Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2024 – 03:01 pm BST

PDB ID	:	5IHE
Title	:	D-family DNA polymerase - DP1 subunit (3'-5' proof-reading exonuclease)
Authors	:	Sauguet, L.; Raia, P.; De Larue, M.
Deposited on	:	2016-02-29
Resolution	:	2.50 Å(reported)

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

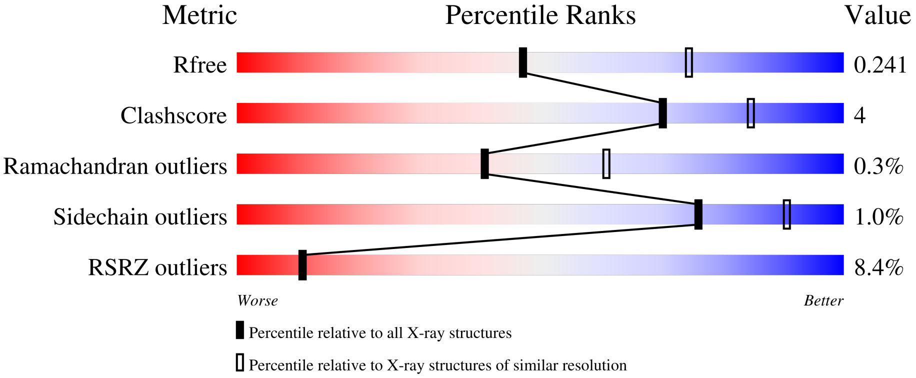
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

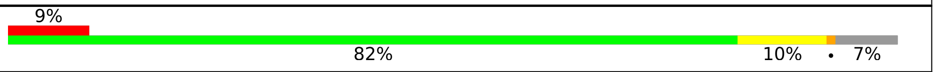
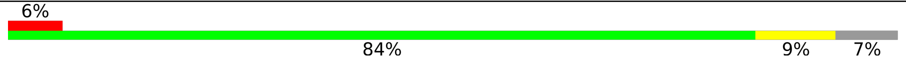
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	475	
1	B	475	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	**Type**	**Chain**	**Res**	**Chirality**	**Geometry**	**Clashes**	**Electron density**
7	EDO	B	706	-	-	-	X

2 Entry composition (i)

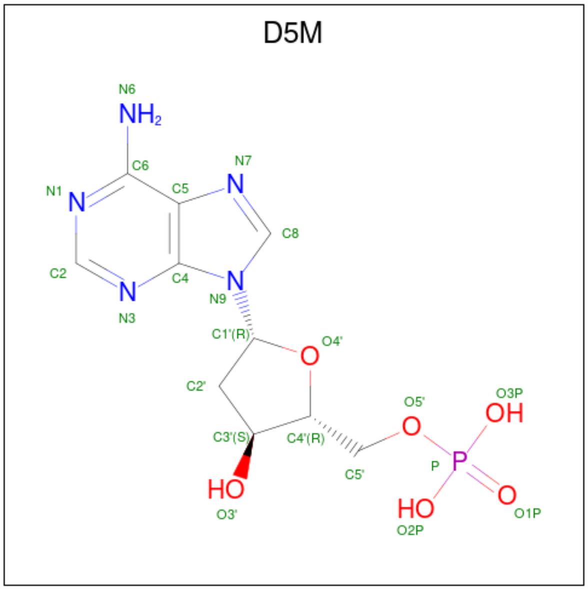
There are 8 unique types of molecules in this entry. The entry contains 7181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA polymerase II small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total 3517	C 2294	N 577	O 639	S 7	0	0	0
1	B	442	Total 3535	C 2307	N 579	O 642	S 7	0	1	0

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	B	1	Total 22	C 10	N 5	O 6	P 1	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	A	1	1	1	0	0
			Total	Fe		
3	B	1	1	1	0	0

