wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 11:26 AM UTC

PDB ID	:	4XSC / pdb_00004xsc
Title	:	Complex structure of thymidylate synthase from varicella zoster virus with a phosphorylated BVDU
Authors	:	Hew, K.
Deposited on	:	2015-01-22
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

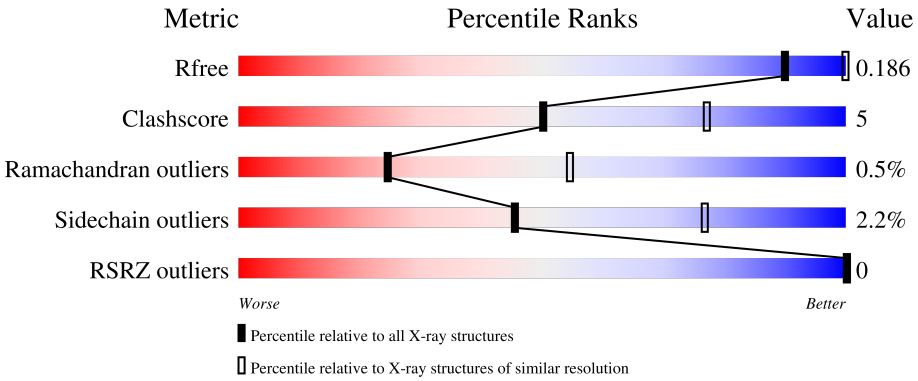
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 <=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	311	70% 14% 15%
1	B	311	79% 13% 9%
1	C	311	74% 10% 15%
1	D	311	76% 13% •• 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9025 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2127	1366	368	383	10			
1	B	284	Total	C	N	O	S	0	0	0
			2303	1481	403	409	10			
1	C	264	Total	C	N	O	S	0	0	0
			2135	1373	369	383	10			
1	D	282	Total	C	N	O	S	0	0	0
			2288	1470	401	407	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q4JQW2
A	-14	HIS	-	expression tag	UNP Q4JQW2
A	-13	HIS	-	expression tag	UNP Q4JQW2
A	-12	HIS	-	expression tag	UNP Q4JQW2
A	-11	HIS	-	expression tag	UNP Q4JQW2
A	-10	HIS	-	expression tag	UNP Q4JQW2
A	-9	HIS	-	expression tag	UNP Q4JQW2
A	-8	SER	-	expression tag	UNP Q4JQW2
A	-7	SER	-	expression tag	UNP Q4JQW2
A	-6	GLY	-	expression tag	UNP Q4JQW2
A	-5	VAL	-	expression tag	UNP Q4JQW2
A	-4	ASP	-	expression tag	UNP Q4JQW2
A	-3	LEU	-	expression tag	UNP Q4JQW2
A	-2	GLY	-	expression tag	UNP Q4JQW2
A	-1	THR	-	expression tag	UNP Q4JQW2
A	0	GLU	-	expression tag	UNP Q4JQW2
A	1	ASN	-	expression tag	UNP Q4JQW2
A	2	LEU	-	expression tag	UNP Q4JQW2
A	3	TYR	-	expression tag	UNP Q4JQW2
A	4	PHE	-	expression tag	UNP Q4JQW2
A	5	GLN	-	expression tag	UNP Q4JQW2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	SER	-	expression tag	UNP Q4JQW2
A	7	MET	-	expression tag	UNP Q4JQW2
B	-15	MET	-	initiating methionine	UNP Q4JQW2
B	-14	HIS	-	expression tag	UNP Q4JQW2
B	-13	HIS	-	expression tag	UNP Q4JQW2
B	-12	HIS	-	expression tag	UNP Q4JQW2
B	-11	HIS	-	expression tag	UNP Q4JQW2
B	-10	HIS	-	expression tag	UNP Q4JQW2
B	-9	HIS	-	expression tag	UNP Q4JQW2
B	-8	SER	-	expression tag	UNP Q4JQW2
B	-7	SER	-	expression tag	UNP Q4JQW2
B	-6	GLY	-	expression tag	UNP Q4JQW2
B	-5	VAL	-	expression tag	UNP Q4JQW2
B	-4	ASP	-	expression tag	UNP Q4JQW2
B	-3	LEU	-	expression tag	UNP Q4JQW2
B	-2	GLY	-	expression tag	UNP Q4JQW2
B	-1	THR	-	expression tag	UNP Q4JQW2
B	0	GLU	-	expression tag	UNP Q4JQW2
B	1	ASN	-	expression tag	UNP Q4JQW2
B	2	LEU	-	expression tag	UNP Q4JQW2
B	3	TYR	-	expression tag	UNP Q4JQW2
B	4	PHE	-	expression tag	UNP Q4JQW2
B	5	GLN	-	expression tag	UNP Q4JQW2
B	6	SER	-	expression tag	UNP Q4JQW2
B	7	MET	-	expression tag	UNP Q4JQW2
C	-15	MET	-	initiating methionine	UNP Q4JQW2
C	-14	HIS	-	expression tag	UNP Q4JQW2
C	-13	HIS	-	expression tag	UNP Q4JQW2
C	-12	HIS	-	expression tag	UNP Q4JQW2
C	-11	HIS	-	expression tag	UNP Q4JQW2
C	-10	HIS	-	expression tag	UNP Q4JQW2
C	-9	HIS	-	expression tag	UNP Q4JQW2
C	-8	SER	-	expression tag	UNP Q4JQW2
C	-7	SER	-	expression tag	UNP Q4JQW2
C	-6	GLY	-	expression tag	UNP Q4JQW2
C	-5	VAL	-	expression tag	UNP Q4JQW2
C	-4	ASP	-	expression tag	UNP Q4JQW2
C	-3	LEU	-	expression tag	UNP Q4JQW2
C	-2	GLY	-	expression tag	UNP Q4JQW2
C	-1	THR	-	expression tag	UNP Q4JQW2
C	0	GLU	-	expression tag	UNP Q4JQW2
C	1	ASN	-	expression tag	UNP Q4JQW2

