



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:43 AM UTC

PDB ID : 8FMG / pdb_00008fmg
Title : Structure of CBASS Cap5 from *Pseudomonas syringae* as an activated tetramer with the cyclic dinucleotide 3'2'-c-diAMP ligand (3 tetramers in the AU)
Authors : Rechkoblit, O.; Kreitler, D.F.; Aggarwal, A.K.
Deposited on : 2022-12-23
Resolution : 1.79 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

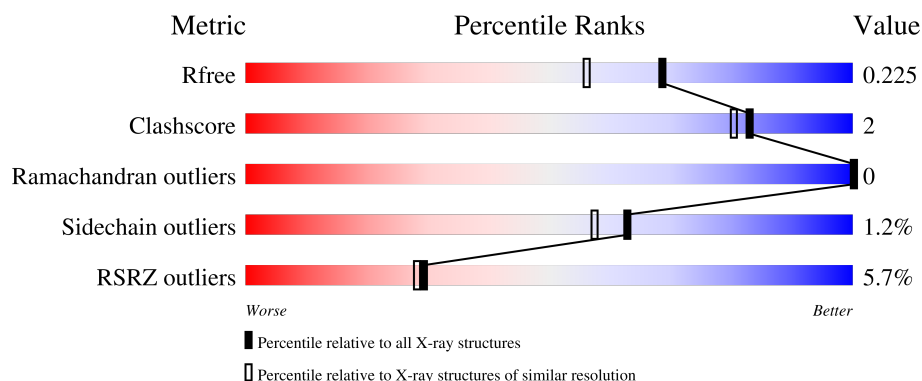
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	388	 4% 89% 5% 5%
1	B	388	 6% 82% 9% 9%
1	C	388	 7% 86% 9% 5%
1	D	388	 6% 86% 5% 9%

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Mol	Chain	Length	Quality of chain
1	E	388	6% 89% 6% 5%
1	F	388	5% 85% 6% 9%
1	G	388	3% 87% 8% 5%
1	H	388	6% 88% 8%
1	K	388	6% 92% 5%
1	L	388	2% 85% 6% 8%
1	M	388	7% 90% 5% 5%
1	N	388	7% 85% 5% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 69460 atoms, of which 32951 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 SAVED domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	H	N	O	S	0	4	0
			5714	1817	2826	520	540	11			
1	B	354	Total	C	H	N	O	S	0	0	0
			5368	1718	2656	482	502	10			
1	C	368	Total	C	H	N	O	S	0	0	0
			5600	1784	2764	512	530	10			
1	D	353	Total	C	H	N	O	S	0	0	0
			5340	1713	2635	481	501	10			
1	E	369	Total	C	H	N	O	S	0	0	0
			5597	1791	2754	510	532	10			
1	F	353	Total	C	H	N	O	S	0	1	0
			5412	1730	2677	485	510	10			
1	G	368	Total	C	H	N	O	S	0	0	0
			5640	1793	2795	514	528	10			
1	H	356	Total	C	H	N	O	S	0	0	0
			5431	1737	2685	486	513	10			
1	K	369	Total	C	H	N	O	S	0	1	0
			5580	1787	2745	508	530	10			
1	L	357	Total	C	H	N	O	S	0	1	0
			5480	1748	2713	491	518	10			
1	M	369	Total	C	H	N	O	S	0	0	0
			5637	1794	2788	514	531	10			
1	N	354	Total	C	H	N	O	S	0	2	0
			5382	1727	2661	484	500	10			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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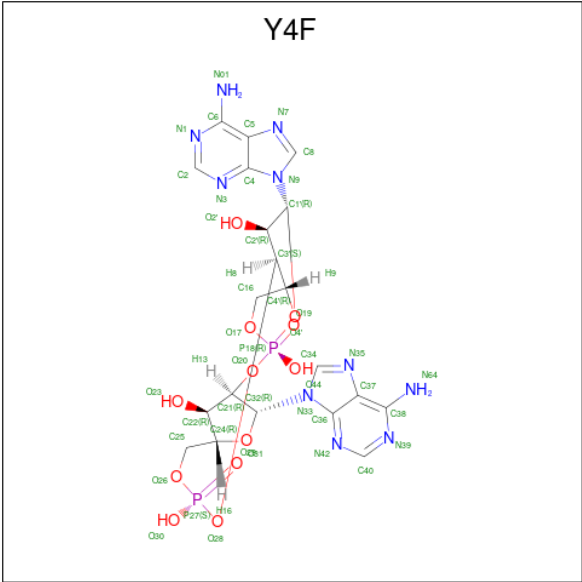
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	L	1	Total	Zn	0	0
			1	1		
2	M	1	Total	Zn	0	0
			1	1		
2	N	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	G	2	Total	Mg	0	0
			2	2		
3	H	1	Total	Mg	0	0
			1	1		
3	K	2	Total	Mg	0	0
			2	2		
3	M	2	Total	Mg	0	0
			2	2		

- Molecule 4 is Cyclic (adenosine-(2'-5')-monophosphate-adenosine-(3'-5')-monophosphate (CCD ID: Y4F) (formula: C₂₀H₂₄N₁₀O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	B	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	C	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	D	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	E	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	F	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	G	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	H	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	K	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	L	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	M	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		
4	N	1	Total	C	H	N	O	P	0	0
			65	20	21	10	12	2		

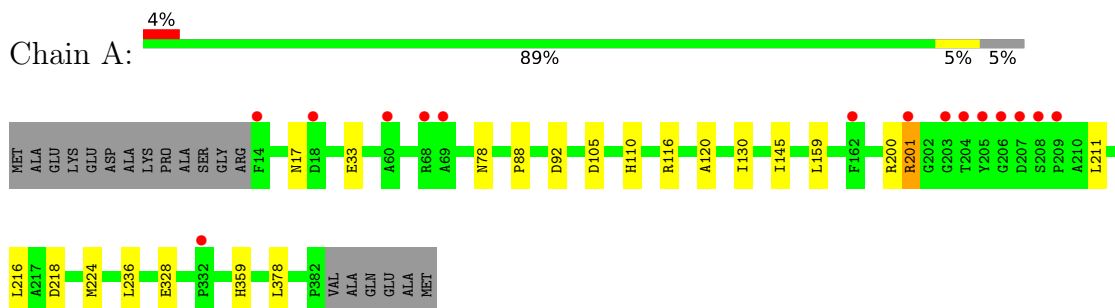
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total 230	O 230	0	0
5	B	218	Total 218	O 218	0	0
5	C	206	Total 206	O 206	0	0
5	D	141	Total 141	O 141	0	0
5	E	252	Total 252	O 252	0	0
5	F	162	Total 162	O 162	0	0
5	G	232	Total 232	O 232	0	0
5	H	212	Total 212	O 212	0	0
5	K	233	Total 233	O 233	0	0
5	L	223	Total 223	O 223	0	0
5	M	202	Total 202	O 202	0	0
5	N	163	Total 163	O 163	0	0

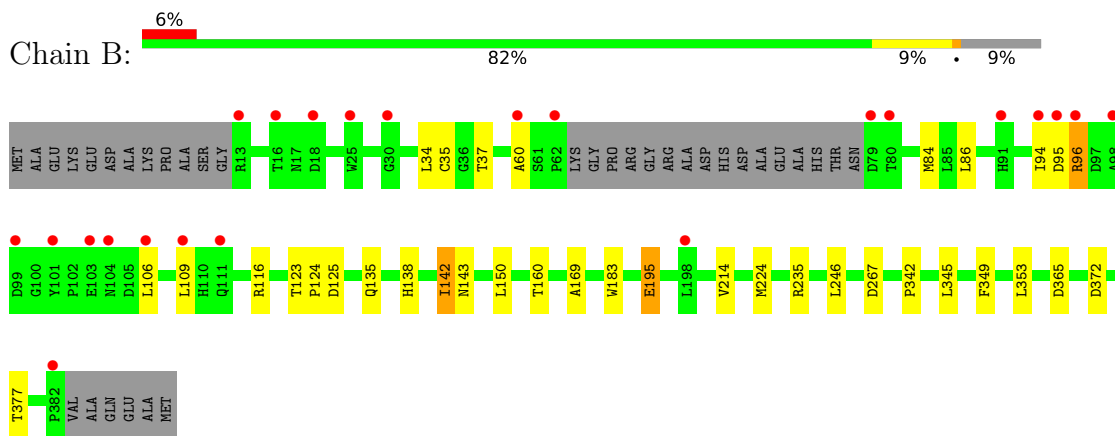
3 Residue-property plots [i](#)

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.

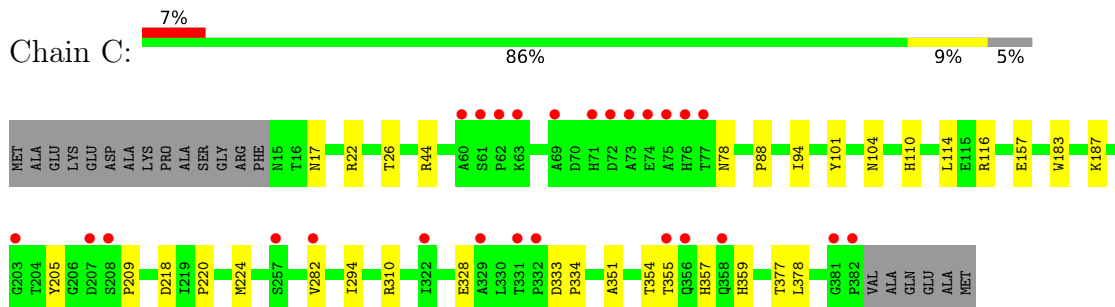
- Molecule 1: SAVED domain-containing protein



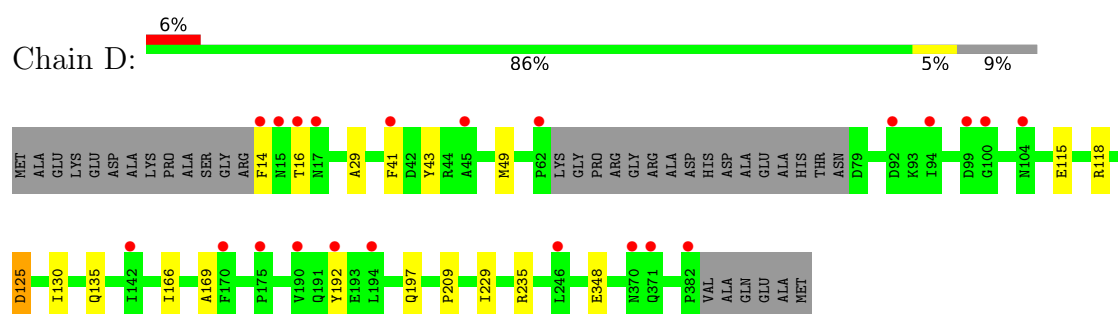
- Molecule 1: SAVED domain-containing protein



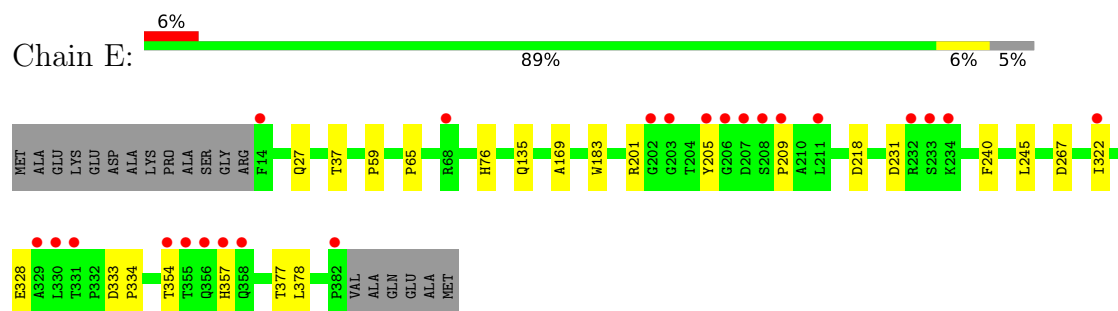
- Molecule 1: SAVED domain-containing protein



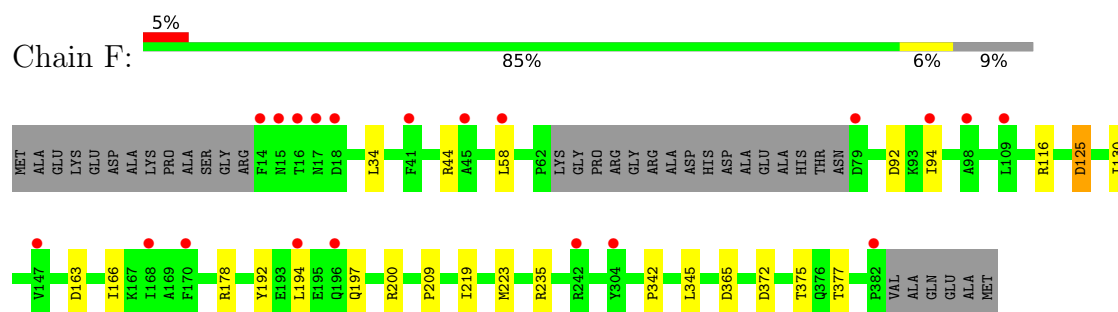
- Molecule 1: SAVED domain-containing protein



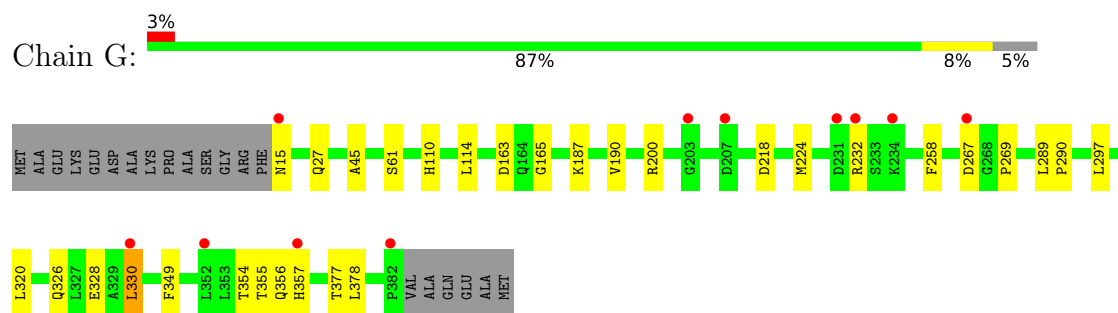
- Molecule 1: SAVED domain-containing protein



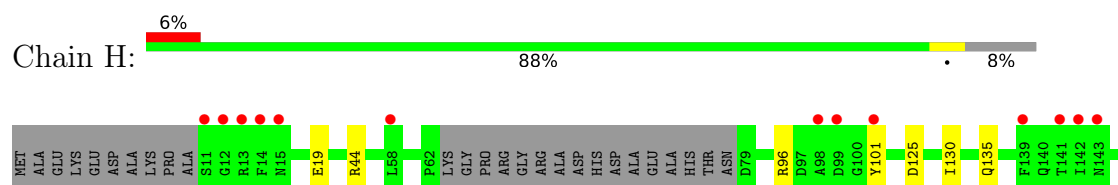
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein

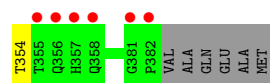
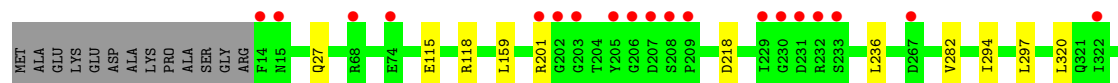


- Molecule 1: SAVED domain-containing protein

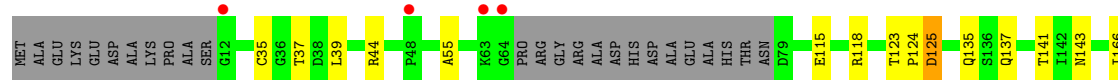
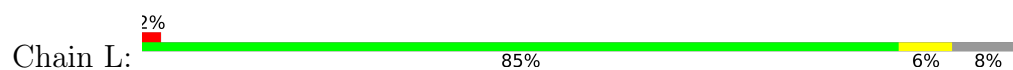