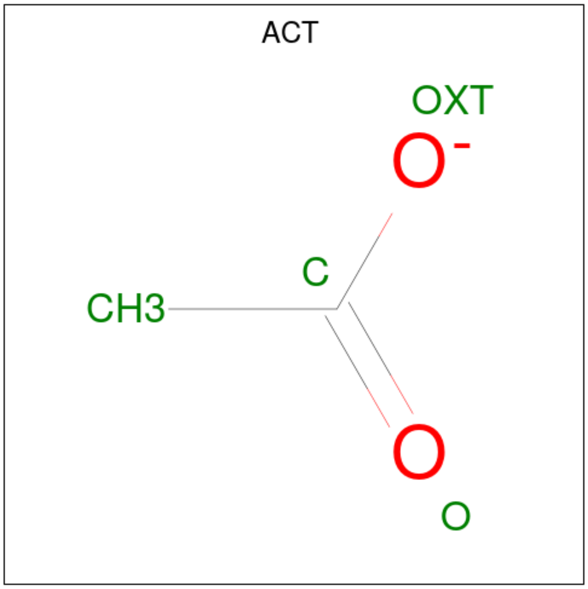
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	1	1	1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	2	2	2	0	0
			Total	Ca		
5	B	1	1	1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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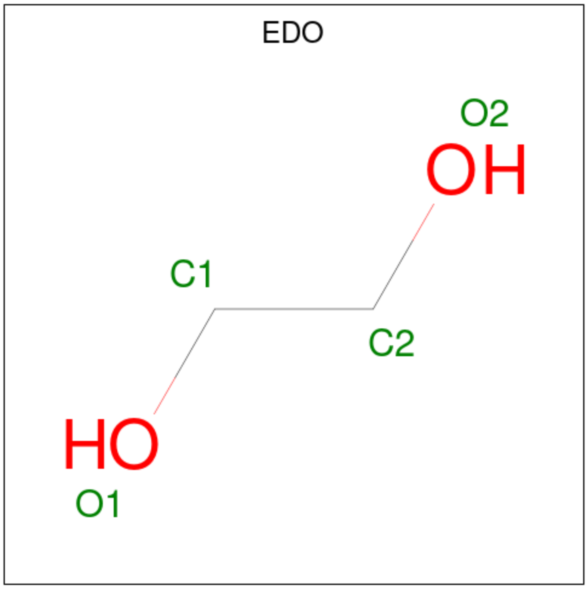
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0

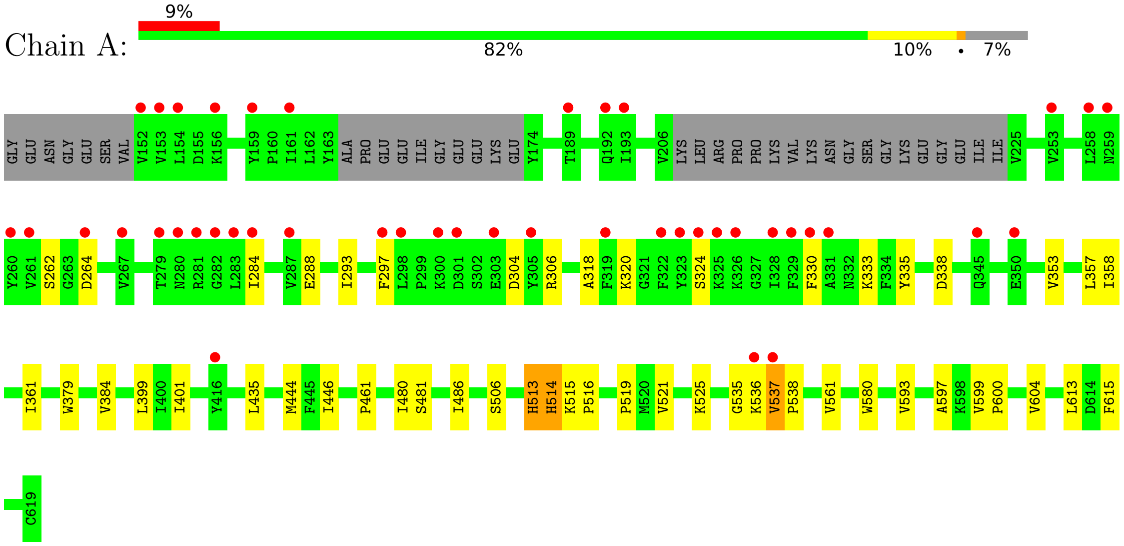
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	37	Total O 37 37	0	0
8	B	29	Total O 29 29	0	0

