



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:43 AM UTC

PDB ID : 5FUY / pdb_00005fuy
Title : catalytic domain of Thymidine kinase from Trypanosoma brucei with dTMP
Authors : Timm, J.; Valente, M.; Castillo-Acosta, V.; Balzarini, T.; Nettleship, J.E.;
Rada, H.; Wilson, K.S.; Gonzalez-Pacanowska, D.
Deposited on : 2016-01-31
Resolution : 2.80 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

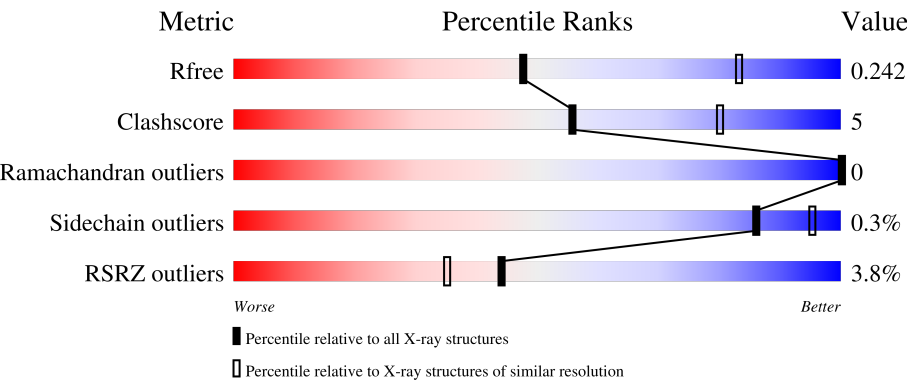
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	183	4% 84% 7% 10%
1	B	183	2% 81% 9% 10%
1	C	183	4% 81% 8% 10%
1	D	183	5% 80% 7% 12%
1	E	183	3% 82% 8% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	183	

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
3	QBT	A	1386	X	-	-	-
3	QBT	B	1385	X	-	-	-
3	QBT	C	1386	X	-	-	-
3	QBT	D	1384	X	-	-	-
3	QBT	E	1387	X	-	-	-
3	QBT	F	1386	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7607 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.

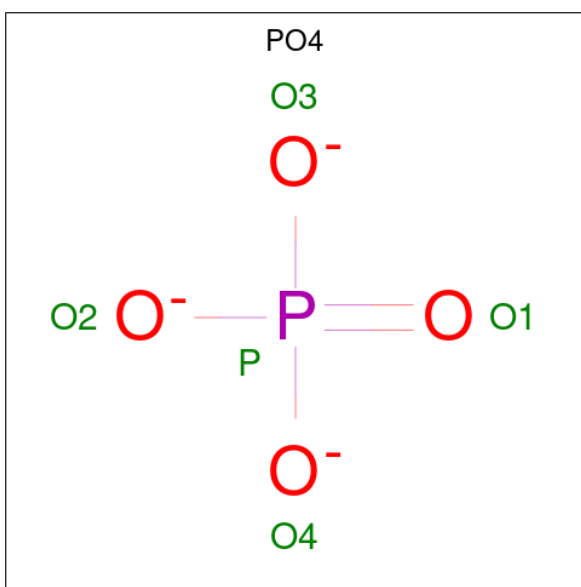
- Molecule 1 is a protein called THYMDINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1238	776	212	238	12			
1	B	164	Total	C	N	O	S	0	0	0
			1248	780	221	235	12			
1	C	164	Total	C	N	O	S	0	0	0
			1199	754	204	229	12			
1	D	161	Total	C	N	O	S	0	0	0
			1182	744	202	226	10			
1	E	167	Total	C	N	O	S	0	0	0
			1261	787	220	242	12			
1	F	167	Total	C	N	O	S	0	0	0
			1276	795	223	246	12			

There are 12 discrepancies between the modelled and reference sequences:

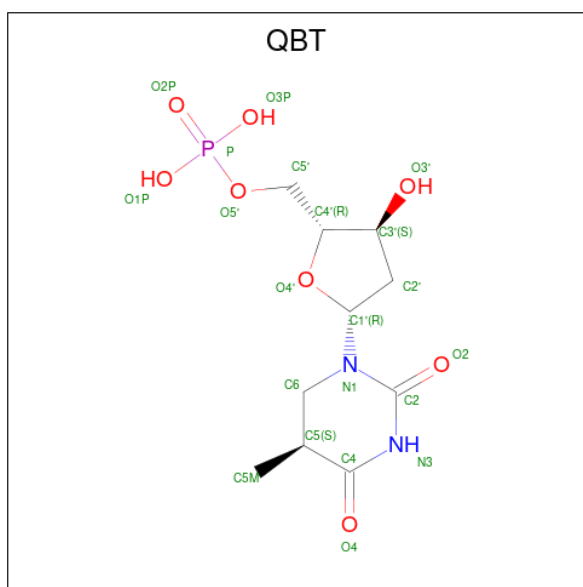
Chain	Residue	Modelled	Actual	Comment	Reference
A	385	ALA	-	expression tag	UNP Q38CF2
A	292	ASP	GLY	engineered mutation	UNP Q38CF2
B	385	ALA	-	expression tag	UNP Q38CF2
B	292	ASP	GLY	engineered mutation	UNP Q38CF2
C	385	ALA	-	expression tag	UNP Q38CF2
C	292	ASP	GLY	engineered mutation	UNP Q38CF2
D	385	ALA	-	expression tag	UNP Q38CF2
D	292	ASP	GLY	engineered mutation	UNP Q38CF2
E	385	ALA	-	expression tag	UNP Q38CF2
E	292	ASP	GLY	engineered mutation	UNP Q38CF2
F	385	ALA	-	expression tag	UNP Q38CF2
F	292	ASP	GLY	engineered mutation	UNP Q38CF2

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is [(2R,3S,5R)-3-HYDROXY-5-[(5S)-5-METHYL-2,4-DIOXO-1,3-DIAZINAN-1-YL]OXOLAN-2-YL]METHYL DIHYDROGEN PHOSPHATE (CCD ID: QBT) (formula: C₁₀H₁₇N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	E	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	F	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

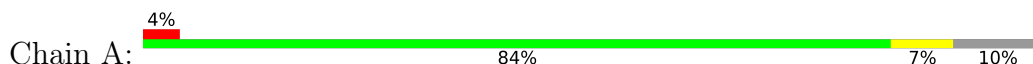
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total 8	O 8	0	0
5	B	7	Total 7	O 7	0	0
5	C	1	Total 1	O 1	0	0
5	D	3	Total 3	O 3	0	0
5	E	11	Total 11	O 11	0	0
5	F	11	Total 11	O 11	0	0

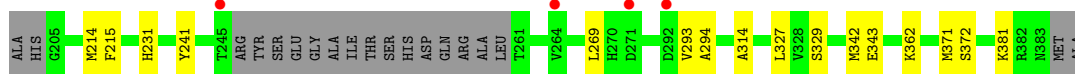
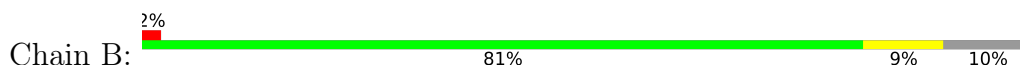
3 Residue-property plots [i](#)

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.

