



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 5DHP / pdb_00005dhp
Title : Crystal structure of NAD kinase 1 from *Listeria monocytogenes* in complex with a novel inhibitor
Authors : Gelin, M.; Paoletti, J.; Assairi, L.; Huteau, V.; Pochet, S.; Labesse, G.
Deposited on : 2015-08-31
Resolution : 2.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

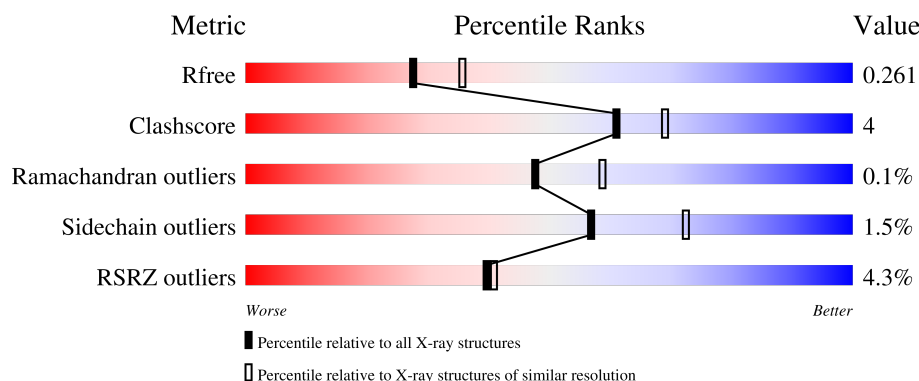
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	272	 4% 90% 7% .
1	B	272	 3% 85% 11% ..
1	C	272	 4% 88% 8% .
1	D	272	 6% 78% 14% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8624 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 NAD kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2064	1322	345	388	9			
1	B	263	Total	C	N	O	S	0	2	0
			2113	1356	354	394	9			
1	C	261	Total	C	N	O	S	0	0	0
			2035	1303	342	381	9			
1	D	250	Total	C	N	O	S	0	1	0
			1953	1249	337	360	7			

There are 32 discrepancies between the modelled and reference sequences:

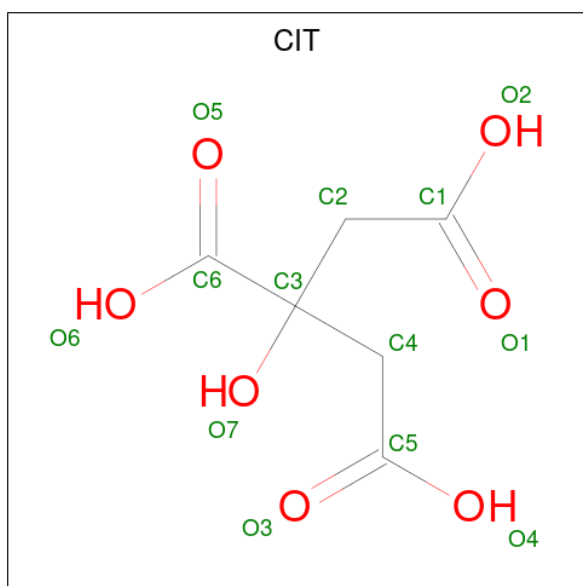
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	LEU	-	expression tag	UNP Q8Y8D7
A	266	GLU	-	expression tag	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	265	LEU	-	expression tag	UNP Q8Y8D7
B	266	GLU	-	expression tag	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	265	LEU	-	expression tag	UNP Q8Y8D7
C	266	GLU	-	expression tag	UNP Q8Y8D7
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7

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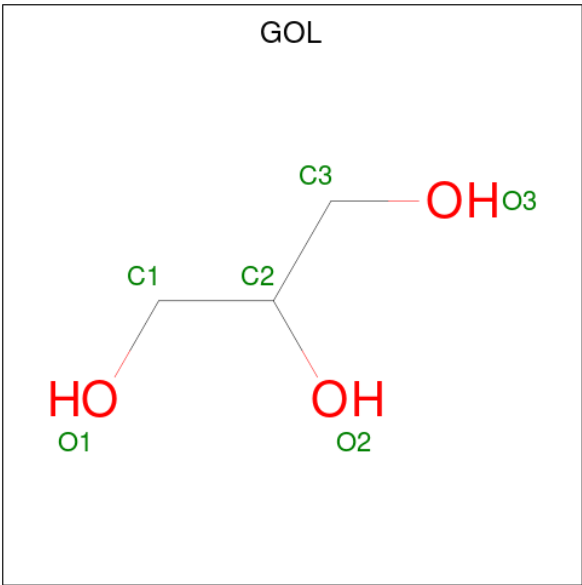
Chain	Residue	Modelled	Actual	Comment	Reference
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	272	HIS	-	expression tag	UNP Q8Y8D7
D	265	LEU	-	expression tag	UNP Q8Y8D7
D	266	GLU	-	expression tag	UNP Q8Y8D7
D	267	HIS	-	expression tag	UNP Q8Y8D7
D	268	HIS	-	expression tag	UNP Q8Y8D7
D	269	HIS	-	expression tag	UNP Q8Y8D7
D	270	HIS	-	expression tag	UNP Q8Y8D7
D	271	HIS	-	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



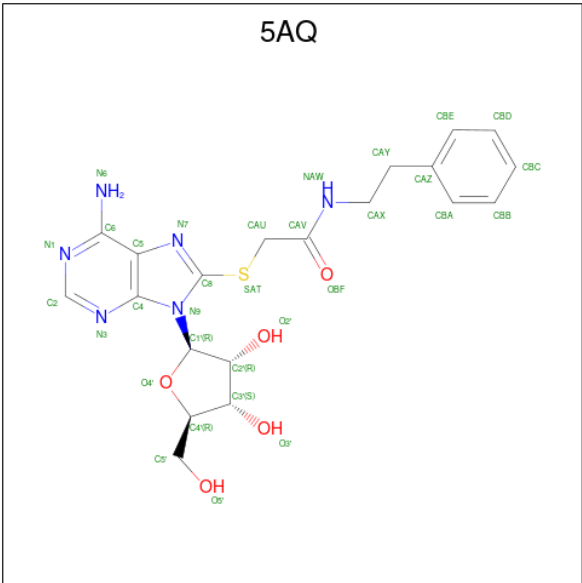
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 8-(2-oxo-2-[(2-phenylethyl)amino]ethyl)sulfanyladenosine (CCD ID: 5AQ) (formula: C₂₀H₂₄N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	20	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			32	20	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			32	20	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			32	20	6	5	1		

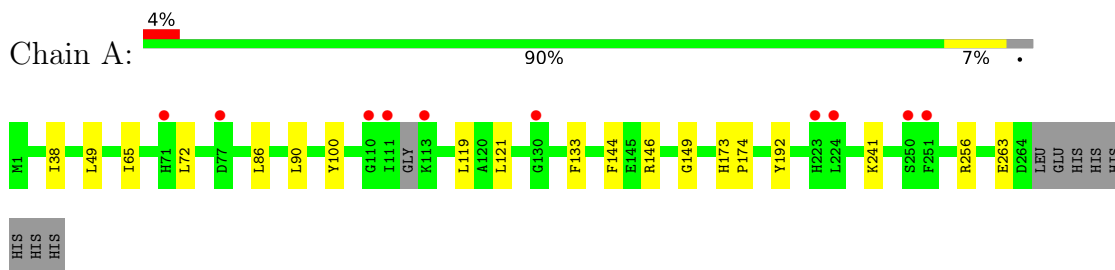
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	60	Total	O	0	1
			61	61		
5	C	72	Total	O	0	0
			72	72		
5	D	67	Total	O	0	0
			67	67		