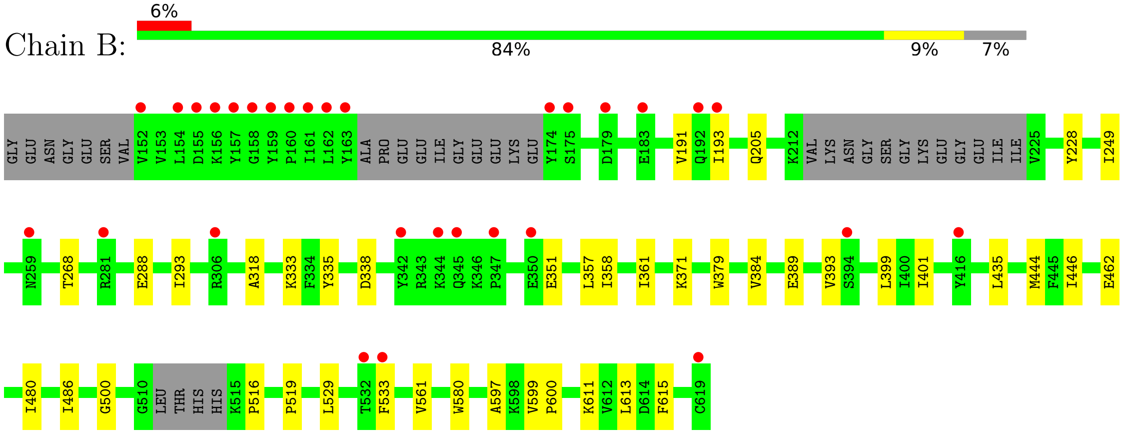
3 Residue-property plots

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: DNA polymerase II small subunit



- Molecule 1: DNA polymerase II small subunit



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.97Å 91.42Å 145.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 2.50 47.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.42-2.50) 98.9 (47.42-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.197 , 0.225 0.209 , 0.241	Depositor DCC
R_{free} test set	1998 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7181	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACT, FE, D5M, EDO, CA

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	0.43	0/3605	0.68	1/4898 (0.0%)
1	B	0.43	0/3625	0.65	0/4923
All	All	0.43	0/7230	0.67	1/9821 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	514	HIS	CB-CA-C	-5.79	98.82	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3517	0	3548	31	0
1	B	3535	0	3574	21	0
2	A	22	0	12	1	0
2	B	22	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
7	B	4	0	6	0	0
8	A	37	0	0	0	0
8	B	29	0	0	0	0
All	All	7181	0	7158	52	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 4.