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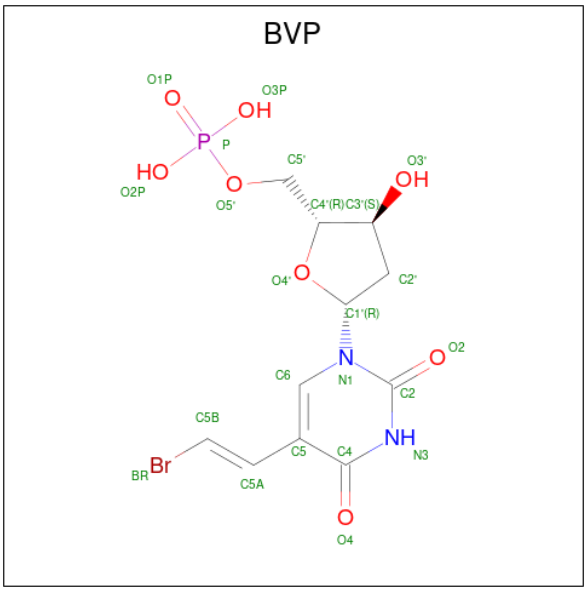
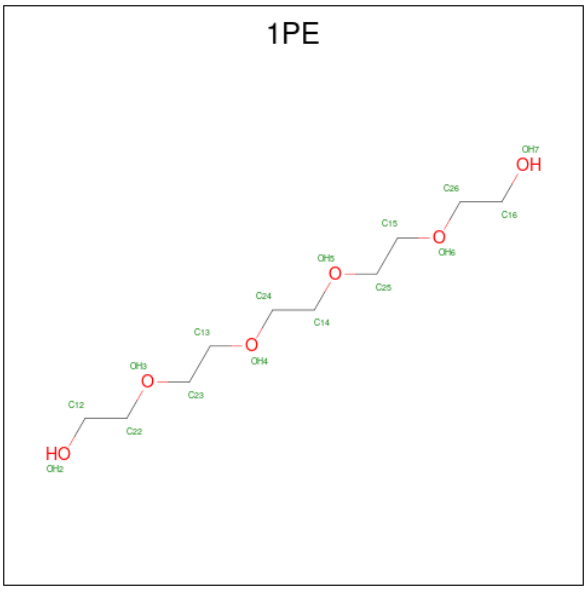
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LEU	-	expression tag	UNP Q4JQW2
C	3	TYR	-	expression tag	UNP Q4JQW2
C	4	PHE	-	expression tag	UNP Q4JQW2
C	5	GLN	-	expression tag	UNP Q4JQW2
C	6	SER	-	expression tag	UNP Q4JQW2
C	7	MET	-	expression tag	UNP Q4JQW2
D	-15	MET	-	initiating methionine	UNP Q4JQW2
D	-14	HIS	-	expression tag	UNP Q4JQW2
D	-13	HIS	-	expression tag	UNP Q4JQW2
D	-12	HIS	-	expression tag	UNP Q4JQW2
D	-11	HIS	-	expression tag	UNP Q4JQW2
D	-10	HIS	-	expression tag	UNP Q4JQW2
D	-9	HIS	-	expression tag	UNP Q4JQW2
D	-8	SER	-	expression tag	UNP Q4JQW2
D	-7	SER	-	expression tag	UNP Q4JQW2
D	-6	GLY	-	expression tag	UNP Q4JQW2
D	-5	VAL	-	expression tag	UNP Q4JQW2
D	-4	ASP	-	expression tag	UNP Q4JQW2
D	-3	LEU	-	expression tag	UNP Q4JQW2
D	-2	GLY	-	expression tag	UNP Q4JQW2
D	-1	THR	-	expression tag	UNP Q4JQW2
D	0	GLU	-	expression tag	UNP Q4JQW2
D	1	ASN	-	expression tag	UNP Q4JQW2
D	2	LEU	-	expression tag	UNP Q4JQW2
D	3	TYR	-	expression tag	UNP Q4JQW2
D	4	PHE	-	expression tag	UNP Q4JQW2
D	5	GLN	-	expression tag	UNP Q4JQW2
D	6	SER	-	expression tag	UNP Q4JQW2
D	7	MET	-	expression tag	UNP Q4JQW2

- Molecule 2 is (E)-5-(2-BROMOVINYL)-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: BVP) (formula: $C_{11}H_{14}BrN_2O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br C N O P 23 1 11 2 8 1	0	0
2	B	1	Total C N O P 20 9 2 8 1	0	0
2	C	1	Total Br C N O P 23 1 11 2 8 1	0	0
2	D	1	Total C N O P 20 9 2 8 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	B	1	Total C O 10 6 4	0	0
3	C	1	Total C O 16 10 6	0	0
3	D	1	Total C O 10 6 4	0	0

- Molecule 4 is water.