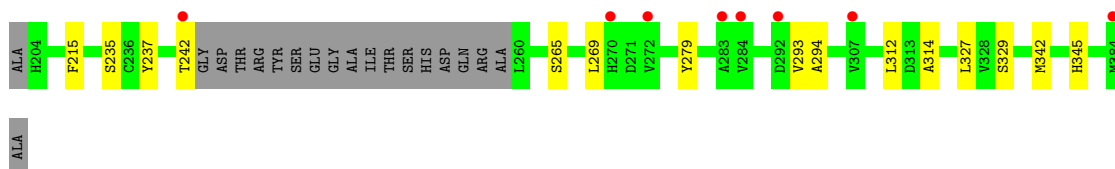
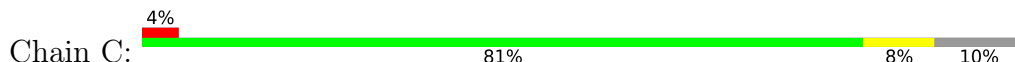
- Molecule 1: THYMDINE KINASE



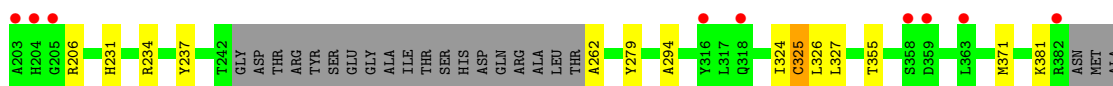
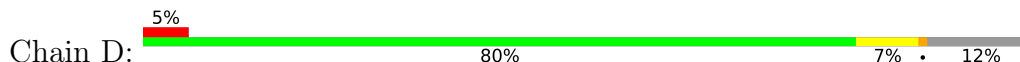
- Molecule 1: THYMDINE KINASE



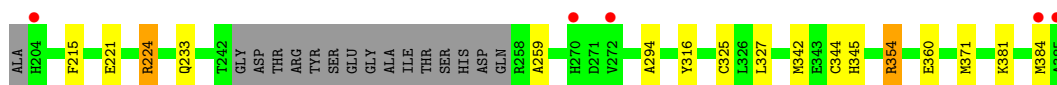
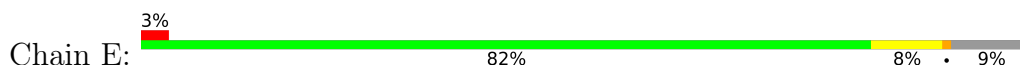
- Molecule 1: THYMDINE KINASE



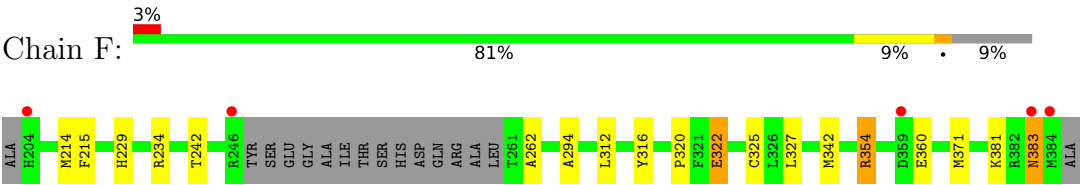
- Molecule 1: THYMDINE KINASE



- Molecule 1: THYMDINE KINASE



● Molecule 1: THYMDINE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.61Å 97.00Å 304.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.22 – 2.80 152.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (152.22-2.80) 95.7 (152.22-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.243 (Not available) , 0.242	Depositor DCC
R_{free} test set	1573 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.3	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	0.93	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.27% 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: PO4, QBT, 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	0.83	0/1257	0.82	0/1702
1	B	0.83	0/1268	0.84	0/1711
1	C	0.77	0/1218	0.84	0/1652
1	D	0.88	1/1201 (0.1%)	0.85	1/1631 (0.1%)
1	E	0.84	0/1280	0.90	2/1731 (0.1%)
1	F	0.93	1/1296 (0.1%)	0.92	4/1750 (0.2%)
All	All	0.85	2/7520 (0.0%)	0.86	7/10177 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	383	ASN	CA-C	5.09	1.59	1.52
1	D	206	ARG	C-O	-5.06	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	354	ARG	CG-CD-NE	9.24	132.33	112.00
1	F	354	ARG	CG-CD-NE	9.18	132.19	112.00
1	E	384	MET	N-CA-C	-8.05	93.65	110.80
1	F	322	GLU	CB-CA-C	-6.25	97.43	110.17
1	F	242	THR	N-CA-C	5.66	117.92	111.02
1	D	325	CYS	CB-CA-C	5.37	121.10	110.42
1	F	262	ALA	CB-CA-C	5.02	118.03	110.50

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	1238	0	1172	11	0
1	B	1248	0	1196	13	0
1	C	1199	0	1103	11	0
1	D	1182	0	1095	16	0
1	E	1261	0	1196	10	0
1	F	1276	0	1213	14	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	21	0	14	0	0
3	B	21	0	14	0	0
3	C	21	0	14	1	0
3	D	21	0	14	0	0
3	E	21	0	14	0	0
3	F	21	0	14	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	8	0	0	0	0
5	B	7	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	E	11	0	0	0	0
5	F	11	0	0	0	0
All	All	7607	0	7059	68	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 5.

