



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:12 pm BST

PDB ID : 6BHV  
Title : Human PARP-1 bound to NAD<sup>+</sup> analog benzamide adenine dinucleotide (BAD)  
Authors : Pascal, J.M.; Langelier, M.F.  
Deposited on : 2017-10-31  
Resolution : 2.30 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

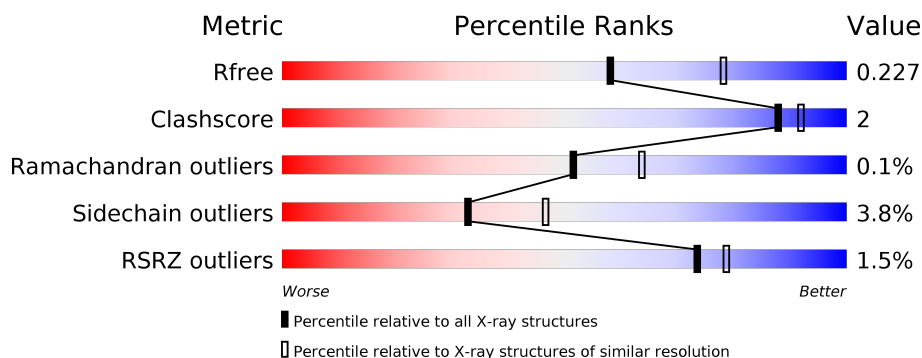
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	271	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 82%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>5%</span> <span>12%</span> </div> </div>
1	B	271	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 6%, green 80%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>80%</span> <span>6%</span> <span>13%</span> </div> </div>
1	C	271	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 7%, green 75%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>75%</span> <span>7%</span> <span>17%</span> </div> </div>
1	D	271	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 80%, yellow 7%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>80%</span> <span>7%</span> <span>12%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7704 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1874	1202	319	347	6			
1	B	237	Total	C	N	O	S	0	1	0
			1877	1205	320	346	6			
1	C	226	Total	C	N	O	S	0	0	0
			1801	1157	307	331	6			
1	D	238	Total	C	N	O	S	0	0	0
			1877	1204	319	348	6			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	742	MET	-	initiating methionine	UNP P09874
A	743	GLY	-	expression tag	UNP P09874
A	744	SER	-	expression tag	UNP P09874
A	745	SER	-	expression tag	UNP P09874
A	746	HIS	-	expression tag	UNP P09874
A	747	HIS	-	expression tag	UNP P09874
A	748	HIS	-	expression tag	UNP P09874
A	749	HIS	-	expression tag	UNP P09874
A	750	HIS	-	expression tag	UNP P09874
A	751	HIS	-	expression tag	UNP P09874
A	752	SER	-	expression tag	UNP P09874
A	753	SER	-	expression tag	UNP P09874
A	754	GLY	-	expression tag	UNP P09874
A	755	LEU	-	expression tag	UNP P09874
A	756	VAL	-	expression tag	UNP P09874
A	757	PRO	-	expression tag	UNP P09874
A	758	ARG	-	expression tag	UNP P09874
A	759	GLY	-	expression tag	UNP P09874
A	760	SER	-	expression tag	UNP P09874
A	761	HIS	-	expression tag	UNP P09874
A	762	MET	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
A	763	THR	-	expression tag	UNP P09874
A	764	LYS	-	expression tag	UNP P09874
A	765	SER	-	expression tag	UNP P09874
A	766	LYS	-	expression tag	UNP P09874
A	767	LEU	-	expression tag	UNP P09874
A	768	PRO	-	expression tag	UNP P09874
A	769	LYS	-	expression tag	UNP P09874
A	770	PRO	-	expression tag	UNP P09874
A	771	VAL	-	expression tag	UNP P09874
A	772	GLN	-	expression tag	UNP P09874
A	773	ASP	-	expression tag	UNP P09874
A	774	LEU	-	expression tag	UNP P09874
A	775	ILE	-	expression tag	UNP P09874
A	776	LYS	-	expression tag	UNP P09874
A	777	MET	-	expression tag	UNP P09874
A	778	ILE	-	expression tag	UNP P09874
A	779	PHE	-	expression tag	UNP P09874
A	780	GLY	-	expression tag	UNP P09874
A	781	SER	-	expression tag	UNP P09874
A	782	GLY	-	expression tag	UNP P09874
A	783	SER	-	expression tag	UNP P09874
A	784	GLY	-	expression tag	UNP P09874
A	785	SER	-	expression tag	UNP P09874
A	786	GLY	-	expression tag	UNP P09874
A	787	GLY	-	expression tag	UNP P09874
B	742	MET	-	initiating methionine	UNP P09874
B	743	GLY	-	expression tag	UNP P09874
B	744	SER	-	expression tag	UNP P09874
B	745	SER	-	expression tag	UNP P09874
B	746	HIS	-	expression tag	UNP P09874
B	747	HIS	-	expression tag	UNP P09874
B	748	HIS	-	expression tag	UNP P09874
B	749	HIS	-	expression tag	UNP P09874
B	750	HIS	-	expression tag	UNP P09874
B	751	HIS	-	expression tag	UNP P09874
B	752	SER	-	expression tag	UNP P09874
B	753	SER	-	expression tag	UNP P09874
B	754	GLY	-	expression tag	UNP P09874
B	755	LEU	-	expression tag	UNP P09874
B	756	VAL	-	expression tag	UNP P09874
B	757	PRO	-	expression tag	UNP P09874
B	758	ARG	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	759	GLY	-	expression tag	UNP P09874
B	760	SER	-	expression tag	UNP P09874
B	761	HIS	-	expression tag	UNP P09874
B	762	MET	-	expression tag	UNP P09874
B	763	THR	-	expression tag	UNP P09874
B	764	LYS	-	expression tag	UNP P09874
B	765	SER	-	expression tag	UNP P09874
B	766	LYS	-	expression tag	UNP P09874
B	767	LEU	-	expression tag	UNP P09874
B	768	PRO	-	expression tag	UNP P09874
B	769	LYS	-	expression tag	UNP P09874
B	770	PRO	-	expression tag	UNP P09874
B	771	VAL	-	expression tag	UNP P09874
B	772	GLN	-	expression tag	UNP P09874
B	773	ASP	-	expression tag	UNP P09874
B	774	LEU	-	expression tag	UNP P09874
B	775	ILE	-	expression tag	UNP P09874
B	776	LYS	-	expression tag	UNP P09874
B	777	MET	-	expression tag	UNP P09874
B	778	ILE	-	expression tag	UNP P09874
B	779	PHE	-	expression tag	UNP P09874
B	780	GLY	-	expression tag	UNP P09874
B	781	SER	-	expression tag	UNP P09874
B	782	GLY	-	expression tag	UNP P09874
B	783	SER	-	expression tag	UNP P09874
B	784	GLY	-	expression tag	UNP P09874
B	785	SER	-	expression tag	UNP P09874
B	786	GLY	-	expression tag	UNP P09874
B	787	GLY	-	expression tag	UNP P09874
C	742	MET	-	initiating methionine	UNP P09874
C	743	GLY	-	expression tag	UNP P09874
C	744	SER	-	expression tag	UNP P09874
C	745	SER	-	expression tag	UNP P09874
C	746	HIS	-	expression tag	UNP P09874
C	747	HIS	-	expression tag	UNP P09874
C	748	HIS	-	expression tag	UNP P09874
C	749	HIS	-	expression tag	UNP P09874
C	750	HIS	-	expression tag	UNP P09874
C	751	HIS	-	expression tag	UNP P09874
C	752	SER	-	expression tag	UNP P09874
C	753	SER	-	expression tag	UNP P09874
C	754	GLY	-	expression tag	UNP P09874