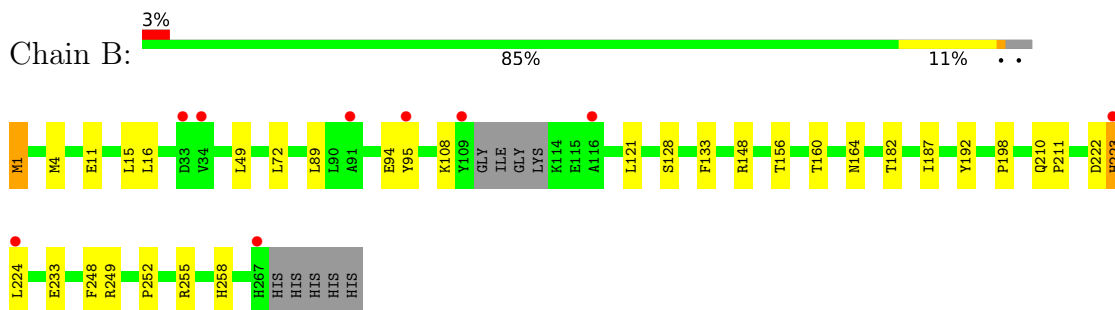
3 Residue-property plots [i](#)

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.

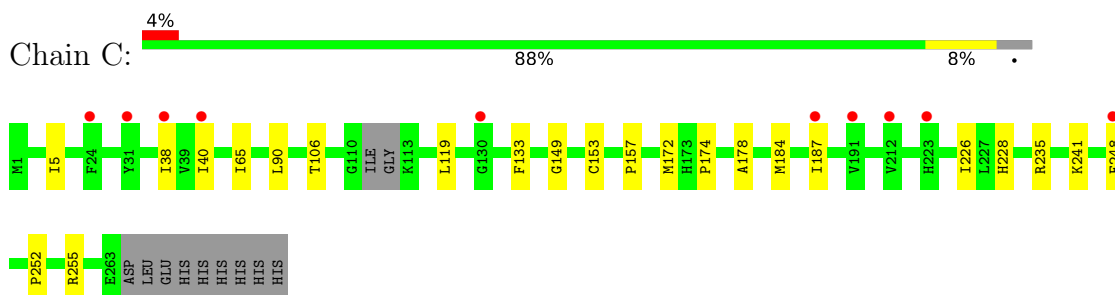
- Molecule 1: NAD kinase 1



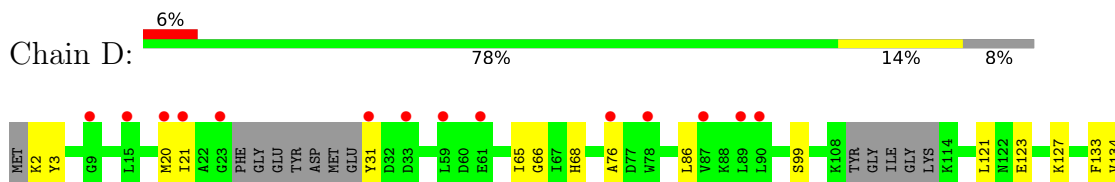
- Molecule 1: NAD kinase 1



- Molecule 1: NAD kinase 1



- Molecule 1: NAD kinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.93Å 119.53Å 67.31Å 90.00° 100.28° 90.00°	Depositor
Resolution (Å)	44.26 – 2.27 44.26 – 2.27	Depositor EDS
% Data completeness (in resolution range)	96.1 (44.26-2.27) 96.0 (44.26-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.217 , 0.259 0.222 , 0.261	Depositor DCC
R_{free} test set	1408 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8624	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, 5AQ, GOL

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	0.26	0/2114	0.69	0/2862
1	B	0.25	0/2168	0.70	0/2929
1	C	0.24	0/2085	0.68	0/2824
1	D	0.25	0/2004	0.67	0/2712
All	All	0.25	0/8371	0.69	0/11327

There are no bond length outliers.

There are no bond angle outliers.

