



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:44 PM EST

PDB ID : 7HL1
Title : Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z3241250482 (DNV2_NS5A-x1037)
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Deposited on : 2024-10-15
Resolution : 1.66 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

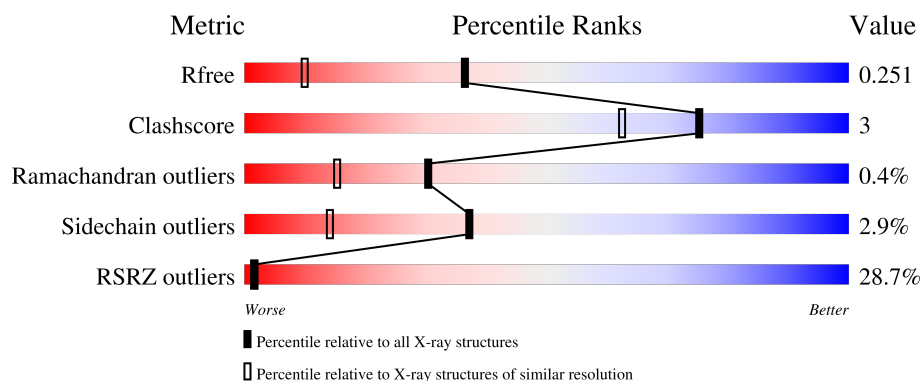
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	637	<div> <div>26%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>

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:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1006	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5313 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	7	0
			4816	3033	864	885	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



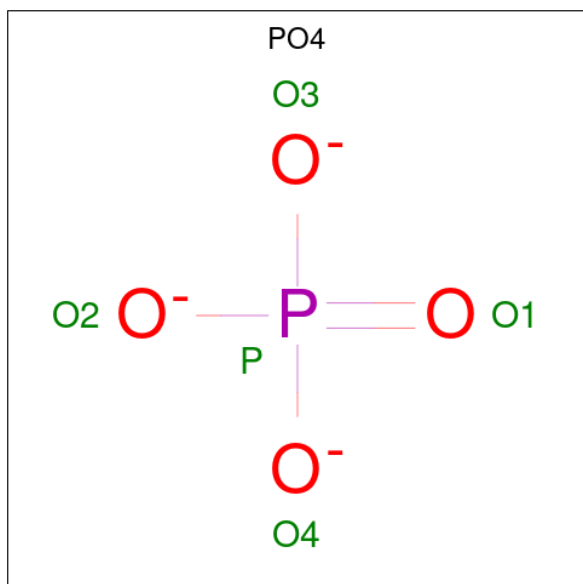
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



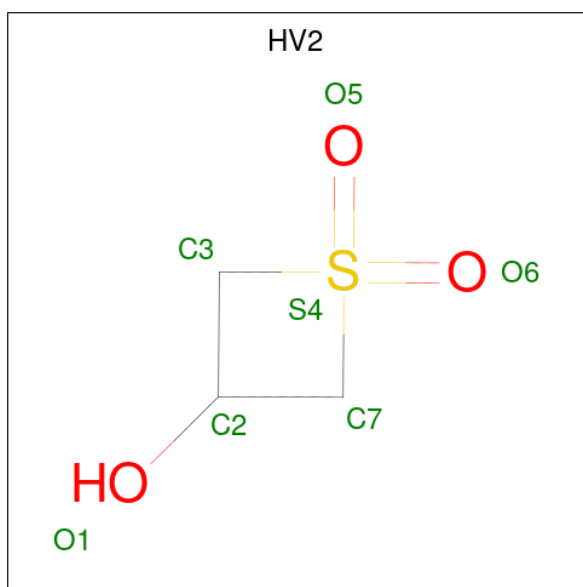
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 1,1-bis(oxidanylidene)thietan-3-ol (three-letter code: HV2) (formula: $C_3H_6O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	3	3	1		
7	A	1	Total	C	O	S	0	0
			7	3	3	1		
7	A	1	Total	C	O	S	0	0
			7	3	3	1		