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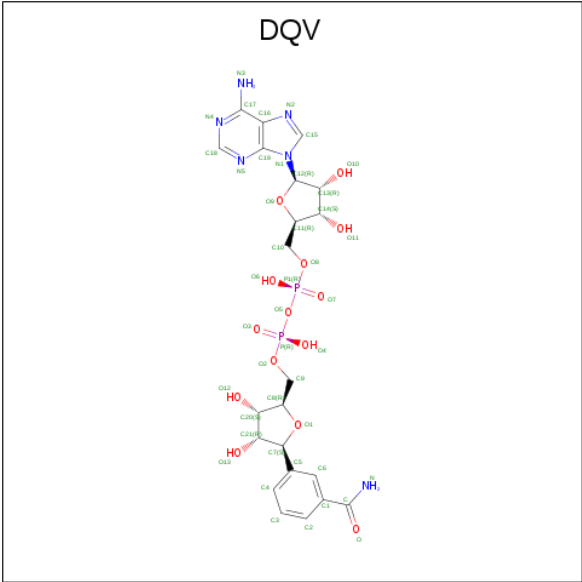
Chain	Residue	Modelled	Actual	Comment	Reference
C	755	LEU	-	expression tag	UNP P09874
C	756	VAL	-	expression tag	UNP P09874
C	757	PRO	-	expression tag	UNP P09874
C	758	ARG	-	expression tag	UNP P09874
C	759	GLY	-	expression tag	UNP P09874
C	760	SER	-	expression tag	UNP P09874
C	761	HIS	-	expression tag	UNP P09874
C	762	MET	-	expression tag	UNP P09874
C	763	THR	-	expression tag	UNP P09874
C	764	LYS	-	expression tag	UNP P09874
C	765	SER	-	expression tag	UNP P09874
C	766	LYS	-	expression tag	UNP P09874
C	767	LEU	-	expression tag	UNP P09874
C	768	PRO	-	expression tag	UNP P09874
C	769	LYS	-	expression tag	UNP P09874
C	770	PRO	-	expression tag	UNP P09874
C	771	VAL	-	expression tag	UNP P09874
C	772	GLN	-	expression tag	UNP P09874
C	773	ASP	-	expression tag	UNP P09874
C	774	LEU	-	expression tag	UNP P09874
C	775	ILE	-	expression tag	UNP P09874
C	776	LYS	-	expression tag	UNP P09874
C	777	MET	-	expression tag	UNP P09874
C	778	ILE	-	expression tag	UNP P09874
C	779	PHE	-	expression tag	UNP P09874
C	780	GLY	-	expression tag	UNP P09874
C	781	SER	-	expression tag	UNP P09874
C	782	GLY	-	expression tag	UNP P09874
C	783	SER	-	expression tag	UNP P09874
C	784	GLY	-	expression tag	UNP P09874
C	785	SER	-	expression tag	UNP P09874
C	786	GLY	-	expression tag	UNP P09874
C	787	GLY	-	expression tag	UNP P09874
D	742	MET	-	initiating methionine	UNP P09874
D	743	GLY	-	expression tag	UNP P09874
D	744	SER	-	expression tag	UNP P09874
D	745	SER	-	expression tag	UNP P09874
D	746	HIS	-	expression tag	UNP P09874
D	747	HIS	-	expression tag	UNP P09874
D	748	HIS	-	expression tag	UNP P09874
D	749	HIS	-	expression tag	UNP P09874
D	750	HIS	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
D	751	HIS	-	expression tag	UNP P09874
D	752	SER	-	expression tag	UNP P09874
D	753	SER	-	expression tag	UNP P09874
D	754	GLY	-	expression tag	UNP P09874
D	755	LEU	-	expression tag	UNP P09874
D	756	VAL	-	expression tag	UNP P09874
D	757	PRO	-	expression tag	UNP P09874
D	758	ARG	-	expression tag	UNP P09874
D	759	GLY	-	expression tag	UNP P09874
D	760	SER	-	expression tag	UNP P09874
D	761	HIS	-	expression tag	UNP P09874
D	762	MET	-	expression tag	UNP P09874
D	763	THR	-	expression tag	UNP P09874
D	764	LYS	-	expression tag	UNP P09874
D	765	SER	-	expression tag	UNP P09874
D	766	LYS	-	expression tag	UNP P09874
D	767	LEU	-	expression tag	UNP P09874
D	768	PRO	-	expression tag	UNP P09874
D	769	LYS	-	expression tag	UNP P09874
D	770	PRO	-	expression tag	UNP P09874
D	771	VAL	-	expression tag	UNP P09874
D	772	GLN	-	expression tag	UNP P09874
D	773	ASP	-	expression tag	UNP P09874
D	774	LEU	-	expression tag	UNP P09874
D	775	ILE	-	expression tag	UNP P09874
D	776	LYS	-	expression tag	UNP P09874
D	777	MET	-	expression tag	UNP P09874
D	778	ILE	-	expression tag	UNP P09874
D	779	PHE	-	expression tag	UNP P09874
D	780	GLY	-	expression tag	UNP P09874
D	781	SER	-	expression tag	UNP P09874
D	782	GLY	-	expression tag	UNP P09874
D	783	SER	-	expression tag	UNP P09874
D	784	GLY	-	expression tag	UNP P09874
D	785	SER	-	expression tag	UNP P09874
D	786	GLY	-	expression tag	UNP P09874
D	787	GLY	-	expression tag	UNP P09874

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl [(2R,3S,4R,5S)-5-(3-carbamoylphenyl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (non-preferred name) (three-letter code: DQV) (formula: C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			52	23	6	20	3		
2	B	1	Total	C	N	O	P	0	1
			55	24	6	21	4		
2	C	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
2	D	1	Total	C	N	O	P	0	1
			52	23	6	20	3		

- Molecule 3 is water.

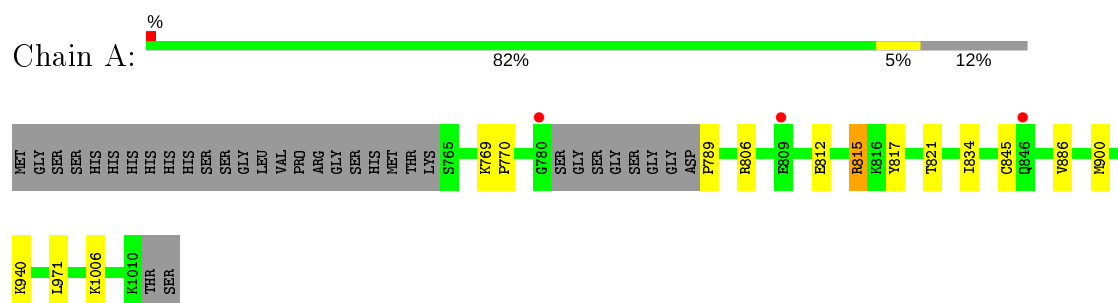
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	16	Total	O	0	0
			16	16		
3	C	11	Total	O	0	0
			11	11		
3	D	24	Total	O	0	0
			24	24		



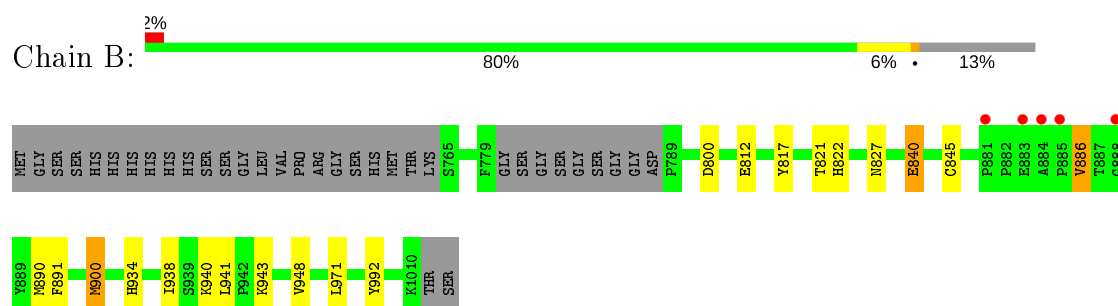
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