All (68) 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:D:371:MET:SD	1:D:381:LYS:NZ	2.06	1.28
1:B:241:TYR:OH	1:B:362:LYS:NZ	1.83	1.10
1:A:342:MET:HE2	1:B:231:HIS:HB3	1.61	0.83
1:C:345:HIS:O	1:D:234:ARG:NH2	2.14	0.81
1:A:230:LYS:CE	1:A:261:THR:OG1	2.30	0.78
1:C:242:THR:CB	1:C:265:SER:HB3	2.16	0.75
1:D:324:ILE:O	1:D:327:LEU:N	2.19	0.74
1:A:231:HIS:HB3	1:B:342:MET:HE2	1.77	0.65
1:F:229:HIS:ND1	1:F:234:ARG:NH1	2.44	0.64
1:A:230:LYS:HE2	1:A:261:THR:OG1	1.98	0.63
1:E:325:CYS:HB3	1:F:325:CYS:HB3	1.82	0.62
1:E:221:GLU:OE2	1:E:224:ARG:NH1	2.34	0.60
1:B:343:GLU:OE1	1:B:381:LYS:NZ	2.31	0.59
1:D:237:TYR:HA	1:D:262:ALA:HB3	1.85	0.58
1:D:355:THR:HG21	1:D:371:MET:HE3	1.86	0.57
1:B:314:ALA:HB2	1:C:329:SER:HB2	1.87	0.56
1:D:294:ALA:HA	1:D:327:LEU:HD13	1.87	0.56
1:B:215:PHE:CD2	1:B:342:MET:HE1	2.42	0.55
1:C:235:SER:HB2	1:C:279:TYR:HD1	1.72	0.55
1:E:354:ARG:NH2	1:E:360:GLU:O	2.40	0.54
1:F:229:HIS:CE1	1:F:234:ARG:NH1	2.75	0.54
1:D:324:ILE:O	1:D:326:LEU:N	2.40	0.53
1:E:233:GLN:HA	1:E:259:ALA:HB2	1.91	0.53
1:F:354:ARG:NH2	1:F:360:GLU:O	2.42	0.53
1:F:312:LEU:HD11	3:F:1386:QBT:H62C	1.91	0.52
1:C:215:PHE:CD2	1:C:342:MET:HE1	2.44	0.52
1:D:237:TYR:CD1	1:D:262:ALA:CB	2.93	0.52
1:A:215:PHE:CD2	1:A:342:MET:HE1	2.45	0.52
1:D:324:ILE:O	1:D:325:CYS:C	2.53	0.51
1:F:312:LEU:CD1	3:F:1386:QBT:H62C	2.40	0.51
1:F:215:PHE:CD2	1:F:342:MET:HE1	2.45	0.51
1:A:230:LYS:HE3	1:A:261:THR:OG1	2.09	0.51
1:A:233:GLN:HA	1:A:259:ALA:HB2	1.92	0.51
1:E:215:PHE:CD2	1:E:342:MET:HE1	2.46	0.50
1:F:229:HIS:CE1	1:F:234:ARG:HH12	2.30	0.50
1:D:237:TYR:CD1	1:D:262:ALA:HB3	2.47	0.50
1:D:324:ILE:C	1:D:326:LEU:N	2.70	0.50
1:F:294:ALA:HA	1:F:327:LEU:HD13	1.92	0.50
1:C:294:ALA:HA	1:C:327:LEU:HD13	1.95	0.49
1:B:294:ALA:HA	1:B:327:LEU:HD13	1.94	0.48
1:F:214:MET:HE3	3:F:1386:QBT:H5'1	1.94	0.48
1:E:344:CYS:O	1:E:345:HIS:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ALA:HA	1:A:327:LEU:HD13	1.95	0.48
1:A:343:GLU:OE1	1:A:381:LYS:NZ	2.47	0.47
1:B:241:TYR:CE2	1:B:362:LYS:HE3	2.49	0.47
1:E:294:ALA:HA	1:E:327:LEU:HD13	1.96	0.47
1:B:371:MET:SD	1:B:381:LYS:HE3	2.54	0.47
1:C:312:LEU:HD11	3:C:1386:QBT:H62C	1.98	0.46
1:E:371:MET:SD	1:E:381:LYS:HE3	2.56	0.46
1:B:214:MET:O	1:B:372:SER:OG	2.32	0.46
1:E:221:GLU:CD	1:E:224:ARG:HH11	2.25	0.45
1:F:371:MET:SD	1:F:381:LYS:HE3	2.56	0.45
1:D:327:LEU:HA	1:D:327:LEU:HD12	1.75	0.44
1:B:329:SER:HB2	1:C:314:ALA:HB2	1.99	0.43
1:F:381:LYS:C	1:F:383:ASN:H	2.26	0.43
1:F:320:PRO:HG2	1:F:322:GLU:OE2	2.18	0.43
1:A:230:LYS:CD	1:A:261:THR:OG1	2.66	0.43
1:F:316:TYR:CE1	1:F:354:ARG:NH2	2.87	0.42
1:A:325:CYS:HB3	1:D:325:CYS:HB3	2.01	0.42
1:C:237:TYR:CD1	1:C:279:TYR:CE2	3.08	0.42
1:C:269:LEU:CD1	1:C:293:VAL:HA	2.50	0.42
1:E:316:TYR:CE1	1:E:354:ARG:NH2	2.88	0.41
1:D:294:ALA:HA	1:D:327:LEU:CD1	2.50	0.41
1:D:262:ALA:HB2	1:D:279:TYR:CZ	2.55	0.41
1:B:269:LEU:CD1	1:B:293:VAL:HA	2.51	0.41
1:B:327:LEU:HD12	1:B:327:LEU:HA	1.92	0.41
1:D:237:TYR:HD1	1:D:262:ALA:CB	2.32	0.41
1:C:327:LEU:HD12	1:C:327:LEU:HA	1.95	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	161/183 (88%)	159 (99%)	2 (1%)	0	100	100
1	B	160/183 (87%)	157 (98%)	3 (2%)	0	100	100
1	C	160/183 (87%)	159 (99%)	1 (1%)	0	100	100
1	D	157/183 (86%)	152 (97%)	5 (3%)	0	100	100
1	E	163/183 (89%)	161 (99%)	2 (1%)	0	100	100
1	F	163/183 (89%)	160 (98%)	3 (2%)	0	100	100
All	All	964/1098 (88%)	948 (98%)	16 (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	129/156 (83%)	129 (100%)	0	100	100
1	B	131/156 (84%)	131 (100%)	0	100	100
1	C	119/156 (76%)	119 (100%)	0	100	100
1	D	118/156 (76%)	117 (99%)	1 (1%)	73	90
1	E	131/156 (84%)	130 (99%)	1 (1%)	73	90
1	F	135/156 (86%)	135 (100%)	0	100	100
All	All	763/936 (82%)	761 (100%)	2 (0%)	86	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	231	HIS
1	E	224	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	346	ASN
1	B	268	ASN
1	B	345	HIS
1	B	346	ASN
1	C	263	ASN
1	E	229	HIS
1	E	263	ASN
1	E	346	ASN
1	F	345	HIS
1	F	346	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 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	$\# Z > 2$
2	PO4	F	1385	-	4,4,4	0.90	0	6,6,6	0.95	0
3	QBT	A	1386	-	20,22,22	2.93	5 (25%)	26,33,33	1.80	7 (26%)
2	PO4	D	1383	-	4,4,4	0.91	0	6,6,6	1.20	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QBT	D	1384	-	20,22,22	2.65	3 (15%)	26,33,33	1.92	7 (26%)
2	PO4	A	1385	-	4,4,4	1.15	0	6,6,6	2.14	3 (50%)
3	QBT	F	1386	-	20,22,22	2.69	4 (20%)	26,33,33	2.02	7 (26%)
2	PO4	B	1384	-	4,4,4	0.96	0	6,6,6	1.32	1 (16%)
2	PO4	C	1385	-	4,4,4	0.96	0	6,6,6	1.38	1 (16%)
3	QBT	C	1386	-	20,22,22	2.76	3 (15%)	26,33,33	2.12	6 (23%)
3	QBT	E	1387	-	20,22,22	2.86	5 (25%)	26,33,33	1.52	4 (15%)
2	PO4	E	1386	-	4,4,4	1.64	2 (50%)	6,6,6	1.22	1 (16%)
3	QBT	B	1385	-	20,22,22	3.02	4 (20%)	26,33,33	1.78	5 (19%)