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	2064	0	1982	10	0
1	B	2113	0	2063	17	0
1	C	2035	0	1937	15	0
1	D	1953	0	1884	23	0
2	A	13	0	5	2	0
2	B	13	0	5	3	0
2	D	13	0	5	0	0
3	A	6	0	8	0	0
4	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	0	1	0
4	C	32	0	0	0	0
4	D	32	0	0	3	0
5	A	86	0	0	2	0
5	B	61	0	0	1	0
5	C	72	0	0	0	0
5	D	67	0	0	2	0
All	All	8624	0	7889	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:CYS:HB2	1:C:184:MET:HE3	1.70	0.72
1:B:252:PRO:HA	2:B:301:CIT:H42	1.76	0.67
1:A:38:ILE:HD13	1:A:90:LEU:HD22	1.79	0.64
1:C:172:MET:HE1	1:C:178:ALA:HB3	1.82	0.60
1:D:160:THR:HG21	1:D:172:MET:HG2	1.84	0.58
1:C:255:ARG:HD2	1:D:142:ILE:HD13	1.86	0.57
4:D:302:5AQ:O5'	4:D:302:5AQ:CBC	2.53	0.57
1:A:100:TYR:OH	2:A:301:CIT:O5	2.18	0.55
1:C:38:ILE:HG21	1:C:90:LEU:HD21	1.89	0.55
1:C:38:ILE:HD13	1:C:90:LEU:HD11	1.87	0.55
1:D:2:LYS:N	5:D:403:HOH:O	2.39	0.55
1:C:106:THR:HG21	1:C:235:ARG:HH11	1.72	0.54
1:B:222:ASP:O	1:B:223[A]:HIS:HB2	2.07	0.54
2:B:301:CIT:O3	5:B:401:HOH:O	2.18	0.54
1:B:182:THR:HG22	1:B:198:PRO:HB3	1.92	0.52
1:B:148:ARG:HG2	1:B:187:ILE:HD13	1.92	0.51
1:C:157:PRO:HB2	1:C:174:PRO:HA	1.92	0.50
1:A:49:LEU:HD23	1:A:121:LEU:HD23	1.94	0.50
1:D:138:VAL:HB	1:D:208:SER:HB3	1.93	0.50
1:C:90:LEU:HD13	1:C:248:PHE:HZ	1.77	0.50
1:C:255:ARG:HH11	1:D:142:ILE:HD13	1.78	0.49
4:D:302:5AQ:NAW	4:D:302:5AQ:C8	2.76	0.49
1:C:252:PRO:HD2	1:C:255:ARG:HD3	1.94	0.49
1:D:146:ARG:HG2	1:D:192:TYR:HD1	1.78	0.48
1:B:1:MET:SD	1:B:1:MET:N	2.71	0.48
1:B:252:PRO:HD2	1:B:255:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:HB3	1:B:248:PHE:CE1	2.50	0.47
1:C:226:ILE:HG13	1:C:228:HIS:CE1	2.49	0.47
1:B:128:SER:HB2	1:B:133:PHE:HB2	1.97	0.47
2:B:301:CIT:O1	2:B:301:CIT:O7	2.28	0.47
1:B:89:LEU:HB3	1:B:248:PHE:CE1	2.50	0.46
1:D:211:PRO:HG3	1:D:217:PHE:HE2	1.80	0.46
1:D:121:LEU:O	1:D:156:THR:OG1	2.30	0.46
1:D:256:ARG:NH2	5:D:407:HOH:O	2.48	0.46
1:B:148:ARG:HD3	1:B:192:TYR:CE2	2.51	0.46
1:B:4:MET:HE2	1:B:4:MET:HB2	1.87	0.46
1:B:160:THR:HA	1:B:164:ASN:HB3	1.98	0.46
1:D:68:HIS:ND1	1:D:68:HIS:O	2.49	0.45
2:A:301:CIT:O3	5:A:401:HOH:O	2.21	0.45
1:D:135:VAL:HG21	1:D:209:LEU:HB3	1.97	0.45
1:D:134:VAL:HG22	1:D:148:ARG:HG3	1.98	0.44
1:B:210:GLN:HA	1:B:211:PRO:HD3	1.82	0.44
1:D:252:PRO:HD2	1:D:255:ARG:HE	1.83	0.44
1:A:133:PHE:HB3	1:A:149:GLY:O	2.18	0.43
1:D:99:SER:HB3	1:D:242[B]:LYS:HD3	2.00	0.43
1:A:144:PHE:O	1:B:258:HIS:HD2	2.00	0.43
1:A:146:ARG:HG2	1:A:192:TYR:HD1	1.83	0.43
1:D:123:GLU:OE2	4:D:302:5AQ:O2'	2.37	0.43
1:D:127:LYS:O	1:D:218:GLN:N	2.48	0.43
1:A:65:ILE:HG21	1:A:86:LEU:HD21	2.01	0.42
1:A:173:HIS:HA	1:A:174:PRO:HD3	1.80	0.42
1:A:256:ARG:NH2	5:A:402:HOH:O	2.31	0.42
1:D:21:ILE:HD11	1:D:31:TYR:CD1	2.54	0.42
1:B:49:LEU:HD23	1:B:121:LEU:HD23	2.02	0.42
1:C:133:PHE:HB3	1:C:149:GLY:O	2.20	0.42
1:C:40:ILE:HG12	1:C:65:ILE:HB	2.01	0.42
1:D:127:LYS:HD2	1:D:184:MET:HE1	2.01	0.42
1:D:220:SER:HA	1:D:225:SER:HA	2.02	0.42
1:D:65:ILE:HG21	1:D:86:LEU:HD21	2.03	0.41
1:D:66:GLY:HA3	1:D:76:ALA:HA	2.03	0.41
1:D:20:MET:HE1	1:D:86:LEU:HD23	2.03	0.40
1:D:133:PHE:HB3	1:D:149:GLY:O	2.21	0.40
1:B:121:LEU:O	1:B:156:THR:OG1	2.37	0.40
1:C:5:ILE:HG12	1:C:40:ILE:HB	2.03	0.40
1:A:119:LEU:HD11	1:A:241:LYS:HD2	2.02	0.40
4:B:302:5AQ:NAW	4:B:302:5AQ:CBA	2.82	0.40
1:C:119:LEU:HD11	1:C:241:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LYS:HE3	1:B:233:GLU:HB3	2.02	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	259/272 (95%)	248 (96%)	11 (4%)	0	100	100
1	B	261/272 (96%)	248 (95%)	11 (4%)	2 (1%)	16	18
1	C	257/272 (94%)	244 (95%)	13 (5%)	0	100	100
1	D	245/272 (90%)	233 (95%)	12 (5%)	0	100	100
All	All	1022/1088 (94%)	973 (95%)	47 (5%)	2 (0%)	48	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223[A]	HIS
1	B	223[B]	HIS

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	219/237 (92%)	217 (99%)	2 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	229/237 (97%)	221 (96%)	8 (4%)	32	45
1	C	213/237 (90%)	212 (100%)	1 (0%)	81	89
1	D	206/237 (87%)	204 (99%)	2 (1%)	68	81
All	All	867/948 (92%)	854 (98%)	13 (2%)	57	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	263	GLU
1	B	1	MET
1	B	11	GLU
1	B	15	LEU
1	B	16	LEU
1	B	72	LEU
1	B	94	GLU
1	B	224	LEU
1	B	249	ARG
1	C	187	ILE
1	D	3	TYR
1	D	223	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	204	HIS
1	B	218	GLN
1	C	143	HIS
1	C	218	GLN
1	C	228	HIS

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 [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
4	5AQ	A	303	-	35,35,35	1.93	8 (22%)	47,49,49	1.72	9 (19%)
2	CIT	D	301	-	12,12,12	1.11	0	17,17,17	1.48	2 (11%)
4	5AQ	C	301	-	35,35,35	1.67	5 (14%)	47,49,49	1.94	12 (25%)
2	CIT	B	301	-	12,12,12	1.13	0	17,17,17	1.58	2 (11%)
4	5AQ	B	302	-	35,35,35	1.91	8 (22%)	47,49,49	1.96	12 (25%)
4	5AQ	D	302	-	35,35,35	1.90	8 (22%)	47,49,49	1.85	12 (25%)
3	GOL	A	302	-	5,5,5	0.38	0	5,5,5	0.23	0
2	CIT	A	301	-	12,12,12	1.04	0	17,17,17	1.65	2 (11%)