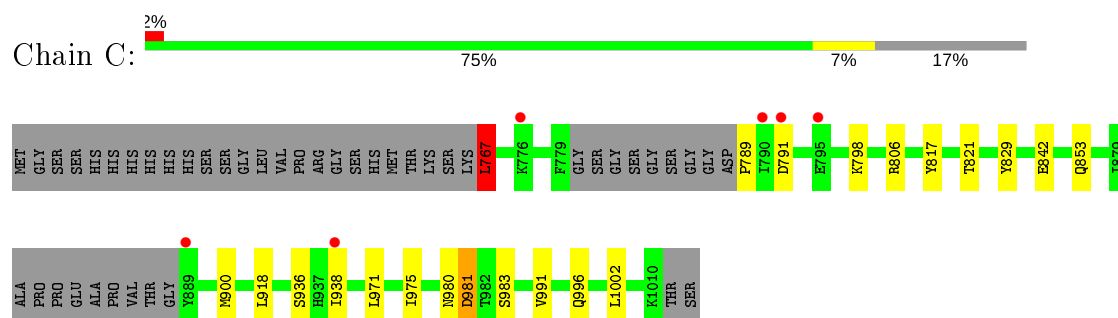
- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 1: Poly [ADP-ribose] polymerase 1

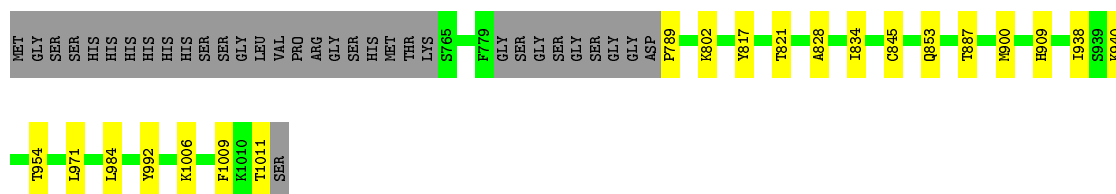


- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 1: Poly [ADP-ribose] polymerase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.51Å 75.36Å 85.61Å 98.66° 104.94° 106.73°	Depositor
Resolution (Å)	20.00 – 2.30 35.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.30) 97.8 (35.39-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.198 , 0.222 0.202 , 0.227	Depositor DCC
$R_{free}$ test set	2141 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DQV

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	0.51	0/1914	0.72	1/2585 (0.0%)
1	B	0.55	0/1921	0.76	1/2595 (0.0%)
1	C	0.52	0/1837	0.74	2/2475 (0.1%)
1	D	0.53	0/1917	0.73	0/2590
All	All	0.53	0/7589	0.74	4/10245 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	900	MET	CG-SD-CE	6.32	110.31	100.20
1	C	767	LEU	CB-CG-CD2	6.09	121.35	111.00
1	A	815	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	981	ASP	CB-CG-OD1	5.38	123.14	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	886	VAL	Peptide

## 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	1874	0	1899	5	0
1	B	1877	0	1903	10	0
1	C	1801	0	1832	13	0
1	D	1877	0	1903	9	0
2	A	52	0	0	0	0
2	B	55	0	0	0	0
2	C	44	0	0	0	0
2	D	52	0	0	0	0
3	A	21	0	0	0	0
3	B	16	0	0	0	0
3	C	11	0	0	0	0
3	D	24	0	0	0	0
All	All	7704	0	7537	30	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 (30) 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:938:ILE:HD11	1:D:992:TYR:CZ	2.11	0.84
1:B:822:HIS:CE1	1:B:827:ASN:HD22	2.09	0.71
1:D:938:ILE:HD11	1:D:992:TYR:CE2	2.32	0.65
1:B:800:ASP:HB3	1:B:840:GLU:HG3	1.80	0.64
1:C:980:ASN:HB3	1:D:828:ALA:HB1	1.84	0.59
1:B:891:PHE:O	1:B:938:ILE:HG22	2.07	0.55
1:C:918:LEU:HD22	1:C:1002:LEU:HD21	1.88	0.55
1:A:769:LYS:HG2	1:A:770:PRO:HD3	1.90	0.54
1:B:938:ILE:HD13	1:B:948:VAL:HG21	1.90	0.53
1:B:938:ILE:HG21	1:B:992:TYR:OH	2.08	0.52
1:D:834:ILE:HD11	1:D:1006:LYS:HB2	1.91	0.52
1:A:769:LYS:CG	1:A:770:PRO:HD3	2.39	0.52
1:A:806:ARG:O	1:A:815:ARG:NH2	2.44	0.51
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.94	0.50
1:B:938:ILE:HA	1:D:1011:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:LYS:CD	1:C:975:ILE:HD12	2.42	0.50
1:C:983:SER:O	1:D:909:HIS:ND1	2.43	0.49
1:C:829:TYR:CE2	1:D:887:THR:HB	2.48	0.48
1:D:821:THR:HB	1:D:900:MET:HA	1.96	0.47
1:C:767:LEU:HD23	1:C:791:ASP:OD2	2.16	0.46
1:B:938:ILE:HD11	1:B:941:LEU:HD23	1.97	0.46
1:A:821:THR:HB	1:A:900:MET:HA	1.98	0.45
1:C:936:SER:O	1:C:938:ILE:HD12	2.16	0.45
1:C:821:THR:HB	1:C:900:MET:HA	1.99	0.44
1:B:943:LYS:HD2	1:C:975:ILE:HD12	1.98	0.44
1:B:821:THR:HB	1:B:900:MET:HA	1.98	0.44
1:C:991:VAL:HG21	1:C:996:GLN:HB2	2.00	0.44
1:C:981:ASP:HA	1:D:1009:PHE:CE1	2.53	0.43
1:C:991:VAL:HG21	1:C:996:GLN:CB	2.48	0.43
1:C:842:GLU:HA	1:C:842:GLU:OE1	2.21	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	234/271 (86%)	228 (97%)	6 (3%)	0	100	100
1	B	234/271 (86%)	227 (97%)	6 (3%)	1 (0%)	34	42
1	C	220/271 (81%)	215 (98%)	5 (2%)	0	100	100
1	D	234/271 (86%)	227 (97%)	7 (3%)	0	100	100
All	All	922/1084 (85%)	897 (97%)	24 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	886	VAL

### 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	206/233 (88%)	199 (97%)	7 (3%)	37	51
1	B	207/233 (89%)	198 (96%)	9 (4%)	29	40
1	C	199/233 (85%)	192 (96%)	7 (4%)	36	50
1	D	207/233 (89%)	198 (96%)	9 (4%)	29	40
All	All	819/932 (88%)	787 (96%)	32 (4%)	33	46

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	PRO
1	A	812	GLU
1	A	817	TYR
1	A	845	CYS
1	A	886	VAL
1	A	940	LYS
1	A	971	LEU
1	B	812	GLU
1	B	817	TYR
1	B	840	GLU
1	B	845	CYS
1	B	890	MET
1	B	934[A]	HIS
1	B	934[B]	HIS
1	B	940	LYS
1	B	971	LEU
1	C	767	LEU
1	C	789	PRO
1	C	798	LYS
1	C	806	ARG
1	C	817	TYR

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Mol	Chain	Res	Type
1	C	853	GLN
1	C	971	LEU
1	D	789	PRO
1	D	802	LYS
1	D	817	TYR
1	D	845	CYS
1	D	853	GLN
1	D	940	LYS
1	D	954	THR
1	D	971	LEU
1	D	984	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	822	HIS
1	D	820	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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$
2	DQV	B	1101[A]	-	43,48,48	0.59	0	54,73,73	0.93	3 (5%)
2	DQV	A	1101[B]	-	43,48,48	0.66	1 (2%)	54,73,73	0.78	2 (3%)
2	DQV	D	1101[B]	-	43,48,48	0.56	0	54,73,73	0.75	2 (3%)
2	DQV	C	1101	-	43,48,48	0.62	0	54,73,73	0.82	3 (5%)
2	DQV	A	1101[A]	-	43,48,48	0.62	0	54,73,73	0.75	1 (1%)
2	DQV	B	1101[B]	-	43,48,48	0.61	0	54,73,73	0.95	4 (7%)
2	DQV	D	1101[A]	-	43,48,48	0.60	0	54,73,73	0.79	2 (3%)