All (52) 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:B:228:TYR:CE2	1:B:533:PHE:HE1	2.14	0.65
1:A:514:HIS:O	1:A:515:LYS:HG2	2.03	0.59
1:B:288:GLU:HG3	1:B:293:ILE:HG12	1.84	0.58
1:B:357:LEU:O	1:B:600:PRO:HD2	2.04	0.57
1:B:435:LEU:HD22	1:B:444:MET:HE3	1.86	0.57
1:A:357:LEU:O	1:A:600:PRO:HD2	2.04	0.56
1:A:597:ALA:HB1	1:A:615:PHE:HB2	1.88	0.56
1:A:461:PRO:O	1:A:481:SER:HB3	2.06	0.56
1:B:318:ALA:HB3	1:B:335:TYR:HB2	1.88	0.55
1:A:318:ALA:HB3	1:A:335:TYR:HB2	1.88	0.55
1:B:597:ALA:HB1	1:B:615:PHE:HB2	1.87	0.55
1:A:288:GLU:HG3	1:A:293:ILE:HG12	1.88	0.54
1:A:561:VAL:HA	2:A:701:D5M:H1	1.89	0.54
1:A:401:ILE:HD12	1:A:446:ILE:HG12	1.90	0.54
1:A:536:LYS:O	1:A:538:PRO:HD3	2.07	0.53
1:B:401:ILE:HD12	1:B:446:ILE:HG12	1.91	0.52
1:A:262:SER:HB2	1:A:264:ASP:OD1	2.09	0.52
1:A:513:HIS:O	1:A:514:HIS:HB2	2.09	0.51
1:A:304:ASP:OD2	1:A:333:LYS:HG3	2.11	0.51
1:B:379:TRP:CD1	1:B:384:VAL:HG12	2.47	0.49
1:A:435:LEU:HD22	1:A:444:MET:HE3	1.93	0.49
1:B:361:ILE:HA	1:B:580:TRP:HB2	1.95	0.48
1:A:361:ILE:HA	1:A:580:TRP:HB2	1.95	0.48
1:A:513:HIS:C	1:A:515:LYS:H	2.17	0.47
1:A:461:PRO:O	1:A:481:SER:CB	2.62	0.47
1:B:599:VAL:HB	1:B:613:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:VAL:HG12	1:A:525:LYS:HE2	1.97	0.47
1:A:537:VAL:O	1:A:537:VAL:HG13	2.16	0.46
1:A:599:VAL:HB	1:A:613:LEU:HB2	1.97	0.46
1:A:320:LYS:HB3	1:A:333:LYS:HB3	1.97	0.46
1:A:379:TRP:CD1	1:A:384:VAL:HG12	2.51	0.45
1:A:480:ILE:HD13	1:A:486:ILE:HD11	1.98	0.45
1:A:324:SER:HB2	1:A:330:PHE:CE1	2.51	0.45
1:A:513:HIS:HE1	1:A:593:VAL:H	1.65	0.44
1:B:480:ILE:HD13	1:B:486:ILE:HD11	1.97	0.44
1:B:399:LEU:HD23	1:B:444:MET:HG2	1.99	0.44
1:A:399:LEU:HD23	1:A:444:MET:HG2	2.00	0.44
1:A:516:PRO:HB3	1:A:561:VAL:HG21	2.00	0.44
1:B:444:MET:HB3	1:B:444:MET:HE2	1.93	0.43
1:B:516:PRO:HB3	1:B:561:VAL:HG21	2.00	0.43
1:B:249:ILE:HG23	1:B:268:THR:HG21	2.01	0.42
1:B:193:ILE:HD11	1:B:351:GLU:HG3	2.02	0.42
1:A:353:VAL:HG13	1:A:604:VAL:HB	2.02	0.42
1:B:358:ILE:HG12	1:B:399:LEU:HD11	2.01	0.42
1:A:535:GLY:C	1:A:537:VAL:N	2.74	0.41
1:B:191:VAL:HG12	1:B:193:ILE:HG13	2.02	0.41
1:A:284:ILE:CD1	1:A:297:PHE:HD1	2.33	0.41
1:B:389:GLU:O	1:B:393:VAL:HG23	2.21	0.41
1:A:516:PRO:C	1:A:519:PRO:HD2	2.41	0.41
1:A:358:ILE:HG12	1:A:399:LEU:HD11	2.02	0.41
1:B:500:GLY:HA3	1:B:529:LEU:O	2.20	0.40
1:B:516:PRO:C	1:B:519:PRO:HD2	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/475 (91%)	415 (96%)	18 (4%)	1 (0%)	47	68
1	B	435/475 (92%)	421 (97%)	12 (3%)	2 (0%)	29	48
All	All	869/950 (92%)	836 (96%)	30 (4%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	VAL
1	B	205	GLN
1	B	462	GLU

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	386/416 (93%)	382 (99%)	4 (1%)	76	90
1	B	388/416 (93%)	384 (99%)	4 (1%)	76	90
All	All	774/832 (93%)	766 (99%)	8 (1%)	76	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ARG
1	A	338	ASP
1	A	506	SER
1	A	513	HIS
1	B	333	LYS
1	B	338	ASP
1	B	371	LYS
1	B	611	LYS

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

Mol	Chain	Res	Type
1	A	513	HIS
1	B	205	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
6	ACT	B	705	-	3,3,3	1.17	0	3,3,3	1.08	0
6	ACT	A	705	-	3,3,3	1.12	0	3,3,3	1.02	0
2	D5M	B	701	4	22,24,24	0.63	0	24,36,36	1.07	3 (12%)
2	D5M	A	701	3,4	22,24,24	0.65	0	24,36,36	0.97	2 (8%)
7	EDO	B	706	-	3,3,3	0.80	0	2,2,2	0.03	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
2	D5M	B	701	4	-	3/6/22/22	0/3/3/3
2	D5M	A	701	3,4	-	3/6/22/22	0/3/3/3
7	EDO	B	706	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	D5M	P-O5'-C5'	3.21	127.13	118.30
2	A	701	D5M	P-O5'-C5'	2.84	126.12	118.30
2	B	701	D5M	C5-C6-N6	2.21	123.72	120.35
2	B	701	D5M	O2P-P-O5'	2.15	112.46	106.73
2	A	701	D5M	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	D5M	C5'-O5'-P-O1P
2	A	701	D5M	C5'-O5'-P-O2P
2	B	701	D5M	C5'-O5'-P-O3P
2	B	701	D5M	C5'-O5'-P-O2P
2	B	701	D5M	C5'-O5'-P-O1P
2	A	701	D5M	C5'-O5'-P-O3P

There are no ring outliers.

