



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:14 pm BST

PDB ID : 4GYZ
Title : Mus Musculus Tdp2 Bound to dAMP and Mg²⁺
Authors : Schellenberg, M.J.; Williams, R.S.
Deposited on : 2012-09-05
Resolution : 2.56 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 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

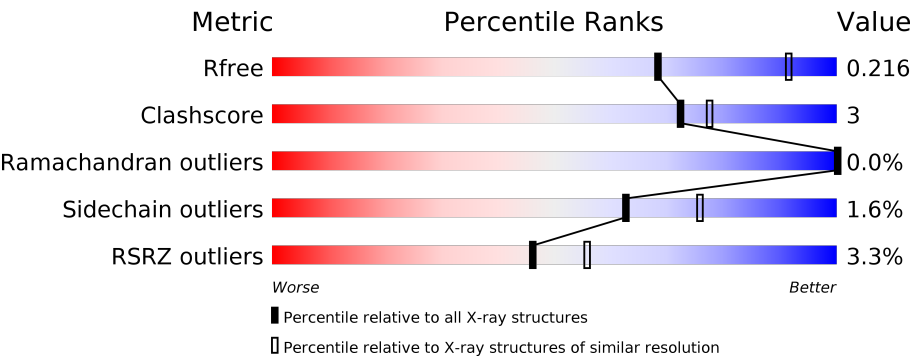
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 ≥ 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	256	<div><div></div><div>89%7%.</div></div>
1	B	256	<div><div>2%</div><div>87%10%.</div></div>
1	C	256	<div><div>2%</div><div>90%7%.</div></div>
1	D	256	<div><div>3%</div><div>83%9%7%</div></div>
1	E	256	<div><div>%</div><div>90%7%.</div></div>
1	F	256	<div><div>12%</div><div>84%11%5%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	256	<div><div></div><div>88%</div><div>7%5%</div></div>
1	H	256	<div><div>5%</div><div></div><div>89%</div><div>7%5%</div></div>
1	I	256	<div><div>3%</div><div></div><div>86%</div><div>10%•</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18120 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 Tyrosyl-DNA phosphodiesterase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	1	0
			1962	1253	342	353	14			
1	B	249	Total	C	N	O	S	0	1	0
			1978	1260	342	361	15			
1	C	248	Total	C	N	O	S	0	0	0
			1969	1255	341	359	14			
1	D	238	Total	C	N	O	S	0	1	0
			1895	1209	326	346	14			
1	E	249	Total	C	N	O	S	0	0	0
			1978	1261	342	361	14			
1	F	244	Total	C	N	O	S	0	0	0
			1937	1235	337	351	14			
1	G	243	Total	C	N	O	S	0	2	0
			1939	1238	336	349	16			
1	H	244	Total	C	N	O	S	0	2	0
			1952	1247	340	350	15			
1	I	246	Total	C	N	O	S	0	1	0
			1964	1252	342	356	14			

There are 27 discrepancies between the modelled and reference sequences:

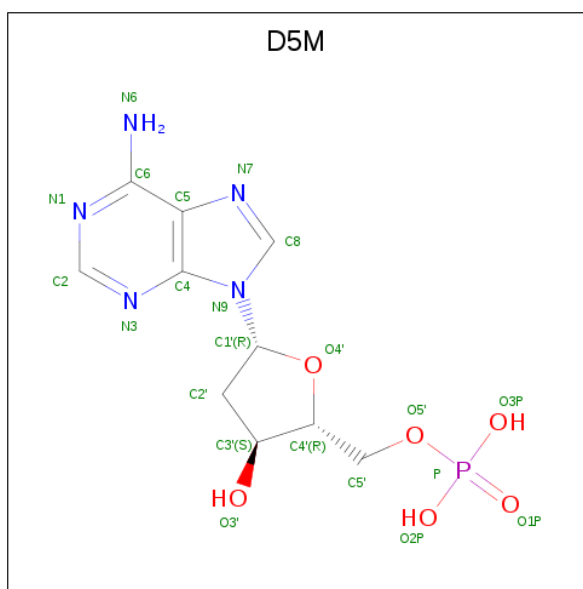
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
A	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
A	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
B	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
B	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
B	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
C	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
C	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
C	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
D	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
D	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
E	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
E	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
E	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
F	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
F	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
F	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
G	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
G	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
G	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
H	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
H	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
H	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7
I	115	SER	-	EXPRESSION TAG	UNP Q9JJX7
I	116	ASN	-	EXPRESSION TAG	UNP Q9JJX7
I	117	GLY	-	EXPRESSION TAG	UNP Q9JJX7