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	QBT	B	1385	-	1/1/8/9	2/10/38/38	0/2/2/2
3	QBT	A	1386	-	1/1/8/9	1/10/38/38	0/2/2/2
3	QBT	D	1384	-	1/1/8/9	2/10/38/38	0/2/2/2
3	QBT	F	1386	-	1/1/8/9	5/10/38/38	0/2/2/2
3	QBT	E	1387	-	1/1/8/9	3/10/38/38	0/2/2/2
3	QBT	C	1386	-	1/1/8/9	2/10/38/38	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1385	QBT	C6-N1	-11.00	1.33	1.46
3	A	1386	QBT	C6-N1	-10.56	1.34	1.46
3	C	1386	QBT	C6-N1	-10.39	1.34	1.46
3	E	1387	QBT	C6-N1	-10.17	1.34	1.46
3	F	1386	QBT	C6-N1	-9.88	1.34	1.46
3	D	1384	QBT	C6-N1	-9.49	1.35	1.46
3	A	1386	QBT	C2-N1	4.87	1.42	1.35
3	B	1385	QBT	C2-N1	4.76	1.42	1.35
3	D	1384	QBT	C2-N1	4.58	1.42	1.35
3	E	1387	QBT	C2-N1	4.57	1.41	1.35
3	C	1386	QBT	C2-N1	4.48	1.41	1.35
3	E	1387	QBT	C6-C5	-4.36	1.38	1.51
3	B	1385	QBT	C6-C5	-4.31	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1384	QBT	C6-C5	-4.18	1.39	1.51
3	F	1386	QBT	C6-C5	-4.05	1.39	1.51
3	A	1386	QBT	C6-C5	-3.82	1.40	1.51
3	F	1386	QBT	C2-N1	3.80	1.40	1.35
3	C	1386	QBT	C6-C5	-3.75	1.40	1.51
3	B	1385	QBT	C4-N3	-2.57	1.32	1.37
3	E	1387	QBT	C4-N3	-2.57	1.32	1.37
3	A	1386	QBT	C4-N3	-2.56	1.32	1.37
3	F	1386	QBT	C4-N3	-2.43	1.32	1.37
3	E	1387	QBT	O2-C2	2.25	1.27	1.23
2	E	1386	PO4	P-O4	-2.20	1.48	1.54
2	E	1386	PO4	P-O2	-2.07	1.48	1.54
3	A	1386	QBT	C2-N3	-2.03	1.34	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1386	QBT	N3-C2-N1	5.56	122.24	116.65
3	F	1386	QBT	C4-N3-C2	-5.16	120.55	126.83
3	C	1386	QBT	C4-N3-C2	-5.02	120.71	126.83
3	D	1384	QBT	C4-N3-C2	-4.66	121.15	126.83
3	D	1384	QBT	N3-C2-N1	4.64	121.31	116.65
3	F	1386	QBT	N3-C2-N1	4.53	121.20	116.65
3	A	1386	QBT	N3-C2-N1	4.48	121.15	116.65
3	B	1385	QBT	C4-N3-C2	-4.45	121.41	126.83
3	C	1386	QBT	C5M-C5-C6	4.40	122.20	112.05
3	B	1385	QBT	N3-C2-N1	4.37	121.04	116.65
3	F	1386	QBT	C5M-C5-C6	4.24	121.83	112.05
3	F	1386	QBT	O2-C2-N1	-4.06	118.22	123.10
3	A	1386	QBT	C5M-C5-C6	3.91	121.07	112.05
3	A	1386	QBT	C4-N3-C2	-3.76	122.25	126.83
3	E	1387	QBT	C5M-C5-C6	3.60	120.36	112.05
3	E	1387	QBT	C4-N3-C2	-3.56	122.49	126.83
3	B	1385	QBT	C5M-C5-C6	3.48	120.09	112.05
2	A	1385	PO4	O3-P-O2	3.46	118.69	107.91
3	D	1384	QBT	O2-C2-N1	-3.42	119.00	123.10
3	D	1384	QBT	C5M-C5-C6	3.36	119.81	112.05
3	E	1387	QBT	N3-C2-N1	3.21	119.88	116.65
3	C	1386	QBT	O2-C2-N1	-3.05	119.44	123.10
2	C	1385	PO4	O4-P-O2	2.86	116.81	107.91
3	A	1386	QBT	C2'-C1'-N1	2.66	118.75	115.59
3	F	1386	QBT	C2'-C1'-N1	-2.66	112.43	115.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1384	PO4	O3-P-O1	-2.53	102.00	110.95
2	A	1385	PO4	O4-P-O3	-2.45	100.29	107.91
2	A	1385	PO4	O2-P-O1	-2.43	102.36	110.95
3	C	1386	QBT	C6-C5-C4	2.42	118.48	111.53
3	D	1384	QBT	C6-C5-C4	2.39	118.38	111.53
3	B	1385	QBT	C6-C5-C4	2.37	118.33	111.53
3	D	1384	QBT	O3P-P-O1P	2.36	116.64	107.80
2	D	1383	PO4	O3-P-O1	-2.23	103.08	110.95
3	C	1386	QBT	O3P-P-O1P	2.21	116.10	107.80
2	E	1386	PO4	O4-P-O1	-2.20	103.18	110.95
3	A	1386	QBT	C6-C5-C4	2.18	117.78	111.53
3	E	1387	QBT	C6-C5-C4	2.17	117.77	111.53
3	F	1386	QBT	O3P-P-O5'	-2.17	101.01	106.67
3	A	1386	QBT	O5'-C5'-C4'	2.16	116.36	108.99
3	B	1385	QBT	O2-C2-N1	-2.15	120.51	123.10
3	A	1386	QBT	O2-C2-N3	-2.15	117.53	121.49
3	D	1384	QBT	O1P-P-O5'	-2.12	101.14	106.67
3	F	1386	QBT	C6-C5-C4	2.09	117.52	111.53

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1386	QBT	C5
3	B	1385	QBT	C5
3	C	1386	QBT	C5
3	D	1384	QBT	C5
3	E	1387	QBT	C5
3	F	1386	QBT	C5

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1387	QBT	C5'-O5'-P-O1P
3	E	1387	QBT	C5'-O5'-P-O3P
3	F	1386	QBT	C5'-O5'-P-O1P
3	F	1386	QBT	C5'-O5'-P-O2P
3	F	1386	QBT	C5'-O5'-P-O3P
3	F	1386	QBT	O4'-C4'-C5'-O5'
3	F	1386	QBT	C3'-C4'-C5'-O5'
3	B	1385	QBT	C3'-C4'-C5'-O5'
3	C	1386	QBT	C3'-C4'-C5'-O5'
3	B	1385	QBT	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

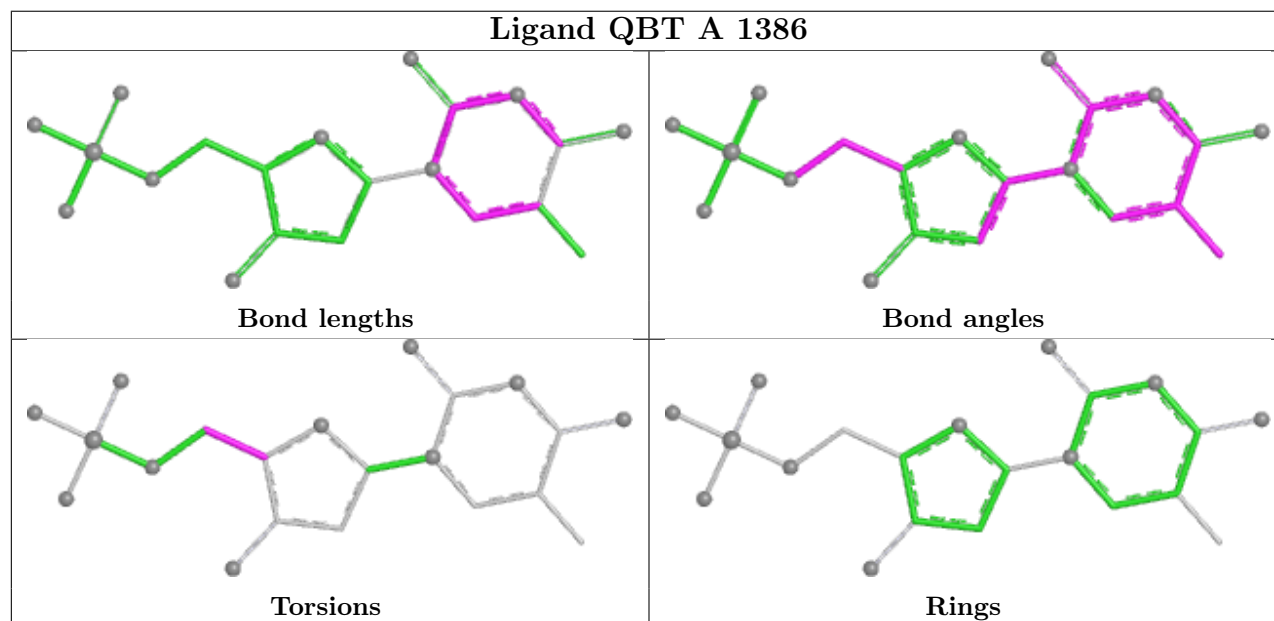
Mol	Chain	Res	Type	Atoms
3	C	1386	QBT	O4'-C4'-C5'-O5'
3	D	1384	QBT	C3'-C4'-C5'-O5'
3	D	1384	QBT	O4'-C4'-C5'-O5'
3	E	1387	QBT	C5'-O5'-P-O2P
3	A	1386	QBT	O4'-C4'-C5'-O5'

There are no ring outliers.