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
2	DQV	B	1101[A]	-	-	5/26/62/62	0/5/5/5
2	DQV	A	1101[B]	-	-	14/26/62/62	0/5/5/5
2	DQV	D	1101[B]	-	-	10/26/62/62	0/5/5/5
2	DQV	C	1101	-	-	3/26/62/62	0/5/5/5
2	DQV	A	1101[A]	-	-	7/26/62/62	0/5/5/5
2	DQV	B	1101[B]	-	-	5/26/62/62	0/5/5/5
2	DQV	D	1101[A]	-	-	9/26/62/62	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101[B]	DQV	P-O4	-2.05	1.45	1.55

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101[A]	DQV	C20-C21-C7	2.91	105.28	101.93
2	B	1101[B]	DQV	C20-C21-C7	2.91	105.28	101.93
2	A	1101[B]	DQV	O8-P1-O7	2.73	119.75	109.07
2	D	1101[A]	DQV	O8-P1-O7	2.70	119.63	109.07
2	C	1101	DQV	C20-C21-C7	2.50	104.82	101.93
2	A	1101[B]	DQV	C16-C17-N3	2.25	123.77	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101[A]	DQV	C16-C17-N3	2.25	123.77	120.35
2	B	1101[A]	DQV	C16-C17-N3	2.24	123.76	120.35
2	B	1101[B]	DQV	C16-C17-N3	2.24	123.76	120.35
2	C	1101	DQV	C16-C17-N3	2.21	123.71	120.35
2	B	1101[A]	DQV	O1-C7-C21	2.20	108.22	104.66
2	B	1101[B]	DQV	O1-C7-C21	2.20	108.22	104.66
2	D	1101[B]	DQV	C16-C17-N3	2.13	123.60	120.35
2	D	1101[A]	DQV	C16-C17-N3	2.13	123.60	120.35
2	C	1101	DQV	O4-P-O2	2.13	117.62	107.75
2	B	1101[B]	DQV	O4-P-O2	2.04	117.20	107.75
2	D	1101[B]	DQV	O8-P1-O7	2.01	116.93	109.07

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101[A]	DQV	C20-C8-C9-O2
2	A	1101[B]	DQV	C9-O2-P-O3
2	D	1101[B]	DQV	C9-O2-P-O3
2	A	1101[A]	DQV	C10-O8-P1-O5
2	A	1101[A]	DQV	C10-O8-P1-O7
2	D	1101[A]	DQV	C9-O2-P-O4
2	D	1101[A]	DQV	C9-O2-P-O5
2	B	1101[A]	DQV	O1-C8-C9-O2
2	A	1101[B]	DQV	O1-C8-C9-O2
2	D	1101[B]	DQV	O1-C8-C9-O2
2	A	1101[B]	DQV	C20-C8-C9-O2
2	D	1101[B]	DQV	P-O5-P1-O7
2	B	1101[B]	DQV	P-O5-P1-O7
2	D	1101[B]	DQV	C20-C8-C9-O2
2	C	1101	DQV	P1-O5-P-O2
2	A	1101[A]	DQV	P-O5-P1-O8
2	B	1101[B]	DQV	P1-O5-P-O2
2	D	1101[A]	DQV	P-O5-P1-O8
2	A	1101[B]	DQV	C6-C5-C7-C21
2	A	1101[A]	DQV	C6-C5-C7-C21
2	A	1101[B]	DQV	C10-O8-P1-O5
2	A	1101[B]	DQV	C9-O2-P-O5
2	D	1101[B]	DQV	C9-O2-P-O5
2	A	1101[A]	DQV	C9-O2-P-O5
2	A	1101[B]	DQV	P-O5-P1-O6
2	A	1101[B]	DQV	C10-O8-P1-O7

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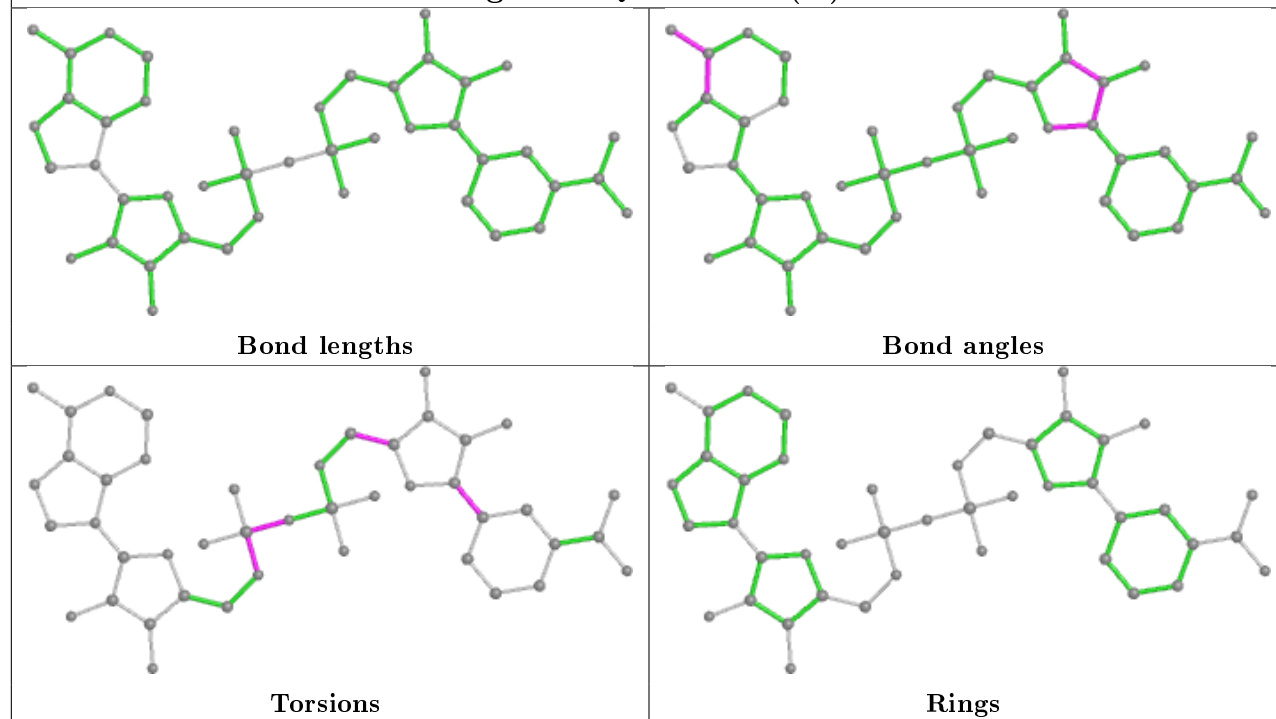
Mol	Chain	Res	Type	Atoms
2	A	1101[B]	DQV	C9-O2-P-O4
2	D	1101[B]	DQV	C9-O2-P-O4
2	D	1101[A]	DQV	C9-O2-P-O3
2	B	1101[A]	DQV	C6-C5-C7-C21
2	B	1101[B]	DQV	C6-C5-C7-C21
2	A	1101[B]	DQV	C8-C9-O2-P
2	D	1101[B]	DQV	C6-C5-C7-C21
2	D	1101[A]	DQV	C6-C5-C7-C21
2	A	1101[B]	DQV	C4-C5-C7-C21
2	D	1101[B]	DQV	C4-C5-C7-C21
2	A	1101[A]	DQV	C4-C5-C7-C21
2	D	1101[A]	DQV	C4-C5-C7-C21
2	C	1101	DQV	C6-C5-C7-C21
2	B	1101[B]	DQV	O8-C10-C11-O9
2	B	1101[A]	DQV	P-O5-P1-O8
2	D	1101[A]	DQV	C10-O8-P1-O5
2	C	1101	DQV	O8-C10-C11-O9
2	A	1101[B]	DQV	P-O5-P1-O7
2	D	1101[B]	DQV	P-O5-P1-O6
2	B	1101[B]	DQV	P-O5-P1-O6
2	B	1101[A]	DQV	C10-O8-P1-O7
2	A	1101[B]	DQV	C10-O8-P1-O6
2	D	1101[A]	DQV	C10-O8-P1-O7
2	A	1101[B]	DQV	O8-C10-C11-O9
2	D	1101[B]	DQV	O8-C10-C11-O9
2	A	1101[A]	DQV	O8-C10-C11-O9
2	D	1101[A]	DQV	O8-C10-C11-O9

There are no ring outliers.