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
4	5AQ	A	303	-	-	3/17/33/33	0/4/4/4
2	CIT	D	301	-	-	6/16/16/16	-
4	5AQ	C	301	-	-	2/17/33/33	0/4/4/4
2	CIT	B	301	-	-	6/16/16/16	-
4	5AQ	B	302	-	-	6/17/33/33	0/4/4/4
4	5AQ	D	302	-	-	5/17/33/33	0/4/4/4
3	GOL	A	302	-	-	2/4/4/4	-
2	CIT	A	301	-	-	3/16/16/16	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	5AQ	C4-N9	-6.54	1.29	1.38
4	B	302	5AQ	C4-N9	-6.15	1.29	1.38
4	C	301	5AQ	C4-N9	-6.02	1.29	1.38
4	D	302	5AQ	C4-N9	-5.65	1.30	1.38
4	A	303	5AQ	C5-N7	-4.66	1.31	1.39
4	C	301	5AQ	C5-N7	-4.62	1.31	1.39
4	D	302	5AQ	C5-N7	-4.50	1.31	1.39
4	B	302	5AQ	C5-N7	-4.20	1.31	1.39
4	D	302	5AQ	C8-SAT	-4.13	1.67	1.74
4	B	302	5AQ	C8-N9	-3.92	1.30	1.37
4	A	303	5AQ	C8-SAT	-3.74	1.68	1.74
4	D	302	5AQ	O4'-C4'	-3.54	1.37	1.45
4	B	302	5AQ	O4'-C4'	-3.52	1.37	1.45
4	A	303	5AQ	C8-N9	-3.36	1.31	1.37
4	D	302	5AQ	C8-N9	-3.21	1.32	1.37
4	B	302	5AQ	C8-SAT	-3.02	1.69	1.74
4	C	301	5AQ	C8-N9	-2.82	1.32	1.37
4	A	303	5AQ	O4'-C4'	-2.76	1.38	1.45
4	D	302	5AQ	C1'-N9	-2.68	1.41	1.45
4	D	302	5AQ	C2-N3	-2.67	1.29	1.33
4	C	301	5AQ	O4'-C4'	-2.61	1.39	1.45
4	B	302	5AQ	C2-N3	-2.50	1.29	1.33
4	A	303	5AQ	C2-N3	-2.36	1.29	1.33
4	B	302	5AQ	C1'-N9	-2.29	1.42	1.45
4	C	301	5AQ	C2-N3	-2.26	1.29	1.33
4	B	302	5AQ	CAU-CAV	-2.23	1.49	1.51
4	A	303	5AQ	C2-N1	2.23	1.37	1.33
4	A	303	5AQ	O2'-C2'	-2.17	1.37	1.43
4	D	302	5AQ	C2-N1	2.11	1.37	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	5AQ	N3-C2-N1	-5.63	120.07	128.58
4	A	303	5AQ	N3-C2-N1	-5.56	120.17	128.58
4	B	302	5AQ	N3-C2-N1	-5.52	120.22	128.58
4	D	302	5AQ	C2'-C1'-N9	-5.48	107.53	115.44
4	D	302	5AQ	N3-C2-N1	-5.06	120.92	128.58
2	A	301	CIT	O6-C6-C3	4.54	121.86	113.14
4	C	301	5AQ	C2'-C1'-N9	-4.50	108.95	115.44
4	A	303	5AQ	C5'-C4'-C3'	-4.27	105.02	115.10
4	C	301	5AQ	N9-C8-N7	-4.15	109.65	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CIT	O6-C6-C3	4.10	121.00	113.14
4	B	302	5AQ	C5-C4-N3	-4.01	121.19	126.72
4	B	302	5AQ	N9-C8-N7	-3.99	109.83	114.01
4	B	302	5AQ	C2-N3-C4	3.95	121.47	111.83
4	C	301	5AQ	C5-C4-N3	-3.91	121.34	126.72
4	C	301	5AQ	C5-C4-N9	3.88	108.07	105.63
4	B	302	5AQ	C5-C4-N9	3.75	107.99	105.63
4	B	302	5AQ	C4-C5-N7	-3.72	107.11	110.91
4	C	301	5AQ	C2-N3-C4	3.70	120.88	111.83
2	D	301	CIT	O6-C6-C3	3.70	120.24	113.14
4	B	302	5AQ	C2'-C1'-N9	-3.66	110.16	115.44
4	D	302	5AQ	C4'-O4'-C1'	-3.47	101.81	109.47
4	B	302	5AQ	C4'-O4'-C1'	-3.41	101.93	109.47
4	C	301	5AQ	C4-C5-N7	-3.35	107.48	110.91
4	B	302	5AQ	C6-C5-N7	3.27	134.97	131.72
4	D	302	5AQ	CAX-NAW-CAV	3.20	128.78	122.82
4	D	302	5AQ	C5-C4-N3	-3.19	122.32	126.72
4	A	303	5AQ	C2-N3-C4	3.18	119.61	111.83
4	D	302	5AQ	C2-N3-C4	3.09	119.37	111.83
4	A	303	5AQ	N9-C8-N7	-3.02	110.84	114.01
4	B	302	5AQ	O4'-C4'-C3'	-2.88	99.43	105.15
4	A	303	5AQ	C5-C4-N3	-2.82	122.83	126.72
4	A	303	5AQ	C4-C5-N7	-2.77	108.08	110.91
4	A	303	5AQ	C5-C4-N9	2.73	107.35	105.63
4	D	302	5AQ	OBF-CAV-NAW	2.63	128.18	123.03
4	C	301	5AQ	SAT-C8-N9	2.60	127.63	122.15
4	A	303	5AQ	C2'-C1'-N9	-2.45	111.91	115.44
4	C	301	5AQ	C6-C5-N7	2.44	134.15	131.72
4	B	302	5AQ	N3-C4-N9	2.42	130.82	127.33
4	C	301	5AQ	C4'-O4'-C1'	-2.38	104.20	109.47
4	B	302	5AQ	O4'-C4'-C5'	-2.36	104.22	109.22
4	D	302	5AQ	N3-C4-N9	2.35	130.72	127.33
4	A	303	5AQ	O4'-C4'-C5'	-2.33	104.28	109.22
4	C	301	5AQ	C4-N9-C1'	-2.30	121.19	126.43
4	D	302	5AQ	O4'-C4'-C3'	-2.30	100.59	105.15
2	B	301	CIT	O4-C5-C4	2.29	121.59	114.35
4	D	302	5AQ	N9-C8-N7	-2.27	111.63	114.01
4	C	301	5AQ	N3-C4-N9	2.27	130.60	127.33
4	D	302	5AQ	SAT-C8-N9	2.16	126.70	122.15
2	A	301	CIT	O4-C5-C4	2.13	121.08	114.35
4	D	302	5AQ	C5-C4-N9	2.11	106.95	105.63
2	D	301	CIT	O2-C1-C2	2.10	120.99	114.35

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	CIT	C1-C2-C3-O7
2	A	301	CIT	C1-C2-C3-C4
2	B	301	CIT	O7-C3-C6-O5
2	B	301	CIT	O7-C3-C6-O6
2	B	301	CIT	C4-C3-C6-O5
2	B	301	CIT	C4-C3-C6-O6
2	D	301	CIT	C2-C3-C6-O5
2	D	301	CIT	C2-C3-C6-O6
2	D	301	CIT	O7-C3-C6-O5
2	D	301	CIT	O7-C3-C6-O6
3	A	302	GOL	O1-C1-C2-C3
4	C	301	5AQ	CAV-CAU-SAT-C8
4	D	302	5AQ	O4'-C4'-C5'-O5'
4	A	303	5AQ	O4'-C4'-C5'-O5'
4	D	302	5AQ	C3'-C4'-C5'-O5'
4	A	303	5AQ	C3'-C4'-C5'-O5'
4	B	302	5AQ	O4'-C4'-C5'-O5'
2	A	301	CIT	C1-C2-C3-C6
3	A	302	GOL	O1-C1-C2-O2
4	D	302	5AQ	CAX-CAY-CAZ-CBA
4	B	302	5AQ	CAX-CAY-CAZ-CBA
4	B	302	5AQ	CAX-CAY-CAZ-CBE
4	D	302	5AQ	CAX-CAY-CAZ-CBE
4	B	302	5AQ	C3'-C4'-C5'-O5'
4	C	301	5AQ	NAW-CAX-CAY-CAZ
4	D	302	5AQ	NAW-CAX-CAY-CAZ
2	B	301	CIT	C3-C4-C5-O4
2	B	301	CIT	C3-C4-C5-O3
4	A	303	5AQ	NAW-CAX-CAY-CAZ
4	B	302	5AQ	NAW-CAX-CAY-CAZ
2	D	301	CIT	O2-C1-C2-C3
4	B	302	5AQ	CAV-CAU-SAT-C8
2	D	301	CIT	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CIT	3	0
4	B	302	5AQ	1	0