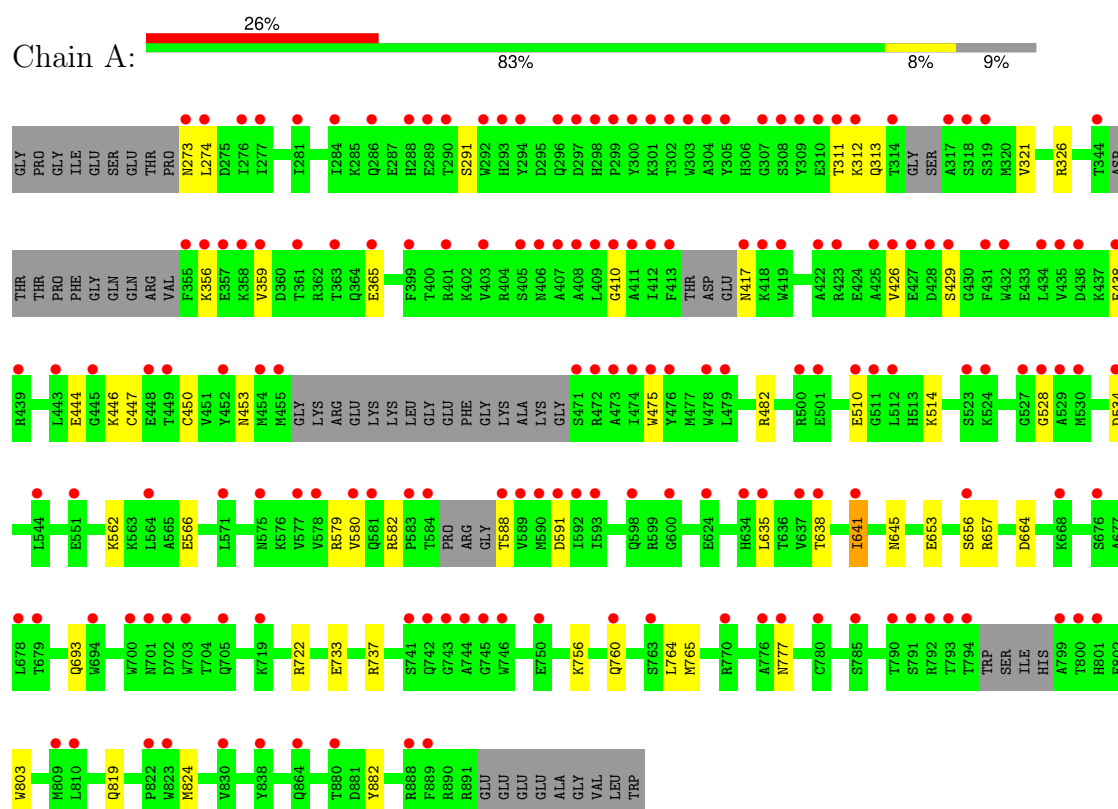
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	425	Total	O	0	0
			425	425		

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. 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. 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: Genome polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.33Å 115.74Å 148.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.18 – 1.66 91.18 – 1.66	Depositor EDS
% Data completeness (in resolution range)	96.6 (91.18-1.66) 96.6 (91.18-1.66)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.201 , 0.231 0.234 , 0.251	Depositor DCC
R_{free} test set	4290 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5313	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: HV2, ZN, PO4, DMS, PEG, MES

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	0.71	0/4923	0.81	1/6637 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ARG	CG-CD-NE	-5.03	101.23	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ASN	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	4816	0	4716	28	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	8	0	12	0	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	21	0	0	1	0
8	A	425	0	0	2	2
All	All	5313	0	4764	28	2

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 3.

All (28) 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:A:534:ASP:OD1	5:A:1006:PO4:O4	1.80	0.99
1:A:664:ASP:OD1	5:A:1006:PO4:O4	1.90	0.89
1:A:764:LEU:HG	1:A:765:MET:HE2	1.73	0.69
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.53	0.67
1:A:638:THR:O	1:A:641:ILE:HG22	1.98	0.64
1:A:764:LEU:HG	1:A:765:MET:CE	2.27	0.63
1:A:534:ASP:OD1	5:A:1006:PO4:P	2.56	0.63
1:A:528:GLY:O	7:A:1010:HV2:O1	2.17	0.62
1:A:562:LYS:O	1:A:566:GLU:HG3	2.02	0.60
1:A:756:LYS:O	1:A:760:GLN:HG3	2.03	0.58
1:A:510:GLU:O	1:A:514:LYS:HG3	2.04	0.58
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.20	0.56
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.08	0.54
1:A:760:GLN:NE2	1:A:803:TRP:O	2.44	0.51
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.54	0.48
1:A:562:LYS:NZ	8:A:1106:HOH:O	2.40	0.47
1:A:777:ASN:HD22	1:A:882:TYR:HB3	1.80	0.47
1:A:582:ARG:O	1:A:588:THR:HA	2.16	0.46
1:A:653:GLU:O	1:A:656:SER:OG	2.29	0.46
1:A:722:ARG:HB3	1:A:824:MET:SD	2.56	0.46
1:A:819:GLN:NE2	8:A:1105:HOH:O	2.39	0.44
1:A:444:GLU:HB3	1:A:446:LYS:HD2	2.00	0.44
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.48	0.43
1:A:475:TRP:CD1	1:A:475:TRP:N	2.87	0.43
1:A:579:ARG:HA	1:A:591:ASP:O	2.18	0.43
1:A:312:LYS:O	1:A:313:GLN:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:O	1:A:313:GLN:HG3	2.21	0.41
1:A:733:GLU:O	1:A:737:ARG:HG3	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1163:HOH:O	8:A:1163:HOH:O[2_445]	1.79	0.41
8:A:1331:HOH:O	8:A:1391:HOH:O[2_545]	1.94	0.26