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C₁₀H₁₄N₅O₆P).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	H	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

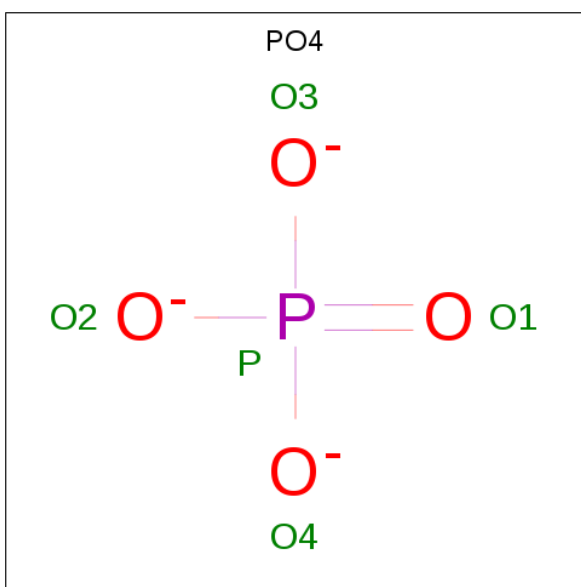
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	55	Total	O	0	1
			56	56		
6	B	30	Total	O	0	0
			30	30		
6	C	63	Total	O	0	0
			63	63		
6	D	38	Total	O	0	0
			38	38		
6	E	49	Total	O	0	0
			49	49		
6	F	23	Total	O	0	0
			23	23		
6	G	62	Total	O	0	0
			62	62		
6	H	39	Total	O	0	0
			39	39		
6	I	37	Total	O	0	0
			37	37		

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.

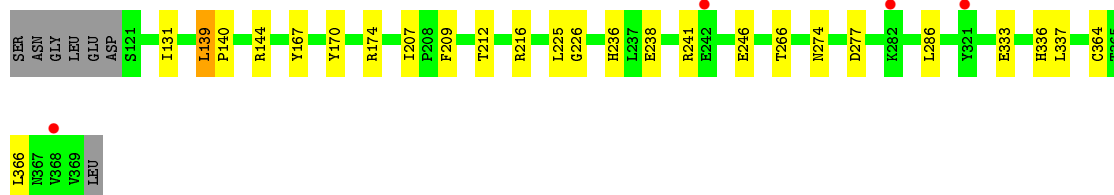
• Molecule 1: Tyrosyl-DNA phosphodiesterase 2

Chain A: 




• Molecule 1: Tyrosyl-DNA phosphodiesterase 2

Chain B: 




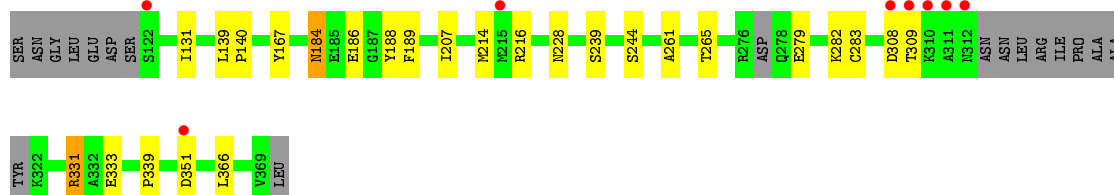
• Molecule 1: Tyrosyl-DNA phosphodiesterase 2

Chain C: 

