



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 6HK1 / pdb_00006hk1
Title : Crystal structure of the Thiazole synthase from Methanothermococcus thermolithotrophicus co-crystallized with Tb-Xo4
Authors : Engilberge, S.; Wagner, T.; Santoni, G.; Breyton, C.; Shima, S.; Franzetti, B.; Riobe, F.; Maury, O.; Girard, E.
Deposited on : 2018-09-05
Resolution : 2.55 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

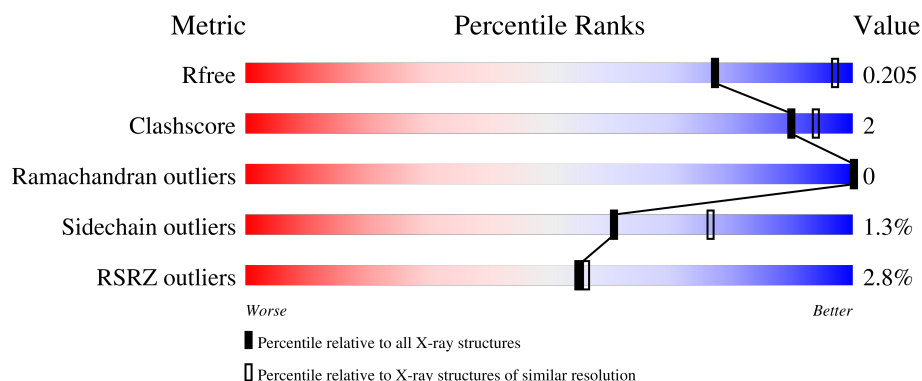
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



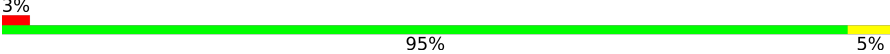
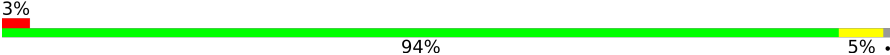
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	261	2% 93% 7%
1	B	261	3% 91% 8% .
1	C	261	2% 92% 6% ..
1	D	261	3% 95% 5%

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Mol	Chain	Length	Quality of chain
1	E	261	
1	F	261	

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
2	TB	A	303	-	-	-	X
2	TB	A	304	-	-	-	X
2	TB	A	307	-	-	-	X
2	TB	A	308	-	-	-	X
2	TB	A	310	-	-	-	X
2	TB	A	311	-	-	-	X
2	TB	B	303	-	-	-	X
2	TB	B	304	-	-	-	X
2	TB	B	305	-	-	-	X
2	TB	C	302	-	-	-	X
2	TB	C	303	-	-	-	X
2	TB	C	304	-	-	-	X
2	TB	C	306	-	-	-	X
2	TB	C	308	-	-	-	X
2	TB	D	303	-	-	-	X
2	TB	D	304	-	-	-	X
2	TB	D	305	-	-	-	X
2	TB	D	306	-	-	-	X
2	TB	D	307	-	-	-	X
2	TB	E	309	-	-	-	X
2	TB	E	310	-	-	-	X
2	TB	E	311	-	-	-	X
2	TB	F	303	-	-	-	X
2	TB	F	304	-	-	-	X
2	TB	F	305	-	-	-	X
2	TB	F	306	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12396 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.

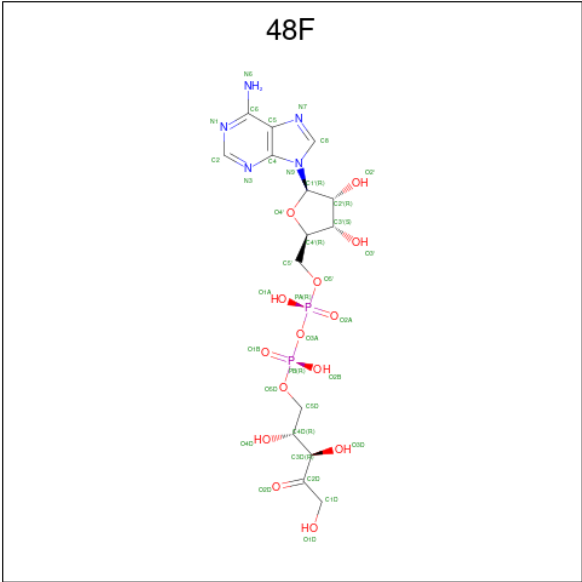
- Molecule 1 is a protein called Thiazole synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1957	1250	323	373	11			
1	B	258	Total	C	N	O	S	0	0	0
			1929	1232	320	367	10			
1	C	257	Total	C	N	O	S	0	0	0
			1920	1226	318	366	10			
1	D	261	Total	C	N	O	S	0	0	0
			1957	1250	323	373	11			
1	E	261	Total	C	N	O	S	0	0	0
			1957	1250	323	373	11			
1	F	258	Total	C	N	O	S	0	0	0
			1932	1235	319	368	10			

- Molecule 2 is TERBIUM(III) ION (CCD ID: TB) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	Tb	0	0
			12	12		
2	B	5	Total	Tb	0	0
			5	5		
2	C	8	Total	Tb	0	0
			8	8		
2	D	7	Total	Tb	0	0
			7	7		
2	E	11	Total	Tb	0	0
			11	11		
2	F	6	Total	Tb	0	0
			6	6		

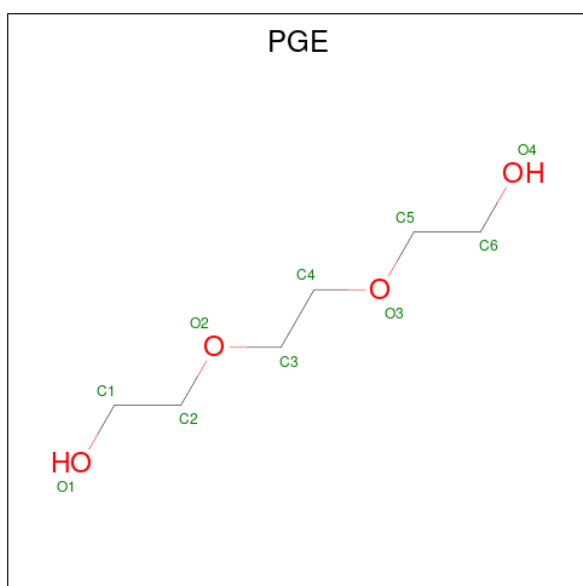
- Molecule 3 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3R)-2,3,5-tris(oxidanyl)-4-oxidanylidene-pentyl] hydrogen phosphate (CCD ID: 48F) (formula: C₁₅H₂₃N₅O₁₄P₂).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



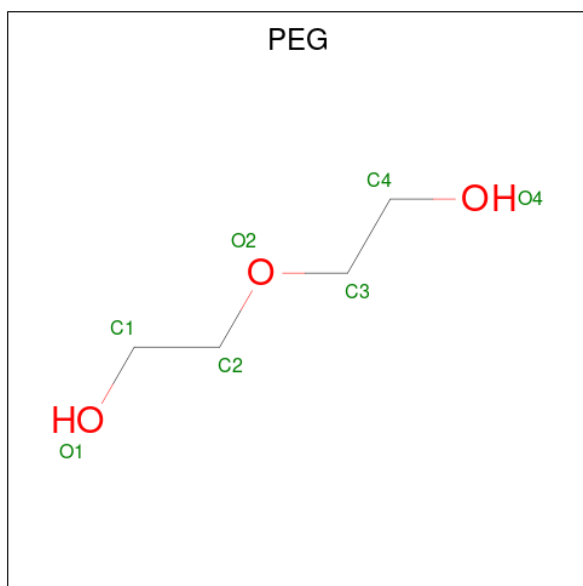
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	94	Total	O	0	0
			94	94		
8	B	59	Total	O	0	0
			59	59		
8	C	72	Total	O	0	0
			72	72		
8	D	64	Total	O	0	0
			64	64		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	88	Total 88	O 88	0	0
8	F	52	Total 52	O 52	0	0

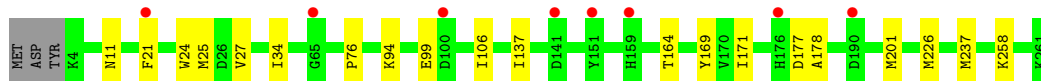
3 Residue-property plots [i](#)

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.