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	575/637 (90%)	549 (96%)	24 (4%)	2 (0%)	37	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	GLY
1	A	291	SER

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	517/554 (93%)	502 (97%)	15 (3%)	37 14

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

Mol	Chain	Res	Type
1	A	274	LEU
1	A	311	THR
1	A	356	LYS
1	A	359	VAL
1	A	365	GLU
1	A	417	ASN
1	A	426	VAL
1	A	429	SER
1	A	438	GLU
1	A	482	ARG
1	A	580	VAL
1	A	635	LEU
1	A	641	ILE
1	A	645	ASN
1	A	693	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	693	GLN
1	A	777	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
7	HV2	A	1011	-	3,7,7	0.04	0	2,11,11	2.41	1 (50%)
3	MES	A	1003[A]	-	12,12,12	0.76	0	15,16,16	0.63	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.29	0
7	HV2	A	1009	-	3,7,7	0.09	0	2,11,11	2.46	1 (50%)
5	PO4	A	1006	-	4,4,4	4.07	3 (75%)	6,6,6	0.59	0
7	HV2	A	1010	-	3,7,7	0.09	0	2,11,11	2.97	2 (100%)
5	PO4	A	1007	-	4,4,4	1.52	1 (25%)	6,6,6	0.39	0
4	DMS	A	1004	-	3,3,3	0.23	0	3,3,3	0.06	0
4	DMS	A	1005	-	3,3,3	0.16	0	3,3,3	0.34	0
6	PEG	A	1008	-	6,6,6	0.17	0	5,5,5	0.08	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
7	HV2	A	1011	-	-	-	0/1/1/1
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
7	HV2	A	1009	-	-	-	0/1/1/1
7	HV2	A	1010	-	-	-	0/1/1/1
6	PEG	A	1008	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	6.52	1.65	1.50
5	A	1006	PO4	P-O2	3.55	1.65	1.54
5	A	1006	PO4	P-O4	-2.96	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	2.90	1.57	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1010	HV2	O1-C2-C7	-3.63	105.92	117.36
7	A	1009	HV2	O1-C2-C7	-3.06	107.72	117.36
7	A	1011	HV2	O1-C2-C7	-2.93	108.14	117.36
7	A	1010	HV2	O1-C2-C3	-2.11	110.72	117.36

There are no chirality outliers.

All (7) torsion outliers are listed below:

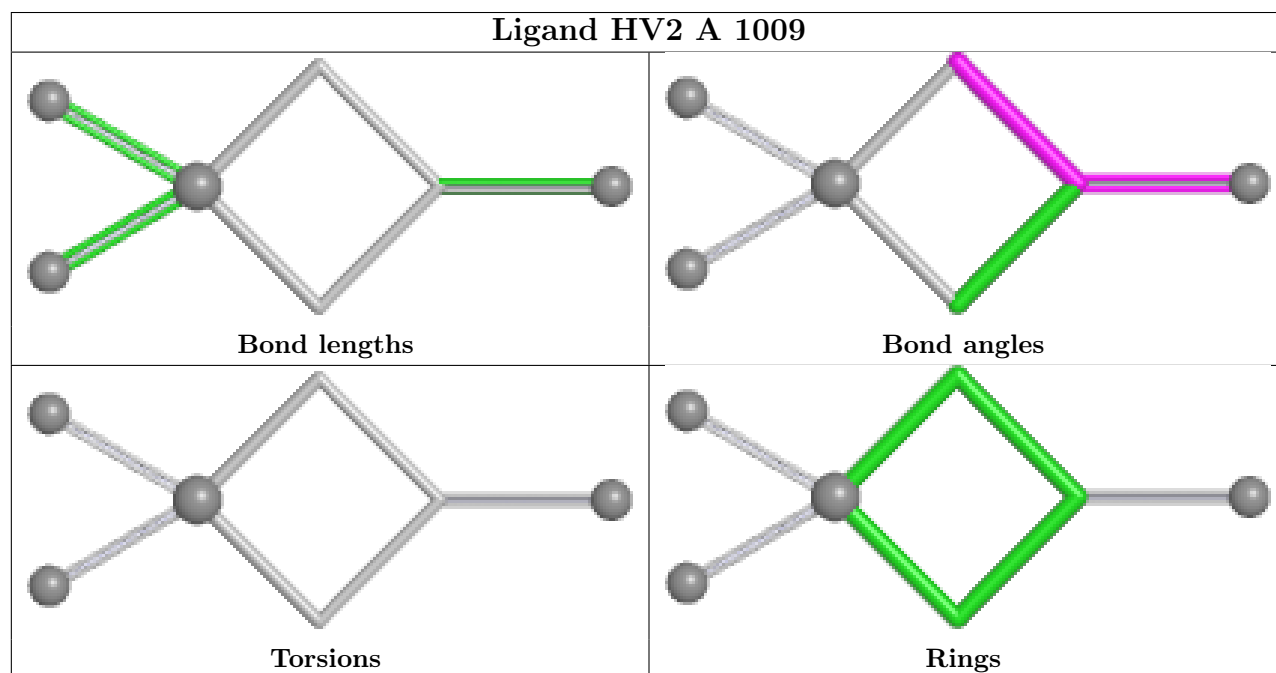
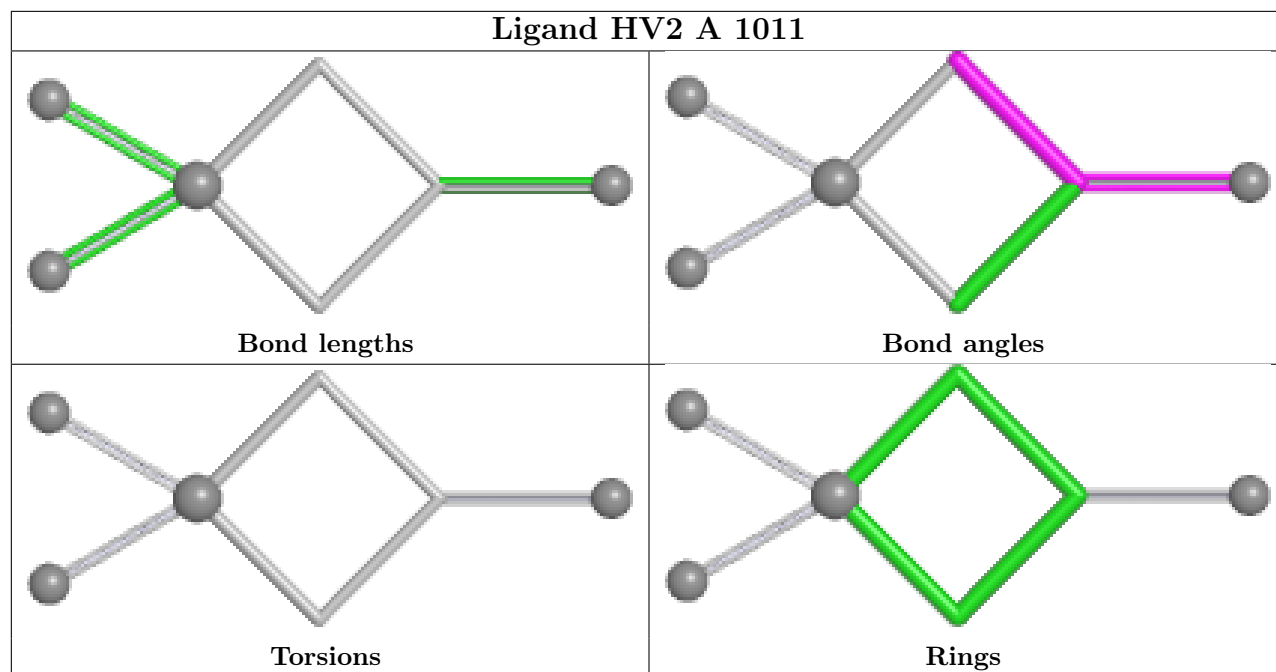
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
6	A	1008	PEG	O1-C1-C2-O2
6	A	1008	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5