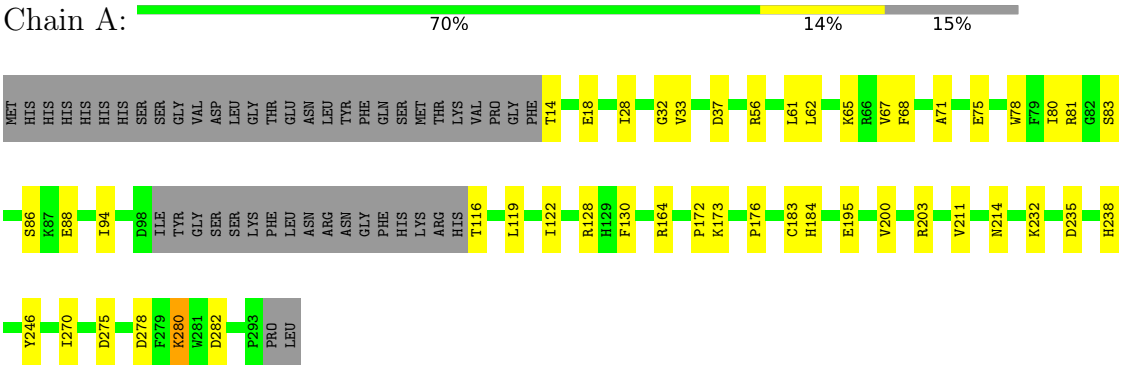
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	4	Total O 4 4	0	0
4	C	9	Total O 9 9	0	0
4	D	13	Total O 13 13	0	0

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.

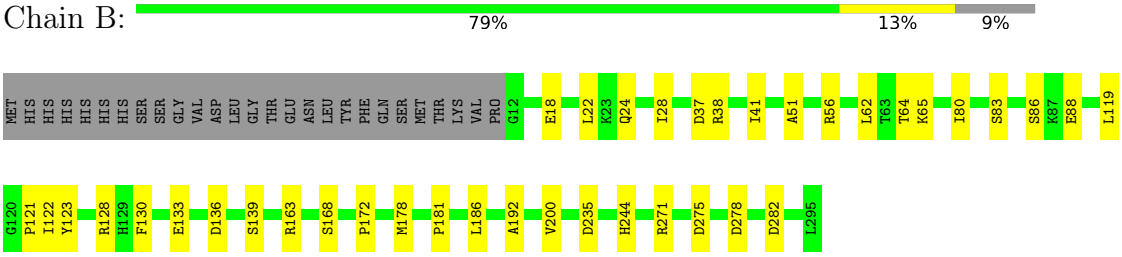
• Molecule 1: Thymidylate synthase

Chain A:



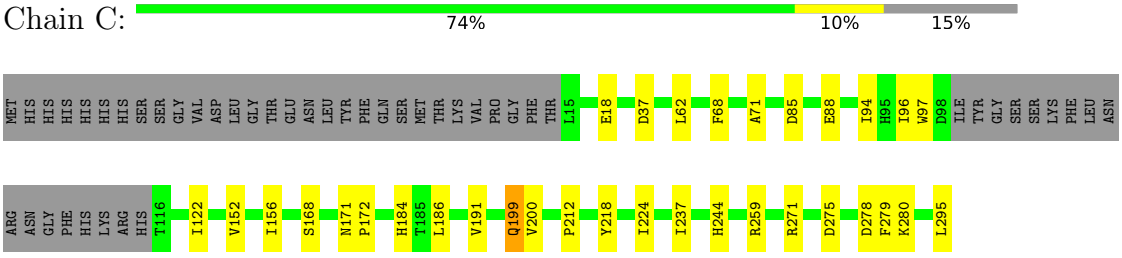
• Molecule 1: Thymidylate synthase

Chain B:



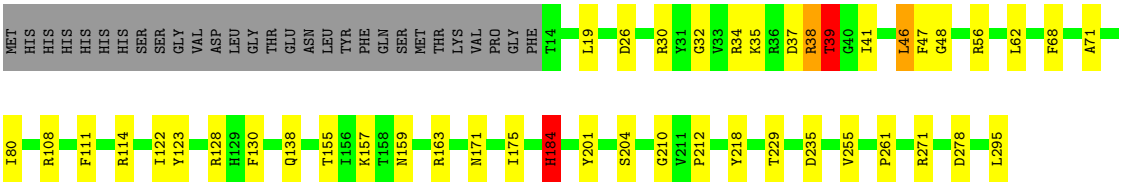
• Molecule 1: Thymidylate synthase

Chain C:



• Molecule 1: Thymidylate synthase

Chain D:


MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET THR LYS VAL PRO GLY PHE T14 L19 D26 R30 Y31 G32 V33 R34 K35 R36 D37 R38 T39 G40 I41 L46 F47 G48 R56 L62 F68 A71
I80 R108 F111 R114 I122 Y123 R128 H129 F130 Q138 T155 I156 K157 T158 N159 R163 N171 I175 H184 Y201 S204 G210 V211 P212 Y218 T229 D235 V255 P261 R271 D278 L295

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	149.51Å 149.51Å 88.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.90 29.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.71-2.90) 99.9 (29.71-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.196 , 0.235 0.154 , 0.186	Depositor DCC
R_{free} test set	2395 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 14.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.270 for -h,-k,l 0.098 for h,-h-k,-l 0.095 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9025	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 1PE, BVP