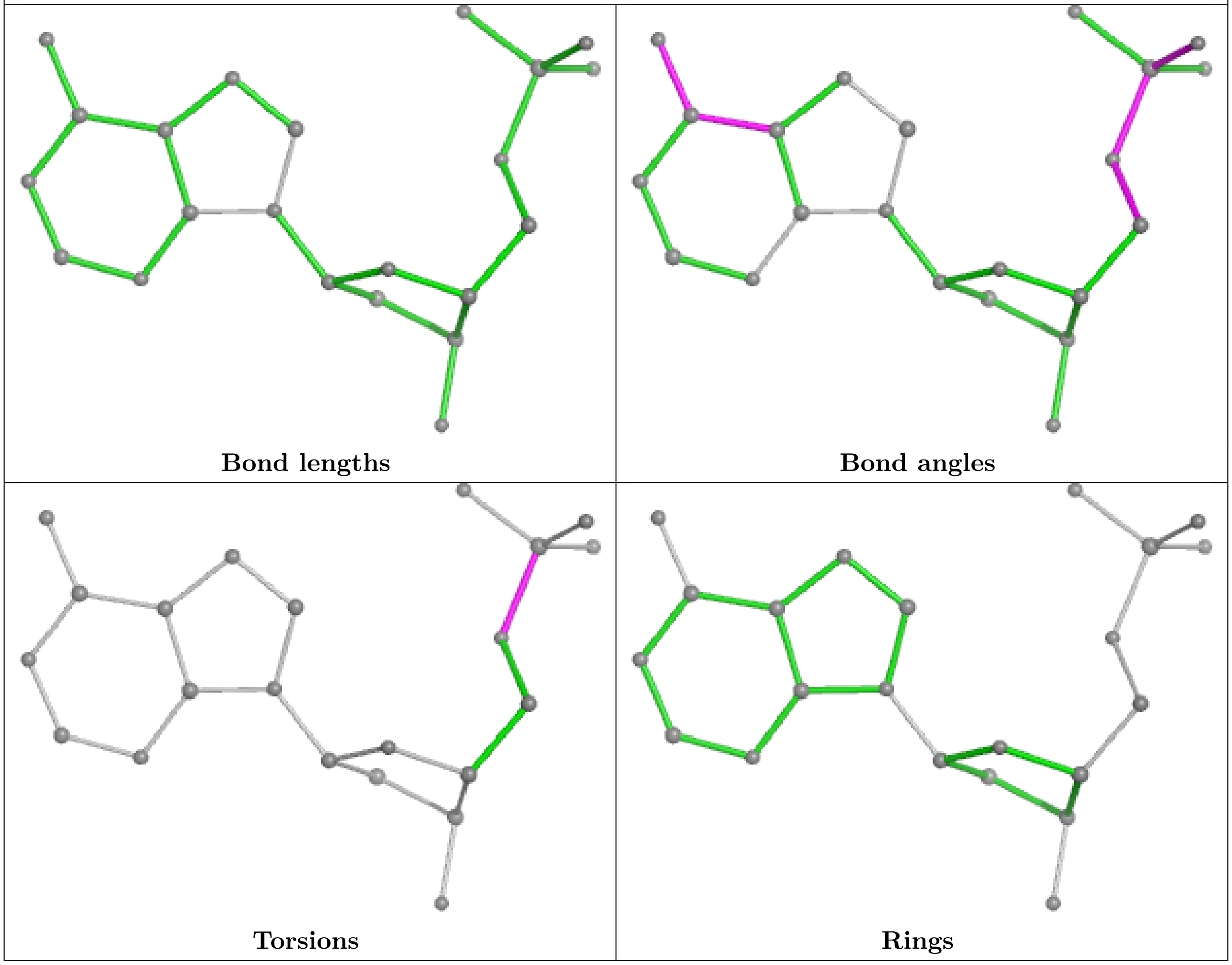
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	D5M	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 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 D5M B 701