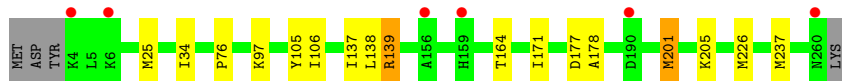
- Molecule 1: Thiazole synthase



- Molecule 1: Thiazole synthase



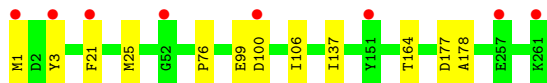
- Molecule 1: Thiazole synthase



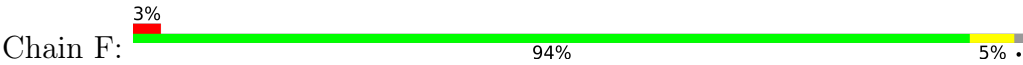
- Molecule 1: Thiazole synthase



- Molecule 1: Thiazole synthase



- Molecule 1: Thiazole synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	216.86Å 216.86Å 207.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.55 49.09 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.09-2.55) 99.0 (49.09-2.55)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.213 0.188 , 0.205	Depositor DCC
R_{free} test set	3959 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12396	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.76% 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: 48F, PEG, PGE, NA, TB, GOL

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	0.55	0/1989	0.94	2/2685 (0.1%)
1	B	0.54	0/1960	0.94	3/2646 (0.1%)
1	C	0.52	0/1951	0.93	2/2635 (0.1%)
1	D	0.52	0/1989	0.91	1/2685 (0.0%)
1	E	0.53	0/1989	0.92	1/2685 (0.0%)
1	F	0.51	0/1964	0.93	3/2653 (0.1%)
All	All	0.53	0/11842	0.93	12/15989 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	99	GLU	N-CA-C	6.75	119.21	111.11
1	A	99	GLU	N-CA-C	6.41	117.92	111.07
1	B	99	GLU	N-CA-C	6.16	118.54	111.02
1	C	76	PRO	N-CA-C	5.71	120.19	112.48
1	B	21	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	76	PRO	N-CA-C	5.59	120.03	112.48
1	F	76	PRO	N-CA-C	5.56	119.99	112.48
1	B	76	PRO	N-CA-C	5.54	119.96	112.48
1	D	76	PRO	N-CA-C	5.49	119.90	112.48
1	E	76	PRO	N-CA-C	5.42	119.80	112.48
1	F	21	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	205	LYS	CG-CD-CE	5.00	122.81	111.30

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	1957	0	1992	10	0
1	B	1929	0	1967	9	0
1	C	1920	0	1954	8	0
1	D	1957	0	1992	6	0
1	E	1957	0	1992	7	0
1	F	1932	0	1963	5	0
2	A	12	0	0	0	0
2	B	5	0	0	0	0
2	C	8	0	0	0	0
2	D	7	0	0	0	0
2	E	11	0	0	0	0
2	F	6	0	0	0	0
3	A	36	0	0	0	0
3	B	36	0	0	1	0
3	C	36	0	0	0	0
3	D	36	0	0	0	0
3	E	36	0	0	0	0
3	F	36	0	0	0	0
4	A	6	0	8	0	0
4	F	6	0	8	0	0
5	A	10	0	14	1	0
5	E	10	0	14	0	0
5	F	10	0	14	0	0
6	C	7	0	10	0	0
7	E	1	0	0	0	0
8	A	94	0	0	0	0
8	B	59	0	0	0	0
8	C	72	0	0	0	0
8	D	64	0	0	0	0
8	E	88	0	0	0	0
8	F	52	0	0	0	0
All	All	12396	0	11928	42	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 (42) 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:E:1:MET:HE3	1:E:3:TYR:CE1	2.33	0.63
1:B:169:TYR:OH	1:B:258:LYS:HD2	2.00	0.62
1:C:226:MET:HE1	1:C:237:MET:SD	2.48	0.54
1:A:210:LEU:HD11	1:A:237:MET:HE2	1.90	0.53
1:B:226:MET:HE2	3:B:306:48F:C1D	2.38	0.53
1:A:99:GLU:H	1:A:99:GLU:CD	2.17	0.53
1:B:226:MET:HE1	1:B:237:MET:SD	2.49	0.52
1:A:21:PHE:CG	1:E:21:PHE:HB2	2.45	0.52
1:C:137:ILE:HD11	1:C:164:THR:HB	1.92	0.51
1:B:137:ILE:HD11	1:B:164:THR:HB	1.93	0.51
1:D:137:ILE:HD11	1:D:164:THR:HB	1.93	0.51
1:E:137:ILE:HD11	1:E:164:THR:HB	1.93	0.50
1:C:138:LEU:O	1:C:139:ARG:HD3	2.12	0.50
1:A:137:ILE:HD11	1:A:164:THR:HB	1.93	0.50
1:C:97:LYS:HG2	1:C:105:TYR:CE2	2.48	0.49
1:B:11:ASN:HB3	1:D:101:VAL:HG21	1.96	0.48
1:F:137:ILE:HD11	1:F:164:THR:HB	1.94	0.48
1:B:25:MET:HE2	1:B:25:MET:HA	1.97	0.46
1:D:25:MET:HA	1:D:25:MET:HE2	1.98	0.46
1:A:95:LEU:HD23	1:A:107:ALA:HB2	1.98	0.46
1:A:25:MET:HA	1:A:25:MET:HE2	1.97	0.46
1:A:21:PHE:CD1	1:E:21:PHE:HB2	2.51	0.45
1:F:25:MET:HE2	1:F:25:MET:HA	1.98	0.45
1:E:25:MET:HA	1:E:25:MET:HE2	1.97	0.45
1:C:25:MET:HA	1:C:25:MET:HE2	1.98	0.45
1:A:219:PRO:HD3	5:A:315:PGE:H3	1.99	0.45
1:E:99:GLU:O	1:E:100:ASP:HB2	2.18	0.43
1:B:24:TRP:HA	1:B:27:VAL:HG12	2.00	0.43
1:C:177:ASP:O	1:C:178:ALA:C	2.62	0.43
1:F:177:ASP:O	1:F:178:ALA:C	2.62	0.43
1:D:177:ASP:O	1:D:178:ALA:C	2.62	0.42
1:F:139:ARG:HD3	1:F:139:ARG:HA	1.92	0.42
1:B:177:ASP:O	1:B:178:ALA:C	2.62	0.42
1:A:81:GLU:OE1	1:A:242:GLY:HA3	2.18	0.42
1:D:99:GLU:O	1:D:100:ASP:HB2	2.19	0.42
1:A:177:ASP:O	1:A:178:ALA:C	2.63	0.42
1:C:201:MET:HE2	1:C:201:MET:HB2	1.96	0.42
1:D:34:ILE:HG12	1:D:171:ILE:HD12	2.01	0.42
1:B:34:ILE:HG12	1:B:171:ILE:HD12	2.01	0.41
1:E:177:ASP:O	1:E:178:ALA:C	2.62	0.41
1:C:34:ILE:HG12	1:C:171:ILE:HD12	2.02	0.41
1:F:34:ILE:HG12	1:F:171:ILE:HD12	2.03	0.41