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	0.32	0/2181	0.74	0/2961
1	B	0.34	0/2365	0.74	0/3208
1	C	0.32	0/2190	0.76	2/2974 (0.1%)
1	D	0.38	0/2349	0.80	2/3187 (0.1%)
All	All	0.34	0/9085	0.76	4/12330 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	38	ARG	N-CA-C	-6.71	103.89	111.07
1	D	184	HIS	CB-CA-C	6.27	121.45	111.73
1	C	171	ASN	CA-C-N	5.12	125.41	119.47
1	C	171	ASN	C-N-CA	5.12	125.41	119.47

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	2127	0	2106	23	0
1	B	2303	0	2280	21	0
1	C	2135	0	2117	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2288	0	2268	38	0
2	A	23	0	11	2	0
2	B	20	0	10	1	0
2	C	23	0	11	1	0
2	D	20	0	10	2	0
3	A	16	0	21	1	0
3	B	10	0	12	0	0
3	C	16	0	21	0	0
3	D	10	0	12	1	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
4	C	9	0	0	0	0
4	D	13	0	0	2	0
All	All	9025	0	8879	94	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.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLN:NE2	1:D:201:TYR:HE2	1.69	0.90
1:D:37:ASP:HB3	1:D:39:THR:HG22	1.61	0.81
1:D:39:THR:HG23	1:D:41:ILE:H	1.46	0.79
1:A:37:ASP:OD1	1:B:163:ARG:NH2	2.18	0.73
1:D:278:ASP:OD2	4:D:1101:HOH:O	2.08	0.71

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	259/311 (83%)	245 (95%)	12 (5%)	2 (1%)	16	44
1	B	282/311 (91%)	266 (94%)	15 (5%)	1 (0%)	30	59
1	C	260/311 (84%)	246 (95%)	13 (5%)	1 (0%)	30	59
1	D	280/311 (90%)	264 (94%)	15 (5%)	1 (0%)	30	59
All	All	1081/1244 (87%)	1021 (94%)	55 (5%)	5 (0%)	24	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	TYR
1	D	39	THR
1	A	68	PHE
1	C	122	ILE
1	A	122	ILE

5.3.2 Protein sidechains (i)

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	231/274 (84%)	224 (97%)	7 (3%)	36	70
1	B	249/274 (91%)	244 (98%)	5 (2%)	48	78
1	C	232/274 (85%)	229 (99%)	3 (1%)	61	86
1	D	248/274 (90%)	242 (98%)	6 (2%)	43	75
All	All	960/1096 (88%)	939 (98%)	21 (2%)	45	77

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	280	LYS
1	D	108	ARG
1	D	295	LEU
1	D	184	HIS
1	D	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	184	HIS
1	D	202	GLN
1	D	249	HIS
1	D	199	GLN
1	B	112	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	1PE	D	1002	-	9,9,15	0.67	0	8,8,14	0.28	0
2	BVP	B	1001	-	21,21,24	3.94	9 (42%)	30,31,35	1.59	5 (16%)
3	1PE	A	1002	-	15,15,15	0.67	0	14,14,14	0.24	0
3	1PE	B	1002	-	9,9,15	0.56	0	8,8,14	0.33	0
2	BVP	A	1001	-	24,24,24	3.59	10 (41%)	32,35,35	1.77	7 (21%)
2	BVP	C	1001	-	24,24,24	3.64	11 (45%)	32,35,35	1.75	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BVP	D	1001	-	21,21,24	3.89	9 (42%)	30,31,35	1.71	5 (16%)
3	1PE	C	1002	-	15,15,15	0.66	0	14,14,14	0.28	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	1PE	D	1002	-	-	2/7/7/13	-
2	BVP	B	1001	-	-	2/10/22/25	0/2/2/2
3	1PE	A	1002	-	-	6/13/13/13	-
3	1PE	B	1002	-	-	4/7/7/13	-
2	BVP	A	1001	-	-	5/13/25/25	0/2/2/2
2	BVP	C	1001	-	-	4/13/25/25	0/2/2/2
2	BVP	D	1001	-	-	2/10/22/25	0/2/2/2
3	1PE	C	1002	-	-	3/13/13/13	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	BVP	O4'-C1'	8.56	1.61	1.42
2	B	1001	BVP	O4'-C1'	8.52	1.61	1.42
2	C	1001	BVP	O4'-C1'	8.44	1.61	1.42
2	D	1001	BVP	O4'-C1'	8.29	1.60	1.42
2	B	1001	BVP	O4'-C4'	-7.41	1.28	1.45

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	BVP	C4-N3-C2	-5.59	120.01	127.34
2	A	1001	BVP	C4-N3-C2	-5.39	120.27	127.34
2	D	1001	BVP	C4-N3-C2	-5.27	120.07	126.61
2	B	1001	BVP	C4-N3-C2	-4.92	120.51	126.61
2	A	1001	BVP	N3-C2-N1	3.86	119.92	114.89

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	BVP	C6-C5-C5A-C5B
2	A	1001	BVP	C4-C5-C5A-C5B
3	A	1002	1PE	OH6-C15-C25-OH5
2	B	1001	BVP	O4'-C4'-C5'-O5'
3	B	1002	1PE	OH4-C13-C23-OH3

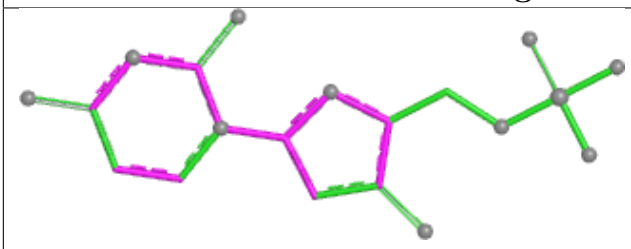
There are no ring outliers.