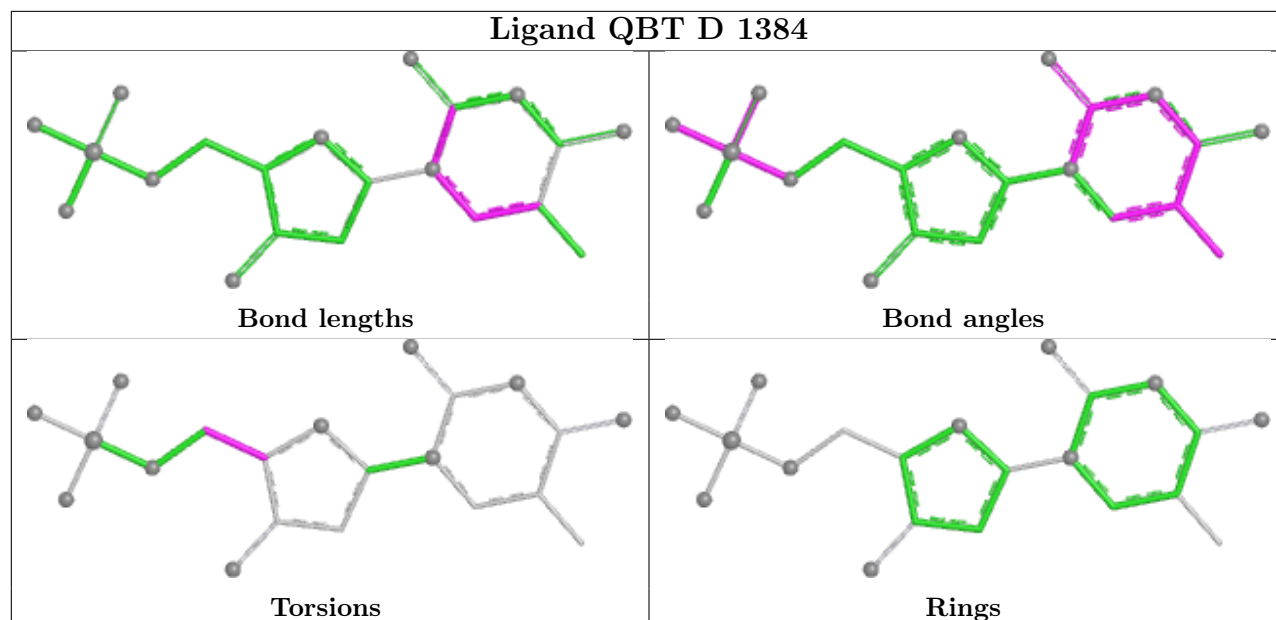
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1386	QBT	3	0
3	C	1386	QBT	1	0

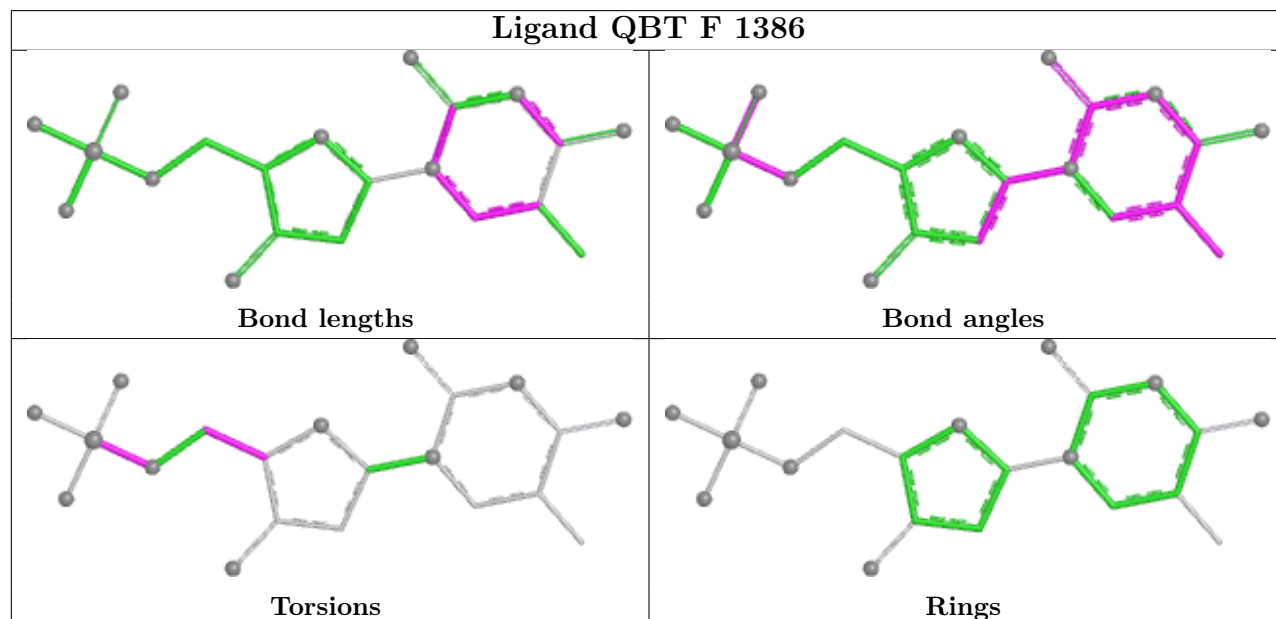
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