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	259/261 (99%)	254 (98%)	5 (2%)	0	100	100
1	B	256/261 (98%)	251 (98%)	5 (2%)	0	100	100
1	C	255/261 (98%)	249 (98%)	6 (2%)	0	100	100
1	D	259/261 (99%)	252 (97%)	7 (3%)	0	100	100
1	E	259/261 (99%)	253 (98%)	6 (2%)	0	100	100
1	F	256/261 (98%)	251 (98%)	5 (2%)	0	100	100
All	All	1544/1566 (99%)	1510 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/201 (100%)	197 (98%)	4 (2%)	48	67
1	B	198/201 (98%)	195 (98%)	3 (2%)	57	74
1	C	197/201 (98%)	194 (98%)	3 (2%)	57	74
1	D	201/201 (100%)	199 (99%)	2 (1%)	68	80
1	E	201/201 (100%)	200 (100%)	1 (0%)	81	88
1	F	198/201 (98%)	196 (99%)	2 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1196/1206 (99%)	1181 (99%)	15 (1%)	61 76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	99	GLU
1	A	106	ILE
1	A	201	MET
1	B	94	LYS
1	B	106	ILE
1	B	201	MET
1	C	106	ILE
1	C	139	ARG
1	C	201	MET
1	D	106	ILE
1	D	201	MET
1	E	106	ILE
1	F	106	ILE
1	F	201	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 62 ligands modelled in this entry, 50 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
3	48F	F	307	-	38,38,38	1.46	7 (18%)	49,57,57	1.70	9 (18%)
3	48F	E	312	-	38,38,38	1.49	6 (15%)	49,57,57	1.67	10 (20%)
5	PGE	E	314	-	9,9,9	0.48	0	8,8,8	0.25	0
5	PGE	A	315	-	9,9,9	0.52	0	8,8,8	0.26	0
6	PEG	C	310	-	6,6,6	0.54	0	5,5,5	0.13	0
3	48F	A	313	-	38,38,38	1.47	5 (13%)	49,57,57	1.68	9 (18%)
3	48F	D	308	-	38,38,38	1.49	7 (18%)	49,57,57	1.67	9 (18%)
4	GOL	F	308	-	5,5,5	0.33	0	5,5,5	0.14	0
4	GOL	A	314	-	5,5,5	0.36	0	5,5,5	0.25	0
3	48F	B	306	-	38,38,38	1.52	6 (15%)	49,57,57	1.70	9 (18%)
3	48F	C	309	-	38,38,38	1.55	6 (15%)	49,57,57	1.73	10 (20%)
5	PGE	F	309	-	9,9,9	0.52	0	8,8,8	0.24	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
3	48F	F	307	-	-	8/32/48/48	0/3/3/3
3	48F	E	312	-	-	12/32/48/48	0/3/3/3
5	PGE	E	314	-	-	5/7/7/7	-
5	PGE	A	315	-	-	4/7/7/7	-
6	PEG	C	310	-	-	1/4/4/4	-
3	48F	A	313	-	-	10/32/48/48	0/3/3/3
3	48F	D	308	-	-	11/32/48/48	0/3/3/3
4	GOL	F	308	-	-	2/4/4/4	-
4	GOL	A	314	-	-	3/4/4/4	-
3	48F	B	306	-	-	8/32/48/48	0/3/3/3
3	48F	C	309	-	-	2/32/48/48	0/3/3/3
5	PGE	F	309	-	-	4/7/7/7	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	312	48F	C5-C4	5.11	1.48	1.39
3	B	306	48F	C5-C4	5.01	1.48	1.39
3	A	313	48F	C5-C4	4.90	1.47	1.39
3	D	308	48F	C5-C4	4.89	1.47	1.39
3	C	309	48F	C5-C4	4.80	1.47	1.39
3	F	307	48F	C5-C4	4.74	1.47	1.39
3	C	309	48F	PA-O3A	3.53	1.63	1.59
3	E	312	48F	PA-O2A	3.25	1.62	1.50
3	D	308	48F	PA-O2A	3.18	1.61	1.50
3	A	313	48F	PA-O2A	3.12	1.61	1.50
3	B	306	48F	PA-O2A	3.10	1.61	1.50
3	C	309	48F	PA-O2A	3.09	1.61	1.50
3	F	307	48F	PA-O2A	3.08	1.61	1.50
3	C	309	48F	PB-O3A	3.00	1.62	1.59
3	B	306	48F	PA-O3A	2.97	1.62	1.59
3	B	306	48F	C5-C6	2.88	1.49	1.41
3	D	308	48F	C5-C6	2.88	1.49	1.41
3	C	309	48F	C5-C6	2.88	1.49	1.41
3	A	313	48F	C5-C6	2.83	1.48	1.41
3	E	312	48F	C5-C6	2.79	1.48	1.41
3	A	313	48F	PA-O3A	2.68	1.62	1.59
3	F	307	48F	PA-O3A	2.65	1.62	1.59
3	F	307	48F	C5-C6	2.61	1.48	1.41
3	E	312	48F	PA-O3A	2.61	1.62	1.59
3	B	306	48F	PB-O3A	2.58	1.62	1.59
3	D	308	48F	PA-O3A	2.58	1.62	1.59
3	E	312	48F	C8-N7	2.43	1.36	1.31
3	F	307	48F	PB-O3A	2.43	1.62	1.59
3	C	309	48F	C8-N7	2.41	1.36	1.31
3	D	308	48F	PB-O3A	2.39	1.62	1.59
3	E	312	48F	PB-O3A	2.38	1.62	1.59
3	B	306	48F	C8-N7	2.38	1.36	1.31
3	A	313	48F	C8-N7	2.37	1.36	1.31
3	D	308	48F	C8-N7	2.35	1.36	1.31
3	F	307	48F	C8-N7	2.33	1.36	1.31
3	F	307	48F	C5-N7	-2.11	1.35	1.39
3	D	308	48F	C5-N7	-2.09	1.35	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	307	48F	C5-C4-N3	-5.54	119.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	313	48F	C5-C4-N3	-5.52	119.12	126.72
3	D	308	48F	C5-C4-N3	-5.48	119.17	126.72
3	B	306	48F	C5-C4-N3	-5.45	119.21	126.72
3	E	312	48F	C5-C4-N3	-5.40	119.28	126.72
3	C	309	48F	C5-C4-N3	-5.40	119.28	126.72
3	B	306	48F	N3-C4-N9	4.75	135.24	127.17
3	F	307	48F	N3-C4-N9	4.68	135.12	127.17
3	E	312	48F	N3-C4-N9	4.62	135.02	127.17
3	A	313	48F	N3-C4-N9	4.61	135.01	127.17
3	D	308	48F	N3-C4-N9	4.53	134.88	127.17
3	C	309	48F	N3-C4-N9	4.34	134.56	127.17
3	C	309	48F	C2-N3-C4	3.76	121.02	111.83
3	C	309	48F	N3-C2-N1	-3.74	122.92	128.58
3	F	307	48F	C2-N3-C4	3.73	120.94	111.83
3	D	308	48F	C2-N3-C4	3.72	120.92	111.83
3	F	307	48F	N3-C2-N1	-3.71	122.96	128.58
3	A	313	48F	C2-N3-C4	3.70	120.87	111.83
3	B	306	48F	C2-N3-C4	3.70	120.86	111.83
3	E	312	48F	C2-N3-C4	3.59	120.61	111.83
3	A	313	48F	N3-C2-N1	-3.58	123.16	128.58
3	C	309	48F	C4-C5-N7	-3.58	106.49	110.58
3	D	308	48F	N3-C2-N1	-3.54	123.23	128.58
3	B	306	48F	N3-C2-N1	-3.52	123.26	128.58
3	E	312	48F	N3-C2-N1	-3.49	123.30	128.58
3	B	306	48F	C4-N9-C8	3.37	109.28	105.74
3	E	312	48F	C4-N9-C8	3.28	109.19	105.74
3	E	312	48F	C4-C5-N7	-3.24	106.88	110.58
3	D	308	48F	C4-C5-N7	-3.23	106.89	110.58
3	C	309	48F	C4-N9-C8	3.13	109.03	105.74
3	B	306	48F	C4-C5-N7	-3.11	107.03	110.58
3	F	307	48F	C4-N9-C8	3.08	108.97	105.74
3	F	307	48F	C4-C5-N7	-3.07	107.07	110.58
3	A	313	48F	C4-C5-N7	-3.02	107.13	110.58
3	D	308	48F	C4-N9-C8	2.86	108.74	105.74
3	A	313	48F	C4-N9-C8	2.86	108.74	105.74
3	C	309	48F	C5-N7-C8	2.64	107.60	103.45
3	C	309	48F	C6-C5-N7	2.46	136.83	132.09
3	D	308	48F	C5-N7-C8	2.44	107.28	103.45
3	B	306	48F	C5-N7-C8	2.41	107.24	103.45
3	E	312	48F	C5-N7-C8	2.40	107.23	103.45
3	F	307	48F	C5-N7-C8	2.35	107.14	103.45
3	C	309	48F	N9-C8-N7	-2.27	110.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	309	48F	C2-N1-C6	2.27	122.45	118.73
3	E	312	48F	C6-C5-N7	2.22	136.38	132.09
3	A	313	48F	C2-N1-C6	2.18	122.31	118.73
3	E	312	48F	C2-N1-C6	2.18	122.31	118.73
3	D	308	48F	C6-C5-N7	2.15	136.23	132.09
3	A	313	48F	C5-N7-C8	2.14	106.81	103.45
3	B	306	48F	N9-C8-N7	-2.14	110.90	113.94
3	B	306	48F	C6-C5-N7	2.14	136.21	132.09
3	E	312	48F	N9-C8-N7	-2.07	111.00	113.94
3	F	307	48F	C2-N1-C6	2.06	122.12	118.73
3	D	308	48F	C2-N1-C6	2.06	122.12	118.73
3	F	307	48F	N9-C8-N7	-2.06	111.02	113.94
3	A	313	48F	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	313	48F	PA-O3A-PB-O5D
3	A	313	48F	C2D-C3D-C4D-C5D
3	A	313	48F	O3D-C3D-C4D-C5D
3	A	313	48F	C2D-C3D-C4D-O4D
3	A	313	48F	O3D-C3D-C4D-O4D
3	A	313	48F	C1D-C2D-C3D-C4D
3	A	313	48F	O2D-C2D-C3D-C4D
3	A	313	48F	O1D-C1D-C2D-O2D
3	B	306	48F	PA-O3A-PB-O5D
3	B	306	48F	C2D-C3D-C4D-O4D
3	B	306	48F	O1D-C1D-C2D-C3D
3	B	306	48F	O1D-C1D-C2D-O2D
3	D	308	48F	C1D-C2D-C3D-C4D
3	D	308	48F	O2D-C2D-C3D-C4D
3	D	308	48F	O2D-C2D-C3D-O3D
3	D	308	48F	O1D-C1D-C2D-O2D
3	E	312	48F	PA-O3A-PB-O5D
3	E	312	48F	C2D-C3D-C4D-C5D
3	E	312	48F	O3D-C3D-C4D-C5D
3	E	312	48F	C2D-C3D-C4D-O4D
3	E	312	48F	O3D-C3D-C4D-O4D
3	E	312	48F	C1D-C2D-C3D-C4D
3	E	312	48F	O2D-C2D-C3D-C4D
3	E	312	48F	O2D-C2D-C3D-O3D