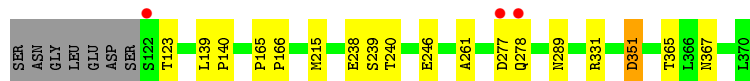
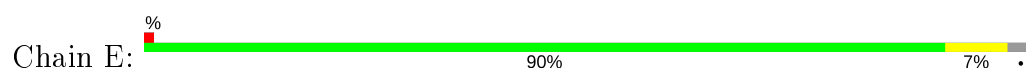


• Molecule 1: Tyrosyl-DNA phosphodiesterase 2

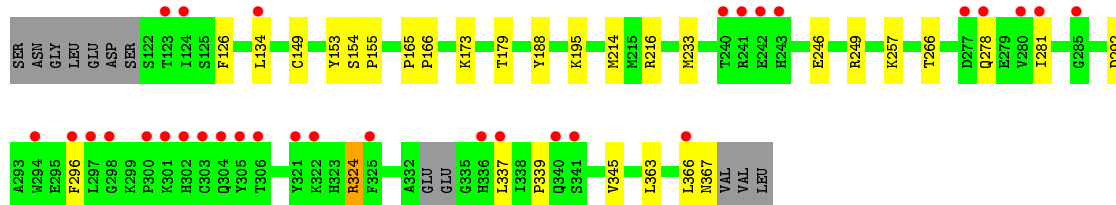
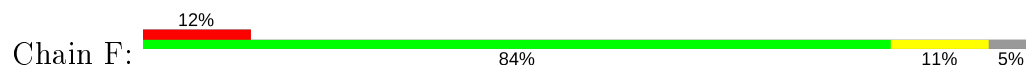
Chain D: 



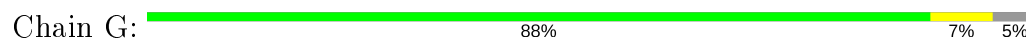
• Molecule 1: Tyrosyl-DNA phosphodiesterase 2



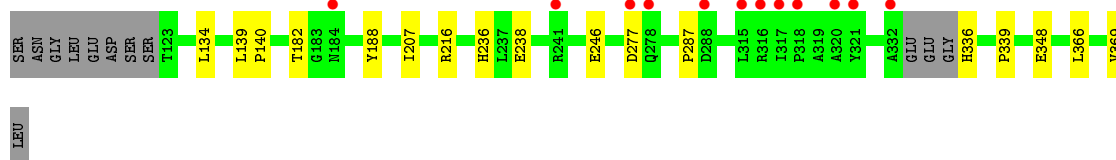
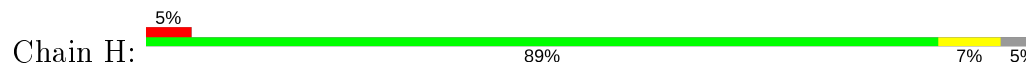
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



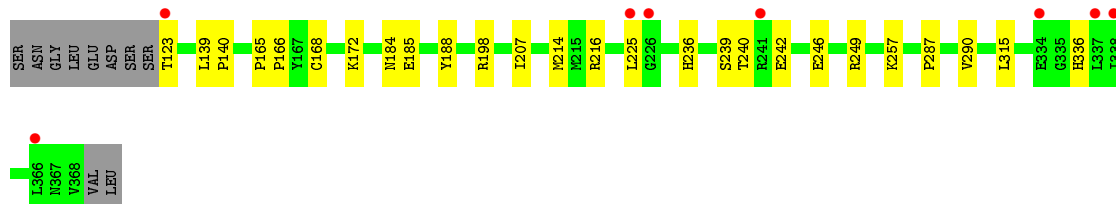
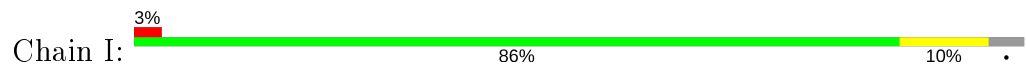
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.35Å 169.33Å 184.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.56 49.98 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.98-2.56) 97.1 (49.98-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928, REFMAC	Depositor
R, R_{free}	0.191 , 0.220 0.187 , 0.216	Depositor DCC
R_{free} test set	4267 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.1	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	0.95	EDS
Total number of atoms	18120	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: MG, CL, PO4, D5M