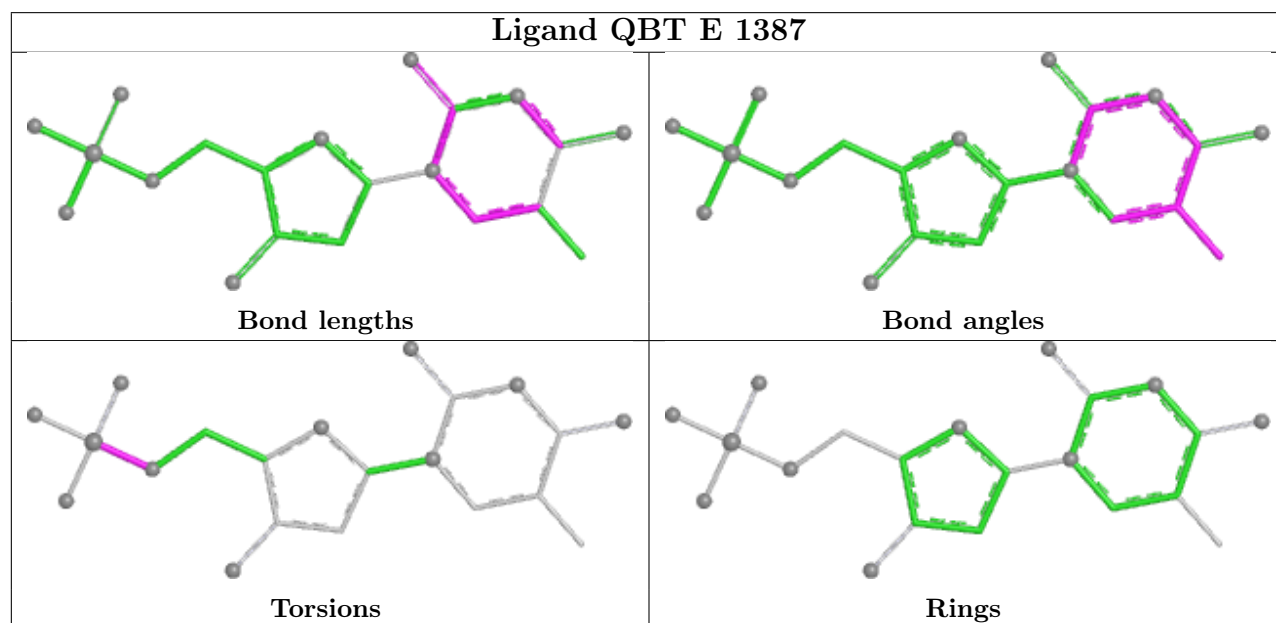
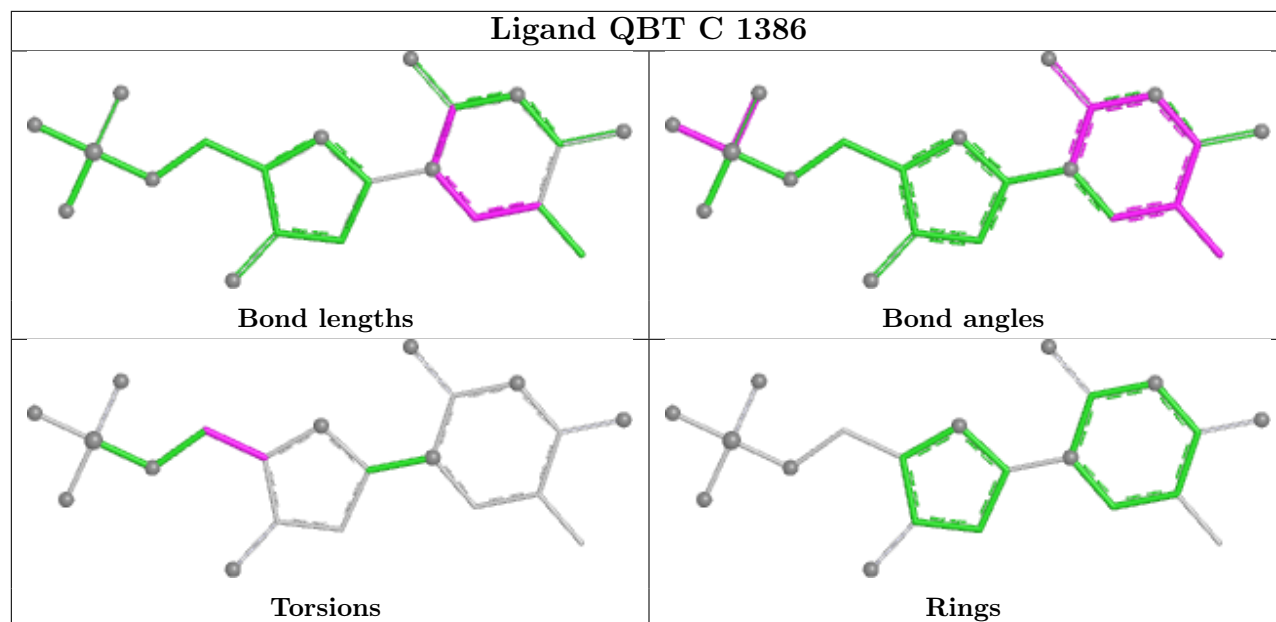