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Mol	Chain	Res	Type	Atoms
3	E	312	48F	O1D-C1D-C2D-O2D
3	F	307	48F	O1D-C1D-C2D-O2D
4	A	314	GOL	C1-C2-C3-O3
5	E	314	PGE	O2-C3-C4-O3
5	F	309	PGE	O1-C1-C2-O2
5	A	315	PGE	O2-C3-C4-O3
4	F	308	GOL	O1-C1-C2-C3
4	A	314	GOL	O2-C2-C3-O3
5	A	315	PGE	O3-C5-C6-O4
6	C	310	PEG	O1-C1-C2-O2
5	E	314	PGE	O1-C1-C2-O2
5	E	314	PGE	O3-C5-C6-O4
5	F	309	PGE	C6-C5-O3-C4
4	F	308	GOL	O1-C1-C2-O2
3	D	308	48F	PA-O3A-PB-O5D
3	F	307	48F	PA-O3A-PB-O5D
3	B	306	48F	O3D-C3D-C4D-C5D
3	D	308	48F	O3D-C3D-C4D-C5D
3	F	307	48F	O3D-C3D-C4D-C5D
5	F	309	PGE	C3-C4-O3-C5
3	E	312	48F	C1D-C2D-C3D-O3D
5	A	315	PGE	O1-C1-C2-O2
3	B	306	48F	C2D-C3D-C4D-C5D
3	D	308	48F	C2D-C3D-C4D-C5D
3	F	307	48F	C2D-C3D-C4D-C5D
5	A	315	PGE	C1-C2-O2-C3
3	C	309	48F	C5D-O5D-PB-O1B
3	D	308	48F	C2D-C3D-C4D-O4D
3	E	312	48F	C5D-O5D-PB-O1B
3	F	307	48F	C2D-C3D-C4D-O4D
3	A	313	48F	O1D-C1D-C2D-C3D
3	D	308	48F	O1D-C1D-C2D-C3D
3	F	307	48F	O4'-C4'-C5'-O5'
3	B	306	48F	O3D-C3D-C4D-O4D
3	D	308	48F	O3D-C3D-C4D-O4D
3	F	307	48F	O3D-C3D-C4D-O4D
5	E	314	PGE	C3-C4-O3-C5
3	C	309	48F	O4'-C4'-C5'-O5'
4	A	314	GOL	O1-C1-C2-O2
3	A	313	48F	PB-O3A-PA-O1A
3	B	306	48F	PB-O3A-PA-O1A
3	E	312	48F	PB-O3A-PA-O1A