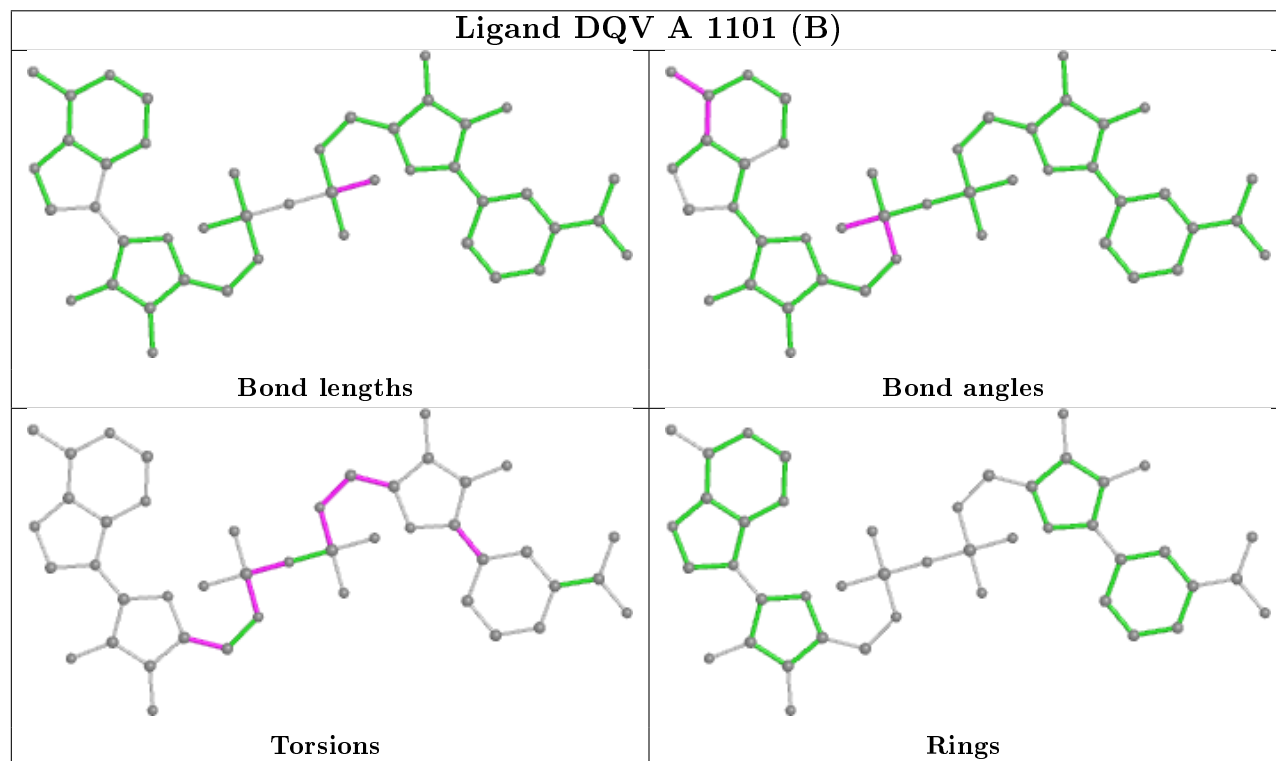
No monomer is involved in short contacts.

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

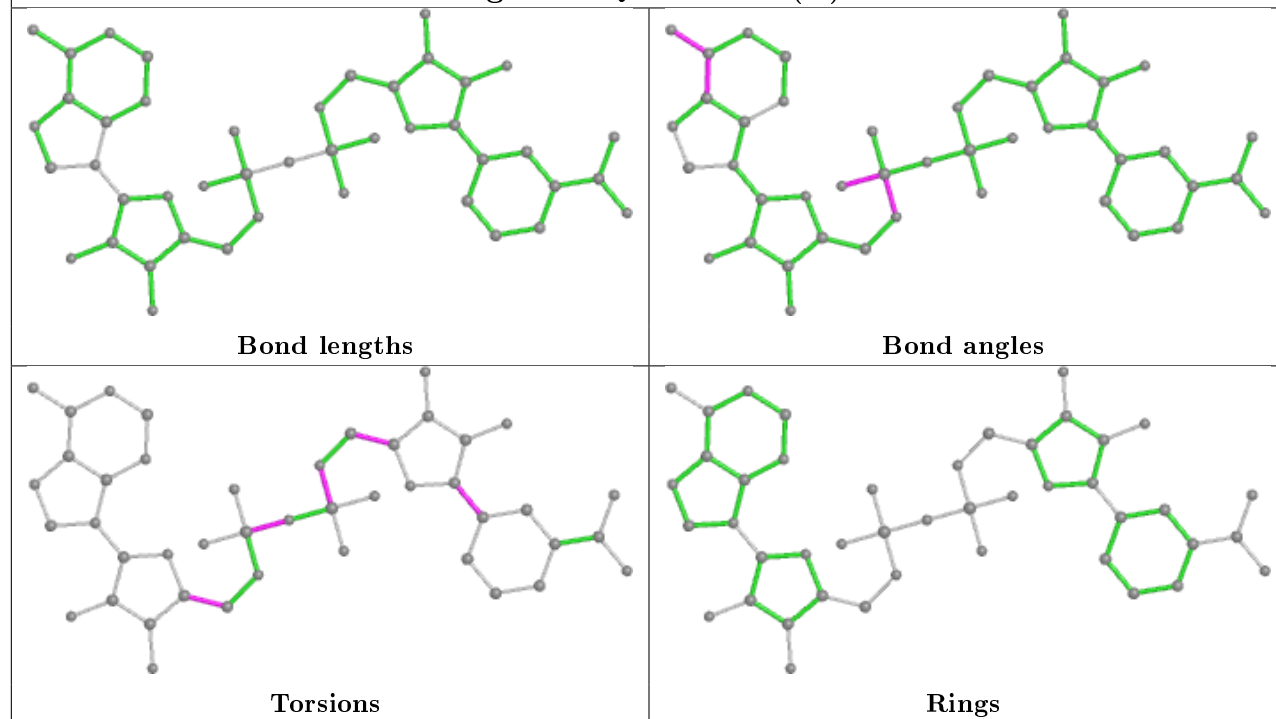
## Ligand DQV B 1101 (A)