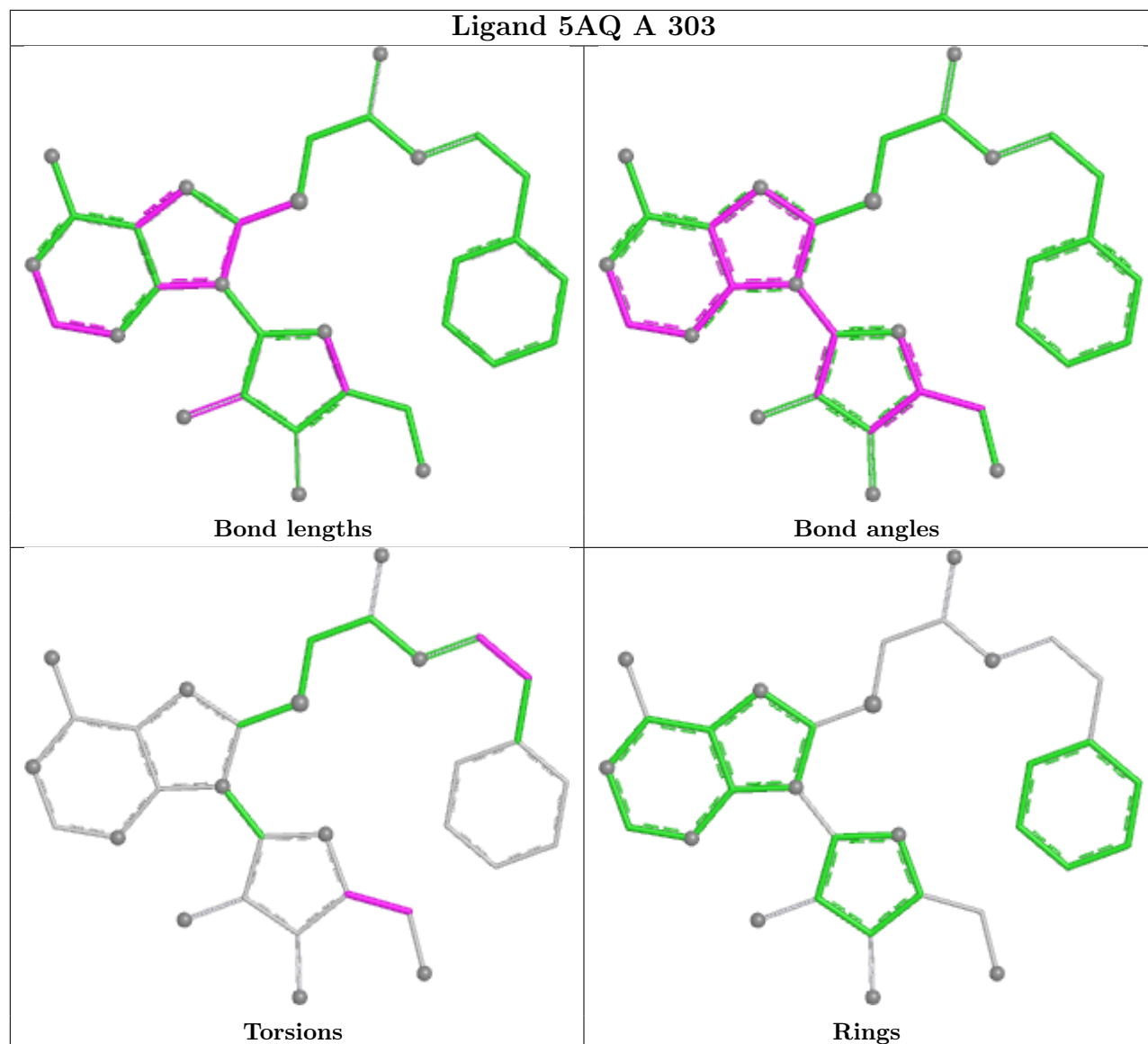
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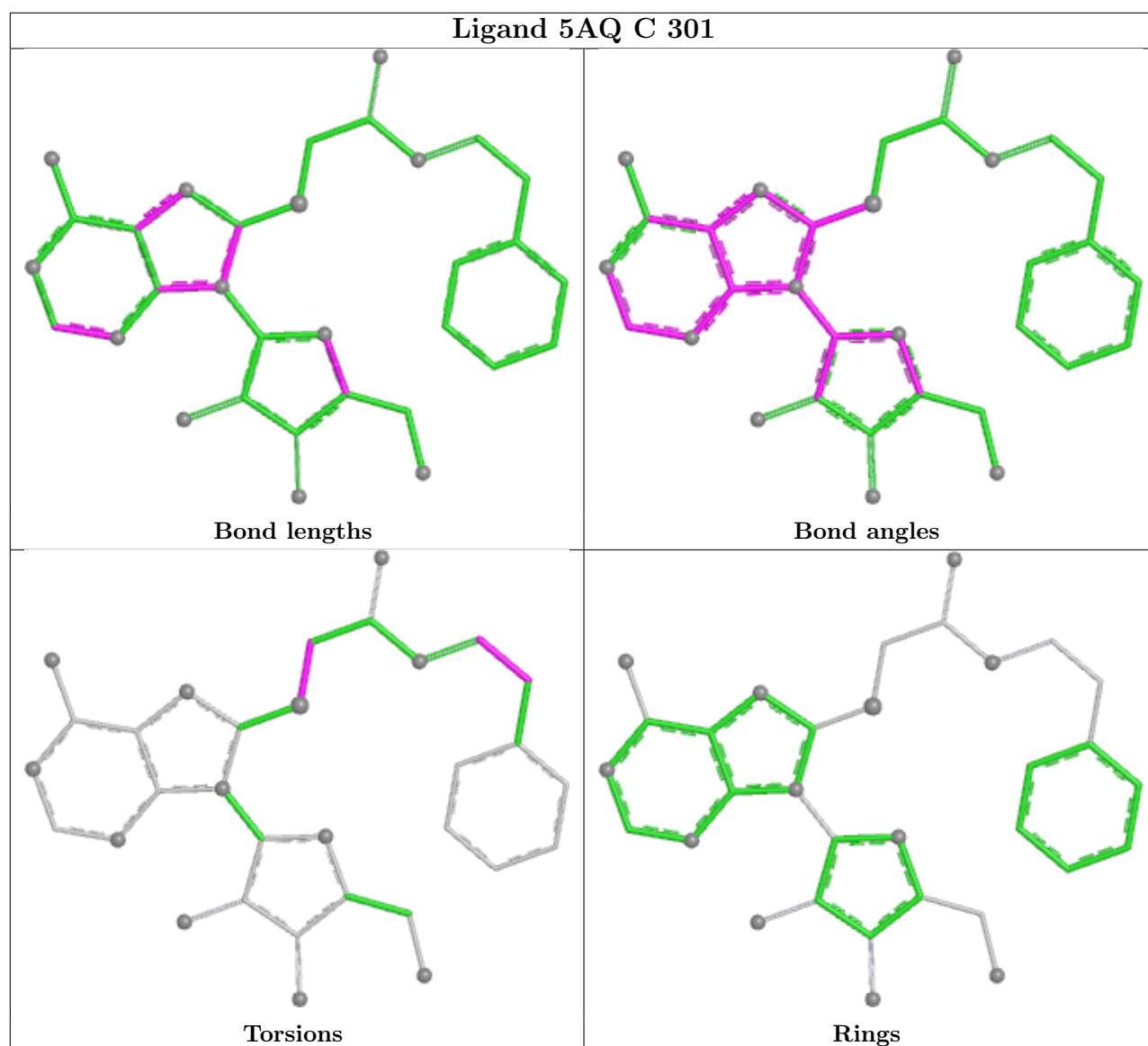
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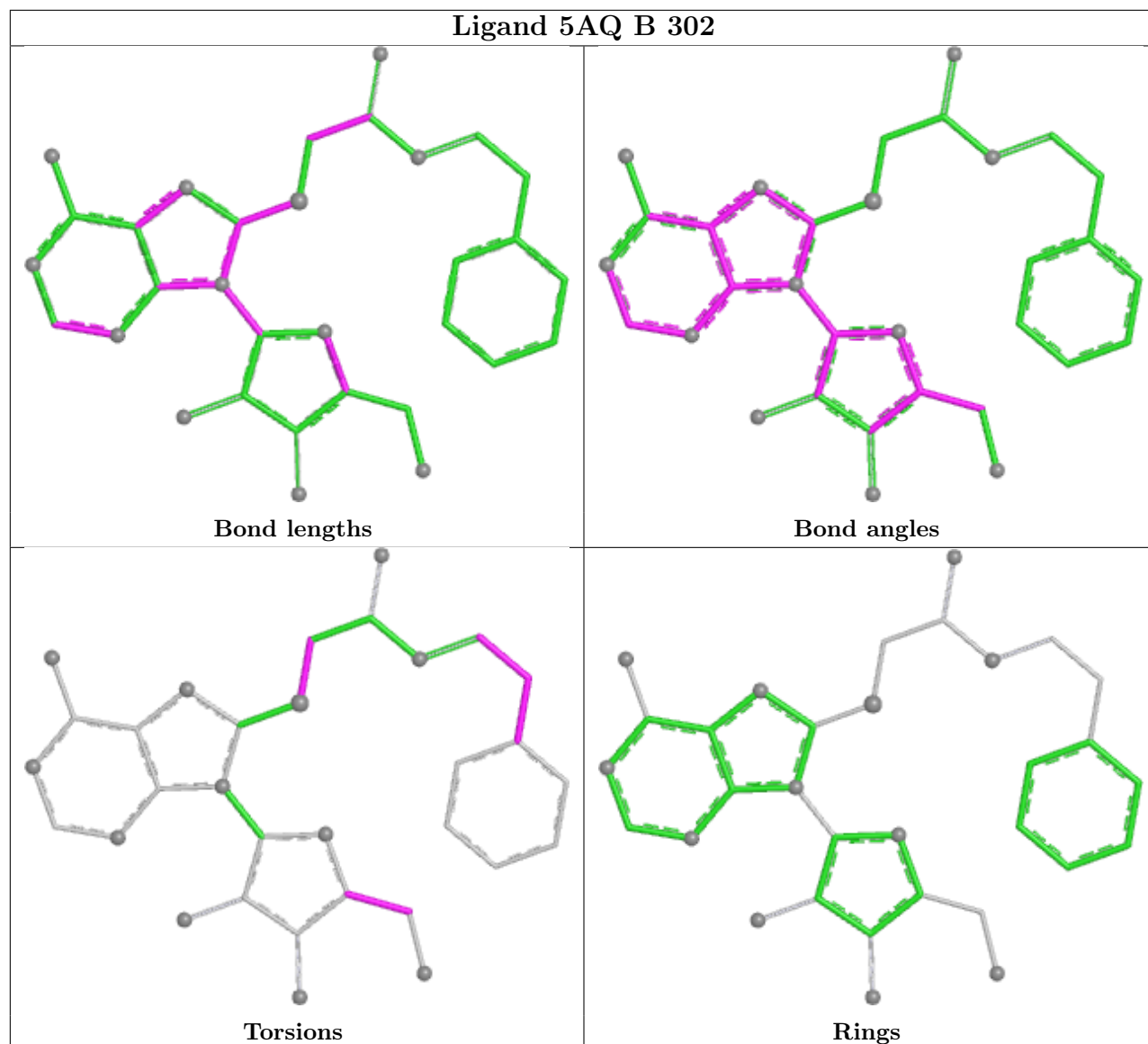
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	5AQ	3	0
2	A	301	CIT	2	0