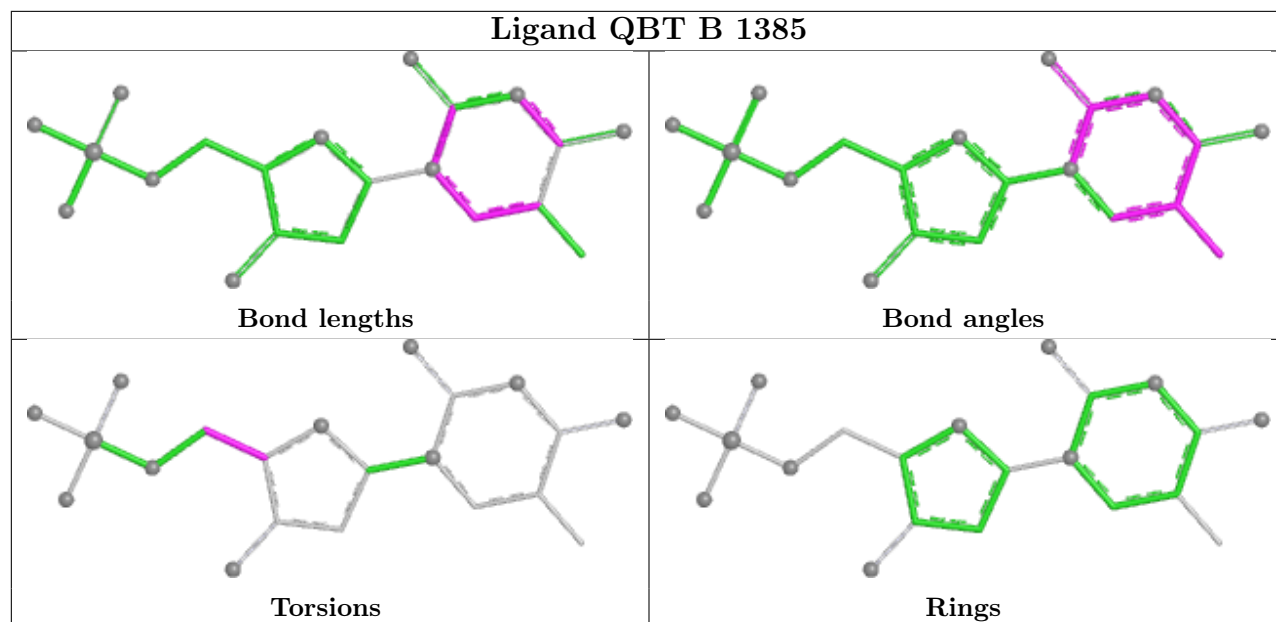
Ligand QBT D 1384



Ligand QBT F 1386







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	165/183 (90%)	0.05	7 (4%) 40 32	41, 63, 102, 130	0
1	B	164/183 (89%)	0.17	4 (2%) 59 49	46, 69, 104, 139	0
1	C	164/183 (89%)	0.45	8 (4%) 35 27	50, 81, 111, 141	0
1	D	161/183 (87%)	0.28	9 (5%) 30 23	41, 66, 119, 141	0
1	E	167/183 (91%)	-0.10	5 (2%) 52 42	33, 57, 99, 125	0
1	F	167/183 (91%)	-0.02	5 (2%) 52 42	33, 53, 90, 136	0
All	All	988/1098 (89%)	0.14	38 (3%) 44 35	33, 65, 109, 141	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	384	MET	5.3
1	D	359	ASP	5.0
1	C	384	MET	4.9
1	D	358	SER	4.3
1	D	203	ALA	3.9
1	A	384	MET	3.6
1	E	385	ALA	3.6
1	C	292	ASP	3.5
1	A	204	HIS	3.4
1	A	272	VAL	3.2
1	B	271	ASP	3.2
1	F	246	ARG	3.2
1	D	204	HIS	3.2
1	C	242	THR	3.1
1	E	384	MET	3.0
1	F	359	ASP	3.0
1	B	245	THR	3.0
1	B	292	ASP	2.9
1	C	284	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	363	LEU	2.9
1	D	205	GLY	2.8
1	D	382	ARG	2.8
1	A	270	HIS	2.8
1	E	272	VAL	2.7
1	E	270	HIS	2.7
1	A	260	LEU	2.5
1	C	283	ALA	2.4
1	D	316	TYR	2.4
1	B	264	VAL	2.4
1	C	270	HIS	2.3
1	E	204	HIS	2.3
1	F	204	HIS	2.3
1	D	318	GLN	2.2
1	A	264	VAL	2.2
1	F	383	ASN	2.1
1	C	272	VAL	2.1
1	C	307	VAL	2.1
1	A	269	LEU	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.

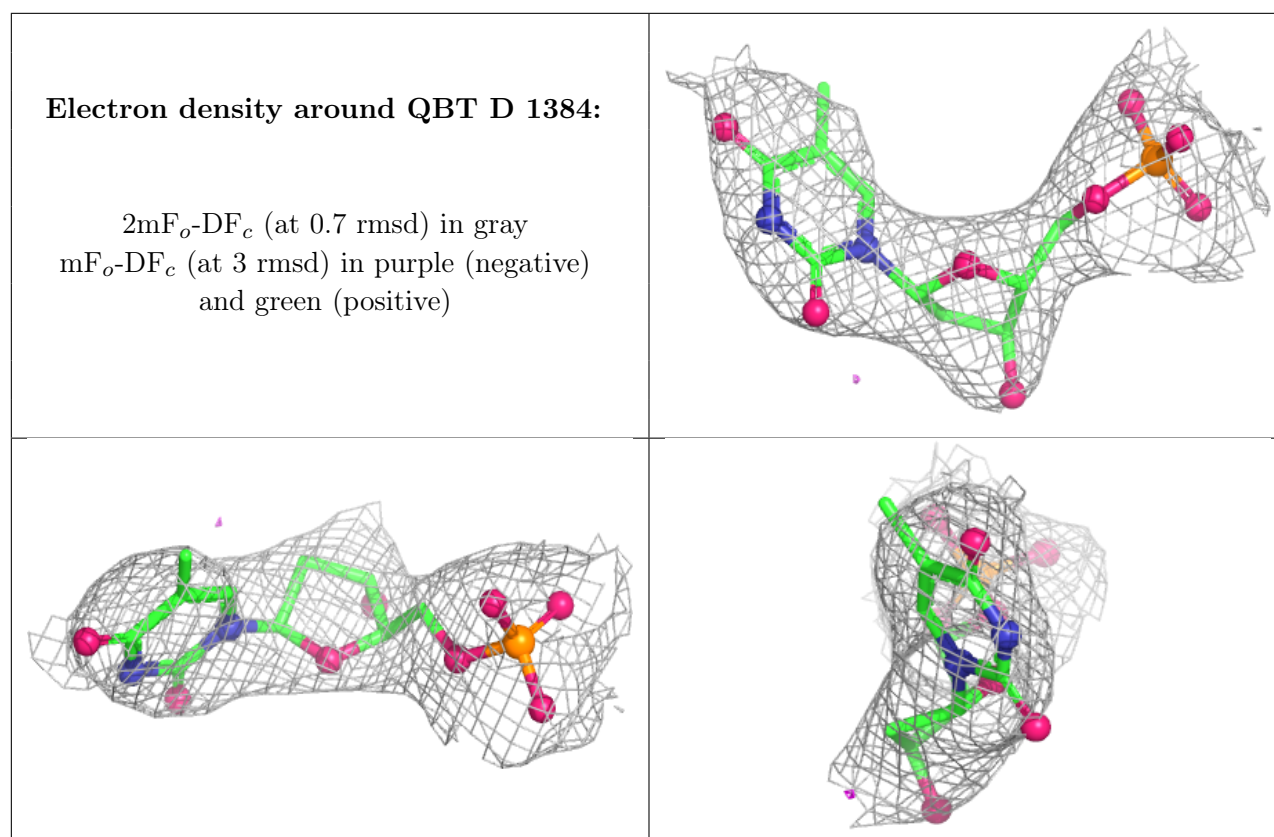
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QBT	D	1384	21/21	0.91	0.08	71,82,93,105	0
3	QBT	C	1386	21/21	0.92	0.09	59,68,89,109	0
3	QBT	B	1385	21/21	0.92	0.08	50,55,79,89	0
3	QBT	F	1386	21/21	0.94	0.08	45,51,72,86	0

Continued on next page...

Continued from previous page...

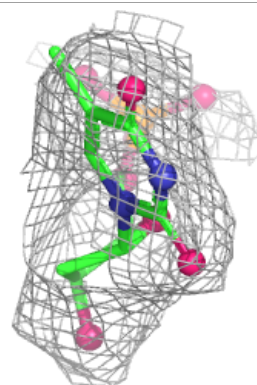
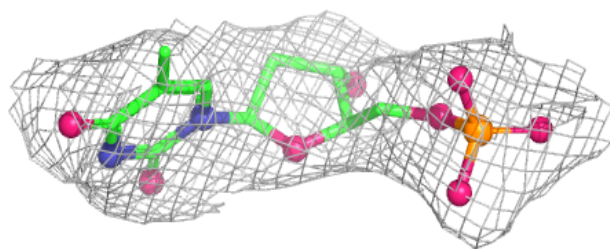
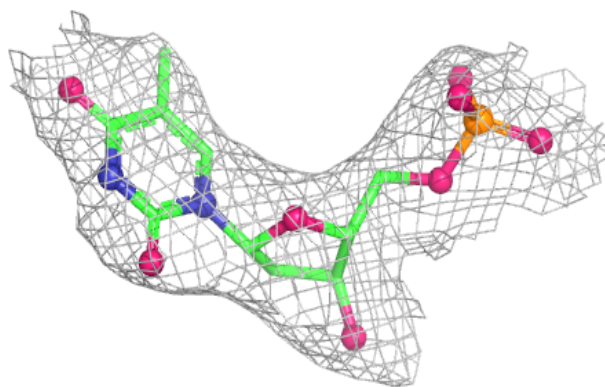
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QBT	E	1387	21/21	0.95	0.07	40,50,62,77	0
3	QBT	A	1386	21/21	0.95	0.07	43,50,65,85	0
2	PO4	C	1385	5/5	0.96	0.07	59,61,65,65	0
2	PO4	D	1383	5/5	0.97	0.04	55,60,62,62	0
2	PO4	B	1384	5/5	0.98	0.05	43,46,51,62	0
2	PO4	A	1385	5/5	0.99	0.04	41,44,52,54	0
2	PO4	E	1386	5/5	0.99	0.04	37,39,40,43	0
2	PO4	F	1385	5/5	0.99	0.04	36,39,40,44	0
4	ZN	C	1387	1/1	0.99	0.05	83,83,83,83	0
4	ZN	D	1385	1/1	0.99	0.03	86,86,86,86	0
4	ZN	F	1387	1/1	0.99	0.02	58,58,58,58	0
4	ZN	B	1386	1/1	1.00	0.02	72,72,72,72	0
4	ZN	E	1388	1/1	1.00	0.02	56,56,56,56	0
4	ZN	A	1387	1/1	1.00	0.02	58,58,58,58	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.