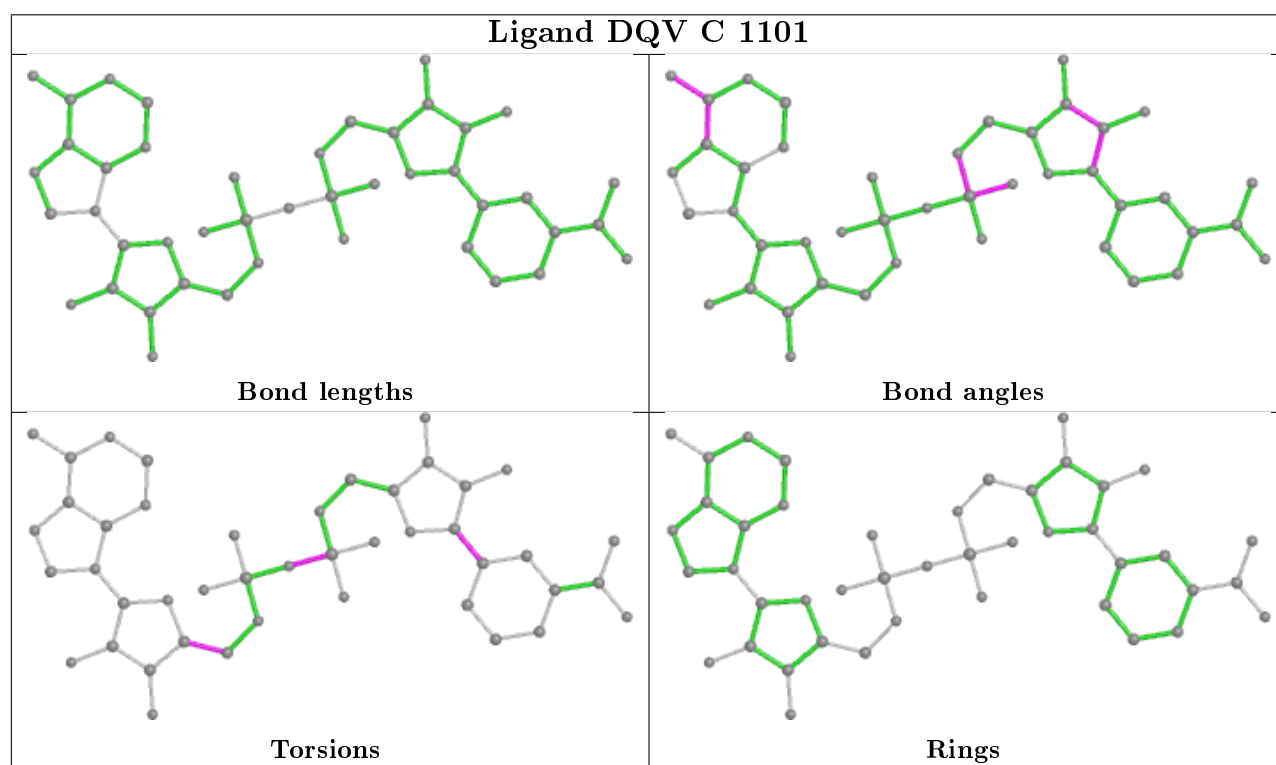
## Ligand DQV A 1101 (B)



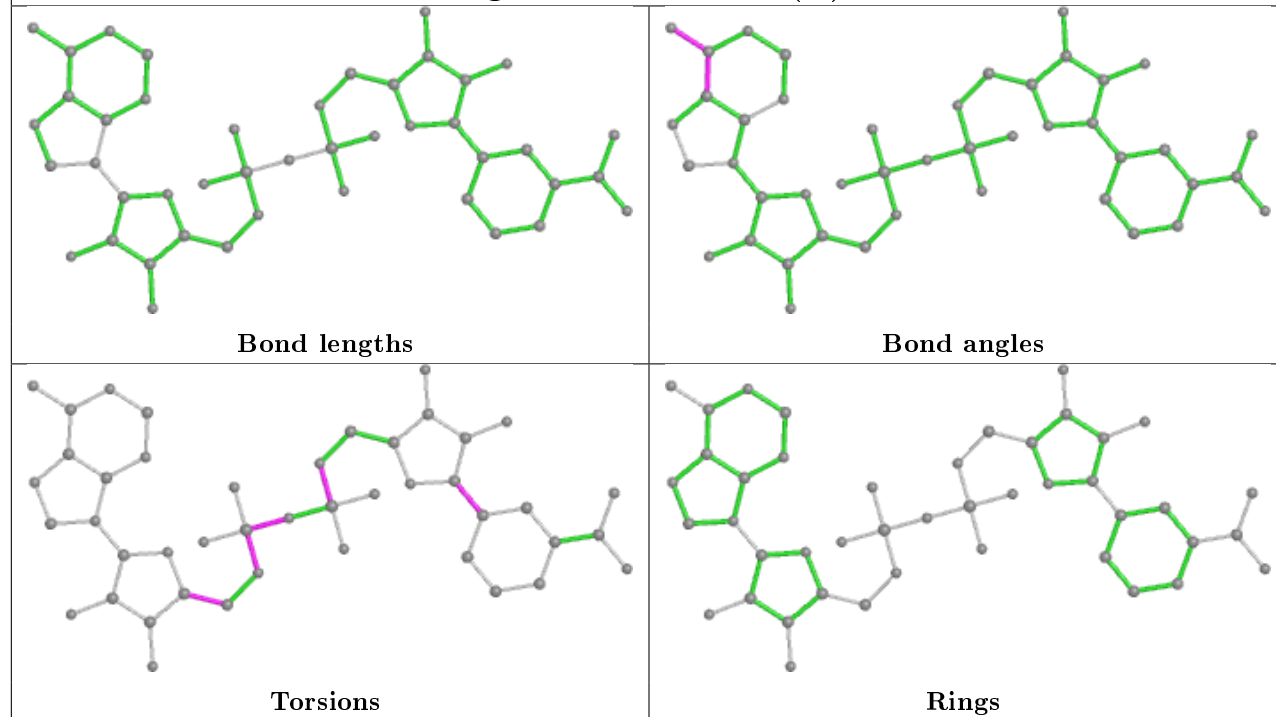
## Ligand DQV D 1101 (B)