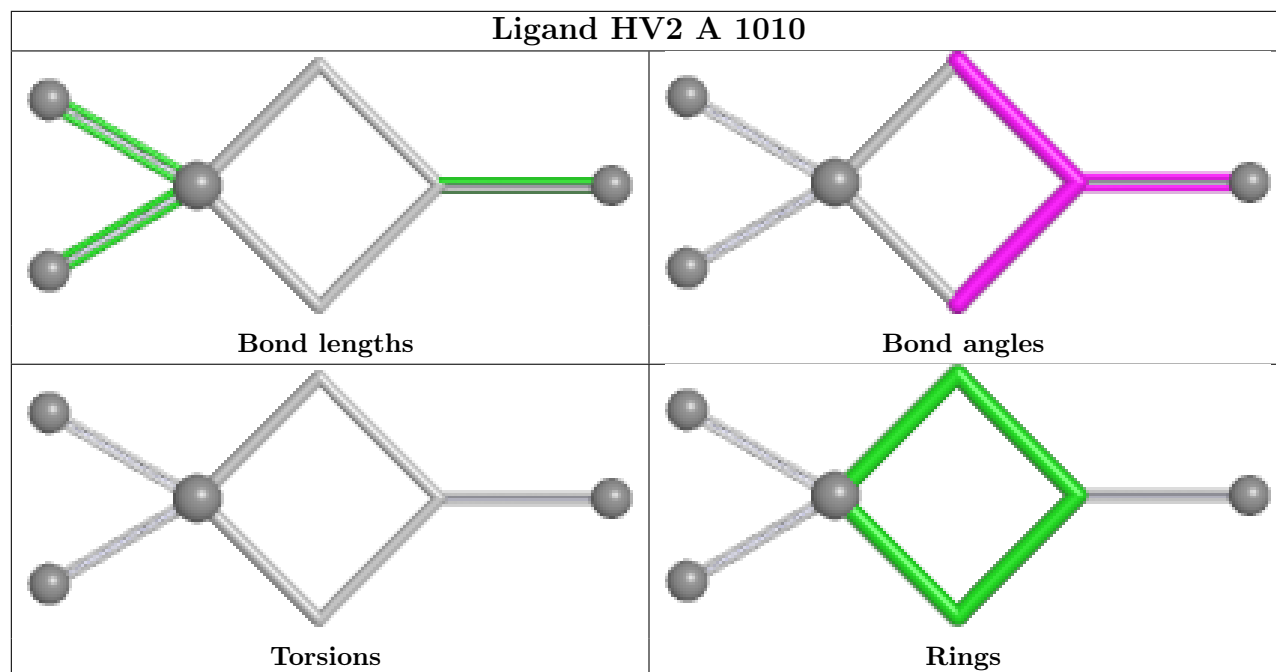
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	PO4	4	0
7	A	1010	HV2	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.





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 ⓘ

Warning: The R factor obtained from EDS is 0.251, which does not match the depositor's R factor of 0.2006. Please interpret the results in this section carefully.

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	582/637 (91%)	1.75	167 (28%) 1 2	6, 35, 104, 158	43 (7%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	838	TYR	16.2
1	A	512[A]	LEU	15.3
1	A	776	ALA	14.5
1	A	810	LEU	14.4
1	A	801[A]	HIS	14.0
1	A	780	CYS	13.7
1	A	700	TRP	13.6
1	A	823	TRP	13.2
1	A	703	TRP	12.4
1	A	719[A]	LYS	12.3
1	A	426	VAL	12.3
1	A	785[A]	SER	12.0
1	A	770	ARG	11.9
1	A	888	ARG	11.0
1	A	777	ASN	10.9
1	A	763	SER	10.8
1	A	822	PRO	10.6
1	A	529	ALA	10.2
1	A	741[A]	SER	9.8
1	A	523	SER	9.4
1	A	527	GLY	9.4
1	A	668	LYS	9.2
1	A	809	MET	9.1
1	A	500	ARG	8.8