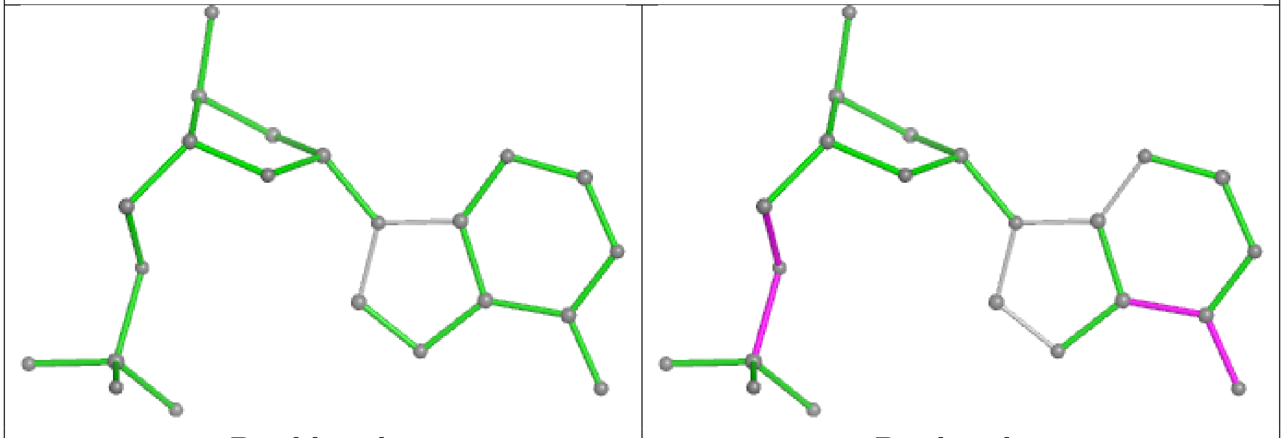
Bond lengths

Bond angles

Torsions

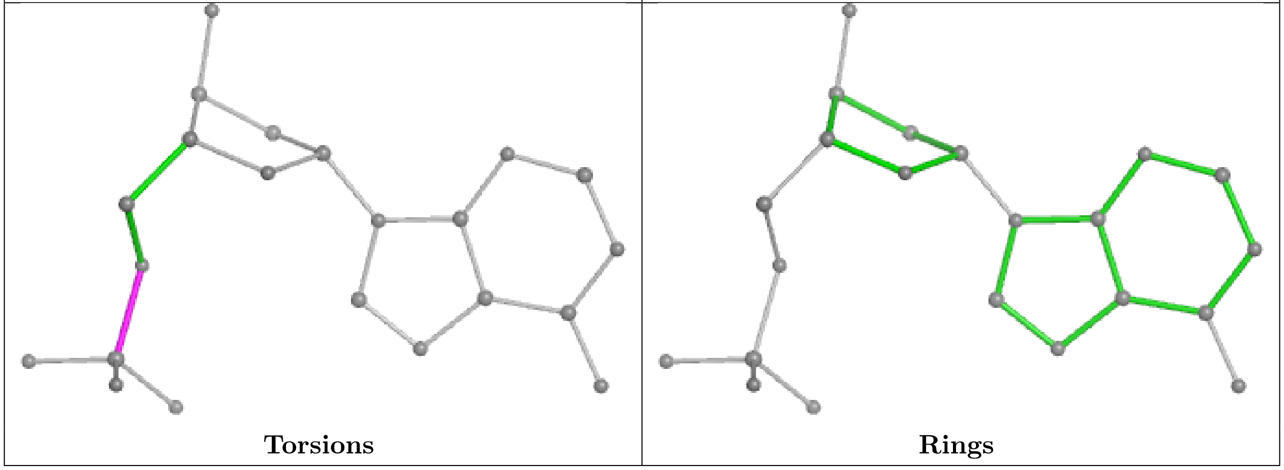
Rings

Ligand D5M A 701



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	440/475 (92%)	0.55	44 (10%)	7	6	53, 79, 128, 166	0
1	B	442/475 (93%)	0.56	30 (6%)	17	17	53, 80, 132, 162	0
All	All	882/950 (92%)	0.56	74 (8%)	11	11	53, 80, 130, 166	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	154	LEU	8.8
1	B	152	VAL	7.1
1	B	162	LEU	6.5
1	B	155	ASP	5.9
1	B	160	PRO	5.5
1	A	154	LEU	5.5
1	B	161	ILE	5.0
1	B	157	TYR	5.0
1	A	537	VAL	4.5
1	A	325	LYS	4.4
1	A	301	ASP	4.2
1	A	329	PHE	4.2
1	A	282	GLY	4.1
1	A	328	ILE	4.1
1	B	342	TYR	3.9
1	A	350	GLU	3.9
1	A	324	SER	3.8
1	A	281	ARG	3.8
1	A	280	ASN	3.7
1	B	175	SER	3.7
1	B	416	TYR	3.6
1	A	156	LYS	3.5
1	B	163	TYR	3.5
1	A	297	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	158	GLY	3.5
1	A	193	ILE	3.4
1	A	326	LYS	3.4
1	A	258	LEU	3.2
1	A	331	ALA	3.2
1	B	174	TYR	3.2
1	A	152	VAL	3.1
1	A	259	ASN	3.1
1	A	260	TYR	3.1
1	B	394	SER	3.0
1	A	536	LYS	3.0
1	A	416	TYR	2.9
1	A	305	TYR	2.9
1	A	267	VAL	2.8
1	A	323	TYR	2.8
1	A	303	GLU	2.8
1	B	193	ILE	2.7
1	A	264	ASP	2.6
1	A	253	VAL	2.6
1	A	345	GLN	2.6
1	A	284	ILE	2.6
1	B	306	ARG	2.6
1	A	330	PHE	2.5
1	B	533	PHE	2.5
1	B	344	LYS	2.5
