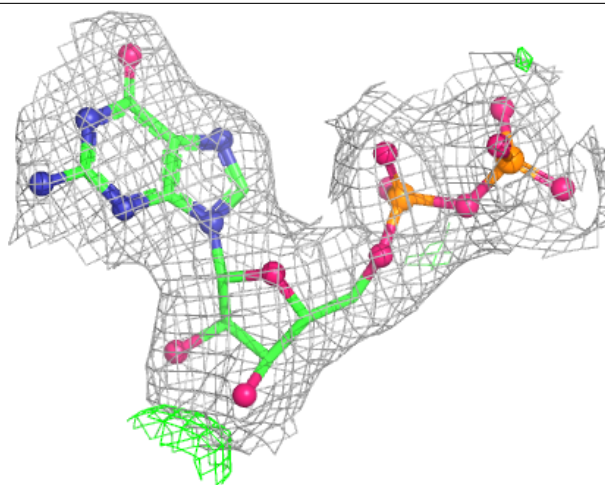
**Electron density around X3H C 1443:**

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



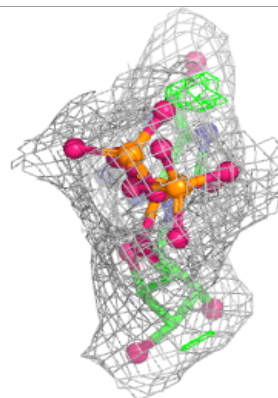
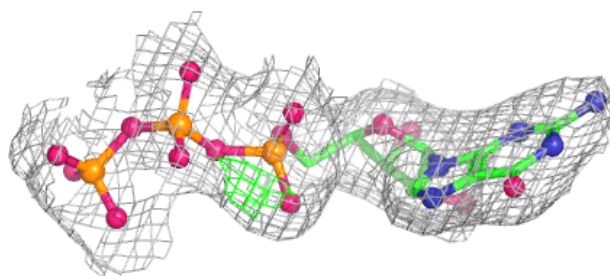
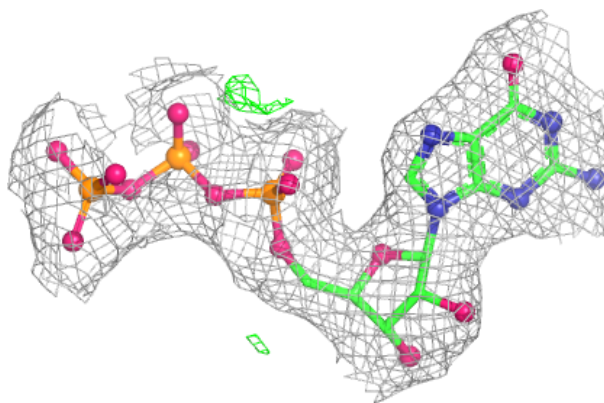
Electron density around GDP B 1429:

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

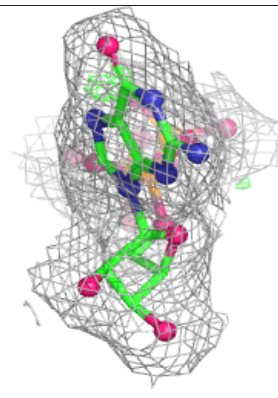
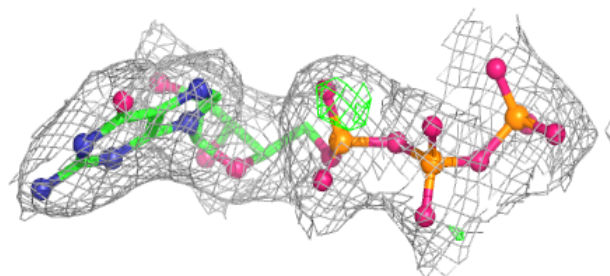
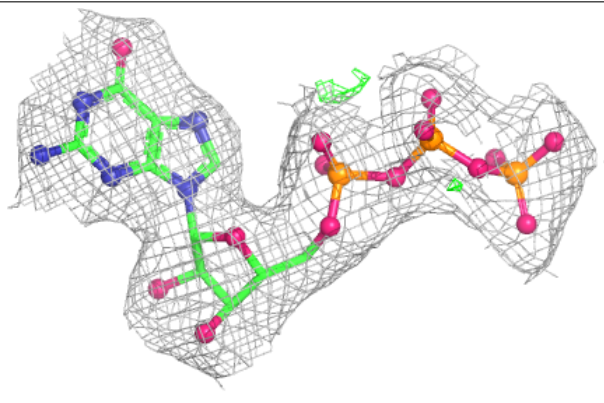


Electron density around GTP C 1440:

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

**Electron density around GTP A 1438:**

$2mF_o-DF_c$ (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.