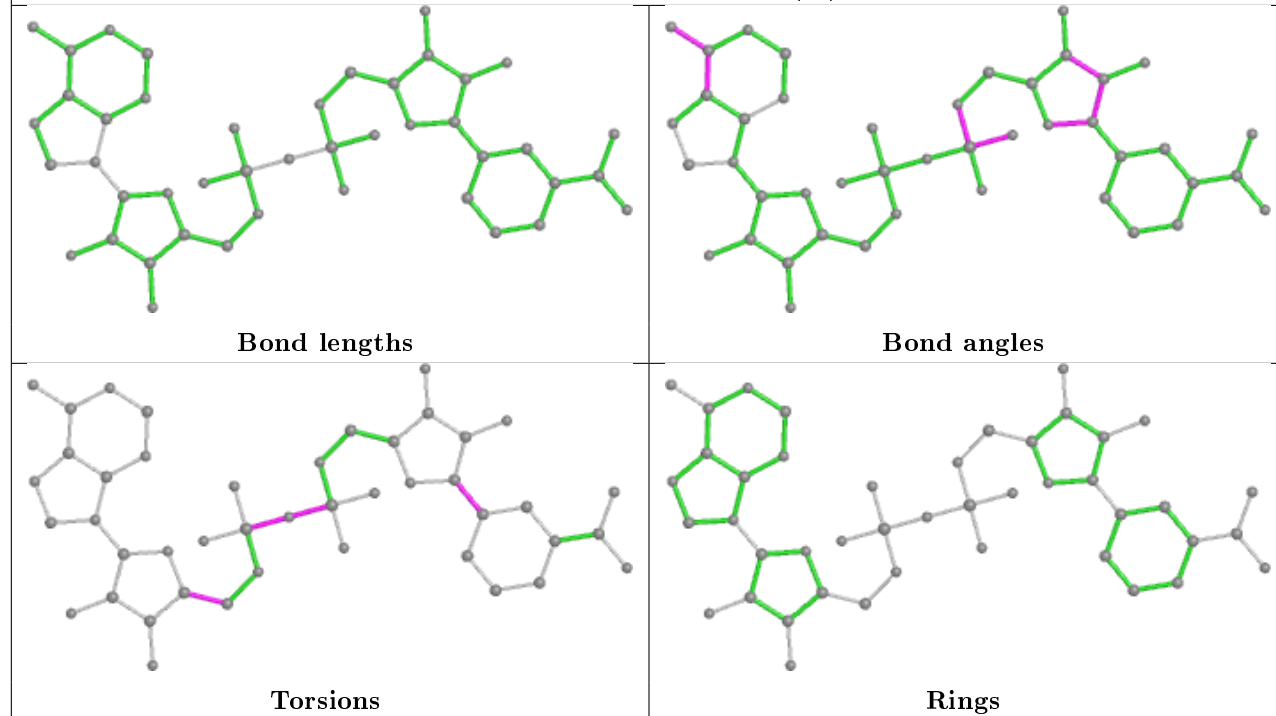
## Ligand DQV C 1101

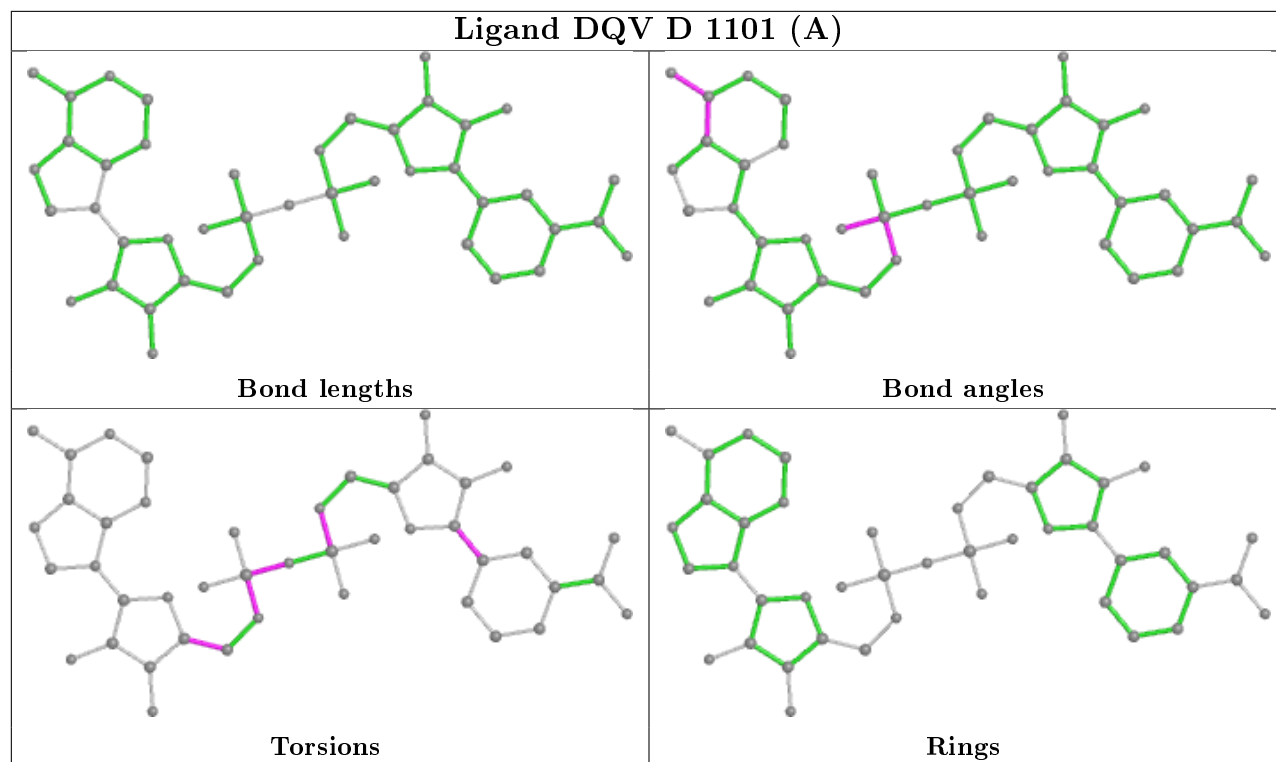


## Ligand DQV A 1101 (A)



## Ligand DQV B 1101 (B)





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	238/271 (87%)	-0.10	3 (1%) 77 81	47, 75, 105, 119	0
1	B	237/271 (87%)	-0.00	5 (2%) 63 70	45, 69, 107, 168	0
1	C	226/271 (83%)	0.04	6 (2%) 54 62	52, 79, 114, 138	0
1	D	238/271 (87%)	-0.11	0 100 100	49, 75, 109, 133	0
All	All	939/1084 (86%)	-0.04	14 (1%) 73 79	45, 74, 109, 168	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	884	ALA	4.1
1	B	881	PRO	4.1
1	B	885	PRO	3.2
1	C	790	ILE	3.2
1	B	888	GLY	3.0
1	C	889	TYR	2.8
1	C	795	GLU	2.7
1	A	846	GLN	2.7
1	A	780	GLY	2.7
1	C	791	ASP	2.3
1	C	938	ILE	2.3
1	C	776	LYS	2.3
1	A	809	GLU	2.2
1	B	883	GLU	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands

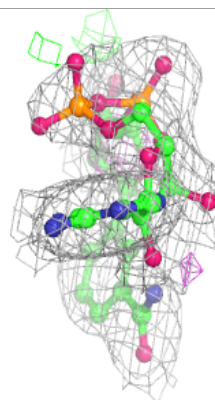
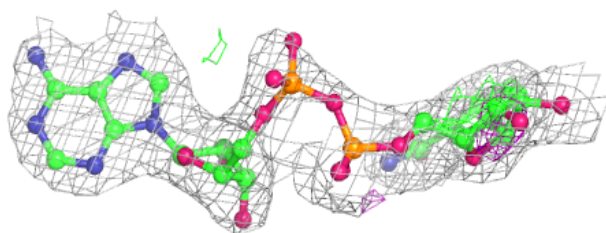
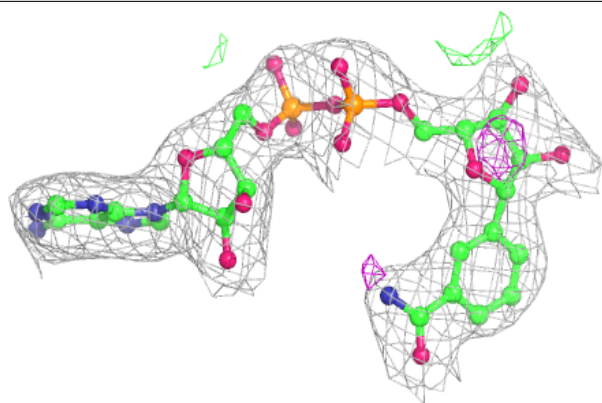
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	DQV	B	1101[A]	44/44	0.94	0.12	44,72,78,81	11
2	DQV	C	1101	44/44	0.94	0.11	58,89,107,111	0
2	DQV	B	1101[B]	44/44	0.94	0.12	44,68,76,78	11
2	DQV	A	1101[A]	44/44	0.95	0.11	47,62,69,70	8
2	DQV	A	1101[B]	44/44	0.95	0.11	47,61,69,69	8
2	DQV	D	1101[B]	44/44	0.96	0.12	44,60,71,76	8
2	DQV	D	1101[A]	44/44	0.96	0.12	44,62,71,76	8

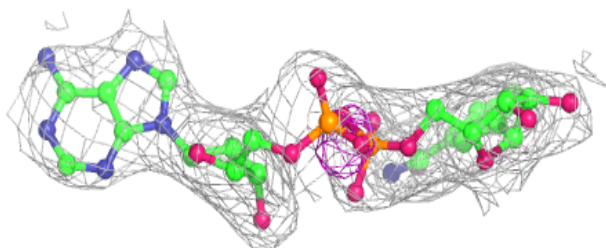
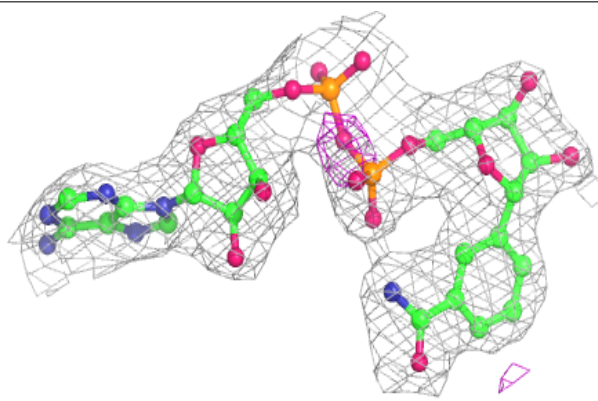
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DQV B 1101 (A):**