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Mol	Chain	Res	Type	RSRZ
1	A	656	SER	8.6
1	A	705	GLN	8.5
1	A	524	LYS	8.5
1	A	551[A]	GLU	8.4
1	A	760	GLN	8.3
1	A	864[A]	GLN	8.2
1	A	528	GLY	7.8
1	A	701	ASN	7.7
1	A	530	MET	7.5
1	A	702	ASP	7.3
1	A	600	GLY	7.2
1	A	355	PHE	7.2
1	A	589	VAL	6.8
1	A	799	ALA	6.6
1	A	598	GLN	6.6
1	A	501	GLU	6.5
1	A	694	TRP	6.4
1	A	510	GLU	6.3
1	A	678	LEU	6.2
1	A	411	ALA	5.9
1	A	413	PHE	5.8
1	A	475	TRP	5.6
1	A	409	LEU	5.5
1	A	317	ALA	5.3
1	A	359	VAL	5.1
1	A	679	THR	5.1
1	A	422	ALA	4.9
1	A	305	TYR	4.9
1	A	412	ILE	4.7
1	A	794	THR	4.6
1	A	407	ALA	4.6
1	A	274	LEU	4.5
1	A	311	THR	4.5
1	A	588	THR	4.4
1	A	292	TRP	4.3
1	A	319	SER	4.2
1	A	791	SER	4.1
1	A	637	VAL	4.1
1	A	419	TRP	4.1
1	A	580	VAL	4.0
1	A	471	SER	4.0
1	A	750	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	284	ILE	4.0
1	A	314	THR	3.9
1	A	474	ILE	3.9
1	A	363	THR	3.9
1	A	431	PHE	3.9
1	A	410	GLY	3.8
1	A	445	GLY	3.8
1	A	294	TYR	3.8
1	A	745	GLY	3.8
1	A	793	THR	3.7
1	A	624	GLU	3.7
1	A	309	TYR	3.7
1	A	403	VAL	3.6
1	A	344	THR	3.6
1	A	584	THR	3.5
1	A	476	TYR	3.5
1	A	473	ALA	3.4
1	A	293	HIS	3.4
1	A	455	MET	3.3
1	A	635	LEU	3.3
1	A	790	THR	3.3
1	A	454	MET	3.3
1	A	290	THR	3.2
1	A	358	LYS	3.2
1	A	301	LYS	3.2
1	A	479	LEU	3.2
1	A	676	SER	3.1
1	A	281	ILE	3.1
1	A	583	PRO	3.1
1	A	296	GLN	3.0
1	A	443	LEU	3.0
1	A	288	HIS	3.0
1	A	634	HIS	3.0
1	A	435	VAL	3.0
1	A	452	TYR	3.0
1	A	298	HIS	3.0
1	A	641	ILE	3.0
1	A	746	TRP	3.0
1	A	356	LYS	3.0
1	A	448	GLU	3.0
1	A	361	THR	2.9
1	A	472	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	439	ARG	2.8
1	A	592	ILE	2.8
1	A	593	ILE	2.8
1	A	428	ASP	2.8
1	A	744	ALA	2.8
1	A	581	GLN	2.7
1	A	478	TRP	2.7
1	A	399	PHE	2.7
1	A	289	GLU	2.6
1	A	590	MET	2.6
1	A	544	LEU	2.6
1	A	417	ASN	2.6
1	A	511	GLY	2.6
1	A	571	LEU	2.5
1	A	578	VAL	2.5
1	A	889	PHE	2.5
1	A	408	ALA	2.5
1	A	425	ALA	2.5
1	A	438	GLU	2.5
1	A	277	ILE	2.5
1	A	303	TRP	2.5
1	A	830	VAL	2.5
1	A	286	GLN	2.4
1	A	302	THR	2.4
1	A	273	ASN	2.4
1	A	418	LYS	2.4
1	A	307	GLY	2.4
1	A	800	THR	2.4
1	A	743	GLY	2.4
1	A	310	GLU	2.4
1	A	534	ASP	2.4
1	A	308	SER	2.3
1	A	434	LEU	2.3
1	A	449	THR	2.3
1	A	406	ASN	2.3
1	A	401	ARG	2.3
1	A	429	SER	2.3
1	A	304	ALA	2.2
1	A	357	GLU	2.2
1	A	792	ARG	2.1
1	A	276	ILE	2.1
1	A	742	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	TYR	2.1
1	A	312	LYS	2.1
1	A	427	GLU	2.1
1	A	299	PRO	2.1
1	A	436	ASP	2.1
1	A	575	ASN	2.1
1	A	405	SER	2.1
1	A	297	ASP	2.1
1	A	432	TRP	2.1
1	A	591	ASP	2.1
1	A	564	LEU	2.1
1	A	638	THR	2.0
1	A	880	THR	2.0
1	A	423	ARG	2.0
1	A	365	GLU	2.0
1	A	577	VAL	2.0
1	A	318	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	1007	5/5	0.63	0.17	60,65,73,90	0
7	HV2	A	1011	7/7	0.66	0.27	82,85,86,88	7
6	PEG	A	1008	7/7	0.70	0.38	46,48,49,50	7
7	HV2	A	1009	7/7	0.76	0.28	20,21,21,22	7
5	PO4	A	1006	5/5	0.76	0.15	30,34,47,51	0
4	DMS	A	1004	4/4	0.82	0.23	74,81,86,90	0