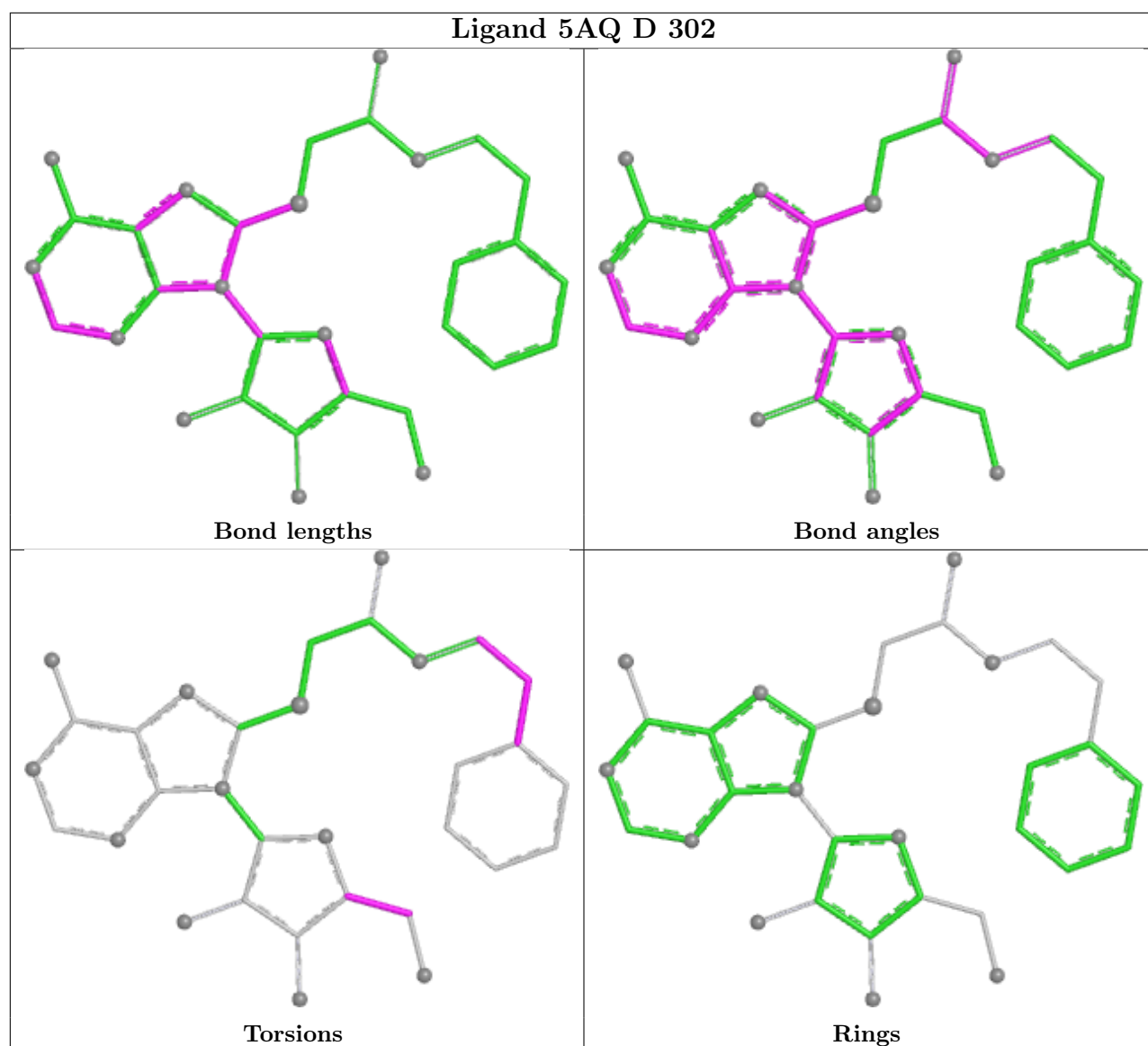
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 5AQ A 303