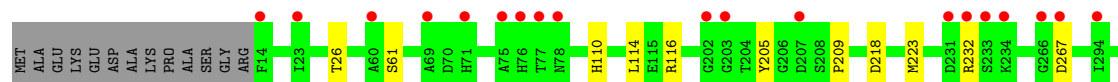
- Molecule 1: SAVED domain-containing protein



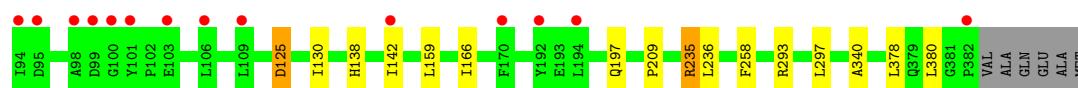
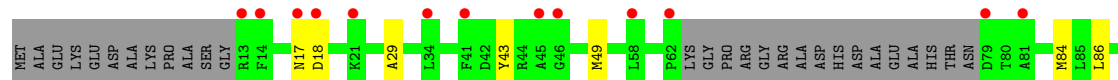
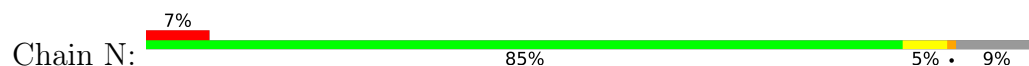
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.19Å 80.52Å 406.84Å 90.00° 90.62° 90.00°	Depositor
Resolution (Å)	58.12 – 1.79 58.12 – 1.79	Depositor EDS
% Data completeness (in resolution range)	61.0 (58.12-1.79) 61.0 (58.12-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.179 , 0.225 0.180 , 0.225	Depositor DCC
R_{free} test set	12884 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.006 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.025 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.020 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.007 for -h,-k,l	Xtriage
F_o , F_c correlation	0.96	EDS
Total number of atoms	69460	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, Y4F, ZN

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	0.19	0/2958	0.38	0/4031
1	B	0.18	0/2777	0.38	0/3788
1	C	0.17	0/2905	0.36	0/3961
1	D	0.15	0/2771	0.35	0/3782
1	E	0.17	0/2913	0.37	0/3975
1	F	0.16	0/2801	0.37	0/3820
1	G	0.17	0/2914	0.36	0/3971
1	H	0.17	0/2812	0.37	0/3832
1	K	0.20	0/2904	0.37	0/3963
1	L	0.18	0/2833	0.38	0/3861
1	M	0.17	0/2918	0.37	0/3978
1	N	0.16	0/2787	0.36	0/3804
All	All	0.17	0/34293	0.37	0/46766

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	2826	2821	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2712	2656	2654	22	0
1	C	2836	2764	2763	21	0
1	D	2705	2635	2633	13	0
1	E	2843	2754	2753	15	0
1	F	2735	2677	2674	15	0
1	G	2845	2795	2794	17	0
1	H	2746	2685	2683	10	0
1	K	2835	2745	2743	8	0
1	L	2767	2713	2710	17	0
1	M	2849	2788	2787	10	0
1	N	2721	2661	2657	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	K	2	0	0	0	0
3	M	2	0	0	0	0
4	A	44	21	0	0	0
4	B	44	21	0	0	0
4	C	44	21	0	0	0
4	D	44	21	0	0	0
4	E	44	21	0	0	0
4	F	44	21	0	0	0
4	G	44	21	0	0	0
4	H	44	21	0	0	0
4	K	44	21	0	0	0
4	L	44	21	0	1	0
4	M	44	21	0	0	0
4	N	44	21	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	230	0	0	4	0
5	B	218	0	0	3	0
5	C	206	0	0	3	0
5	D	141	0	0	0	0
5	E	252	0	0	3	0
5	F	162	0	0	3	0
5	G	232	0	0	3	0
5	H	212	0	0	1	0
5	K	233	0	0	1	0
5	L	223	0	0	1	0
5	M	202	0	0	1	0
5	N	163	0	0	0	0
All	All	36509	32951	32672	163	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 2.

All (163) 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:F:166:ILE:HD11	1:F:197:GLN:HG3	1.60	0.83
1:C:224:MET:HE3	1:C:378:LEU:HD13	1.67	0.77
1:D:166:ILE:HD11	1:D:197:GLN:HG3	1.73	0.70
1:A:159:LEU:HD11	1:A:236:LEU:HD22	1.76	0.67
1:B:365:ASP:OD2	5:B:501:HOH:O	2.14	0.65
1:N:166:ILE:HD11	1:N:197:GLN:HG3	1.79	0.64
1:L:166:ILE:HD11	1:L:197:GLN:HG3	1.80	0.63
1:M:267:ASP:O	5:M:501:HOH:O	2.15	0.63
1:B:84:MET:HE1	1:B:106:LEU:HD12	1.83	0.61
1:N:43:TYR:HB2	1:N:49:MET:HG2	1.83	0.61
1:D:235:ARG:NH2	1:D:348:GLU:OE1	2.33	0.60
1:G:354:THR:HG23	1:G:355:THR:HG23	1.85	0.58
1:H:166:ILE:HD11	1:H:197:GLN:HG3	1.85	0.58
1:L:115:GLU:OE1	1:L:118:ARG:NH1	2.36	0.58
1:C:17:ASN:OD1	1:C:78:ASN:ND2	2.37	0.57
1:B:116:ARG:NH2	5:B:504:HOH:O	2.38	0.57
1:D:229:ILE:HD12	1:D:235:ARG:HD2	1.87	0.56
1:L:166:ILE:HD11	1:L:197:GLN:CG	2.35	0.56
1:A:92:ASP:OD1	5:A:501:HOH:O	2.18	0.56
1:F:194:LEU:HD21	5:F:601:HOH:O	2.06	0.56
1:F:125:ASP:OD1	1:F:125:ASP:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:TYR:O	5:H:501:HOH:O	2.18	0.55
1:F:34:LEU:HD11	1:F:94:ILE:HD11	1.89	0.54
1:B:195:GLU:HG3	5:B:614:HOH:O	2.08	0.54
1:G:320:LEU:HD21	1:G:349:PHE:CD2	2.42	0.54
1:A:88:PRO:HB2	1:C:88:PRO:HB2	1.90	0.54
1:B:125:ASP:OD1	1:B:125:ASP:C	2.50	0.54
1:C:187:LYS:HG2	1:C:224:MET:HE1	1.88	0.54
1:L:39:LEU:HD13	1:L:55:ALA:HB2	1.88	0.54
1:L:194:LEU:HD11	1:L:229:ILE:HG22	1.91	0.53
1:D:115:GLU:OE2	1:D:118:ARG:NH1	2.41	0.53
1:C:116:ARG:NH1	5:C:503:HOH:O	2.33	0.53
1:L:281:PRO:HG2	1:L:284:ASP:OD2	2.09	0.52
1:K:354:THR:O	5:K:501:HOH:O	2.19	0.52
1:N:125:ASP:OD1	1:N:125:ASP:C	2.53	0.52
1:F:116:ARG:NH2	5:F:506:HOH:O	2.42	0.51
1:B:214:VAL:HG21	1:B:246:LEU:HD21	1.92	0.51
1:C:22:ARG:NH1	5:C:501:HOH:O	2.28	0.51
1:L:35:CYS:SG	1:L:37:THR:HG23	2.50	0.51
1:L:125:ASP:OD1	1:L:125:ASP:C	2.53	0.51
1:D:166:ILE:HD11	1:D:197:GLN:CG	2.38	0.51
1:E:27:GLN:CG	1:F:44:ARG:HH22	2.24	0.50
1:A:105:ASP:OD2	5:A:502:HOH:O	2.19	0.50
1:A:159:LEU:CD1	1:A:236:LEU:HD22	2.39	0.50
1:N:138:HIS:NE2	1:N:142:ILE:HD12	2.26	0.50
1:H:125:ASP:OD1	1:H:125:ASP:C	2.55	0.50
1:M:223:MET:HE2	1:M:349:PHE:HD2	1.78	0.49
1:D:41:PHE:CE1	1:E:322:ILE:HD11	2.47	0.49
1:H:150:LEU:HA	1:H:246:LEU:HD12	1.94	0.49
1:G:328:GLU:OE2	1:G:357:HIS:HB3	2.13	0.49
1:N:159:LEU:HD11	1:N:236[B]:LEU:HD12	1.94	0.48
1:C:328:GLU:OE2	1:C:357:HIS:HB3	2.13	0.48
1:C:333:ASP:HB3	1:C:334:PRO:CD	2.44	0.47
1:C:220:PRO:HB2	1:C:378:LEU:HD12	1.96	0.47
1:G:377:THR:OG1	1:G:378:LEU:N	2.47	0.47
1:B:135:GLN:O	1:B:169:ALA:HA	2.14	0.47
1:E:201:ARG:HB2	1:E:201:ARG:NH1	2.30	0.47
1:H:150:LEU:CA	1:H:246:LEU:HD12	2.45	0.47
1:B:235:ARG:HD2	1:B:235:ARG:C	2.40	0.46
1:E:59:PRO:HD3	1:E:65:PRO:O	2.15	0.46
1:N:84:MET:HE2	1:N:86:LEU:HD21	1.98	0.46
1:A:33:GLU:OE1	1:A:110:HIS:ND1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:GLU:OE2	1:E:357:HIS:HB3	2.16	0.46
4:L:402:Y4F:N3	5:L:505:HOH:O	2.36	0.46
1:M:334:PRO:CB	1:M:362:LEU:HD13	2.46	0.46
1:N:378:LEU:HD21	1:N:380:LEU:HD21	1.97	0.46
1:C:205:TYR:HB3	1:C:209:PRO:HB3	1.98	0.45
1:E:27:GLN:HG2	1:F:44:ARG:HH22	1.81	0.45
1:B:349:PHE:HE1	1:B:353:LEU:HD11	1.80	0.45
1:L:137:GLN:O	1:L:141:THR:HG23	2.16	0.45
1:B:183:TRP:CE3	1:B:224:MET:HG3	2.52	0.45
1:H:96:ARG:HA	1:H:101:TYR:O	2.16	0.45
1:L:135:GLN:O	1:L:169:ALA:HA	2.17	0.45
1:B:94:ILE:O	1:B:96:ARG:NE	2.41	0.45
1:M:110:HIS:CE1	1:M:114:LEU:HD11	2.51	0.45
1:K:115[A]:GLU:OE1	1:K:118:ARG:NH1	2.49	0.45
1:G:110:HIS:CE1	1:G:114:LEU:HD11	2.52	0.44
1:M:334:PRO:HB2	1:M:362:LEU:HD13	1.98	0.44
1:C:282:VAL:HG23	1:C:294:ILE:CD1	2.47	0.44
1:K:297:LEU:HD22	1:K:320:LEU:HD13	2.00	0.44
1:N:340:ALA:HA	4:N:402:Y4F:O4'	2.17	0.44
1:D:130:ILE:HD11	1:D:209:PRO:HG2	2.00	0.44
1:F:163:ASP:OD2	1:F:200:ARG:NH1	2.37	0.44
1:G:258:PHE:HB3	1:G:297:LEU:HD11	2.00	0.44
1:B:35:CYS:SG	1:B:37:THR:OG1	2.62	0.44
1:C:26:THR:O	1:D:29:ALA:HA	2.18	0.43
1:H:135:GLN:O	1:H:169:ALA:HA	2.18	0.43
1:C:104:ASN:ND2	5:C:513:HOH:O	2.46	0.43
1:G:326:GLN:O	1:G:330:LEU:HD13	2.18	0.43
1:L:235:ARG:HD2	1:L:235:ARG:C	2.43	0.43
1:E:76:HIS:O	5:E:501:HOH:O	2.21	0.43
1:M:333:ASP:HB3	1:M:334:PRO:CD	2.48	0.43
1:A:201:ARG:CZ	1:D:192:TYR:HE1	2.31	0.43
1:D:125:ASP:OD1	1:D:125:ASP:C	2.62	0.43
1:F:130:ILE:HD11	1:F:209:PRO:HG2	2.01	0.43
1:L:123:THR:N	1:L:124:PRO:CD	2.81	0.43
1:A:17:ASN:ND2	1:A:78:ASN:OD1	2.52	0.43
1:B:138:HIS:CE1	1:B:142:ILE:HD13	2.54	0.43
1:G:190:VAL:HG11	1:G:224:MET:HG2	2.00	0.43
5:A:574:HOH:O	1:B:160:THR:HG21	2.19	0.43
1:K:27:GLN:OE1	1:L:44:ARG:NH1	2.50	0.43
1:A:116:ARG:NH2	5:A:506:HOH:O	2.36	0.43
1:D:135:GLN:O	1:D:169:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:TYR:HB2	1:G:200:ARG:CG	2.49	0.43
1:F:365:ASP:OD1	5:F:501:HOH:O	2.21	0.43
1:K:282:VAL:HG23	1:K:294:ILE:HD13	2.01	0.43
1:M:342:PRO:HD2	1:M:345:LEU:HD12	2.01	0.43
1:A:200:ARG:HG2	1:D:192:TYR:HB2	2.01	0.43
1:B:60:ALA:HA	1:B:84:MET:HE2	2.01	0.43
1:C:377:THR:OG1	1:C:378:LEU:N	2.51	0.42
1:B:150:LEU:HA	1:B:246:LEU:HD13	2.02	0.42
1:C:110:HIS:CE1	1:C:114:LEU:HD11	2.54	0.42
1:A:328:GLU:HB3	1:A:359[A]:HIS:CE1	2.54	0.42
1:A:145:ILE:HD11	1:A:216:LEU:HB2	2.00	0.42
1:G:269:PRO:HB2	1:G:289:LEU:HD21	2.01	0.42
1:N:258:PHE:HB3	1:N:297:LEU:HD11	2.02	0.42
1:H:178:ARG:NH2	1:H:218:ASP:OD2	2.47	0.42
1:N:130:ILE:HD11	1:N:209:PRO:HG2	2.01	0.42
1:N:235:ARG:HG3	1:N:236[B]:LEU:N	2.33	0.42
1:E:205:TYR:HB3	1:E:209:PRO:HB3	2.01	0.42
1:G:27:GLN:OE1	1:H:44:ARG:NH2	2.50	0.42
1:G:45:ALA:HB3	5:G:546:HOH:O	2.19	0.42
1:F:178:ARG:HH21	1:F:377:THR:HG21	1.83	0.42
1:F:235:ARG:HD2	1:F:235:ARG:C	2.45	0.42
1:G:15:ASN:N	5:G:527:HOH:O	2.52	0.42
1:C:157:GLU:OE1	1:C:310:ARG:NH2	2.40	0.41
1:E:377:THR:OG1	1:E:378:LEU:N	2.53	0.41
1:K:27:GLN:HG3	1:L:44:ARG:HH22	1.85	0.41
1:H:130:ILE:HD11	1:H:209:PRO:HG2	2.01	0.41
1:N:235:ARG:HG3	1:N:236[A]:LEU:N	2.33	0.41
1:E:240:PHE:CE2	1:E:245:LEU:HD23	2.55	0.41
1:G:290:PRO:O	5:G:501:HOH:O	2.21	0.41
1:M:354:THR:O	1:M:354:THR:HG22	2.20	0.41
1:A:120:ALA:O	1:B:116:ARG:NH1	2.54	0.41
1:B:34:LEU:HD12	1:B:86:LEU:HD22	2.02	0.41
1:G:187:LYS:HG2	1:G:224:MET:HE1	2.02	0.41
1:A:224:MET:HE3	1:A:378:LEU:HD13	2.03	0.41
1:B:342:PRO:HD2	1:B:345:LEU:HD22	2.02	0.41
1:E:183:TRP:CE3	1:E:378:LEU:HD21	2.55	0.41
1:F:342:PRO:HD2	1:F:345:LEU:HD22	2.02	0.41
1:M:205:TYR:HB3	1:M:209:PRO:HB3	2.02	0.41
1:D:43:TYR:HB2	1:D:49:MET:HG2	2.02	0.41
1:B:160:THR:HG22	1:C:44:ARG:CZ	2.51	0.41
1:C:183:TRP:CH2	1:C:220:PRO:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:GLN:OE1	1:L:44:ARG:NH2	2.54	0.41
1:K:159:LEU:HD11	1:K:236:LEU:HD22	2.02	0.41
1:M:26:THR:O	1:N:29:ALA:HA	2.20	0.41
1:C:354:THR:HG23	1:C:355:THR:N	2.36	0.41
1:L:309:ASN:OD1	1:L:311:ARG:HB2	2.21	0.40
1:C:94:ILE:HA	1:C:101:TYR:CD2	2.56	0.40
1:E:135:GLN:O	1:E:169:ALA:HA	2.21	0.40
1:A:130:ILE:HB	1:A:211:LEU:HD23	2.02	0.40
1:B:349:PHE:CE1	1:B:353:LEU:HD11	2.56	0.40
1:C:351:ALA:O	1:C:354:THR:HG22	2.22	0.40
1:E:37:THR:HG22	5:E:540:HOH:O	2.21	0.40
1:E:267:ASP:OD2	5:E:502:HOH:O	2.22	0.40
1:E:333:ASP:HB3	1:E:334:PRO:HD2	2.03	0.40
1:F:219:ILE:O	1:F:223:MET:HG3	2.21	0.40
1:G:224:MET:HE3	1:G:378:LEU:HD13	2.03	0.40
1:B:123:THR:N	1:B:124:PRO:CD	2.85	0.40
1:G:163:ASP:OD2	1:G:165:GLY:N	2.50	0.40
1:L:240:PHE:HA	1:L:246:LEU:HD23	2.03	0.40
1:N:17:ASN:OD1	1:N:18:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/388 (96%)	356 (96%)	15 (4%)	0	100	100
1	B	350/388 (90%)	337 (96%)	13 (4%)	0	100	100
1	C	366/388 (94%)	355 (97%)	11 (3%)	0	100	100
1	D	349/388 (90%)	337 (97%)	12 (3%)	0	100	100
1	E	367/388 (95%)	351 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	350/388 (90%)	342 (98%)	8 (2%)	0	100	100
1	G	366/388 (94%)	353 (96%)	13 (4%)	0	100	100
1	H	352/388 (91%)	340 (97%)	12 (3%)	0	100	100
1	K	368/388 (95%)	350 (95%)	18 (5%)	0	100	100
1	L	354/388 (91%)	348 (98%)	6 (2%)	0	100	100
1	M	367/388 (95%)	355 (97%)	12 (3%)	0	100	100
1	N	352/388 (91%)	338 (96%)	14 (4%)	0	100	100
All	All	4312/4656 (93%)	4162 (96%)	150 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/317 (96%)	302 (99%)	2 (1%)	76	73
1	B	283/317 (89%)	274 (97%)	9 (3%)	34	22
1	C	296/317 (93%)	294 (99%)	2 (1%)	76	73
1	D	281/317 (89%)	278 (99%)	3 (1%)	65	60
1	E	295/317 (93%)	292 (99%)	3 (1%)	68	64
1	F	288/317 (91%)	283 (98%)	5 (2%)	53	45
1	G	298/317 (94%)	292 (98%)	6 (2%)	48	38
1	H	288/317 (91%)	287 (100%)	1 (0%)	86	86
1	K	292/317 (92%)	290 (99%)	2 (1%)	76	73
1	L	292/317 (92%)	290 (99%)	2 (1%)	76	73
1	M	298/317 (94%)	293 (98%)	5 (2%)	53	45
1	N	282/317 (89%)	279 (99%)	3 (1%)	65	60
All	All	3497/3804 (92%)	3454 (99%)	43 (1%)	63	57