1	B	281	ARG	2.5
1	B	183	GLU	2.5
1	A	283	LEU	2.4
1	B	532	THR	2.4
1	B	159	TYR	2.4
1	A	261	VAL	2.4
1	A	279	THR	2.3
1	B	156	LYS	2.3
1	A	287	VAL	2.3
1	B	619	CYS	2.3
1	A	159	TYR	2.2
1	B	345	GLN	2.2
1	A	153	VAL	2.2
1	A	319	PHE	2.2
1	A	298	LEU	2.2
1	B	259	ASN	2.2
1	A	189	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	GLN	2.2
1	A	322	PHE	2.2
1	A	161	ILE	2.1
1	B	350	GLU	2.1
1	B	347	PRO	2.1
1	B	192	GLN	2.1
1	B	179	ASP	2.0
1	A	300	LYS	2.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

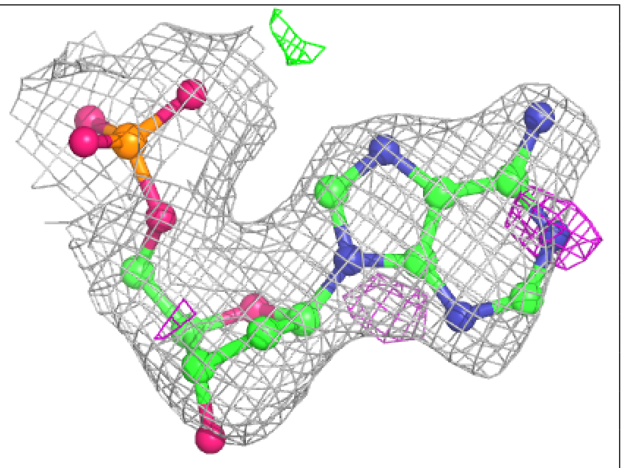
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled '$Q < 0.9$'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

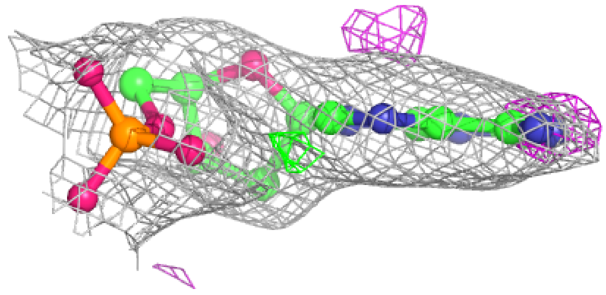
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
7	EDO	B	706	4/4	0.43	0.68	89,90,91,92	0
5	CA	A	704	1/1	0.71	0.25	128,128,128,128	0
5	CA	B	704	1/1	0.73	0.30	130,130,130,130	0
5	CA	A	706	1/1	0.88	0.35	138,138,138,138	0
2	D5M	B	701	22/22	0.91	0.19	86,89,91,93	0
2	D5M	A	701	22/22	0.92	0.22	78,93,98,99	0
6	ACT	B	705	4/4	0.98	0.21	65,66,68,69	0
4	ZN	B	703	1/1	0.98	0.15	70,70,70,70	0
3	FE	A	702	1/1	0.99	0.21	60,60,60,60	0
6	ACT	A	705	4/4	0.99	0.20	65,65,66,67	0
3	FE	B	702	1/1	0.99	0.20	62,62,62,62	0
4	ZN	A	703	1/1	0.99	0.16	66,66,66,66	0