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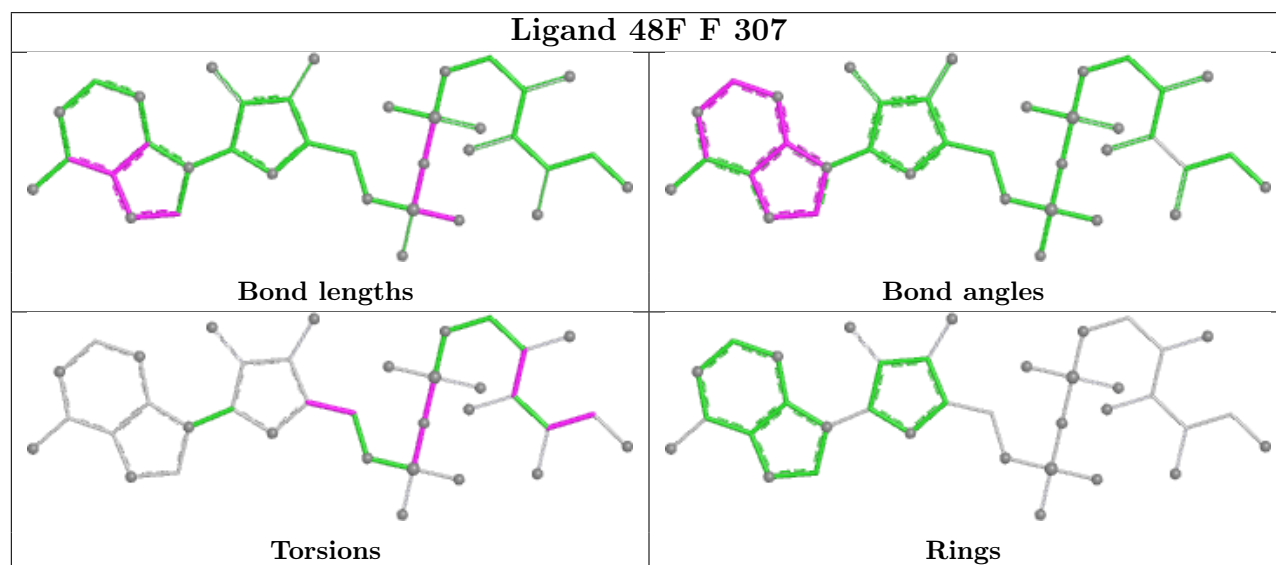
Mol	Chain	Res	Type	Atoms
3	F	307	48F	PB-O3A-PA-O1A
5	F	309	PGE	O2-C3-C4-O3
5	E	314	PGE	C4-C3-O2-C2
3	D	308	48F	PB-O3A-PA-O1A

There are no ring outliers.

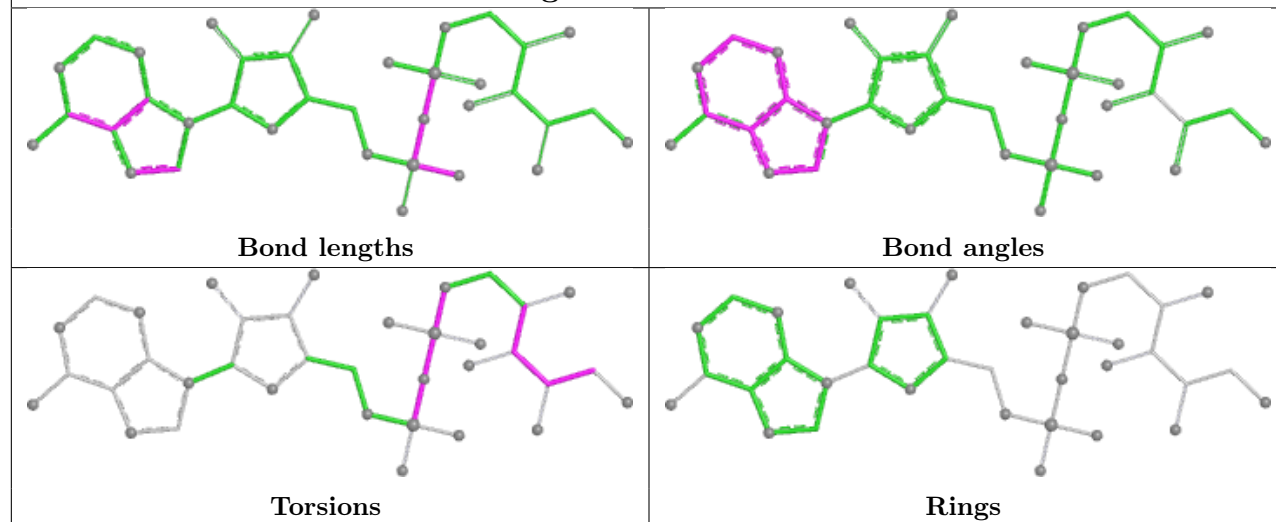
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	315	PGE	1	0
3	B	306	48F	1	0

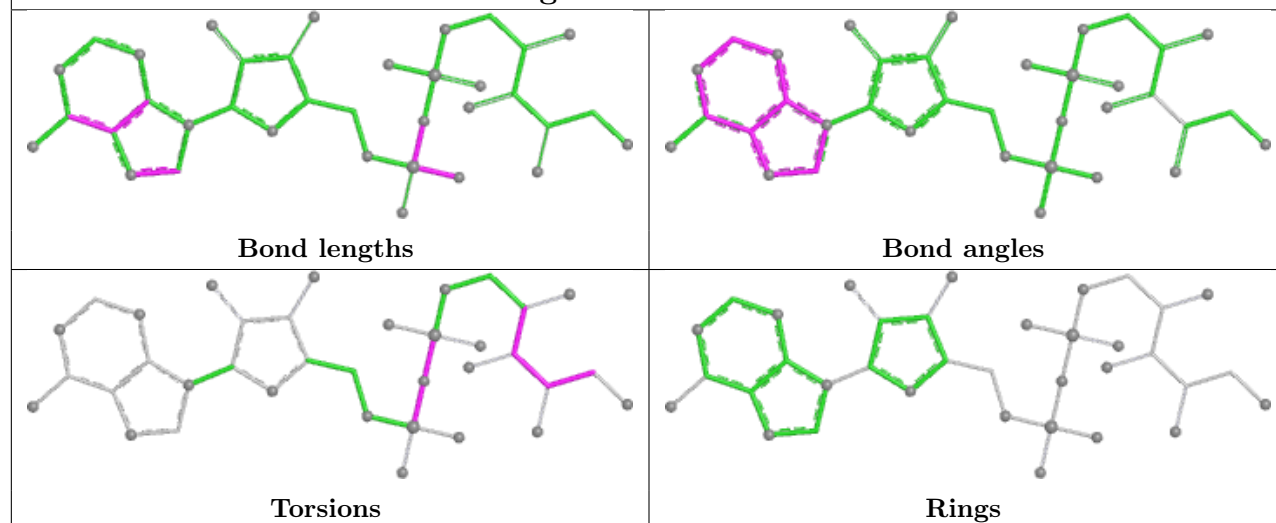
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