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ARG
1	A	218	ASP
1	B	95	ASP
1	B	96	ARG
1	B	109	LEU
1	B	142	ILE
1	B	143	ASN
1	B	195	GLU
1	B	267	ASP
1	B	372	ASP
1	B	377	THR
1	C	218	ASP
1	C	359	HIS
1	D	14	PHE
1	D	16	THR
1	D	125	ASP
1	E	218	ASP
1	E	231	ASP
1	E	354	THR
1	F	58	LEU
1	F	92	ASP
1	F	125	ASP
1	F	372	ASP
1	F	375	THR
1	G	61	SER
1	G	218	ASP
1	G	232	ARG
1	G	267	ASP
1	G	330	LEU
1	G	356	GLN
1	H	19	GLU
1	K	201	ARG
1	K	218	ASP
1	L	125	ASP
1	L	143	ASN
1	M	61	SER
1	M	116	ARG
1	M	218	ASP
1	M	232	ARG
1	M	317	ARG
1	N	125	ASP
1	N	235	ARG

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Mol	Chain	Res	Type
1	N	293	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	56	HIS
1	A	76	HIS
1	A	137	GLN
1	A	184	GLN
1	A	185	ASN
1	A	314	HIS
1	A	371	GLN
1	B	197	GLN
1	B	244	HIS
1	C	184	GLN
1	C	185	ASN
1	C	241	HIS
1	C	308	GLN
1	C	371	GLN
1	D	197	GLN
1	D	241	HIS
1	E	137	GLN
1	E	184	GLN
1	E	185	ASN
1	E	308	GLN
1	F	91	HIS
1	F	137	GLN
1	F	244	HIS
1	G	56	HIS
1	G	76	HIS
1	G	137	GLN
1	G	185	ASN
1	G	356	GLN
1	G	358	GLN
1	G	379	GLN
1	H	138	HIS
1	H	140	GLN
1	H	143	ASN
1	H	196	GLN
1	K	56	HIS
1	K	137	GLN

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Mol	Chain	Res	Type
1	K	164	GLN
1	K	185	ASN
1	K	321	GLN
1	L	138	HIS
1	M	137	GLN
1	M	164	GLN
1	M	184	GLN
1	M	185	ASN
1	M	241	HIS
1	N	308	GLN

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 37 ligands modelled in this entry, 25 are monoatomic - leaving 12 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	$\# Z > 2$
4	Y4F	G	404	-	50,50,50	0.48	0	74,78,78	1.22	4 (5%)
4	Y4F	L	402	-	50,50,50	0.49	0	74,78,78	1.17	4 (5%)
4	Y4F	E	404	-	50,50,50	0.48	0	74,78,78	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Y4F	A	404	-	50,50,50	0.51	0	74,78,78	1.27	5 (6%)
4	Y4F	K	404	-	50,50,50	0.48	0	74,78,78	1.16	4 (5%)
4	Y4F	D	402	-	50,50,50	0.47	0	74,78,78	1.15	4 (5%)
4	Y4F	F	402	-	50,50,50	0.50	0	74,78,78	1.19	5 (6%)
4	Y4F	M	404	-	50,50,50	0.49	0	74,78,78	1.16	4 (5%)
4	Y4F	B	402	-	50,50,50	0.47	0	74,78,78	1.16	4 (5%)
4	Y4F	N	402	-	50,50,50	0.50	0	74,78,78	1.20	5 (6%)
4	Y4F	C	404	-	50,50,50	0.49	0	74,78,78	1.17	4 (5%)
4	Y4F	H	403	-	50,50,50	0.48	0	74,78,78	1.19	5 (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
4	Y4F	G	404	-	-	3/30/62/62	0/6/7/7
4	Y4F	L	402	-	-	1/30/62/62	0/6/7/7
4	Y4F	E	404	-	-	2/30/62/62	0/6/7/7
4	Y4F	A	404	-	-	3/30/62/62	0/6/7/7
4	Y4F	K	404	-	-	3/30/62/62	0/6/7/7
4	Y4F	D	402	-	-	5/30/62/62	0/6/7/7
4	Y4F	F	402	-	-	6/30/62/62	0/6/7/7
4	Y4F	M	404	-	-	3/30/62/62	0/6/7/7
4	Y4F	B	402	-	-	3/30/62/62	0/6/7/7
4	Y4F	N	402	-	-	7/30/62/62	0/6/7/7
4	Y4F	C	404	-	-	3/30/62/62	0/6/7/7
4	Y4F	H	403	-	-	3/30/62/62	0/6/7/7

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	402	Y4F	C37-C36-N42	-5.29	119.43	126.72
4	L	402	Y4F	C37-C36-N42	-5.19	119.56	126.72
4	G	404	Y4F	C37-C36-N42	-5.18	119.58	126.72
4	H	403	Y4F	C37-C36-N42	-5.17	119.59	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	404	Y4F	C37-C36-N42	-5.15	119.63	126.72
4	A	404	Y4F	C37-C36-N42	-5.11	119.68	126.72
4	N	402	Y4F	C37-C36-N42	-5.08	119.72	126.72
4	C	404	Y4F	C37-C36-N42	-5.07	119.73	126.72
4	E	404	Y4F	C37-C36-N42	-5.07	119.73	126.72
4	D	402	Y4F	C37-C36-N42	-5.06	119.75	126.72
4	B	402	Y4F	C37-C36-N42	-5.02	119.81	126.72
4	K	404	Y4F	C37-C36-N42	-4.86	120.03	126.72
4	G	404	Y4F	N42-C40-N39	-4.26	122.13	128.58
4	E	404	Y4F	N42-C40-N39	-4.22	122.19	128.58
4	L	402	Y4F	N42-C40-N39	-4.20	122.22	128.58
4	N	402	Y4F	N42-C40-N39	-4.19	122.24	128.58
4	H	403	Y4F	N42-C40-N39	-4.16	122.29	128.58
4	B	402	Y4F	N42-C40-N39	-4.15	122.30	128.58
4	F	402	Y4F	N42-C40-N39	-4.15	122.31	128.58
4	A	404	Y4F	N42-C40-N39	-4.11	122.36	128.58
4	M	404	Y4F	N42-C40-N39	-4.11	122.36	128.58
4	K	404	Y4F	N42-C40-N39	-4.11	122.37	128.58
4	D	402	Y4F	N42-C40-N39	-4.10	122.37	128.58
4	G	404	Y4F	N42-C36-N33	4.03	134.03	127.17
4	C	404	Y4F	N42-C40-N39	-4.02	122.50	128.58
4	E	404	Y4F	N42-C36-N33	4.02	134.00	127.17
4	N	402	Y4F	N42-C36-N33	4.01	133.99	127.17
4	M	404	Y4F	N42-C36-N33	3.99	133.95	127.17
4	B	402	Y4F	N42-C36-N33	3.99	133.95	127.17
4	A	404	Y4F	N42-C36-N33	3.97	133.93	127.17
4	F	402	Y4F	N42-C36-N33	3.95	133.88	127.17
4	H	403	Y4F	N42-C36-N33	3.89	133.78	127.17
4	L	402	Y4F	N42-C36-N33	3.88	133.77	127.17
4	C	404	Y4F	N42-C36-N33	3.87	133.75	127.17
4	D	402	Y4F	N42-C36-N33	3.84	133.70	127.17
4	K	404	Y4F	N42-C36-N33	3.66	133.40	127.17
4	L	402	Y4F	C40-N42-C36	3.23	119.71	111.83
4	F	402	Y4F	C40-N42-C36	3.21	119.67	111.83
4	G	404	Y4F	C40-N42-C36	3.17	119.58	111.83
4	H	403	Y4F	C40-N42-C36	3.16	119.54	111.83
4	M	404	Y4F	C40-N42-C36	3.13	119.48	111.83
4	E	404	Y4F	C40-N42-C36	3.08	119.35	111.83
4	A	404	Y4F	C40-N42-C36	3.07	119.34	111.83
4	N	402	Y4F	C40-N42-C36	3.07	119.34	111.83
4	D	402	Y4F	C40-N42-C36	3.07	119.33	111.83
4	B	402	Y4F	C40-N42-C36	3.04	119.25	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	404	Y4F	C40-N42-C36	3.03	119.24	111.83
4	C	404	Y4F	C40-N42-C36	3.03	119.23	111.83
4	A	404	Y4F	O2'-C2'-C3'	2.50	118.18	111.19
4	N	402	Y4F	C2'-C3'-C4'	2.37	107.39	103.24
4	H	403	Y4F	O2'-C2'-C3'	2.22	117.41	111.19
4	F	402	Y4F	C2'-C1'-N9	2.18	118.71	113.30
4	E	404	Y4F	C22-C21-C32	-2.04	98.90	102.81

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	Y4F	C3'-O28-P27-O26
4	B	402	Y4F	C3'-O28-P27-O30
4	C	404	Y4F	C3'-O28-P27-O30
4	H	403	Y4F	C3'-O28-P27-O30
4	K	404	Y4F	C3'-O28-P27-O30
4	N	402	Y4F	C3'-O28-P27-O26
4	N	402	Y4F	C3'-O28-P27-O30
4	N	402	Y4F	O17-C16-C4'-O4'
4	D	402	Y4F	O17-C16-C4'-O4'
4	N	402	Y4F	O17-C16-C4'-C3'
4	H	403	Y4F	C4'-C16-O17-P18
4	K	404	Y4F	C4'-C16-O17-P18
4	A	404	Y4F	C3'-O28-P27-O30
4	E	404	Y4F	C3'-O28-P27-O30
4	G	404	Y4F	C3'-O28-P27-O30
4	M	404	Y4F	C3'-O28-P27-O30
4	C	404	Y4F	C4'-C16-O17-P18
4	M	404	Y4F	C4'-C16-O17-P18
4	N	402	Y4F	C2'-C3'-O28-P27
4	A	404	Y4F	C4'-C16-O17-P18
4	E	404	Y4F	C4'-C16-O17-P18
4	F	402	Y4F	C4'-C16-O17-P18
4	G	404	Y4F	C4'-C16-O17-P18
4	L	402	Y4F	C4'-C16-O17-P18
4	D	402	Y4F	C2'-C1'-N9-C4
4	D	402	Y4F	C2'-C1'-N9-C8
4	D	402	Y4F	C4'-C16-O17-P18
4	D	402	Y4F	O4'-C1'-N9-C8
4	F	402	Y4F	C2'-C1'-N9-C4
4	F	402	Y4F	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
4	A	404	Y4F	C3'-O28-P27-O29
4	B	402	Y4F	C3'-O28-P27-O29
4	C	404	Y4F	C3'-O28-P27-O29
4	F	402	Y4F	C3'-O28-P27-O30
4	G	404	Y4F	C3'-O28-P27-O29
4	H	403	Y4F	C3'-O28-P27-O29
4	K	404	Y4F	C3'-O28-P27-O29
4	M	404	Y4F	C3'-O28-P27-O29
4	N	402	Y4F	C3'-O28-P27-O29
4	F	402	Y4F	O4'-C1'-N9-C8
4	F	402	Y4F	O17-C16-C4'-O4'
4	N	402	Y4F	C4'-C3'-O28-P27