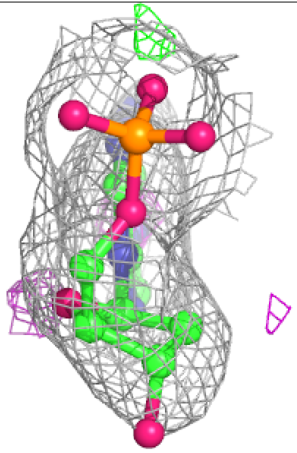
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

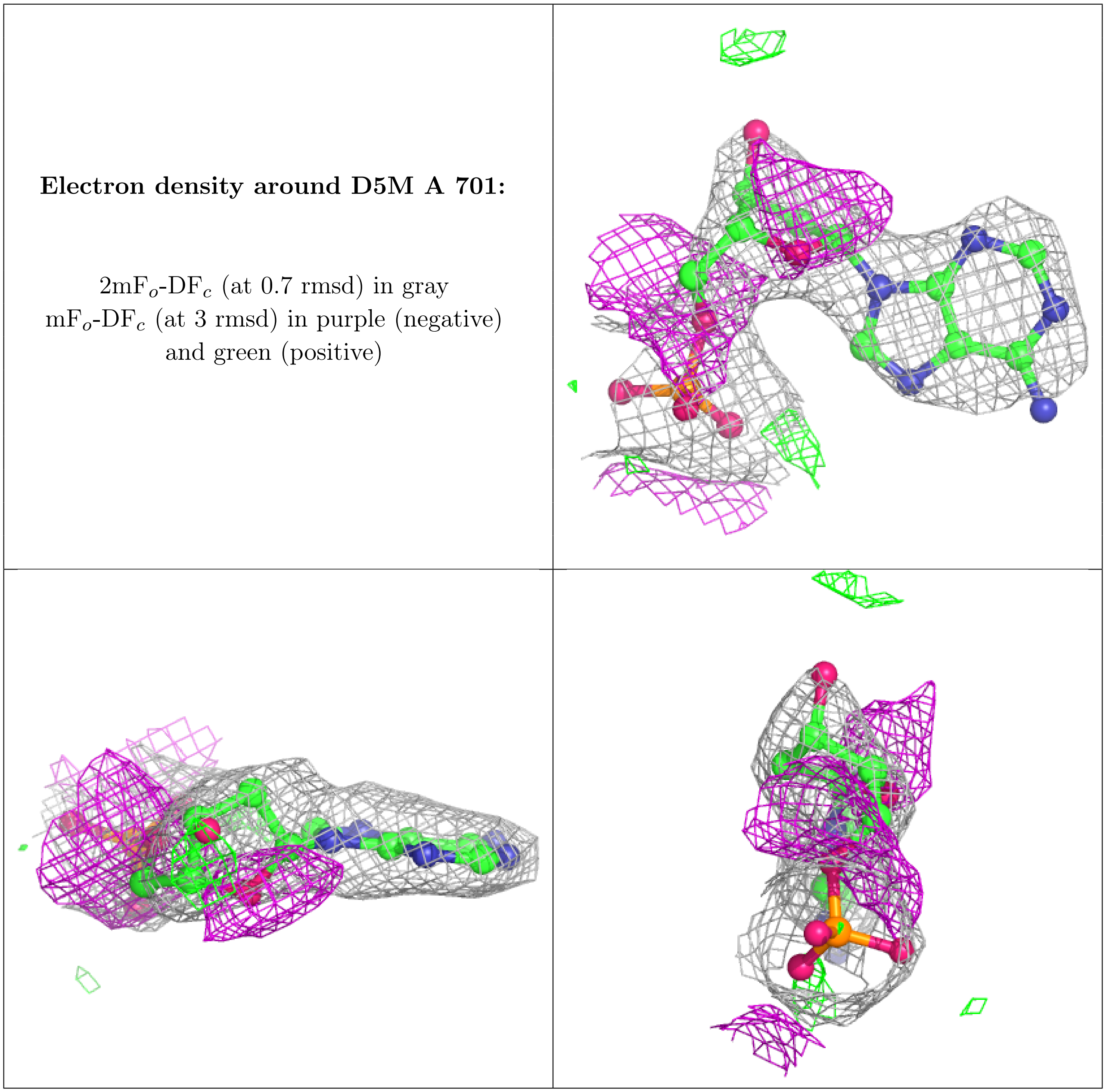
Electron density around D5M B 701:

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









Electron density around D5M A 701:

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.