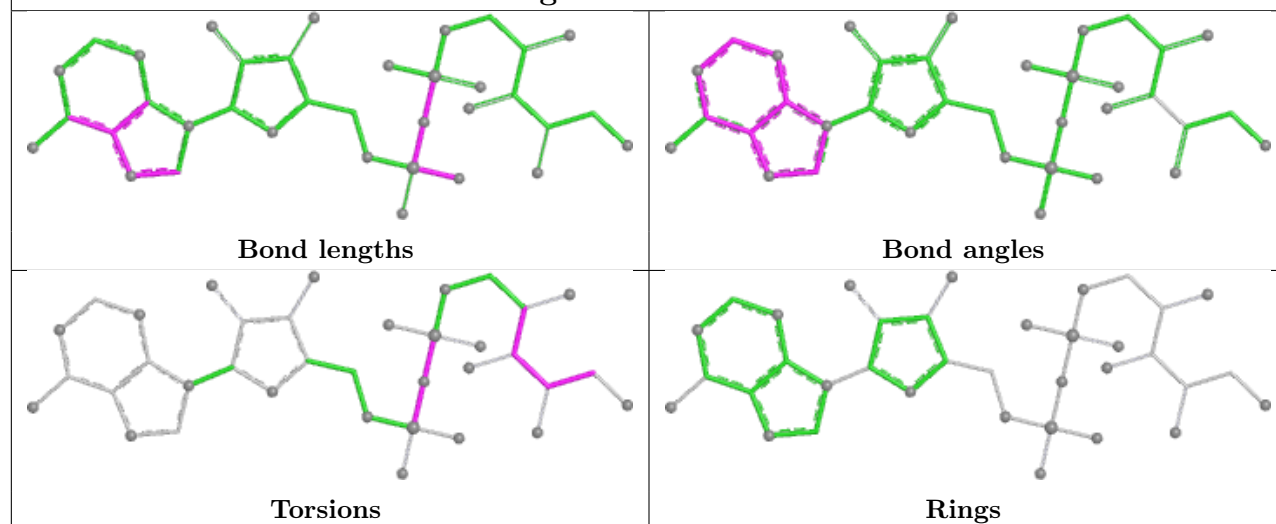
Ligand 48F E 312

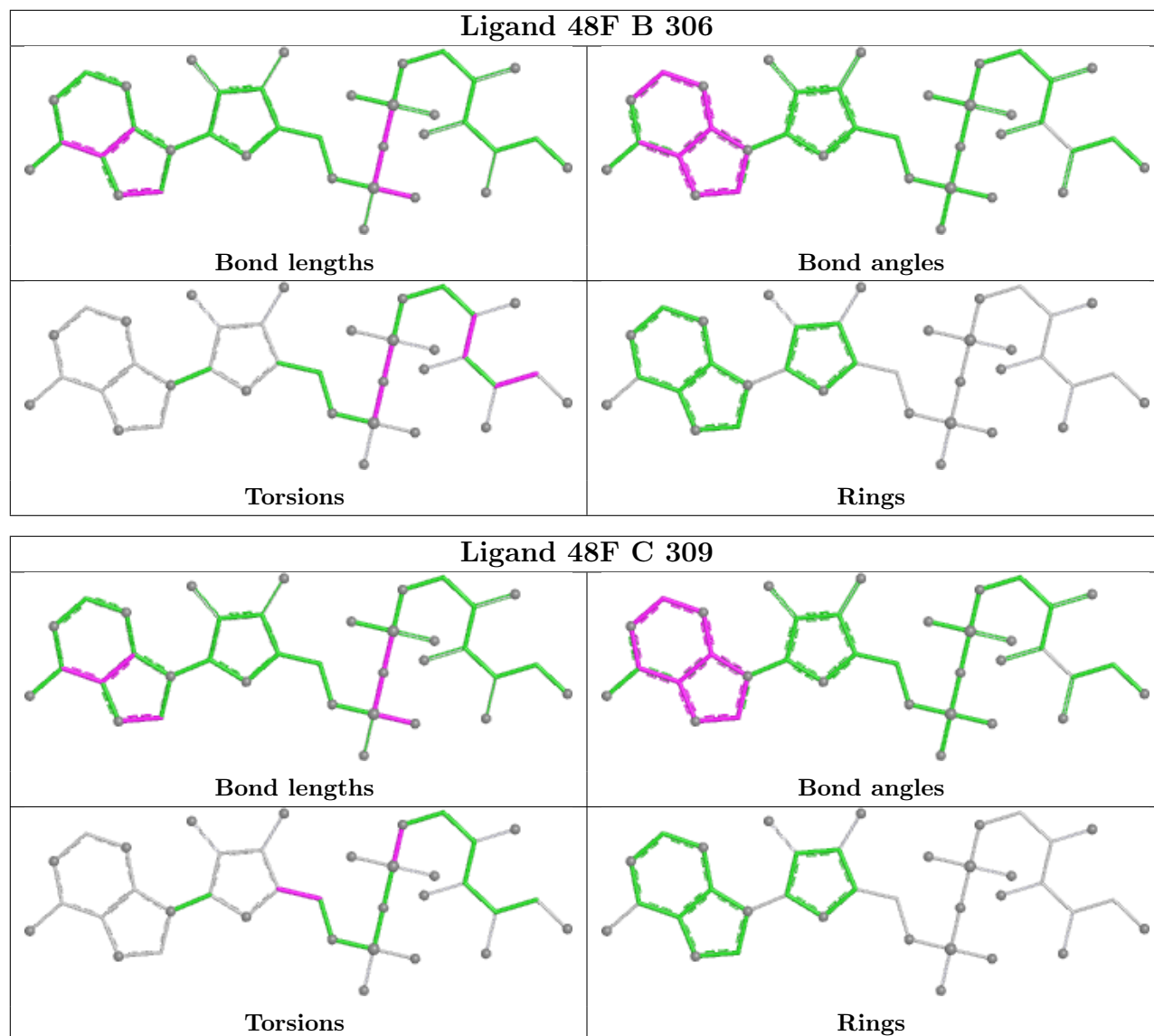


Ligand 48F A 313



Ligand 48F D 308





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	261/261 (100%)	-0.02	6 (2%) 61 62	36, 45, 78, 107	0
1	B	258/261 (98%)	0.21	8 (3%) 51 52	44, 55, 82, 103	0
1	C	257/261 (98%)	0.12	6 (2%) 61 62	43, 54, 83, 103	0
1	D	261/261 (100%)	0.16	8 (3%) 51 52	40, 52, 78, 105	0
1	E	261/261 (100%)	-0.04	8 (3%) 51 52	36, 46, 78, 117	0
1	F	258/261 (98%)	0.19	7 (2%) 56 57	45, 57, 85, 122	0
All	All	1556/1566 (99%)	0.10	43 (2%) 55 56	36, 52, 81, 122	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	TYR	7.9
1	B	100	ASP	4.0
1	D	1	MET	4.0
1	E	21	PHE	4.0
1	A	100	ASP	3.4
1	F	3	TYR	3.4
1	B	21	PHE	3.4
1	A	3	TYR	3.3
1	D	2	ASP	3.3
1	A	21	PHE	3.2
1	F	21	PHE	3.2
1	A	261	LYS	3.2
1	F	100	ASP	3.0
1	D	6	LYS	2.9
1	D	67	GLY	2.8
1	E	52	GLY	2.7
1	C	159	HIS	2.7
1	E	3	TYR	2.7
1	E	151	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	159	HIS	2.7
1	C	156	ALA	2.6
1	F	67	GLY	2.6
1	F	260	ASN	2.6
1	E	100	ASP	2.6
1	C	190	ASP	2.5
1	D	190	ASP	2.5
1	C	4	LYS	2.5
1	E	1	MET	2.4
1	C	6	LYS	2.3
1	C	260	ASN	2.2
1	D	4	LYS	2.2
1	A	99	GLU	2.2
1	E	261	LYS	2.2
1	E	257	GLU	2.2
1	B	176	HIS	2.1
1	B	141	ASP	2.1
1	B	190	ASP	2.1
1	B	65	GLY	2.1
1	A	151	TYR	2.1
1	F	190	ASP	2.1
1	B	159	HIS	2.1
1	D	159	HIS	2.1
1	B	151	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TB	C	306	1/1	-0.51	0.71	81,81,81,81	1
2	TB	C	302	1/1	-0.35	0.61	77,77,77,77	1
2	TB	F	305	1/1	-0.30	0.78	78,78,78,78	1
2	TB	E	311	1/1	-0.05	0.73	85,85,85,85	1
2	TB	F	303	1/1	0.06	0.58	66,66,66,66	1
2	TB	E	310	1/1	0.20	0.75	69,69,69,69	1
2	TB	D	306	1/1	0.32	0.45	62,62,62,62	1
2	TB	C	303	1/1	0.33	0.46	54,54,54,54	1
2	TB	B	303	1/1	0.34	0.58	50,50,50,50	1
2	TB	D	303	1/1	0.35	0.56	55,55,55,55	1
2	TB	E	306	1/1	0.41	0.32	79,79,79,79	1
2	TB	D	304	1/1	0.47	0.41	39,39,39,39	1
2	TB	A	304	1/1	0.51	0.42	43,43,43,43	1
2	TB	C	308	1/1	0.53	0.70	65,65,65,65	1
2	TB	B	304	1/1	0.62	0.44	92,92,92,92	1
2	TB	E	307	1/1	0.62	0.28	49,49,49,49	1
2	TB	A	308	1/1	0.63	0.40	49,49,49,49	1