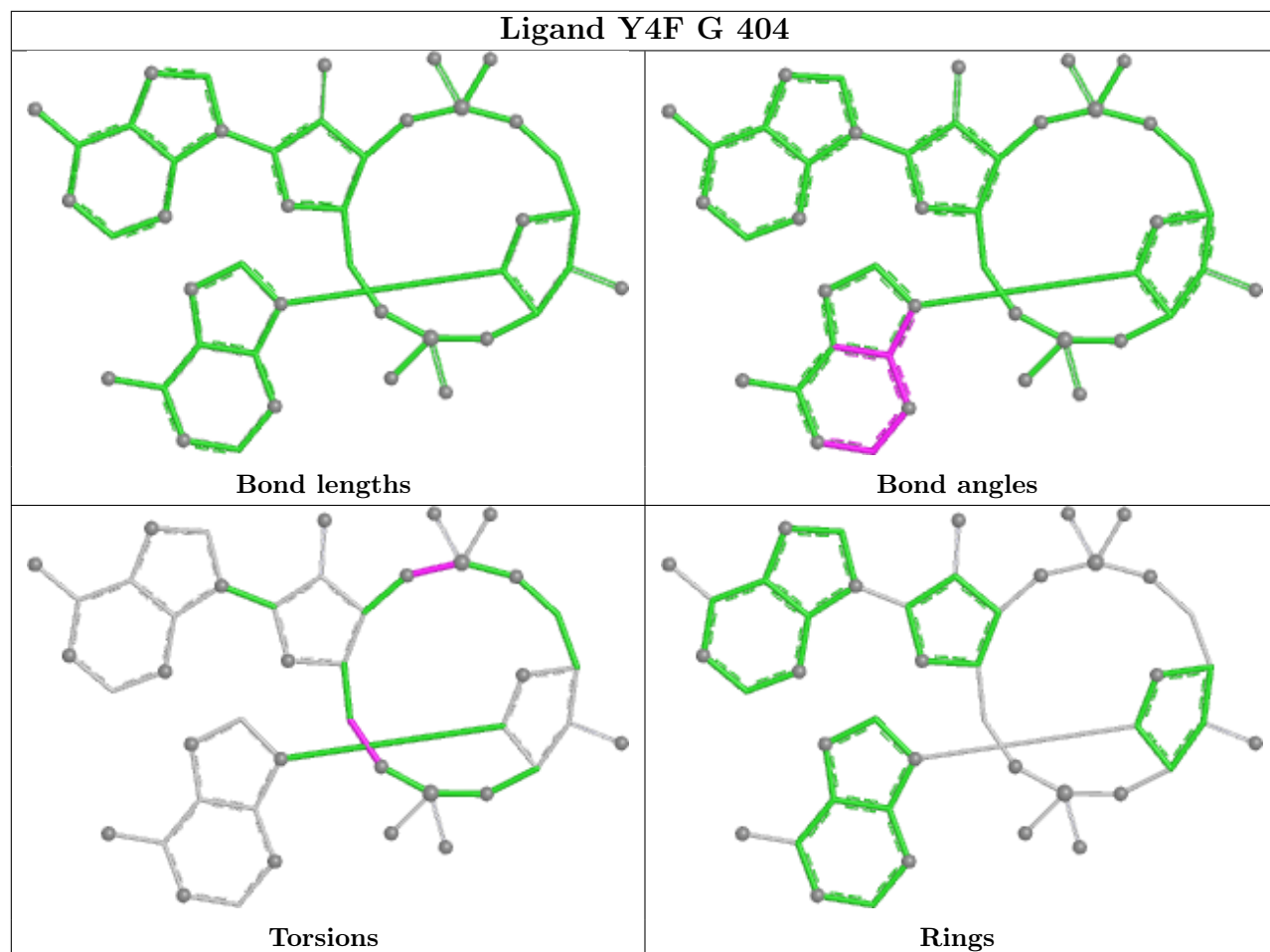
There are no ring outliers.

2 monomers are involved in 2 short contacts:

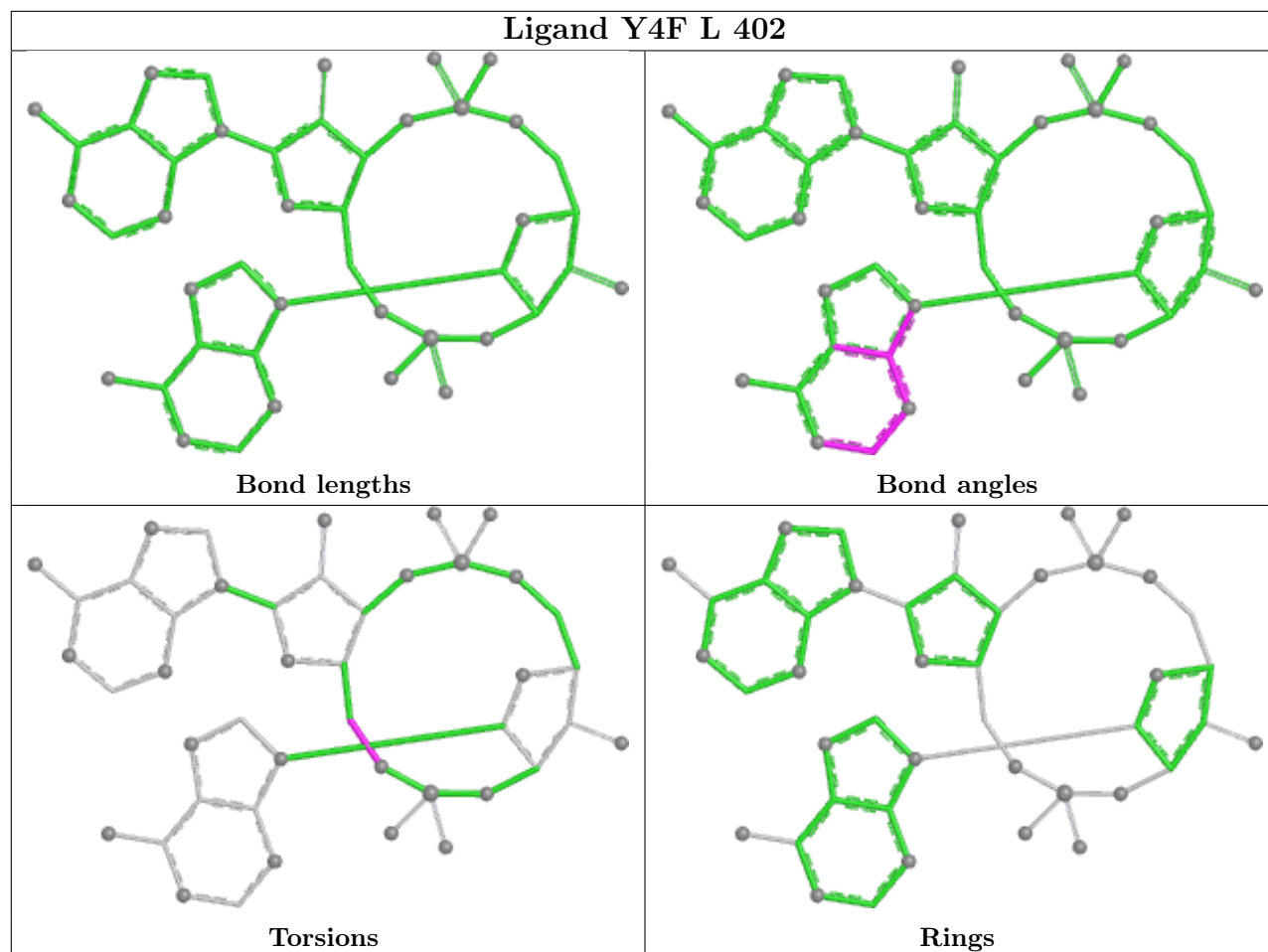
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	402	Y4F	1	0
4	N	402	Y4F	1	0

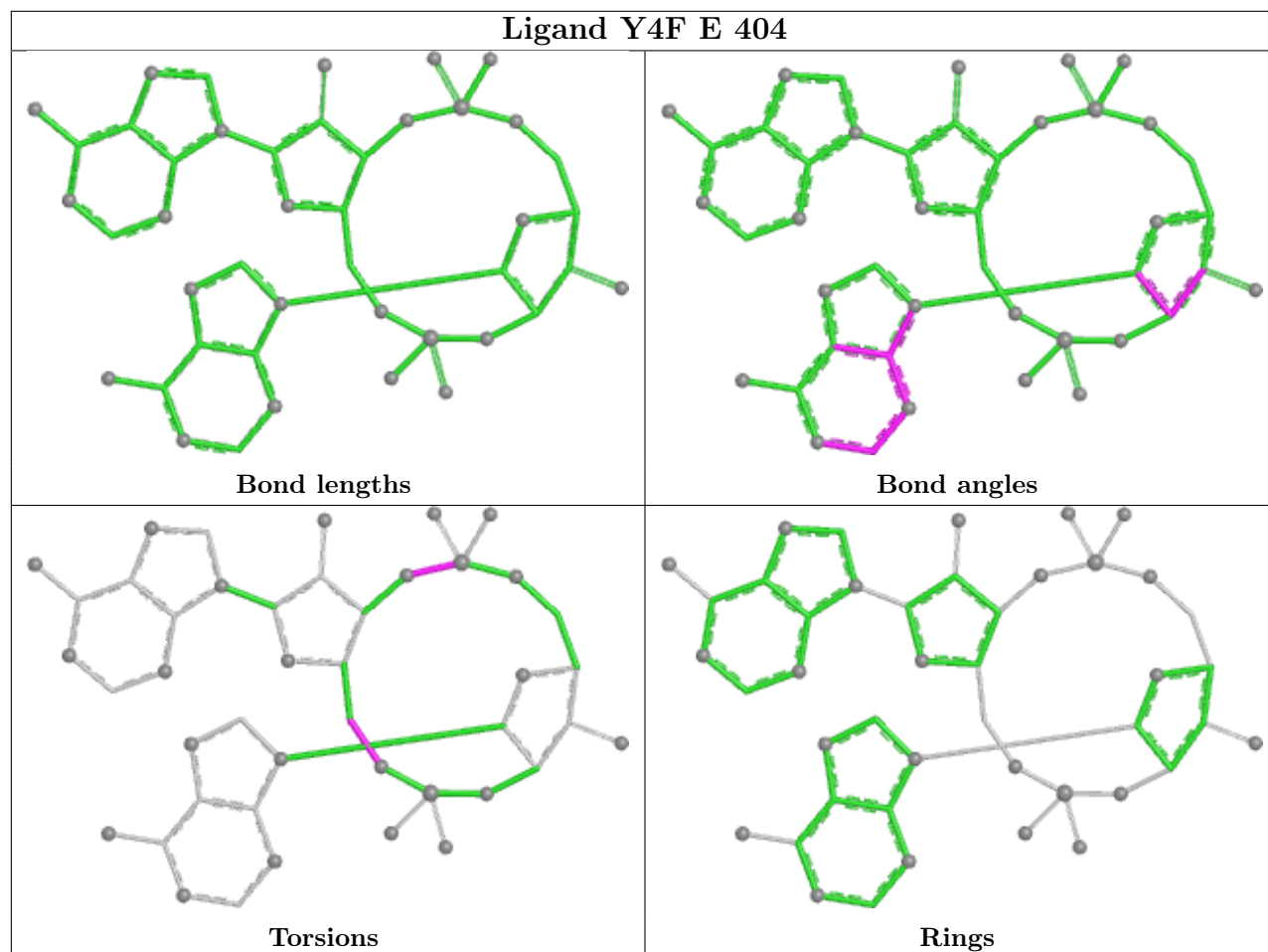
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