6 monomers are involved in 7 short contacts:

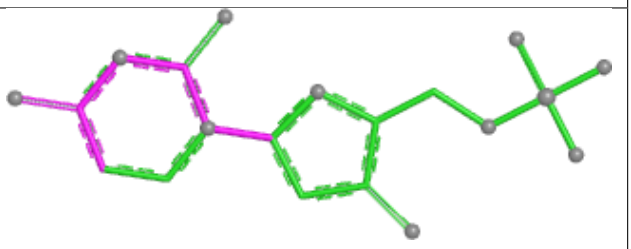
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	1PE	1	0
2	B	1001	BVP	1	0
3	A	1002	1PE	1	0
2	A	1001	BVP	2	0
2	C	1001	BVP	1	0
2	D	1001	BVP	2	0

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 then 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.

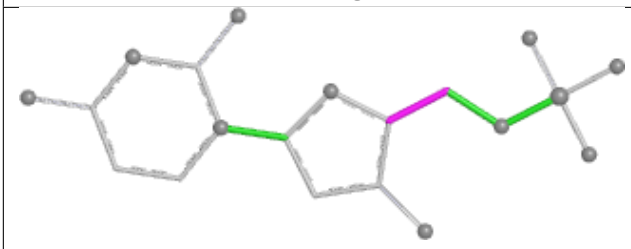
Ligand BVP B 1001



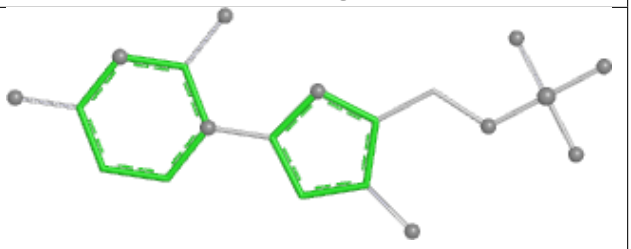
Bond lengths



Bond angles

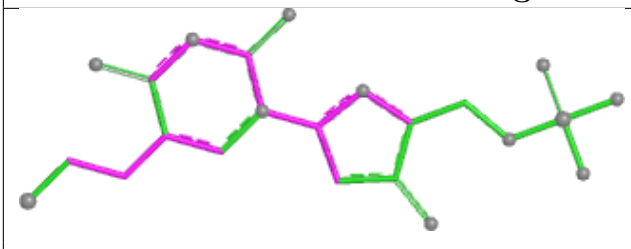


Torsions

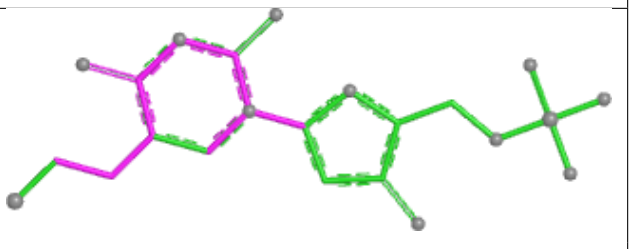


Rings

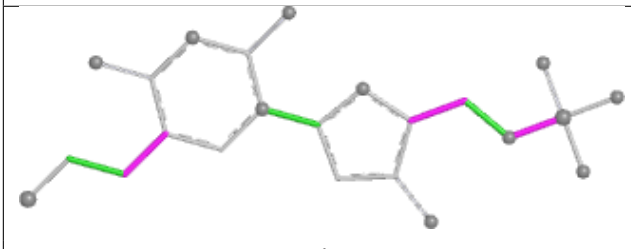
Ligand BVP A 1001



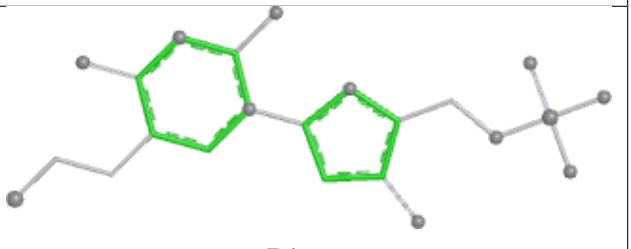
Bond lengths



Bond angles