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/272 (96%)	0.25	10 (3%) 44 46	20, 43, 75, 113	40 (15%)
1	B	263/272 (96%)	0.45	9 (3%) 48 50	20, 51, 84, 104	48 (18%)
1	C	261/272 (95%)	0.53	10 (3%) 44 46	24, 55, 102, 129	35 (13%)
1	D	250/272 (91%)	0.73	16 (6%) 25 26	30, 62, 117, 135	35 (14%)
All	All	1037/1088 (95%)	0.49	45 (4%) 40 41	20, 52, 100, 135	158 (15%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	GLY	6.2
1	D	20	MET	5.6
1	B	223[A]	HIS	5.2
1	B	267	HIS	4.4
1	D	78	TRP	3.9
1	D	9	GLY	3.7
1	C	212	VAL	3.7
1	B	224	LEU	3.2
1	A	71	HIS	3.1
1	D	248	PHE	3.0
1	A	111	ILE	3.0
1	C	24	PHE	2.9
1	C	40	ILE	2.7
1	A	130	GLY	2.7
1	C	191	VAL	2.7
1	D	31	TYR	2.7
1	B	116	ALA	2.6
1	A	110	GLY	2.5
1	A	224	LEU	2.4
1	B	34	VAL	2.4
1	C	248	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	76	ALA	2.4
1	C	38	ILE	2.4
1	D	21	ILE	2.4
1	A	223	HIS	2.3
1	B	109	TYR	2.3
1	D	61	GLU	2.3
1	D	87	VAL	2.3
1	D	89	LEU	2.3
1	B	91	ALA	2.3
1	C	223	HIS	2.3
1	C	187	ILE	2.3
1	D	33	ASP	2.2
1	A	113	LYS	2.2
1	D	90	LEU	2.2
1	A	251	PHE	2.2
1	B	33	ASP	2.1
1	C	130	GLY	2.1
1	D	59	LEU	2.1
1	C	31	TYR	2.1
1	A	250	SER	2.0
1	D	15	LEU	2.0
1	B	95	TYR	2.0
1	A	77	ASP	2.0
1	D	249	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

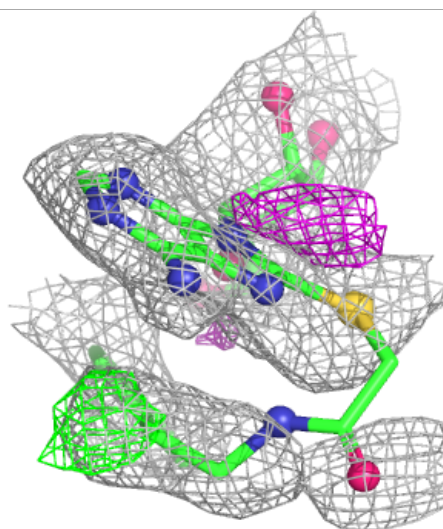
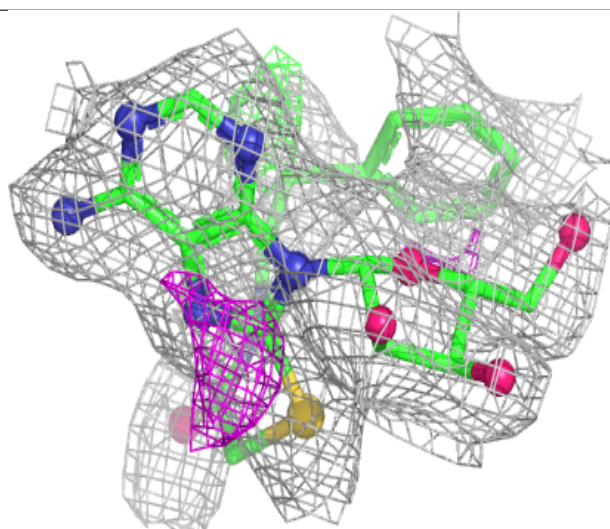
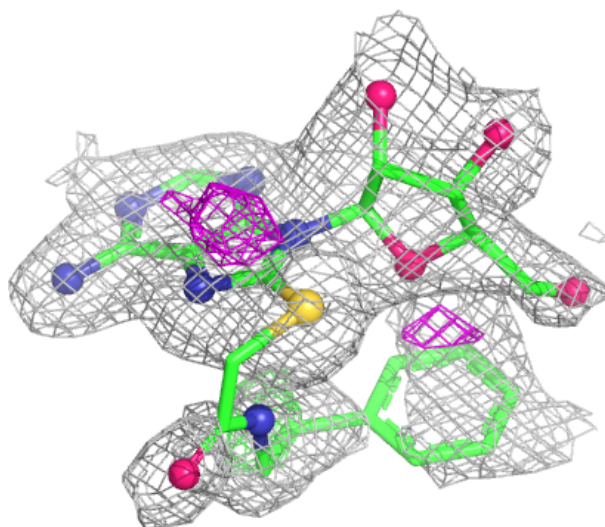
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	A	301	13/13	0.74	0.16	60,64,67,68	13
4	5AQ	D	302	32/32	0.77	0.17	67,71,110,111	0
2	CIT	D	301	13/13	0.79	0.19	51,52,54,55	13
2	CIT	B	301	13/13	0.80	0.17	77,78,79,80	0
3	GOL	A	302	6/6	0.87	0.17	72,73,73,73	0
4	5AQ	C	301	32/32	0.91	0.11	37,41,66,66	0
4	5AQ	B	302	32/32	0.92	0.10	37,43,63,63	0
4	5AQ	A	303	32/32	0.94	0.08	29,43,60,60	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.

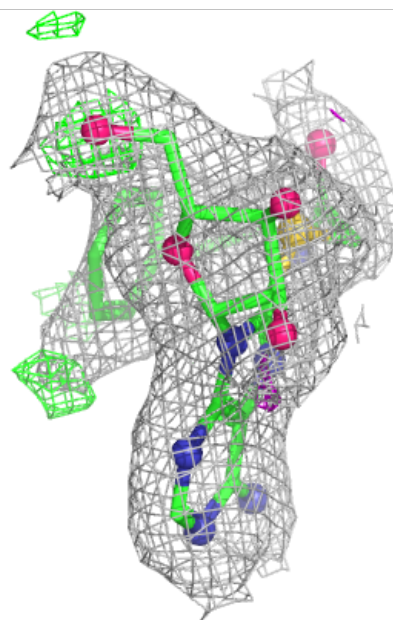
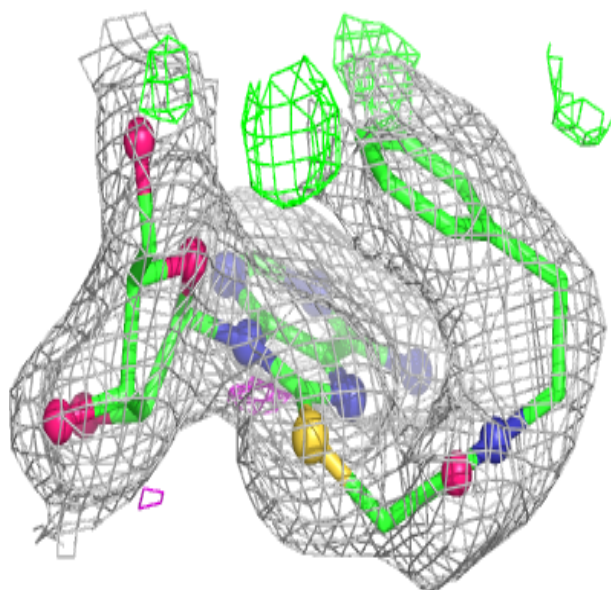
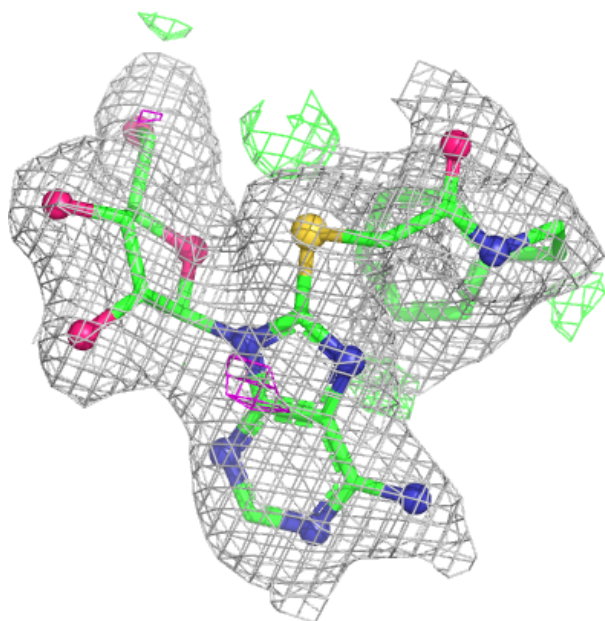
Electron density around 5AQ D 302:

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



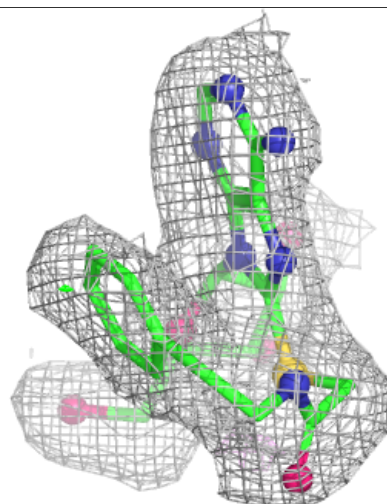
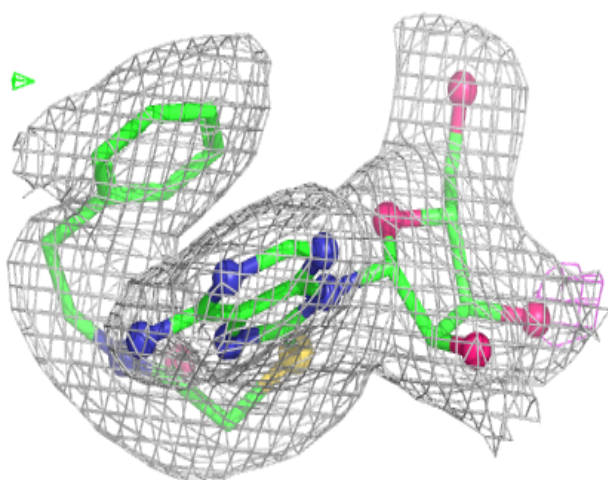
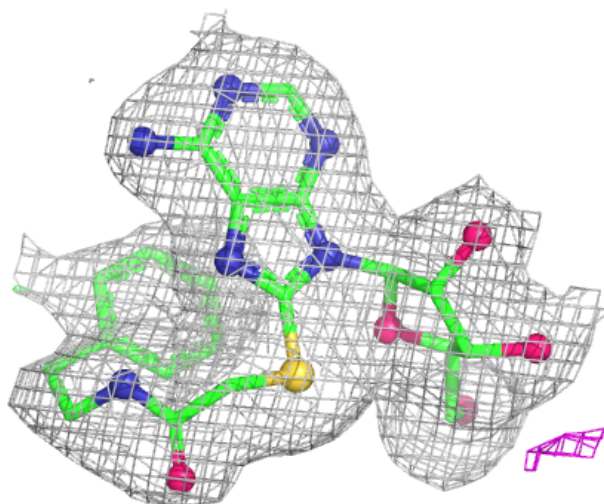
Electron density around 5AQ C 301:

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



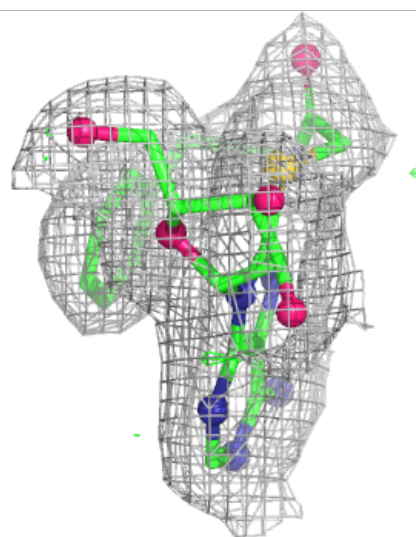
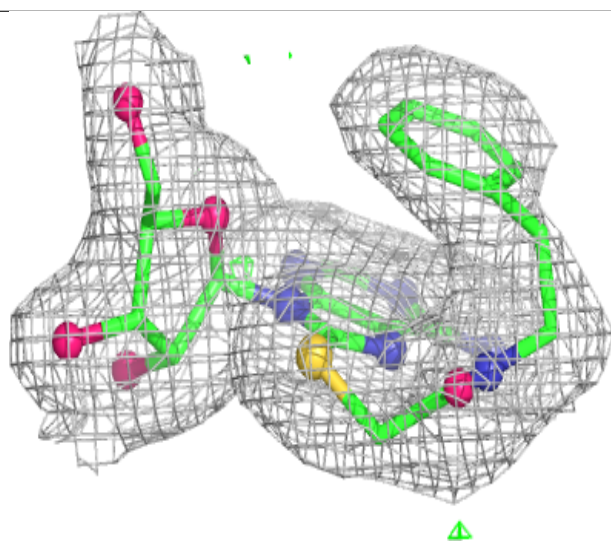
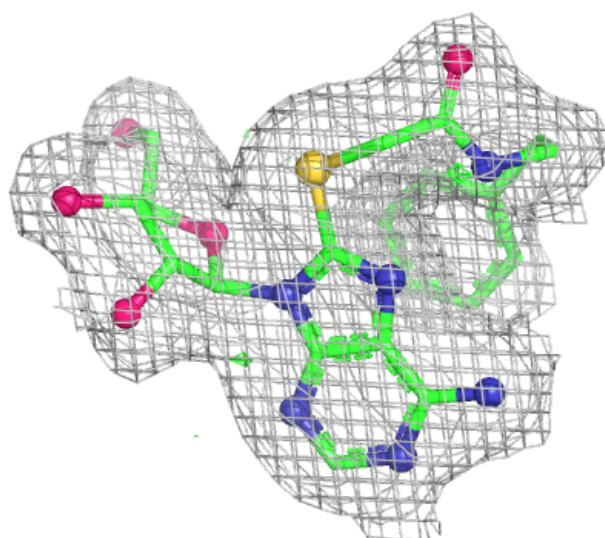
Electron density around 5AQ B 302:

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



Electron density around 5AQ A 303:

$2mF_o-DF_c$ (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.