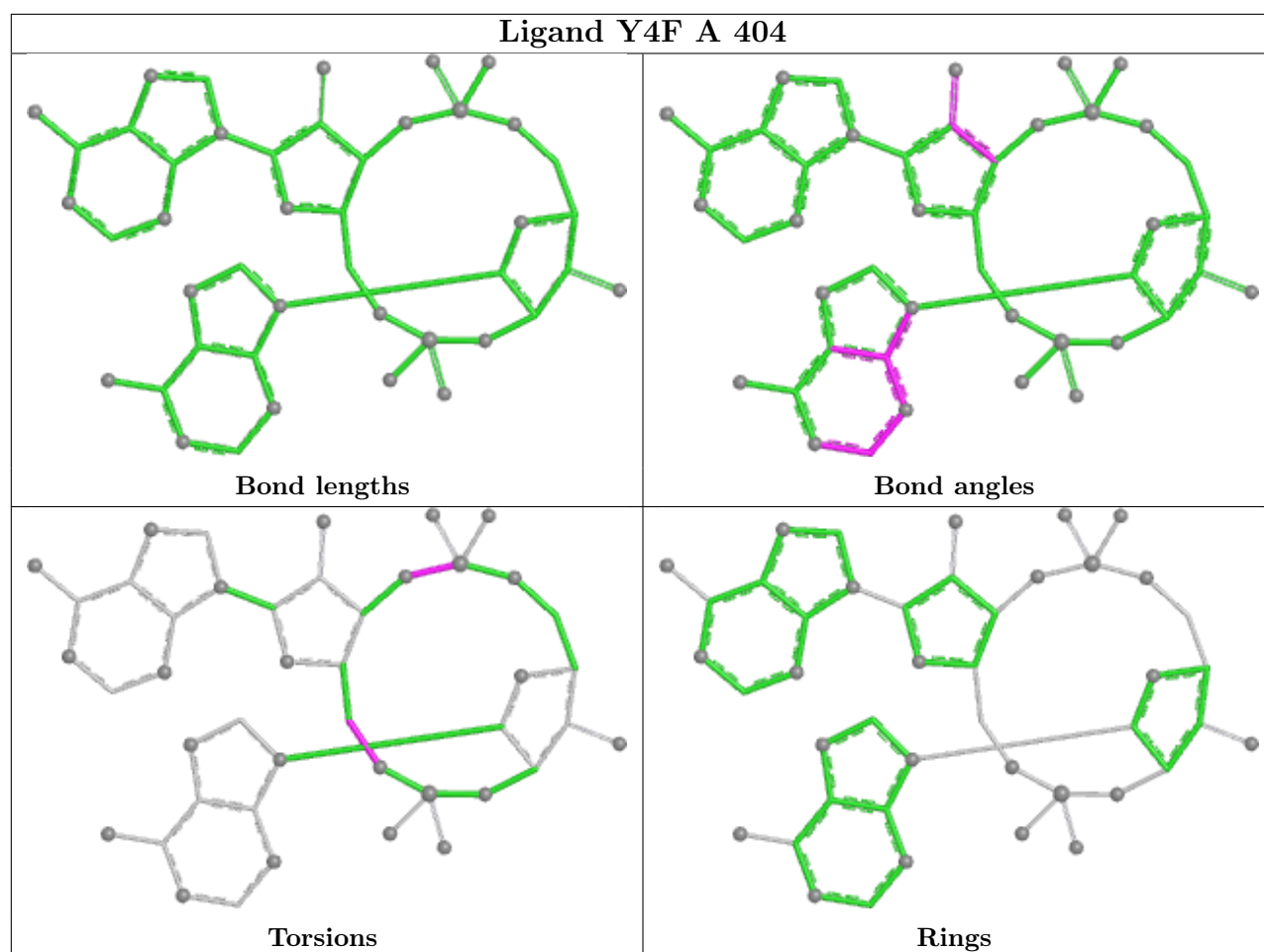
Ligand Y4F G 404



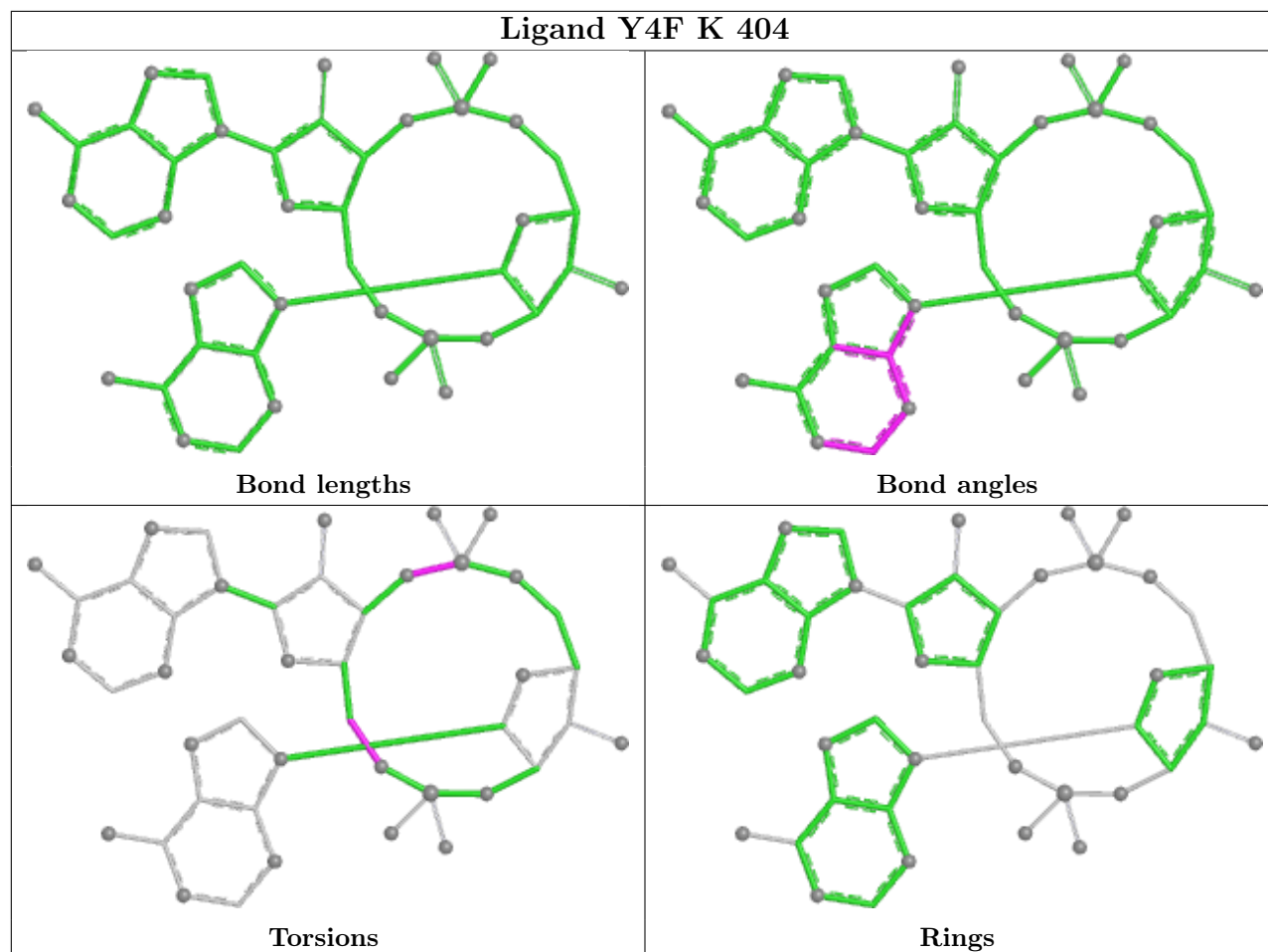
Ligand Y4F L 402



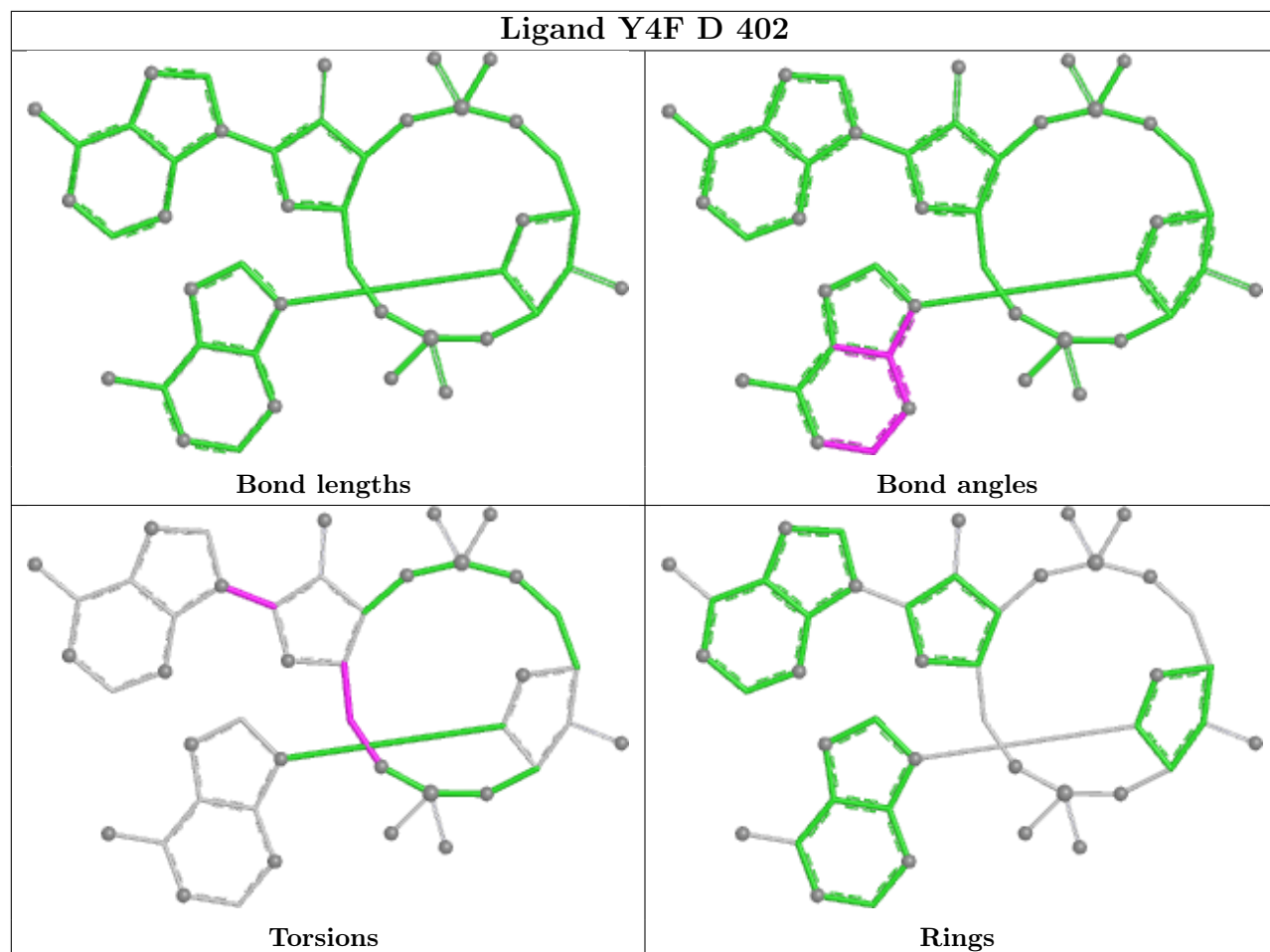




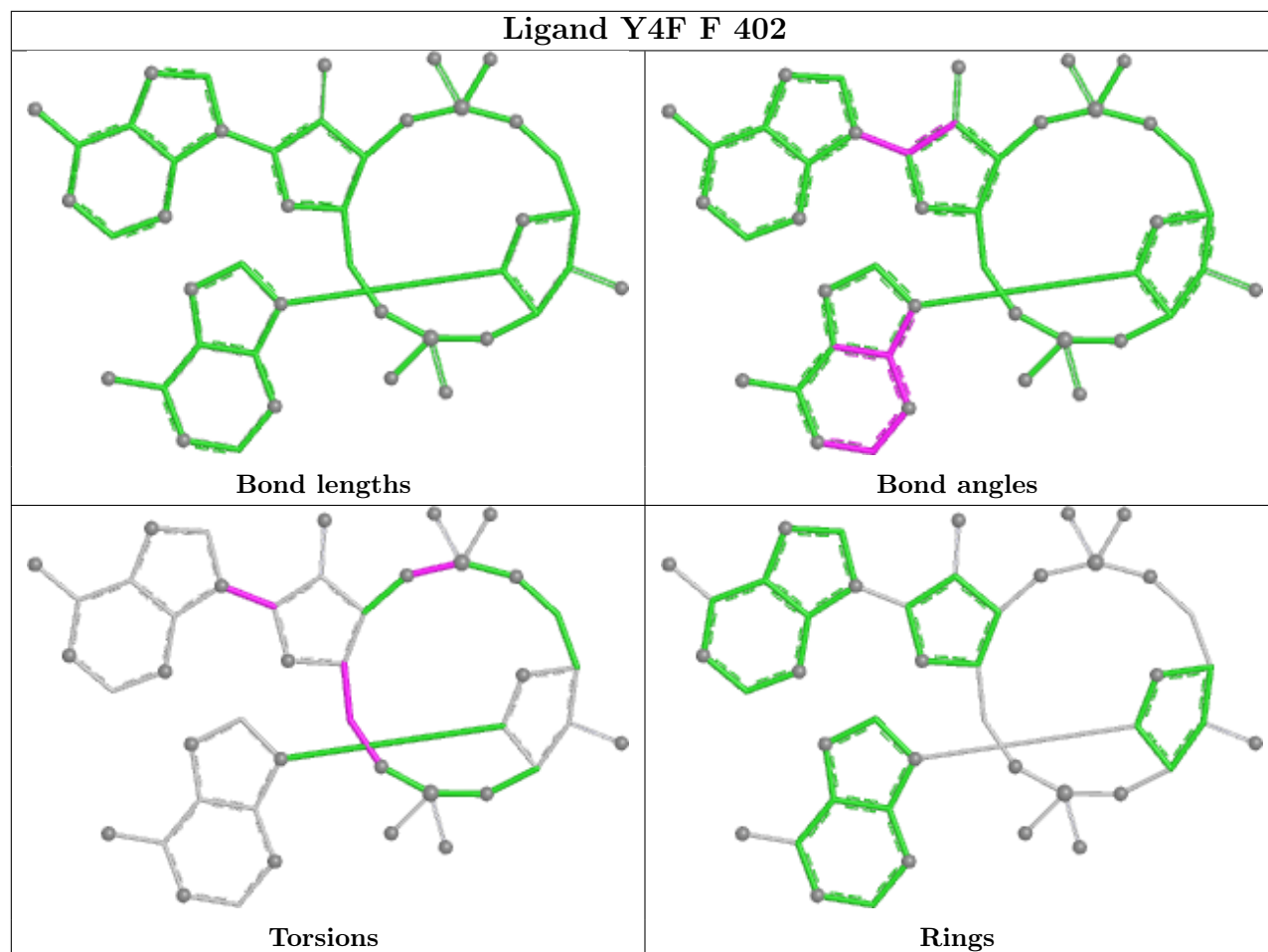
Ligand Y4F K 404

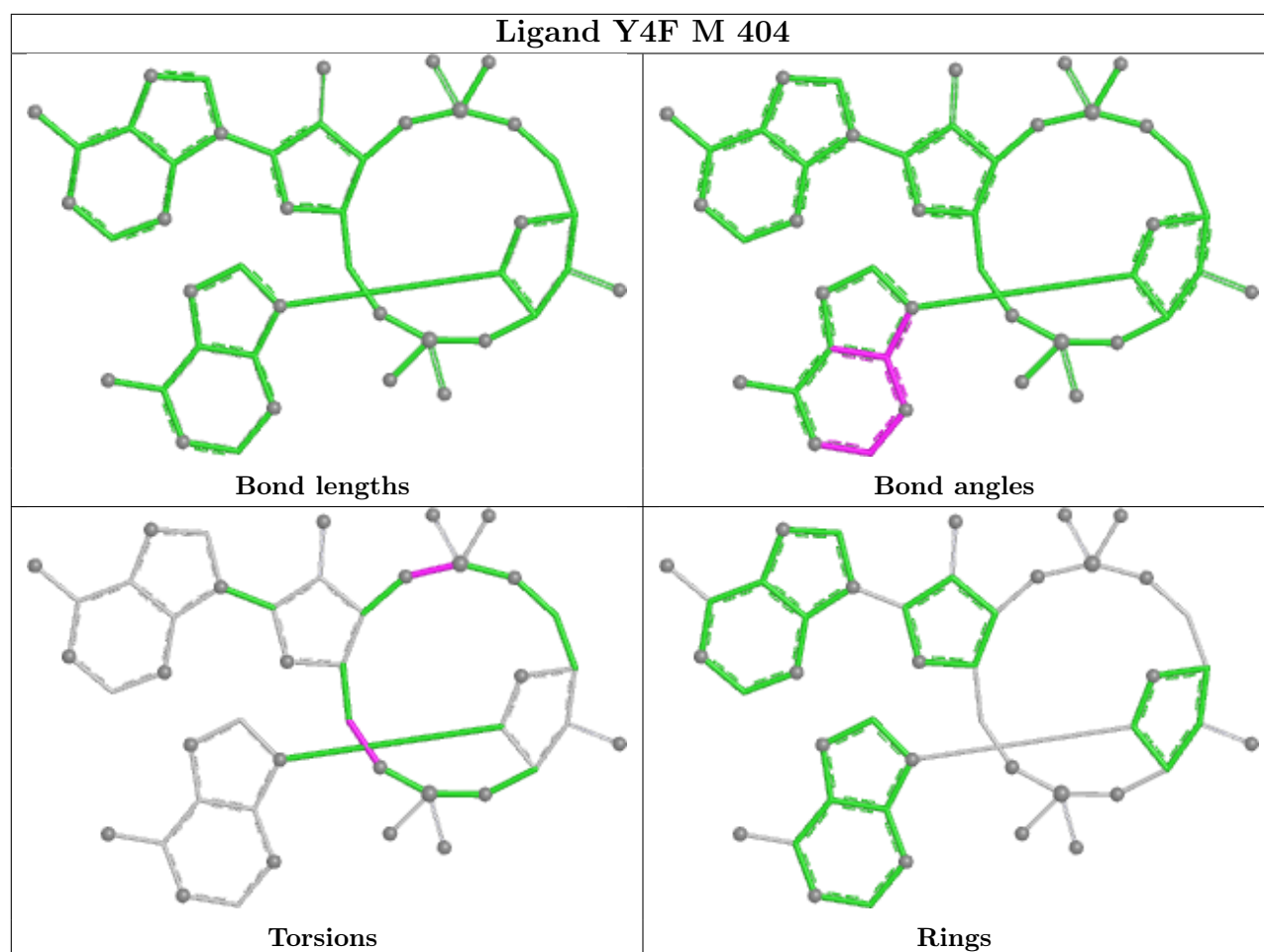


Ligand Y4F D 402

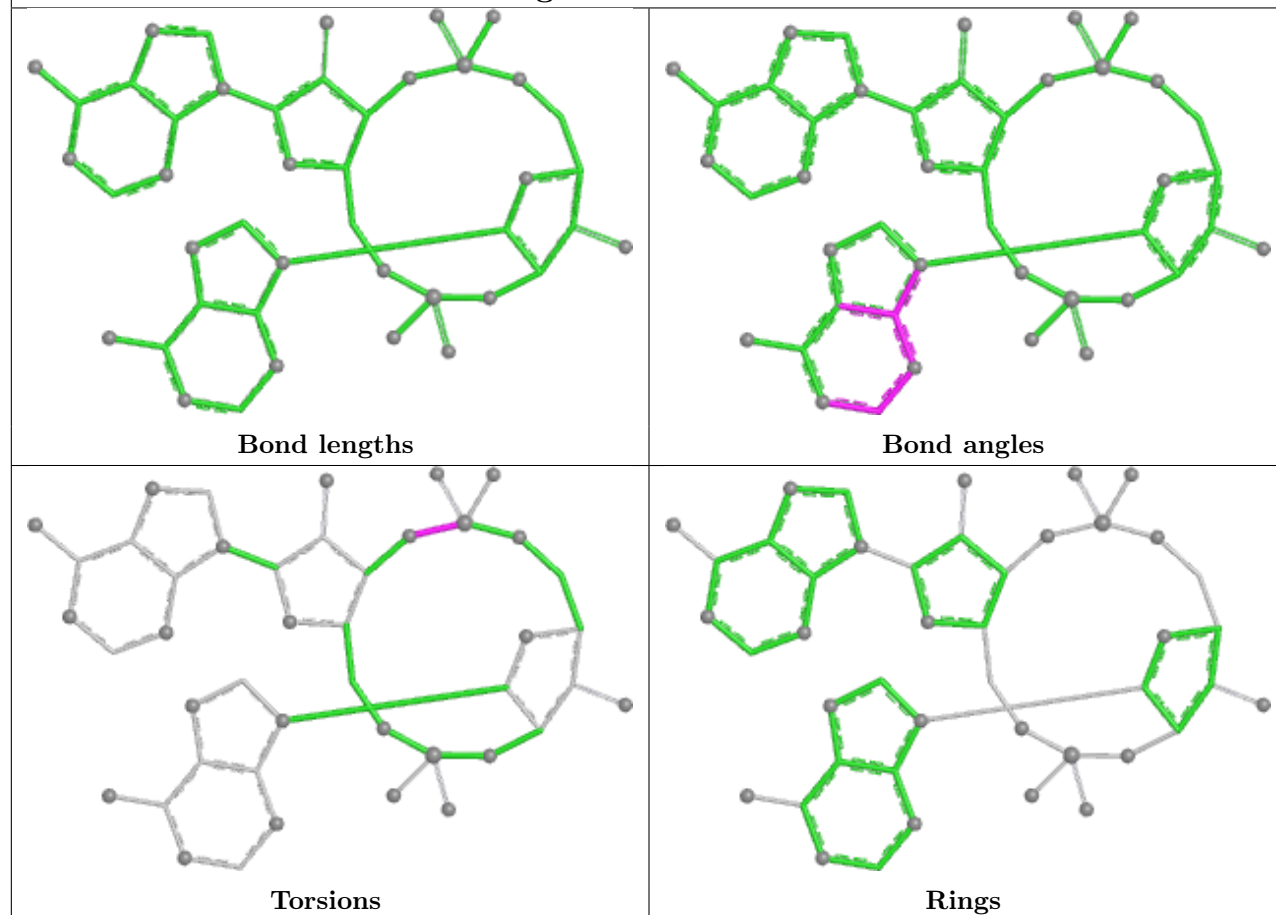


Ligand Y4F F 402

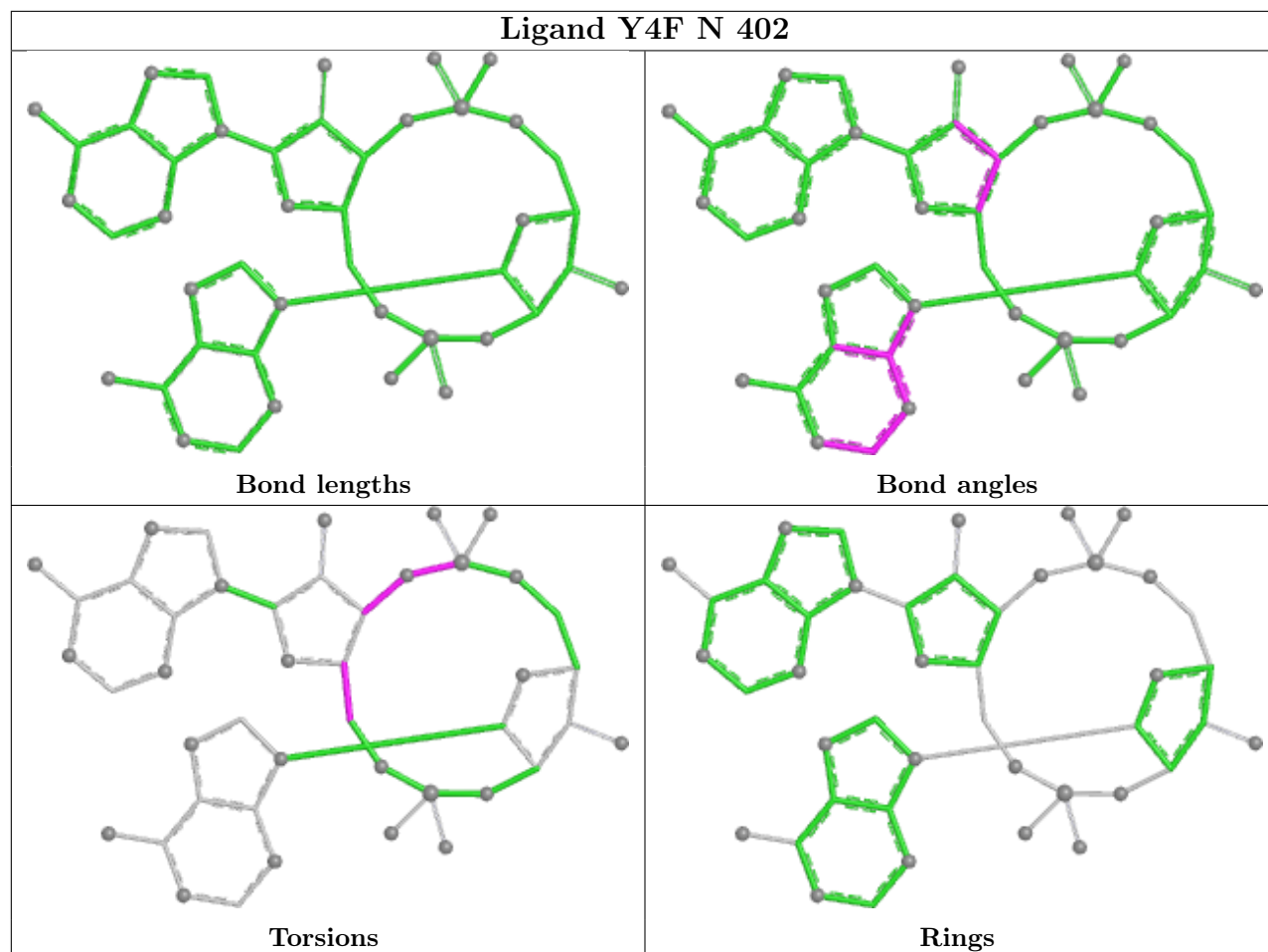




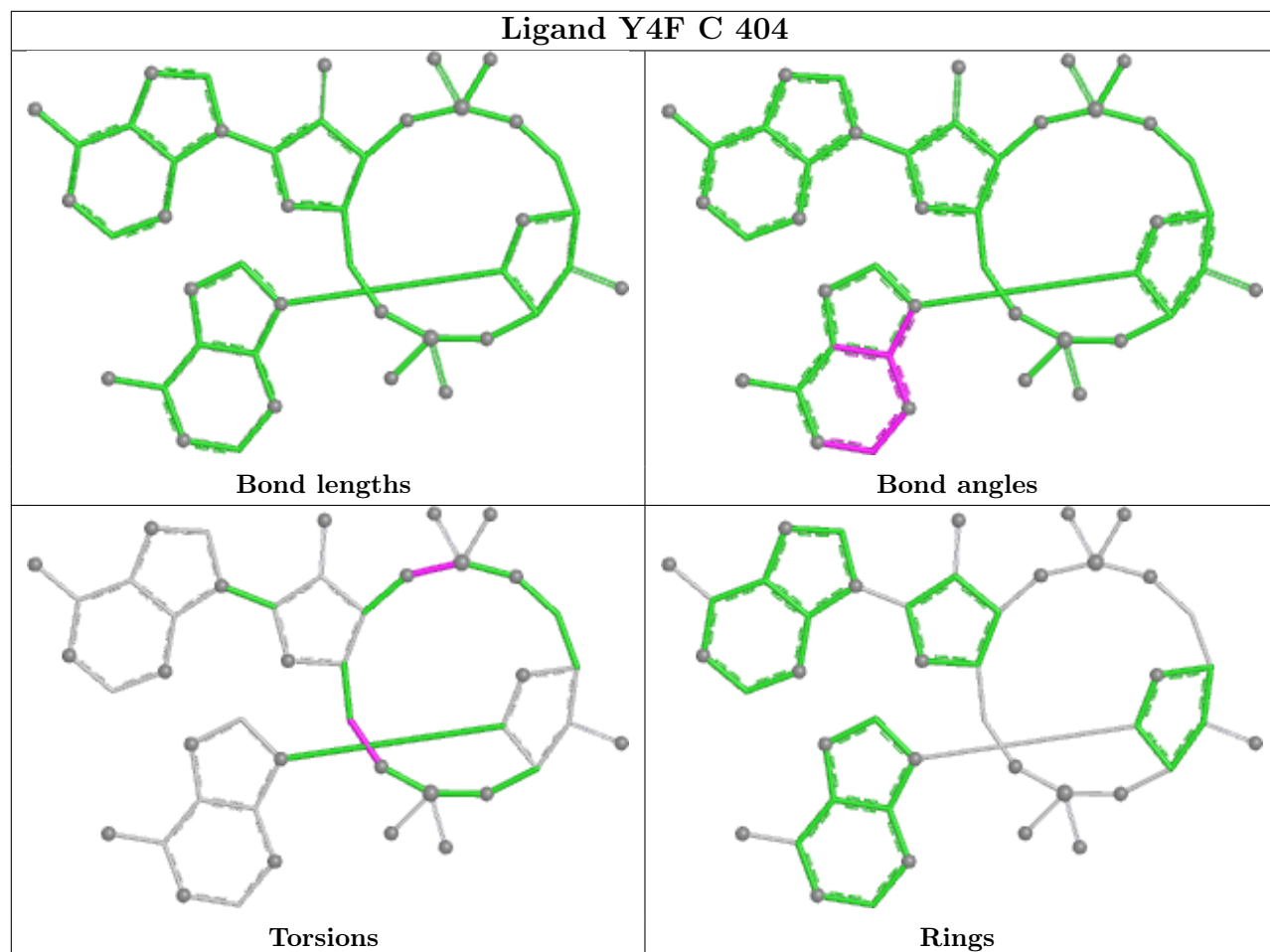
Ligand Y4F B 402

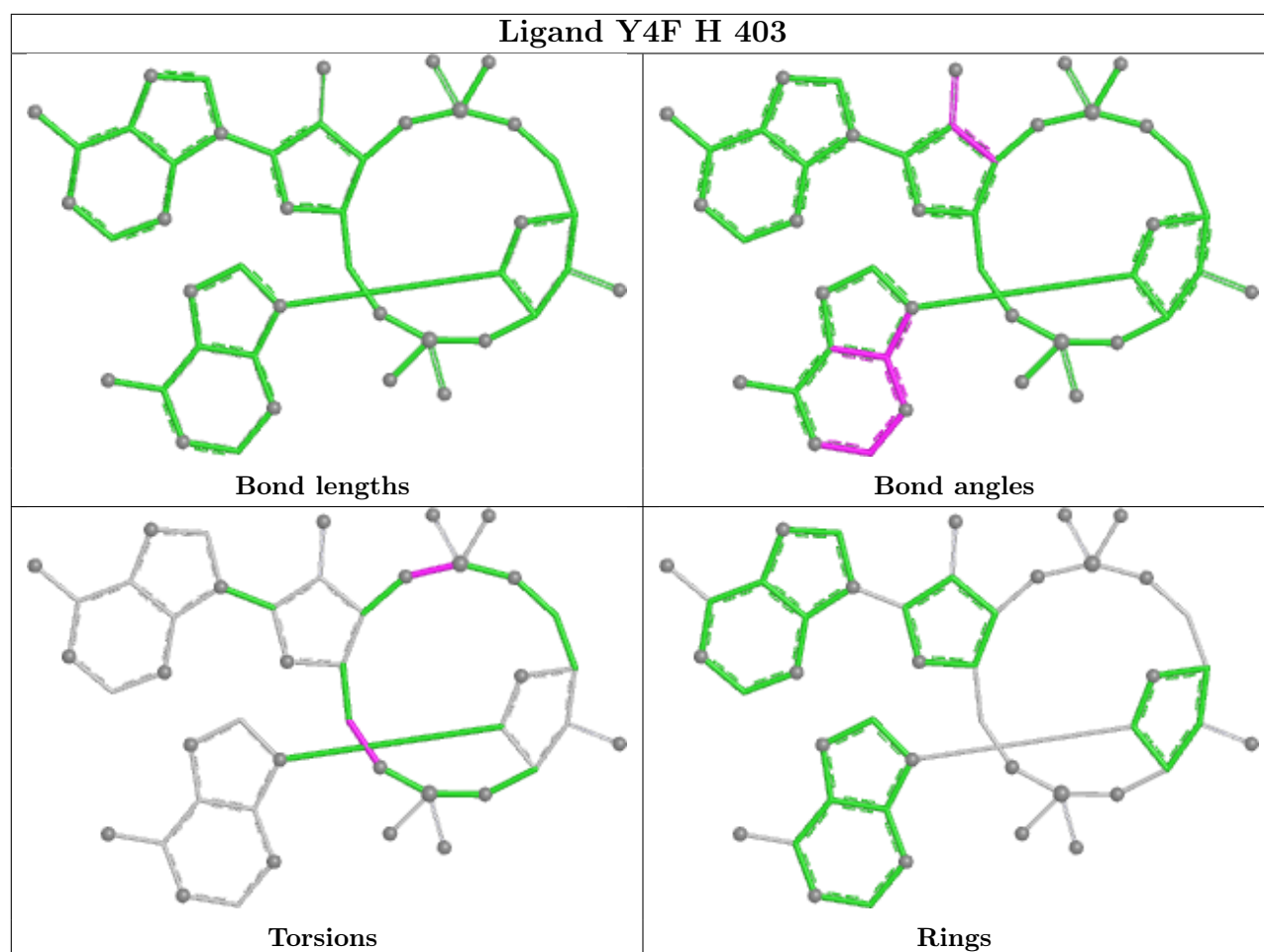


Ligand Y4F N 402



Ligand Y4F C 404





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	369/388 (95%)	0.11	15 (4%)	41	41	12, 30, 65, 132	4 (1%)
1	B	354/388 (91%)	0.28	23 (6%)	25	23	18, 31, 78, 106	0
1	C	368/388 (94%)	0.34	26 (7%)	22	20	20, 33, 72, 103	0
1	D	353/388 (90%)	0.51	22 (6%)	26	25	24, 39, 73, 107	0
1	E	369/388 (95%)	0.25	23 (6%)	26	25	22, 32, 64, 118	0
1	F	353/388 (90%)	0.35	20 (5%)	29	28	18, 35, 70, 97	1 (0%)
1	G	368/388 (94%)	0.12	11 (2%)	52	52	20, 31, 60, 105	0
1	H	356/388 (91%)	0.25	22 (6%)	26	25	20, 31, 68, 106	0
1	K	369/388 (95%)	0.25	25 (6%)	23	22	13, 31, 68, 98	1 (0%)
1	L	357/388 (92%)	0.05	8 (2%)	62	62	12, 30, 57, 88	1 (0%)
1	M	369/388 (95%)	0.35	26 (7%)	22	21	23, 34, 69, 106	0
1	N	354/388 (91%)	0.47	27 (7%)	20	18	15, 36, 77, 104	2 (0%)
All	All	4339/4656 (93%)	0.28	248 (5%)	29	28	12, 33, 70, 132	9 (0%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	14	PHE	5.7
1	B	94	ILE	5.2
1	D	14	PHE	5.2
1	E	355	THR	4.9
1	M	267	ASP	4.8
1	N	382	PRO	4.8
1	H	382	PRO	4.6
1	K	355	THR	4.5
1	A	14	PHE	4.5
1	E	207	ASP	4.4
1	A	205	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	170	PHE	4.4
1	F	194	LEU	4.3
1	B	99	ASP	4.3
1	L	198	LEU	4.2
1	A	332	PRO	4.2
1	M	233	SER	4.1
1	N	99	ASP	4.1
1	H	142	ILE	4.1
1	F	14	PHE	4.0
1	K	233	SER	4.0
1	L	64	GLY	4.0
1	N	100	GLY	4.0
1	B	18	ASP	3.9
1	A	206	GLY	3.9
1	K	207	ASP	3.9
1	K	322	ILE	3.9
1	K	231	ASP	3.9
1	N	101	TYR	3.9
1	H	368	LYS	3.8
1	G	382	PRO	3.8
1	D	15	ASN	3.8
1	F	58	LEU	3.7
1	C	355	THR	3.7
1	C	282	VAL	3.7
1	D	99	ASP	3.7
1	E	233	SER	3.7
1	C	62	PRO	3.5
1	E	382	PRO	3.5
1	A	207	ASP	3.5
1	H	194	LEU	3.5
1	N	106	LEU	3.5
1	C	60	ALA	3.5
1	N	194	LEU	3.5
1	K	382	PRO	3.5
1	K	357	HIS	3.4
1	B	101	TYR	3.4
1	C	69	ALA	3.4
1	N	14	PHE	3.4
1	H	242	ARG	3.4
1	K	208	SER	3.4
1	N	94	ILE	3.3
1	D	370	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	98	ALA	3.3
1	B	382	PRO	3.3
1	E	208	SER	3.3
1	C	63	LYS	3.3
1	D	194	LEU	3.3
1	H	139	PHE	3.3
1	C	72	ASP	3.2
1	K	15	ASN	3.2
1	N	95	ASP	3.2
1	N	62	PRO	3.2
1	G	234	LYS	3.2
1	C	203	GLY	3.2
1	N	41	PHE	3.2
1	E	205	TYR	3.1
1	F	109	LEU	3.1
1	H	11	SER	3.1
1	K	381	GLY	3.1
1	M	203	GLY	3.1
1	N	98	ALA	3.1
1	B	62	PRO	3.1
1	K	209	PRO	3.1