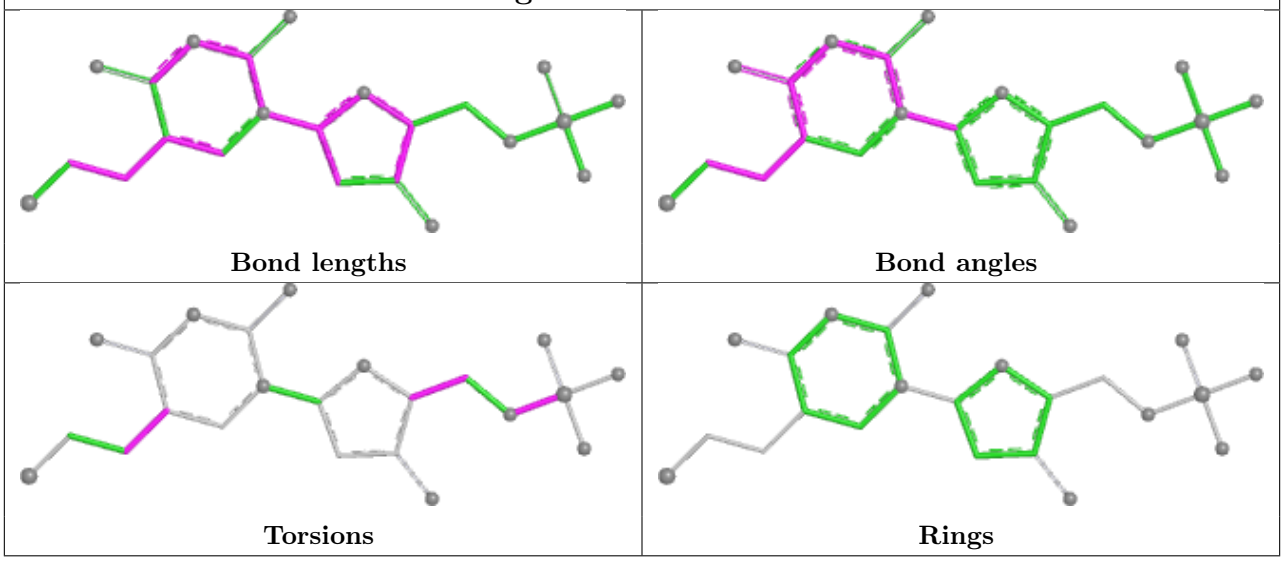


Torsions

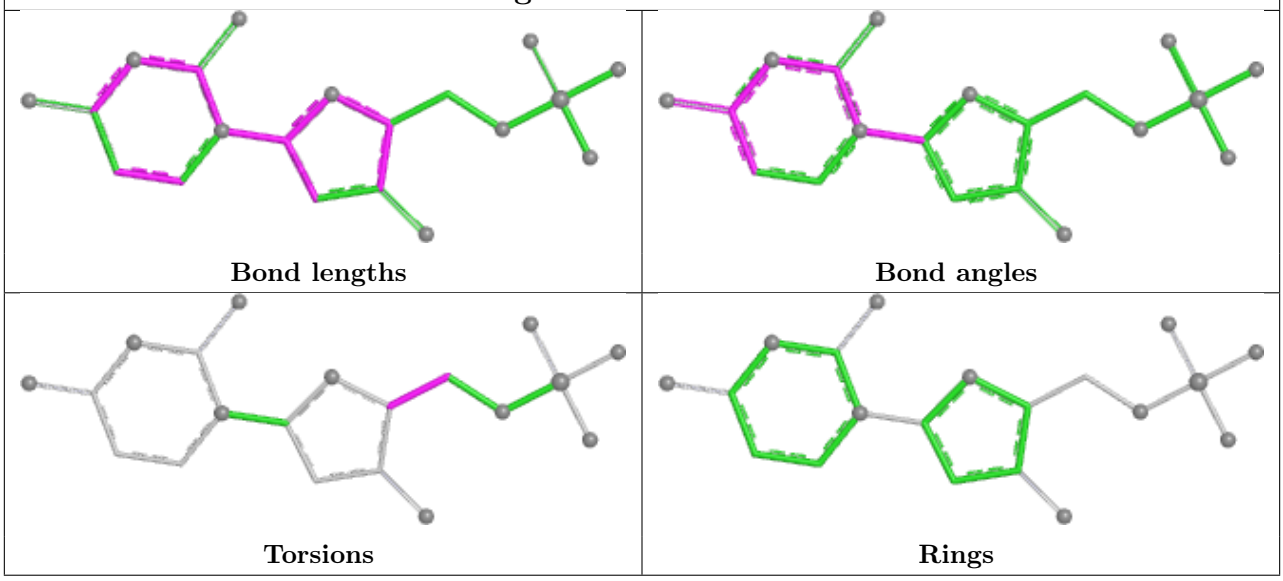


Rings

Ligand BVP C 1001



Ligand BVP D 1001



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, 95^{th} 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	263/311 (84%)	-1.86	0	100	100	22, 37, 56, 76	0
1	B	284/311 (91%)	-1.88	0	100	100	19, 35, 58, 82	0
1	C	264/311 (84%)	-1.86	0	100	100	21, 35, 51, 84	0
1	D	282/311 (90%)	-1.86	0	100	100	19, 35, 58, 85	0
All	All	1093/1244 (87%)	-1.86	0	100	100	19, 36, 57, 85	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	1PE	A	1002	16/16	0.99	0.05	41,63,75,83	0
3	1PE	C	1002	16/16	0.99	0.04	42,57,82,92	0
3	1PE	D	1002	10/16	0.99	0.04	34,53,58,59	0
2	BVP	D	1001	20/23	1.00	0.02	32,45,58,60	0