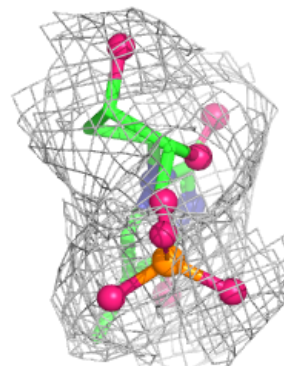
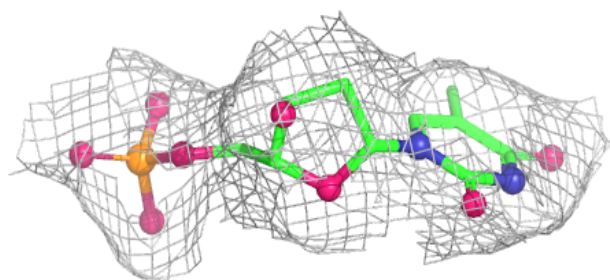
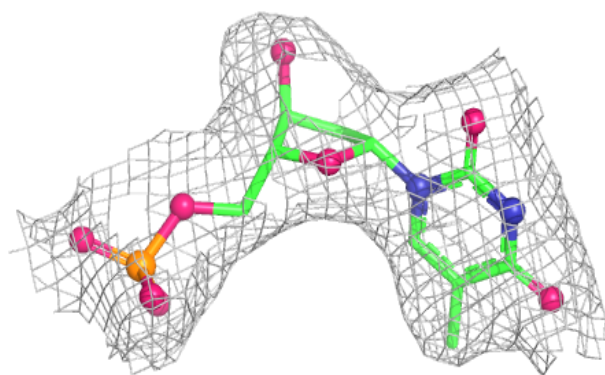


Electron density around QBT C 1386:

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

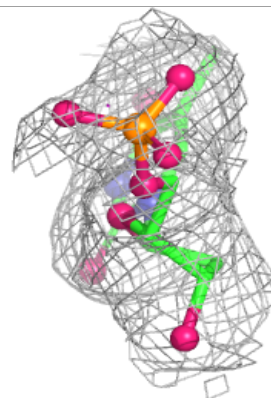
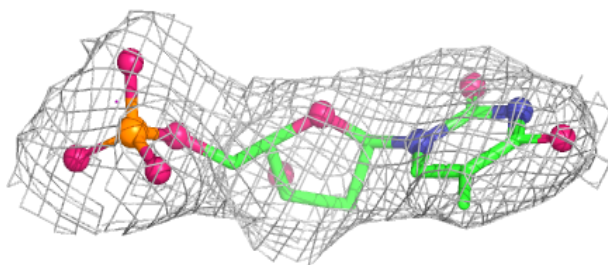
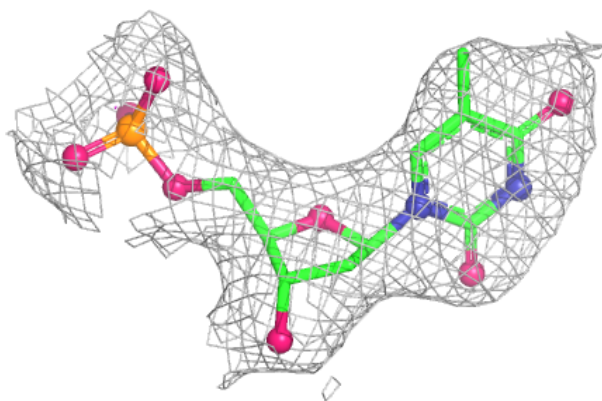
**Electron density around QBT B 1385:**

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

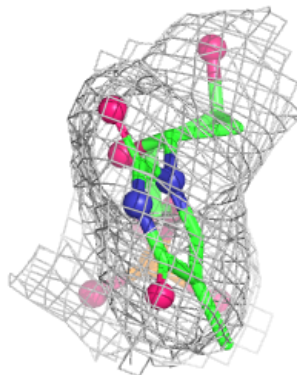
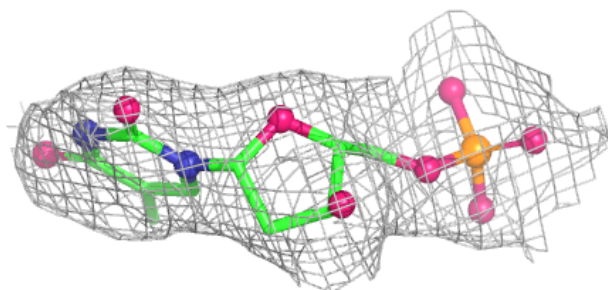
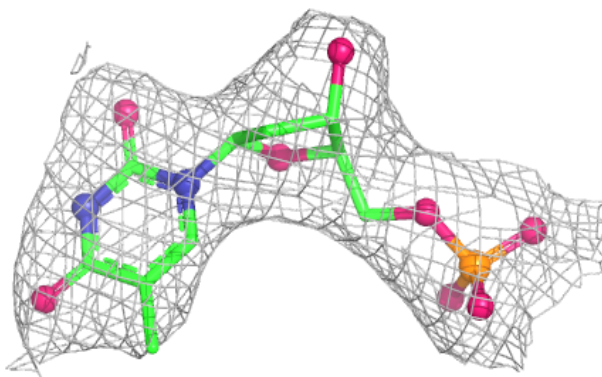


Electron density around QBT F 1386:

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

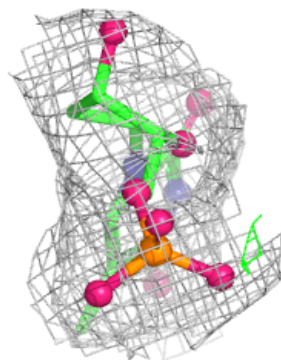
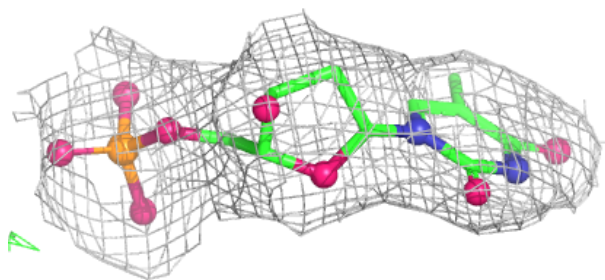
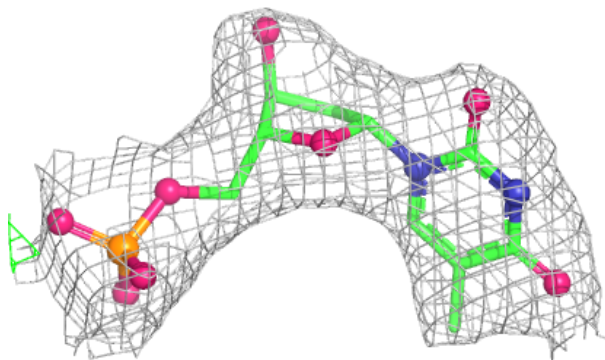
**Electron density around QBT E 1387:**

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



Electron density around QBT A 1386:

$2mF_o - DF_c$ (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.