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

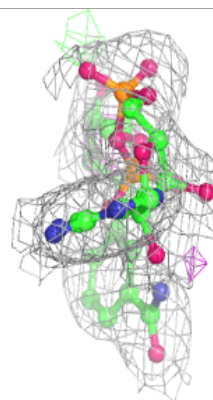
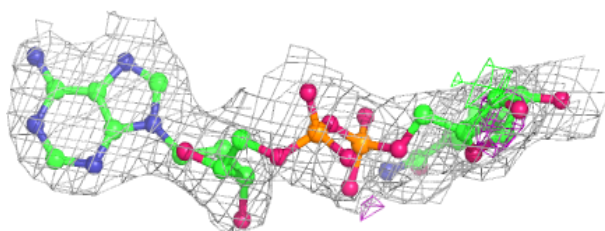
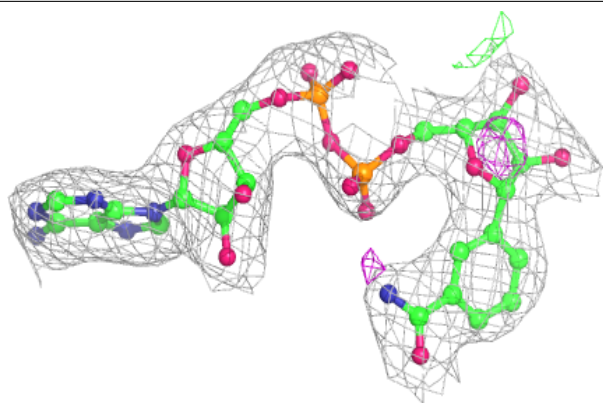
**Electron density around DQV C 1101:**

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

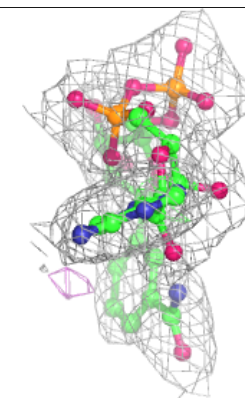
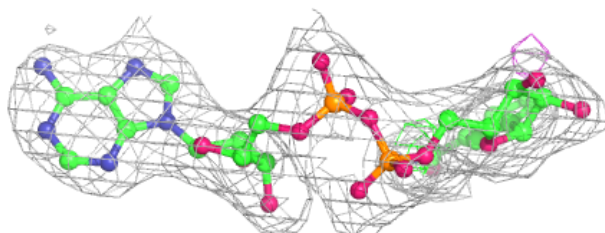
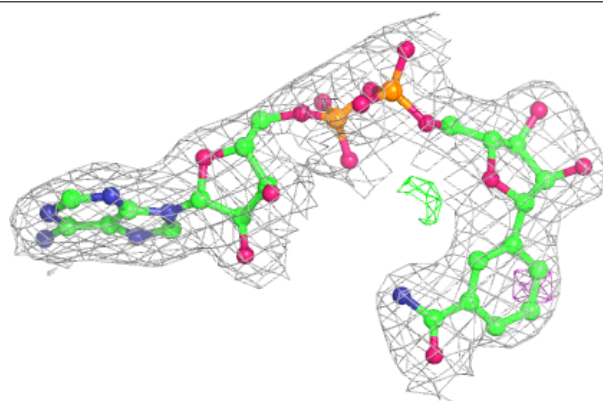


**Electron density around DQV B 1101 (B):**

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

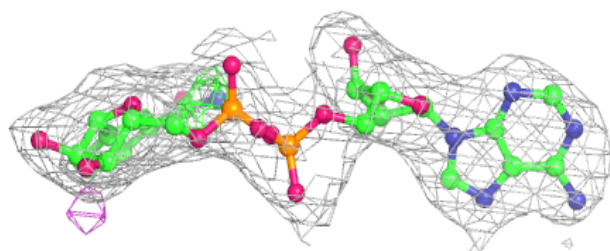
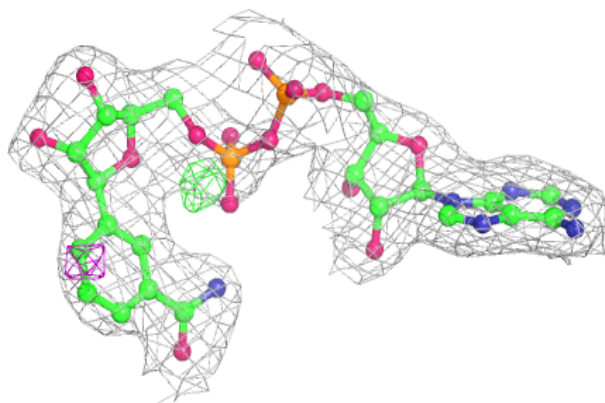
**Electron density around DQV A 1101 (A):**

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

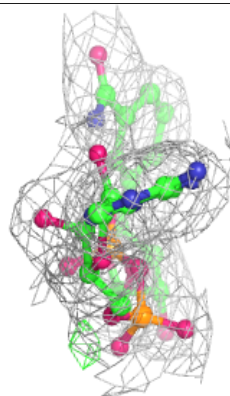
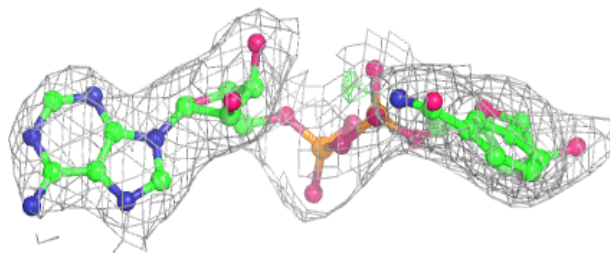
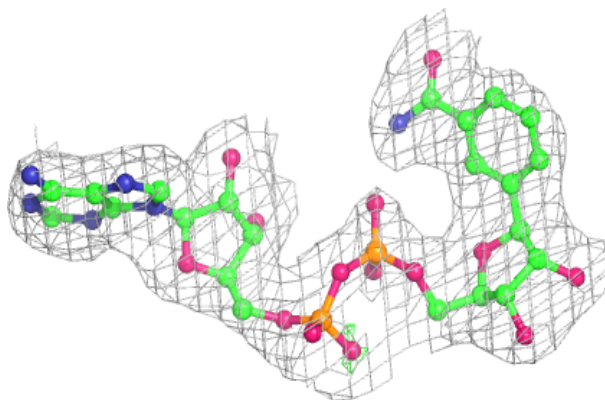


**Electron density around DQV A 1101 (B):**

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

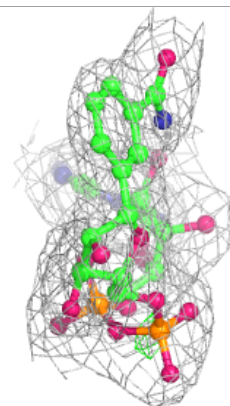
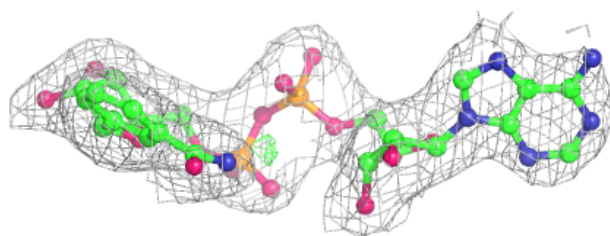
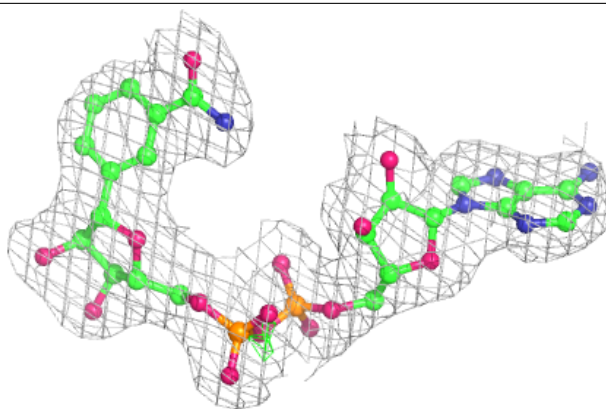
**Electron density around DQV D 1101 (B):**

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



**Electron density around DQV D 1101 (A):**

$2mF_o - DF_c$  (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.