2	TB	F	304	1/1	0.64	0.50	100,100,100,100	1
2	TB	A	311	1/1	0.64	0.65	53,53,53,53	1
2	TB	E	309	1/1	0.66	0.75	63,63,63,63	1
2	TB	C	304	1/1	0.66	0.68	64,64,64,64	1
2	TB	D	307	1/1	0.67	0.74	73,73,73,73	1
2	TB	A	310	1/1	0.68	0.59	52,52,52,52	1
2	TB	D	305	1/1	0.68	0.56	50,50,50,50	1
2	TB	F	301	1/1	0.71	0.27	79,79,79,79	1
2	TB	A	302	1/1	0.74	0.30	61,61,61,61	1
2	TB	B	305	1/1	0.75	0.70	61,61,61,61	1
2	TB	A	307	1/1	0.77	0.57	51,51,51,51	1
2	TB	A	303	1/1	0.77	0.51	73,73,73,73	1
2	TB	F	306	1/1	0.77	0.74	64,64,64,64	1
2	TB	B	301	1/1	0.78	0.28	88,88,88,88	1
2	TB	C	305	1/1	0.82	0.66	60,60,60,60	1
2	TB	E	305	1/1	0.82	0.51	92,92,92,92	1
2	TB	C	307	1/1	0.84	0.72	58,58,58,58	1
2	TB	A	312	1/1	0.84	0.58	58,58,58,58	1
2	TB	E	301	1/1	0.86	0.39	60,60,60,60	1
2	TB	E	308	1/1	0.86	0.68	55,55,55,55	1
2	TB	E	304	1/1	0.87	0.24	66,66,66,66	1
5	PGE	F	309	10/10	0.87	0.15	68,74,80,80	0
6	PEG	C	310	7/7	0.87	0.16	67,69,74,74	0
2	TB	A	305	1/1	0.88	0.46	76,76,76,76	1
5	PGE	A	315	10/10	0.88	0.14	59,65,69,69	0

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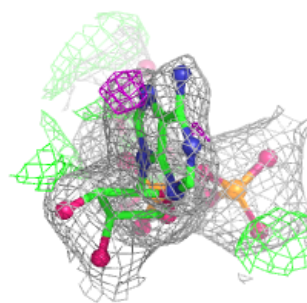
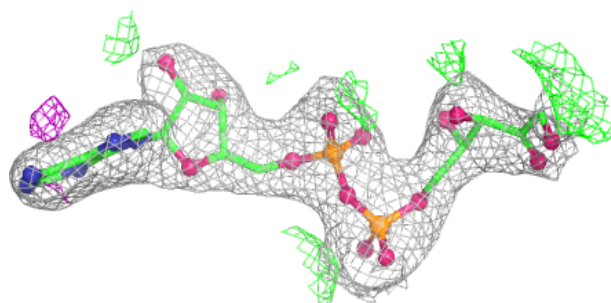
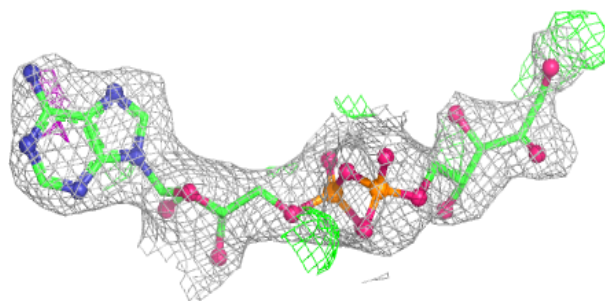
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TB	D	302	1/1	0.89	0.42	58,58,58,58	1
5	PGE	E	314	10/10	0.89	0.14	52,65,74,76	0
2	TB	A	309	1/1	0.89	0.62	50,50,50,50	1
4	GOL	A	314	6/6	0.89	0.22	98,100,107,108	0
2	TB	B	302	1/1	0.90	0.31	89,89,89,89	1
2	TB	A	306	1/1	0.90	0.60	46,46,46,46	1
2	TB	C	301	1/1	0.91	0.30	86,86,86,86	1
4	GOL	F	308	6/6	0.91	0.23	107,109,113,113	0
2	TB	D	301	1/1	0.91	0.31	83,83,83,83	1
2	TB	A	301	1/1	0.92	0.26	85,85,85,85	1
3	48F	D	308	36/36	0.92	0.12	53,60,85,87	0
3	48F	B	306	36/36	0.93	0.11	54,62,93,95	0
2	TB	F	302	1/1	0.93	0.27	91,91,91,91	1
3	48F	C	309	36/36	0.94	0.10	48,58,96,99	0
3	48F	F	307	36/36	0.94	0.10	49,59,94,99	0
3	48F	E	312	36/36	0.95	0.09	44,51,83,84	0
2	TB	E	303	1/1	0.95	0.16	69,69,69,69	1
3	48F	A	313	36/36	0.96	0.08	44,52,78,80	0
7	NA	E	313	1/1	0.96	0.22	62,62,62,62	0
2	TB	E	302	1/1	0.98	0.23	78,78,78,78	1