1	M	207	ASP	3.1
1	D	170	PHE	3.1
1	F	16	THR	3.1
1	E	232	ARG	3.1
1	M	202	GLY	3.0
1	F	304	TYR	3.0
1	M	234	LYS	3.0
1	K	14	PHE	3.0
1	C	329	ALA	3.0
1	C	322	ILE	3.0
1	L	63	LYS	3.0
1	D	62	PRO	3.0
1	D	100	GLY	3.0
1	N	79	ASP	2.9
1	C	77	THR	2.9
1	F	45	ALA	2.9
1	B	109	LEU	2.9
1	D	175	PRO	2.9
1	L	382	PRO	2.9
1	C	76	HIS	2.9
1	F	41	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	16	THR	2.9
1	B	111	GLN	2.9
1	N	142	ILE	2.9
1	C	75	ALA	2.8
1	F	94	ILE	2.8
1	E	354	THR	2.8
1	F	196	GLN	2.8
1	K	356	GLN	2.8
1	H	12	GLY	2.8
1	N	81	ALA	2.8
1	B	25	TRP	2.8
1	A	203	GLY	2.8
1	B	198	LEU	2.8
1	M	77	THR	2.8
1	M	357	HIS	2.8
1	N	109	LEU	2.7
1	D	192	TYR	2.7
1	H	192	TYR	2.7
1	G	232	ARG	2.7
1	C	207	ASP	2.7
1	D	41	PHE	2.7
1	M	349	PHE	2.7
1	B	103	GLU	2.7
1	A	204	THR	2.7
1	H	282	VAL	2.7
1	M	322	ILE	2.7
1	M	60	ALA	2.7
1	H	13	ARG	2.6
1	D	16	THR	2.6
1	M	355	THR	2.6
1	E	356	GLN	2.6
1	E	209	PRO	2.6
1	A	208	SER	2.6
1	G	231	ASP	2.6
1	C	71	HIS	2.6
1	C	61	SER	2.6
1	A	162	PHE	2.6
1	F	170	PHE	2.6
1	N	170	PHE	2.6
1	D	104	ASN	2.6
1	C	382	PRO	2.6
1	E	202	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	230	GLY	2.5
1	C	332	PRO	2.5
1	M	382	PRO	2.5
1	K	206	GLY	2.5
1	C	74	GLU	2.5
1	F	17	ASN	2.5
1	H	15	ASN	2.5
1	D	371	GLN	2.5
1	L	12	GLY	2.5
1	D	142	ILE	2.5
1	M	76	HIS	2.5
1	N	103	GLU	2.5
1	N	18	ASP	2.4
1	B	106	LEU	2.4
1	D	94	ILE	2.4
1	D	17	ASN	2.4
1	A	68	ARG	2.4
1	E	357	HIS	2.4
1	E	206	GLY	2.4
1	H	174	GLY	2.4
1	K	203	GLY	2.4
1	C	358	GLN	2.4
1	N	192	TYR	2.4
1	F	147	VAL	2.4
1	B	95	ASP	2.4
1	F	79	ASP	2.4
1	E	234	LYS	2.4
1	B	91	HIS	2.4
1	B	30	GLY	2.4
1	C	208	SER	2.4
1	G	352	LEU	2.4
1	K	74	GLU	2.4
1	H	143	ASN	2.3
1	B	13	ARG	2.3
1	E	211	LEU	2.3
1	E	329	ALA	2.3
1	K	68	ARG	2.3
1	M	232	ARG	2.3
1	M	320	LEU	2.3
1	G	357	HIS	2.3
1	N	17	ASN	2.3
1	H	99	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	48	PRO	2.3
1	B	80	THR	2.3
1	H	141	THR	2.3
1	A	60	ALA	2.3
1	N	58	LEU	2.3
1	F	168	ILE	2.3
1	M	294	ILE	2.3
1	B	60	ALA	2.3
1	A	209	PRO	2.2
1	F	382	PRO	2.2
1	M	71	HIS	2.2
1	B	98	ALA	2.2
1	F	15	ASN	2.2
1	G	15	ASN	2.2
1	N	34	LEU	2.2
1	A	69	ALA	2.2
1	F	98	ALA	2.2
1	M	69	ALA	2.2
1	D	246	LEU	2.2
1	H	58	LEU	2.2
1	G	203	GLY	2.2
1	M	358	GLN	2.2
1	E	14	PHE	2.2
1	H	14	PHE	2.2
1	E	68	ARG	2.2
1	H	101	TYR	2.2
1	B	104	ASN	2.2
1	K	202	GLY	2.2
1	A	201	ARG	2.2
1	K	232	ARG	2.2
1	K	229	ILE	2.2
1	C	331	THR	2.2
1	G	207	ASP	2.1
1	K	267	ASP	2.1
1	F	242	ARG	2.1
1	M	231	ASP	2.1
1	E	322	ILE	2.1
1	D	190	VAL	2.1
1	B	79	ASP	2.1
1	C	356	GLN	2.1
1	E	358	GLN	2.1
1	L	196	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	331	THR	2.1
1	K	205	TYR	2.1
1	C	381	GLY	2.1
1	L	174	GLY	2.1
1	M	75	ALA	2.1
1	E	330	LEU	2.1
1	G	330	LEU	2.1
1	N	13	ARG	2.1
1	E	203	GLY	2.0