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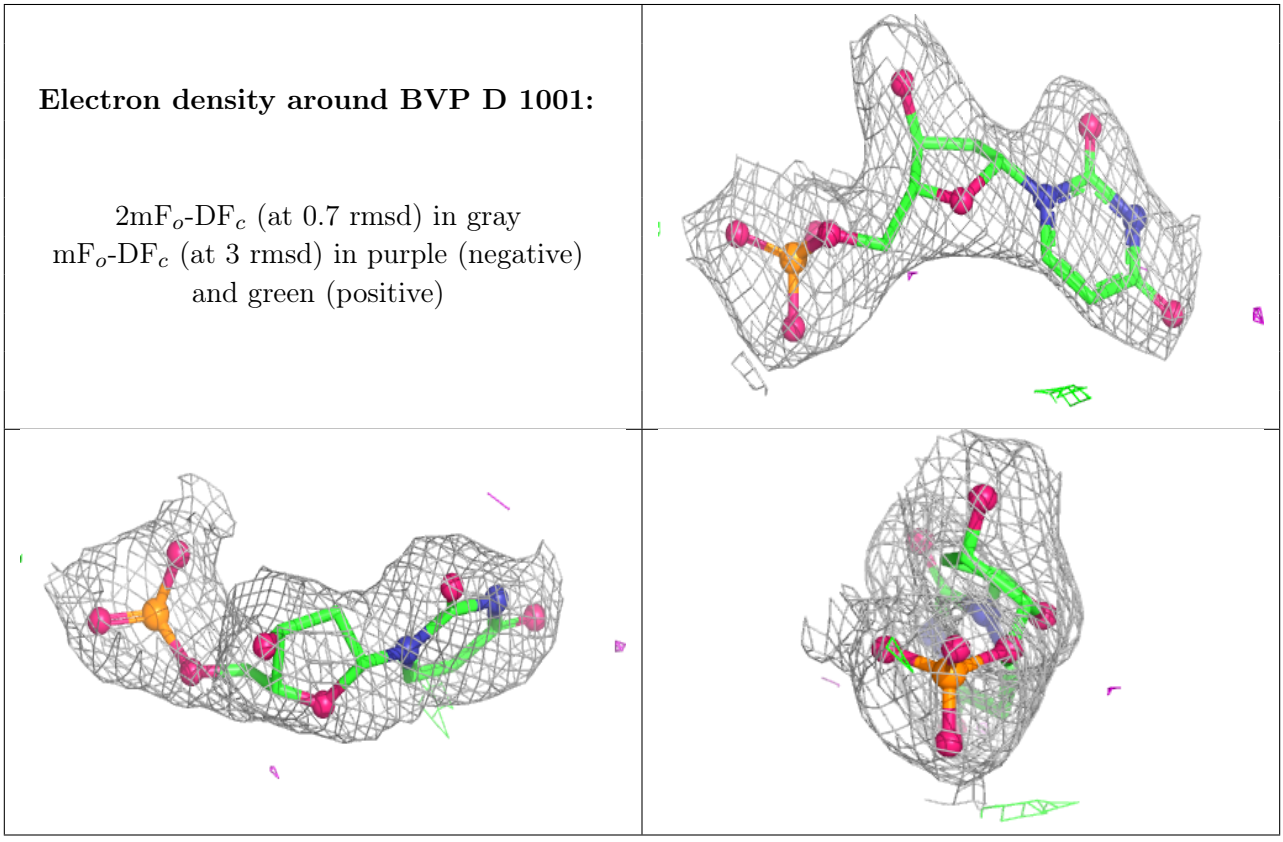
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BVP	A	1001	23/23	1.00	0.03	23,37,61,146	0
3	1PE	B	1002	10/16	1.00	0.04	22,31,49,49	0
2	BVP	B	1001	20/23	1.00	0.02	28,41,54,56	0
2	BVP	C	1001	23/23	1.00	0.02	26,40,74,135	0

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.

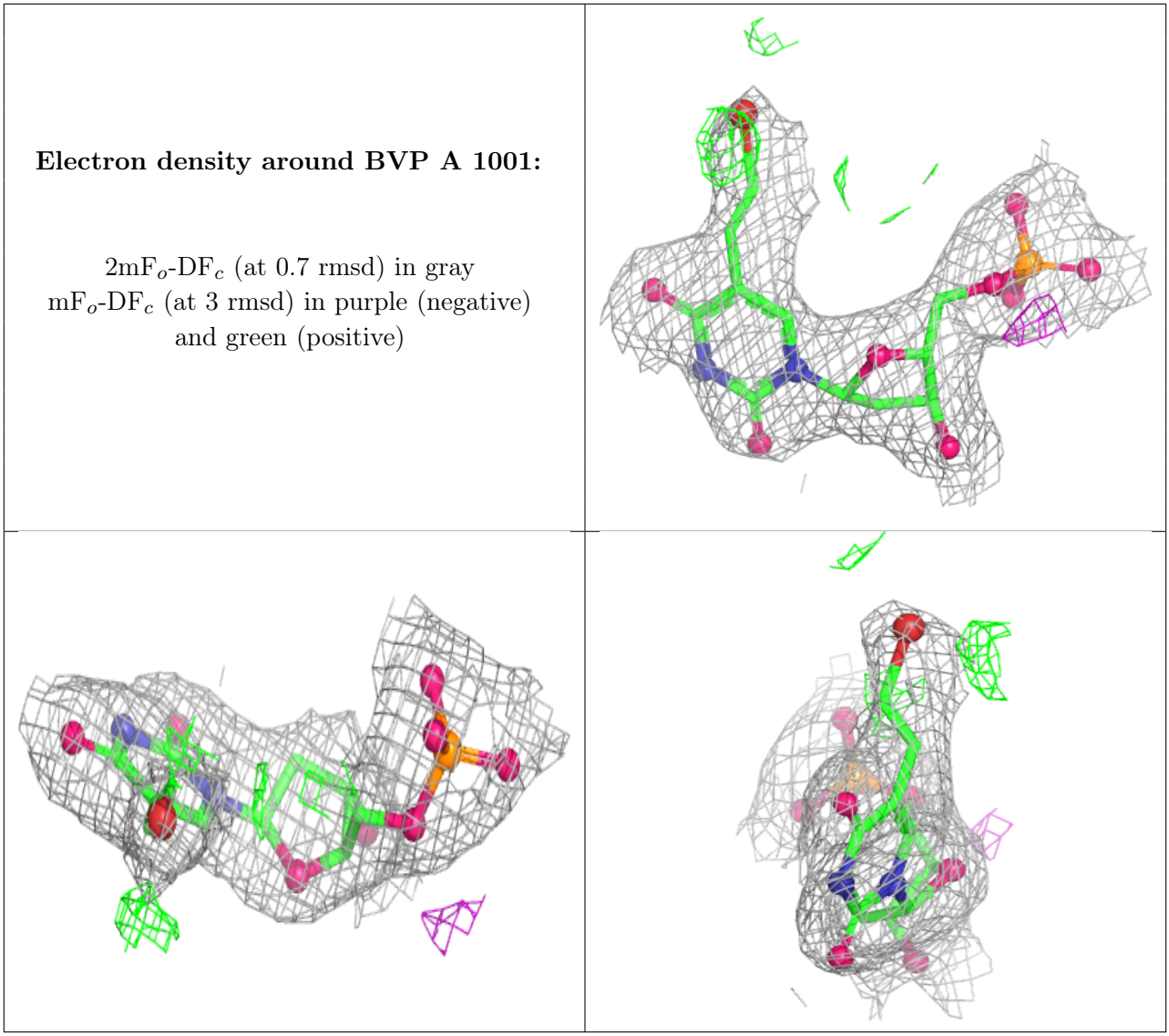
Electron density around BVP D 1001:

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



Electron density around BVP A 1001:

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



Electron density around BVP B 1001:

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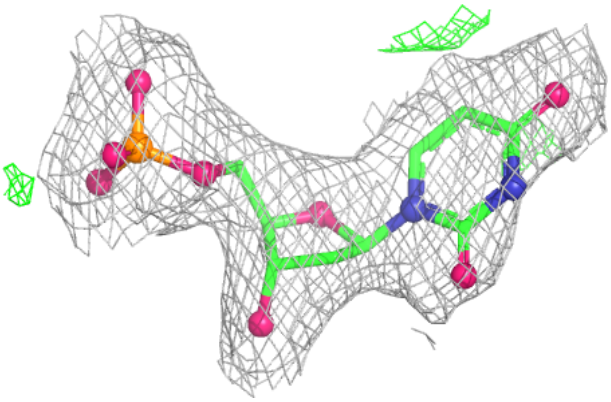
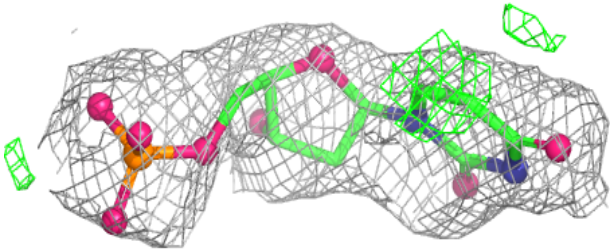
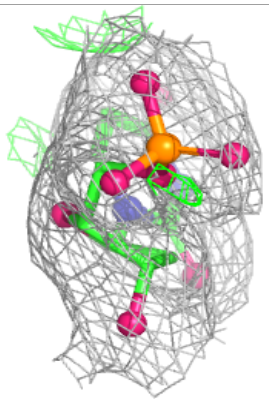
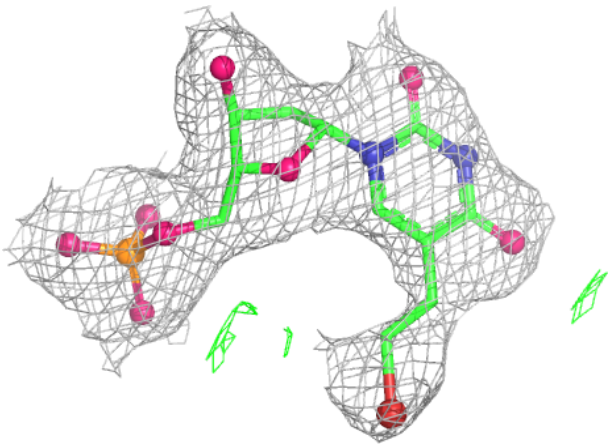


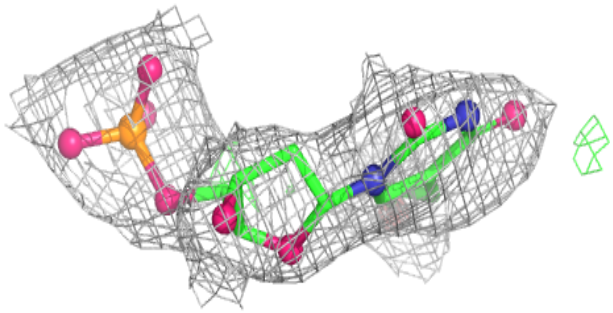


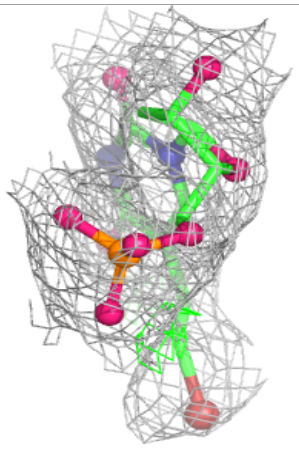


Electron density around BVP C 1001:

$2mF_o$-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.