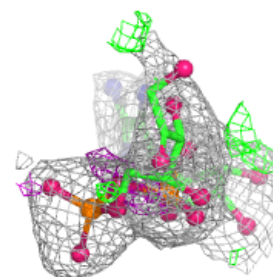
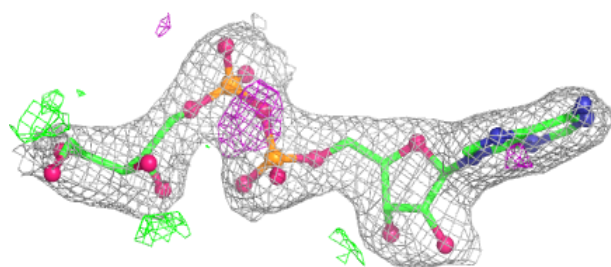
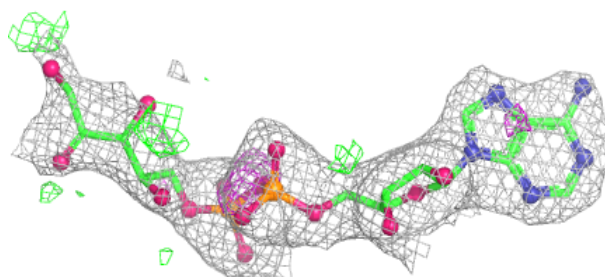
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 48F D 308:

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

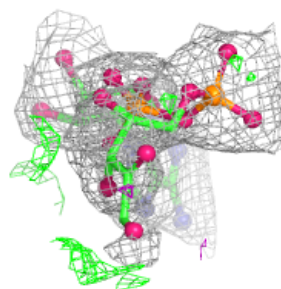
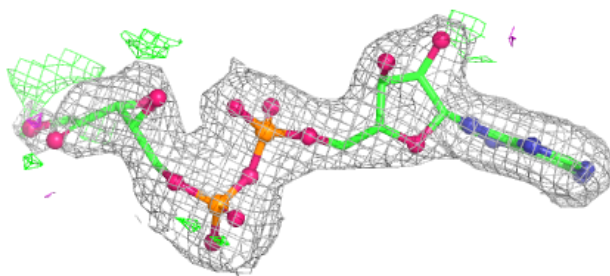
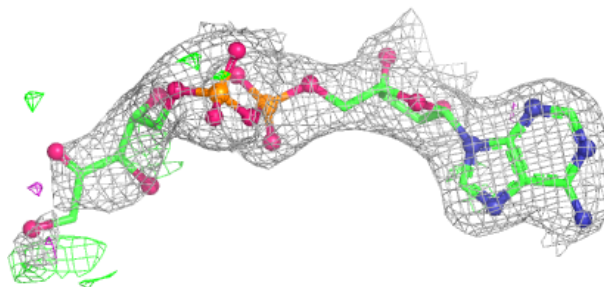
**Electron density around 48F B 306:**

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

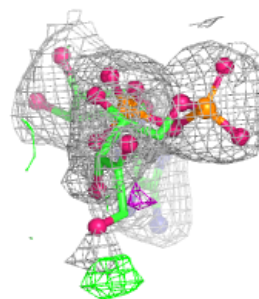
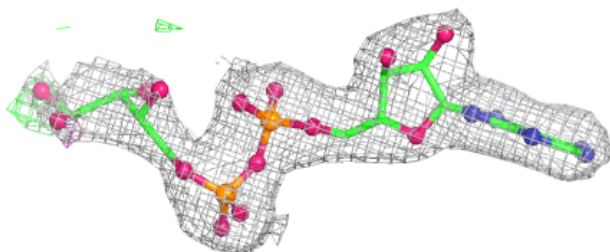
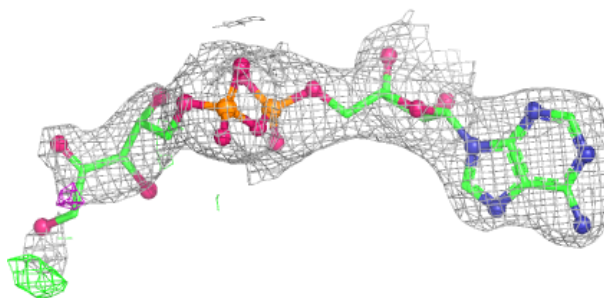


Electron density around 48F C 309:

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

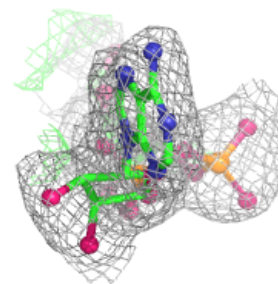
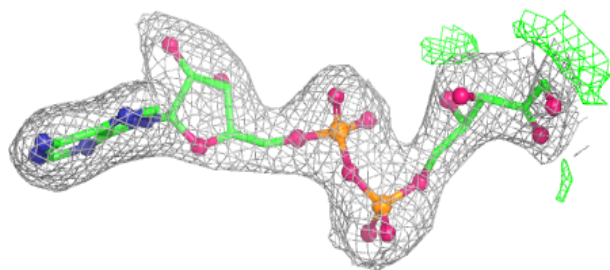
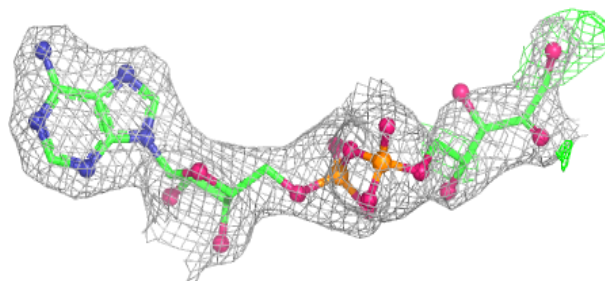
**Electron density around 48F F 307:**

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

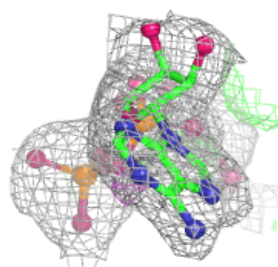
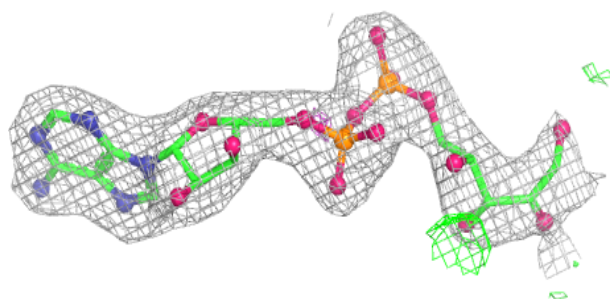
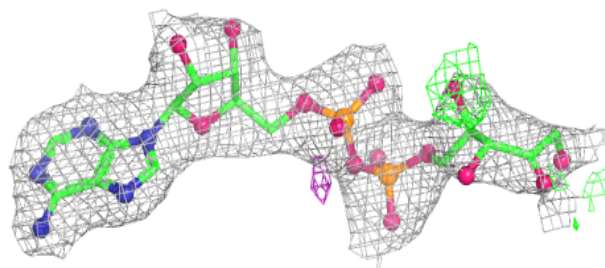


Electron density around 48F E 312:

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

**Electron density around 48F A 313:**

$2mF_o-DF_c$ (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.