1	N	46	GLY	2.0
1	C	73	ALA	2.0
1	D	45	ALA	2.0
1	M	78	ASN	2.0
1	A	18	ASP	2.0
1	G	267	ASP	2.0
1	B	96	ARG	2.0
1	C	257	SER	2.0
1	K	201	ARG	2.0
1	D	382	PRO	2.0
1	H	175	PRO	2.0
1	K	358	GLN	2.0
1	M	266	GLY	2.0
1	M	23	ILE	2.0
1	D	92	ASP	2.0
1	F	18	ASP	2.0
1	N	45	ALA	2.0
1	N	21	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

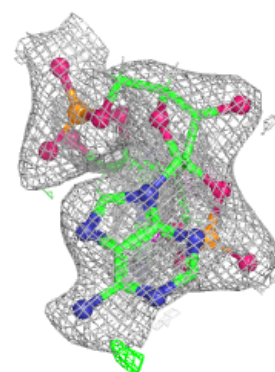
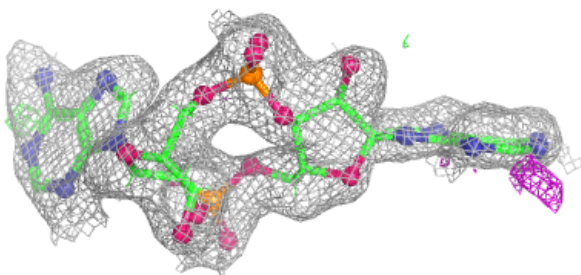
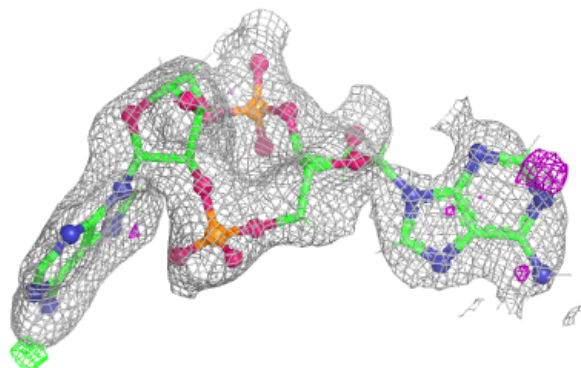
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	Y4F	L	402	44/44	0.87	0.11	35,56,70,77	0
4	Y4F	F	402	44/44	0.90	0.10	35,49,73,79	0
3	MG	E	403	1/1	0.90	0.08	66,66,66,66	0
3	MG	M	403	1/1	0.92	0.10	45,45,45,45	0
4	Y4F	D	402	44/44	0.92	0.09	31,45,62,69	0
3	MG	E	402	1/1	0.94	0.06	23,23,23,23	0
3	MG	G	402	1/1	0.94	0.04	27,27,27,27	0
3	MG	K	403	1/1	0.95	0.08	43,43,43,43	0
3	MG	C	402	1/1	0.95	0.05	38,38,38,38	0
3	MG	A	402	1/1	0.95	0.04	28,28,28,28	0
3	MG	G	403	1/1	0.95	0.09	43,43,43,43	0
4	Y4F	H	403	44/44	0.95	0.07	28,36,45,49	0
3	MG	K	402	1/1	0.95	0.06	28,28,28,28	0
4	Y4F	N	402	44/44	0.95	0.09	24,35,52,63	0
4	Y4F	B	402	44/44	0.96	0.07	20,30,49,53	0
3	MG	M	402	1/1	0.96	0.05	30,30,30,30	0
3	MG	A	403	1/1	0.96	0.12	44,44,44,44	0
3	MG	C	403	1/1	0.97	0.06	44,44,44,44	0
3	MG	H	402	1/1	0.97	0.06	33,33,33,33	0
4	Y4F	E	404	44/44	0.98	0.05	14,21,30,36	0
4	Y4F	A	404	44/44	0.98	0.05	11,17,21,26	0
4	Y4F	G	404	44/44	0.98	0.05	13,20,26,27	0
2	ZN	N	401	1/1	0.98	0.04	35,35,35,35	0
4	Y4F	K	404	44/44	0.98	0.04	14,20,25,29	0
4	Y4F	C	404	44/44	0.98	0.05	15,22,31,37	0
4	Y4F	M	404	44/44	0.98	0.04	17,23,31,34	0
2	ZN	D	401	1/1	0.98	0.04	35,35,35,35	0
2	ZN	A	401	1/1	0.99	0.05	26,26,26,26	0
2	ZN	F	401	1/1	0.99	0.04	33,33,33,33	0
2	ZN	G	401	1/1	0.99	0.09	29,29,29,29	0
2	ZN	H	401	1/1	0.99	0.02	30,30,30,30	0
2	ZN	L	401	1/1	0.99	0.02	32,32,32,32	0
2	ZN	M	401	1/1	0.99	0.02	23,23,23,23	0
2	ZN	B	401	1/1	0.99	0.03	42,42,42,42	0
2	ZN	C	401	1/1	0.99	0.04	26,26,26,26	0
2	ZN	E	401	1/1	1.00	0.03	24,24,24,24	0
2	ZN	K	401	1/1	1.00	0.01	20,20,20,20	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.

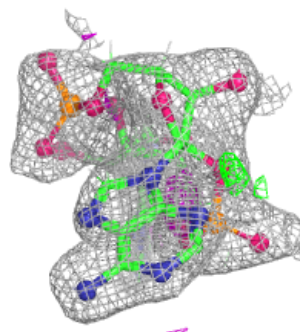
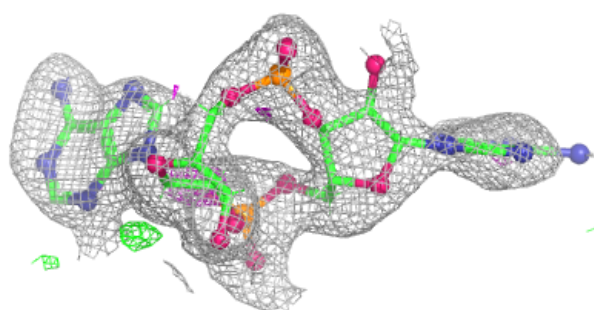
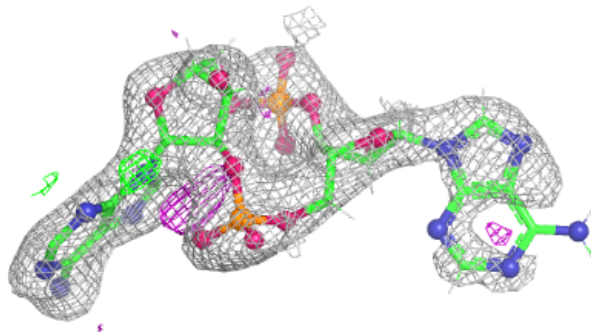
Electron density around Y4F L 402:

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

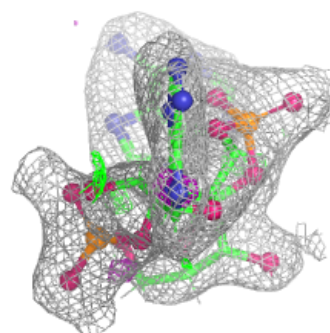
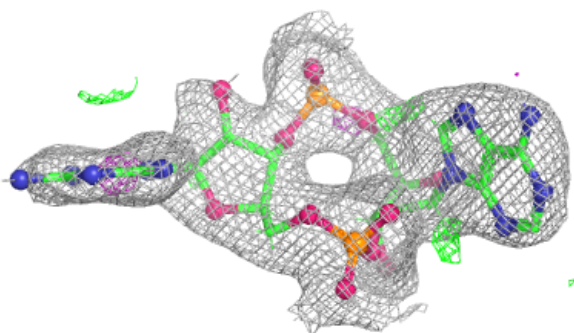
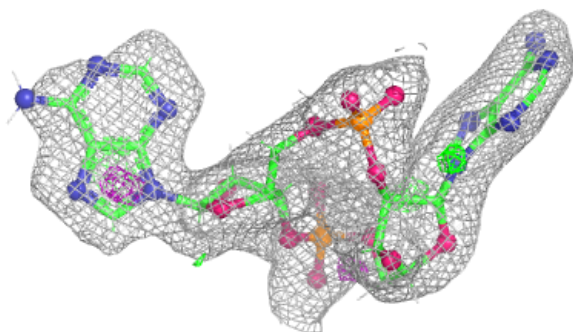


Electron density around Y4F F 402:

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

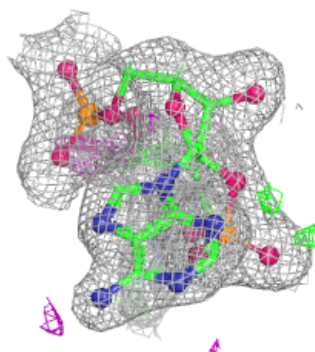
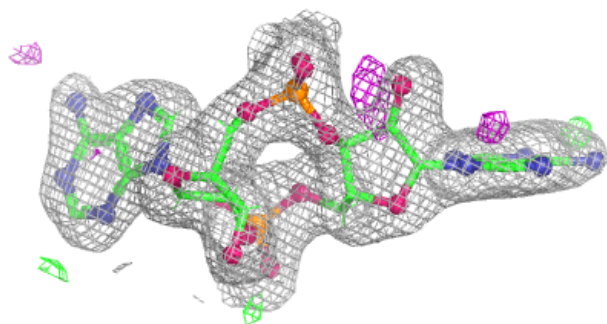
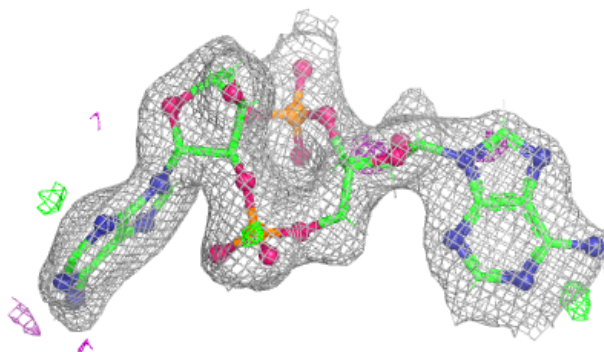
**Electron density around Y4F D 402:**