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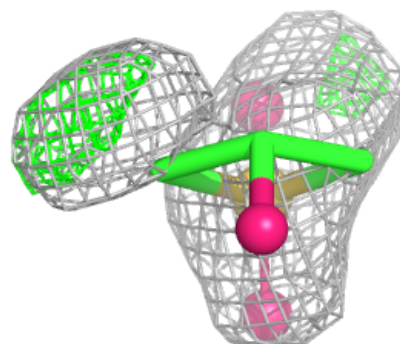
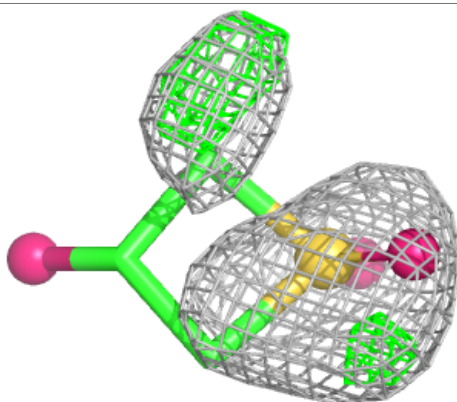
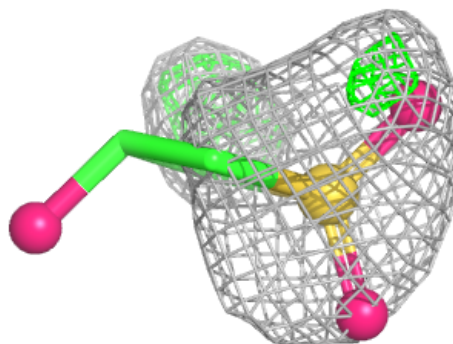
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	HV2	A	1010	7/7	0.88	0.20	34,37,38,39	7
4	DMS	A	1005	4/4	0.92	0.15	49,53,56,57	0
3	MES	A	1003[A]	12/12	0.98	0.33	20,23,25,26	12
3	MES	A	1003[B]	12/12	0.98	0.33	593,610,646,649	12
2	ZN	A	1002	1/1	0.99	0.07	47,47,47,47	0
2	ZN	A	1001	1/1	1.00	0.02	21,21,21,21	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.

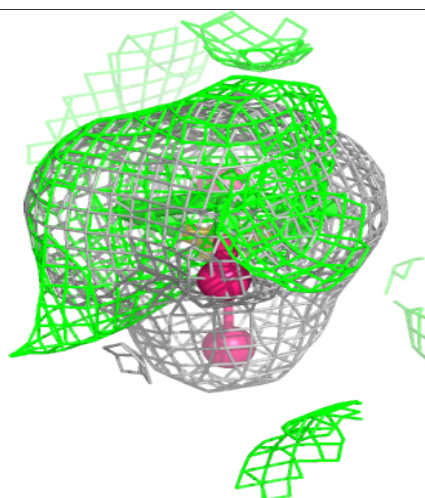
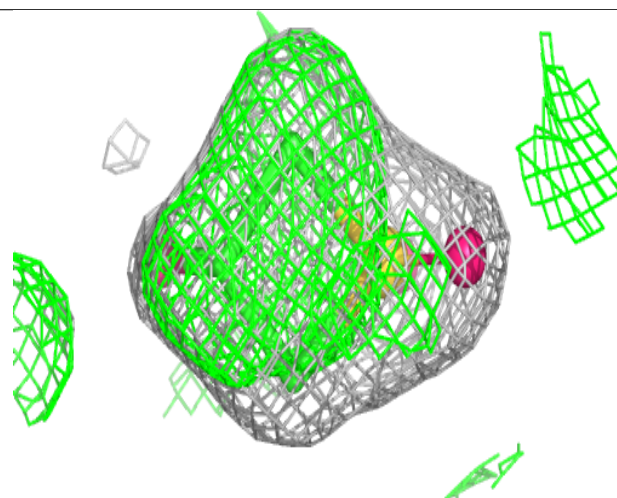
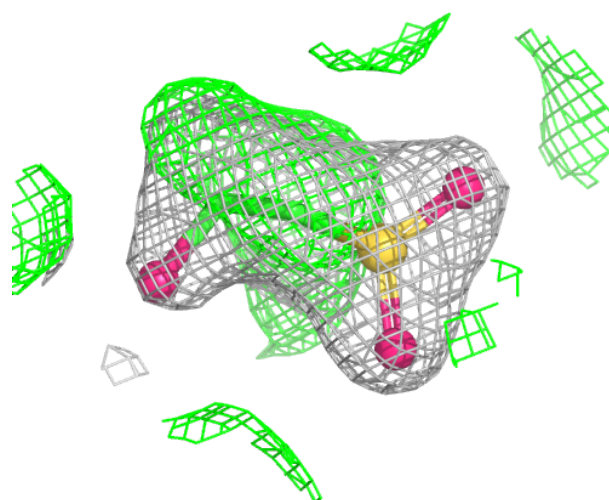
Electron density around HV2 A 1011:

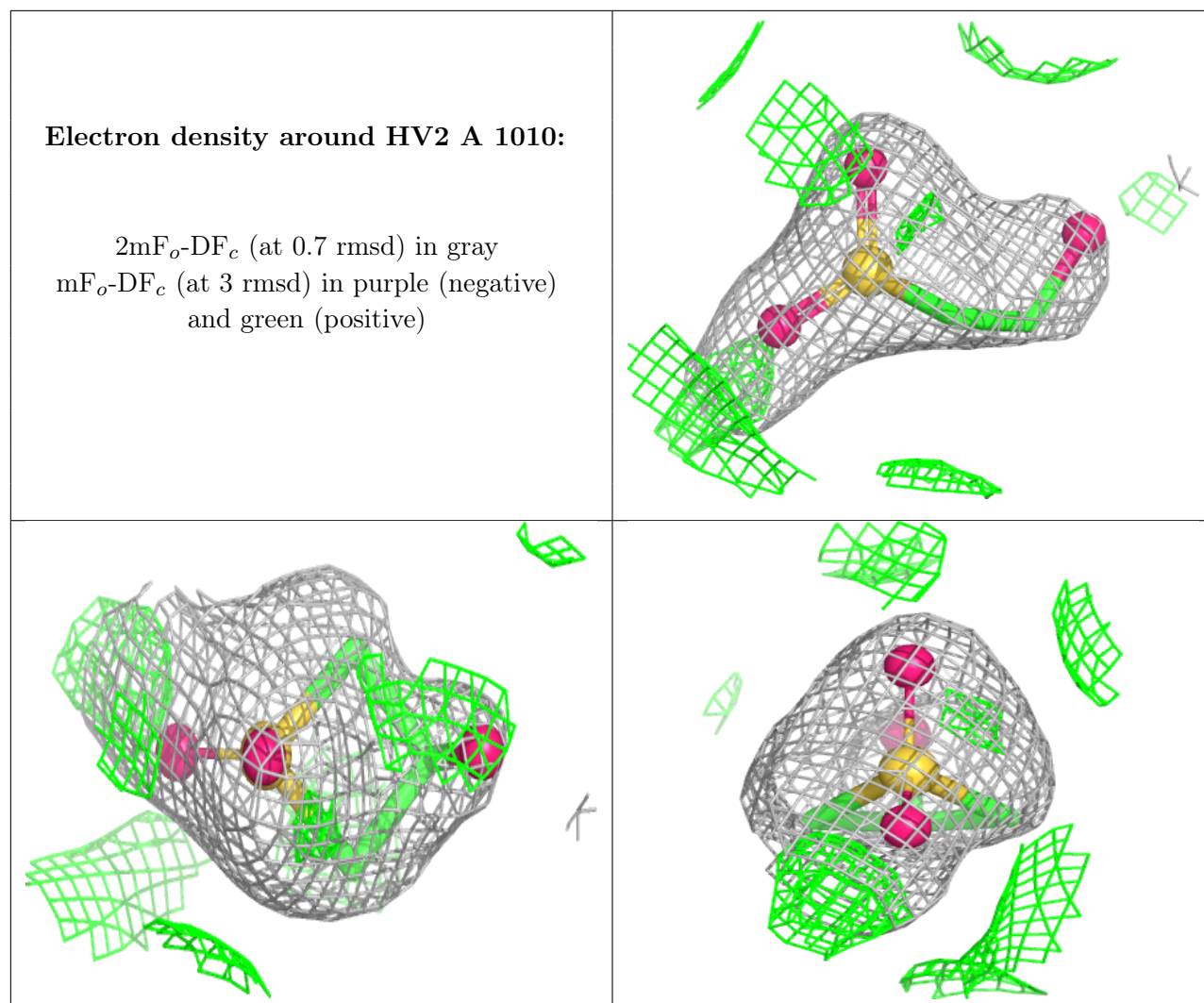
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HV2 A 1009:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.