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

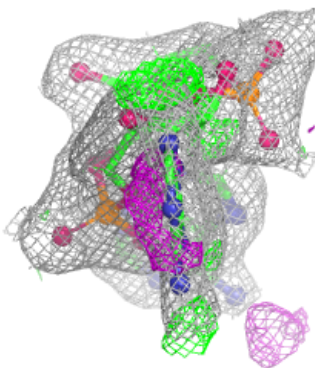
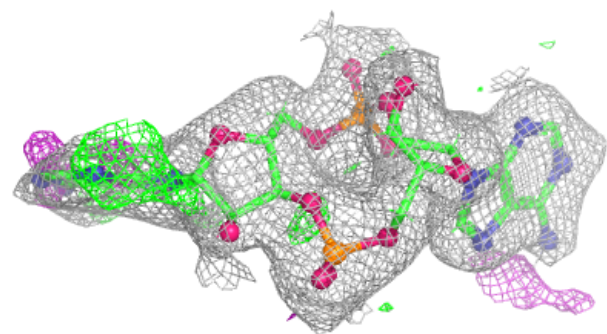
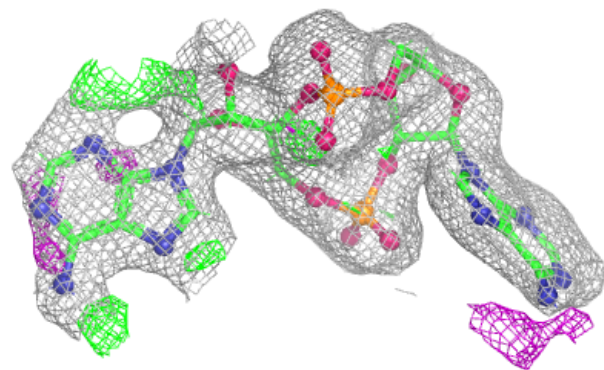


Electron density around Y4F H 403:

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

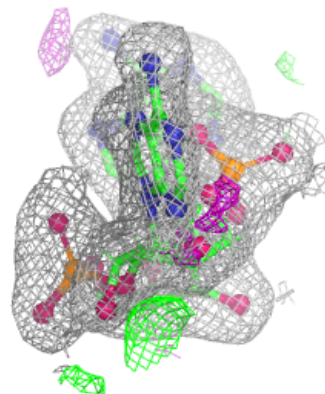
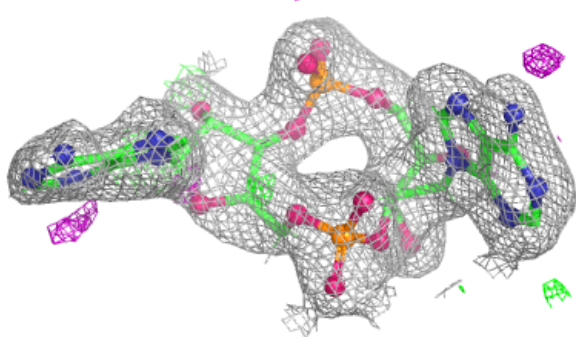
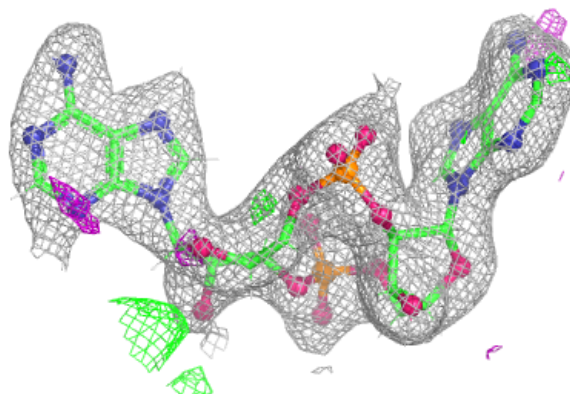
**Electron density around Y4F N 402:**

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

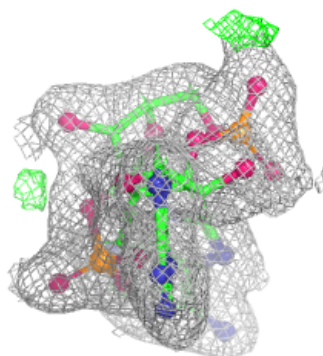
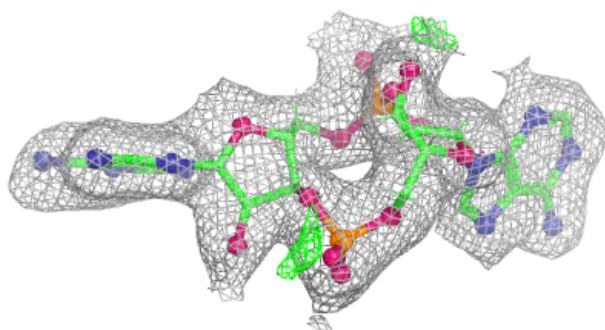
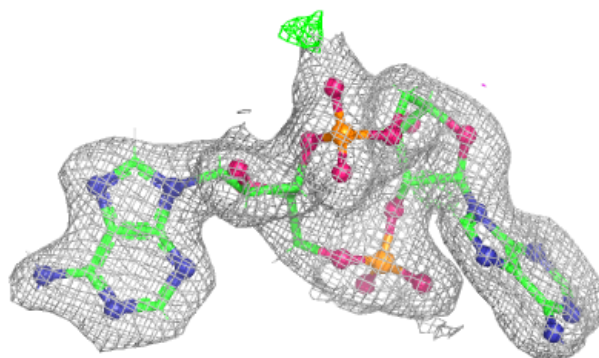


Electron density around Y4F B 402:

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

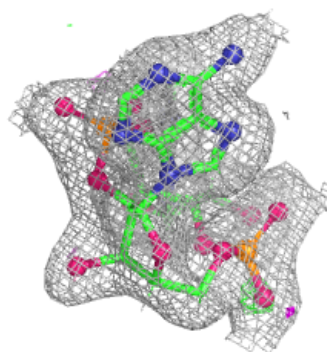
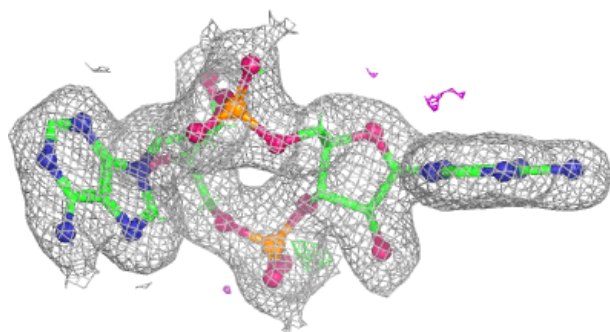
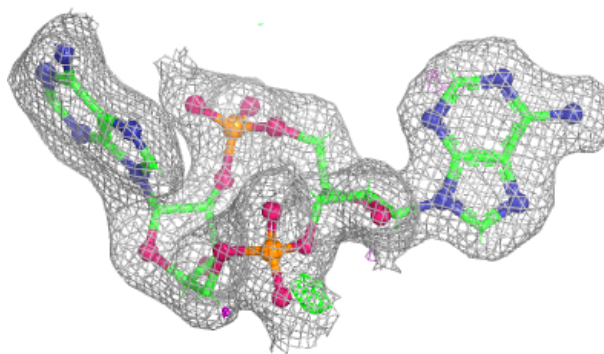
**Electron density around Y4F E 404:**

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

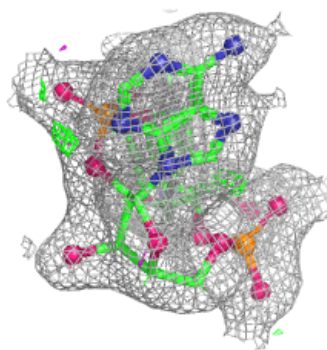
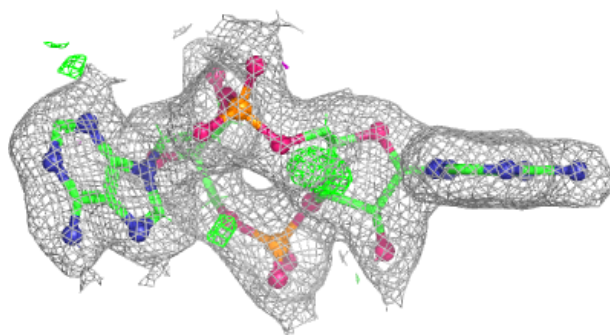
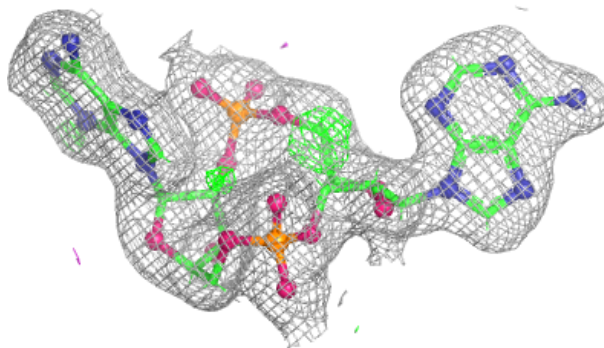


Electron density around Y4F A 404:

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

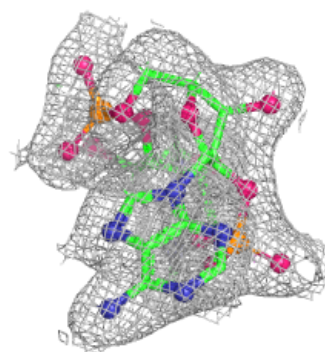
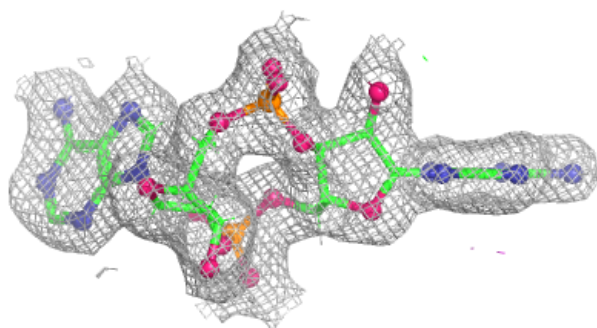
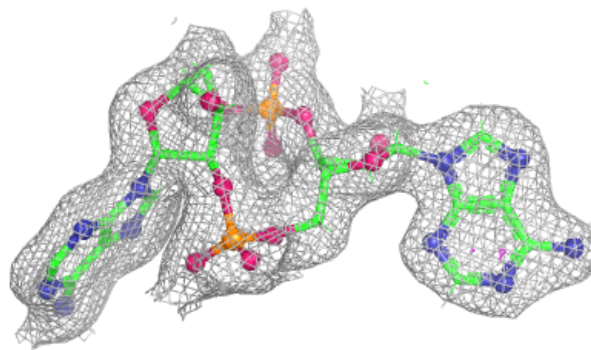
**Electron density around Y4F G 404:**

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

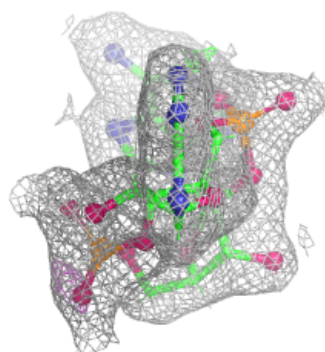
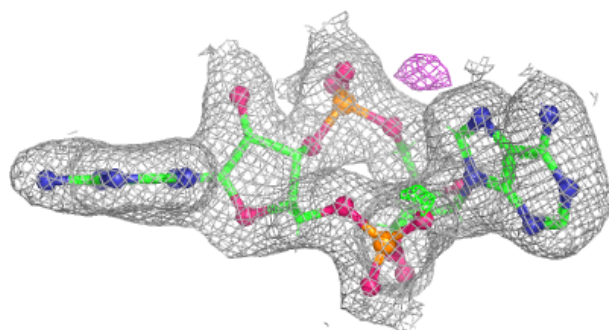
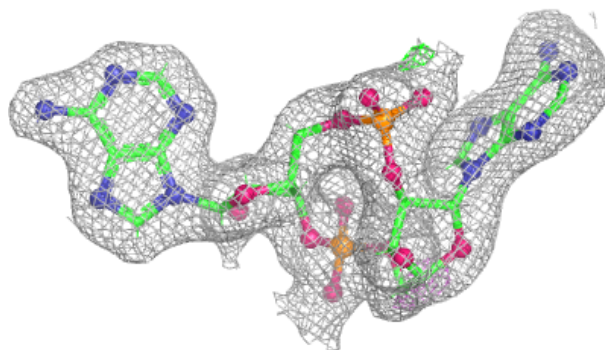


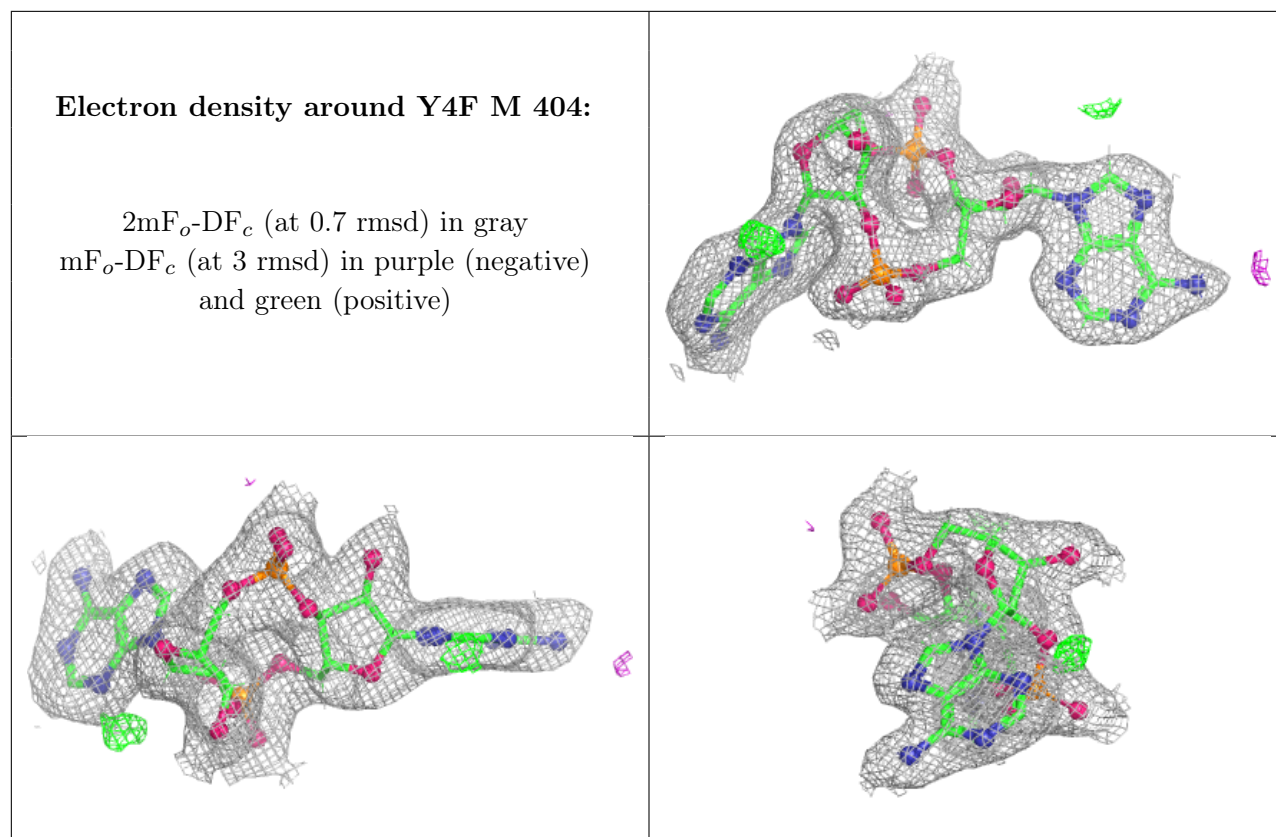
Electron density around Y4F K 404:

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

**Electron density around Y4F C 404:**

$2mF_o-DF_c$ (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.