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	0.23	0/2009	0.41	0/2717
1	B	0.22	0/2026	0.39	0/2743
1	C	0.23	0/2014	0.41	0/2727
1	D	0.23	0/1939	0.40	0/2620
1	E	0.23	0/2023	0.39	0/2738
1	F	0.22	0/1981	0.40	0/2680
1	G	0.22	0/1989	0.40	0/2691
1	H	0.22	0/2002	0.39	0/2709
1	I	0.22	0/2012	0.40	0/2723
All	All	0.22	0/17995	0.40	0/24348

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	1962	0	1969	10	0
1	B	1978	0	1973	18	0
1	C	1969	0	1963	7	0
1	D	1895	0	1890	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1978	0	1974	13	0
1	F	1937	0	1932	17	0
1	G	1939	0	1941	12	0
1	H	1952	0	1960	11	0
1	I	1964	0	1962	16	0
2	A	22	0	12	0	0
2	B	22	0	12	0	0
2	C	22	0	12	0	0
2	D	22	0	12	0	0
2	E	22	0	12	0	0
2	H	22	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	1	0	0	0	0
5	F	5	0	0	0	0
6	A	56	0	0	1	0
6	B	30	0	0	0	0
6	C	63	0	0	0	0
6	D	38	0	0	0	0
6	E	49	0	0	1	0
6	F	23	0	0	0	0
6	G	62	0	0	1	0
6	H	39	0	0	0	0
6	I	37	0	0	1	0
All	All	18120	0	17636	119	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 3.

All (119) 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:324[A]:ARG:NH2	6:A:536:HOH:O	1.95	0.97
1:G:162:GLU:OE1	6:G:538:HOH:O	1.85	0.93
1:G:242:GLU:N	1:G:242:GLU:OE1	2.17	0.78
1:F:154:SER:OG	1:F:195:LYS:NZ	2.18	0.77
1:I:185:GLU:N	1:I:185:GLU:OE1	2.24	0.71
1:F:292:ASP:OD2	1:F:324:ARG:NH2	2.25	0.68
1:D:186:GLU:OE1	1:D:186:GLU:N	2.27	0.67
1:D:188:TYR:OH	1:D:216:ARG:NH1	2.29	0.66
1:A:188:TYR:OH	1:A:216:ARG:NH1	2.28	0.65
1:I:188:TYR:OH	1:I:216:ARG:NH1	2.30	0.64
1:A:246:GLU:OE1	1:A:249:ARG:NH1	2.30	0.64
1:B:170:TYR:CZ	1:B:174:ARG:HG3	2.33	0.63
1:G:246:GLU:OE1	1:G:249:ARG:NH1	2.34	0.61
1:D:139:LEU:N	1:D:140:PRO:HD2	2.20	0.57
1:G:238:GLU:HG3	1:G:246:GLU:CG	2.34	0.57
1:I:198:ARG:HG3	1:I:225:LEU:HD11	1.87	0.56
1:E:239:SER:O	1:E:240:THR:HB	2.06	0.54
1:I:242:GLU:N	1:I:242:GLU:OE1	2.38	0.54
1:B:364:CYS:SG	1:B:366:LEU:CD1	2.96	0.54
1:G:238:GLU:HG3	1:G:246:GLU:HG3	1.90	0.54
1:I:123:THR:N	6:I:531:HOH:O	2.41	0.53
1:A:238:GLU:HG3	1:A:246:GLU:CG	2.40	0.52
1:F:188:TYR:OH	1:F:216:ARG:NH1	2.43	0.52
1:D:261:ALA:O	1:D:331:ARG:NH2	2.43	0.51
1:H:216:ARG:CD	1:H:236:HIS:O	2.58	0.51
1:I:214:MET:HB3	1:I:216:ARG:NH1	2.26	0.51
1:I:246:GLU:OE1	1:I:249:ARG:NH1	2.44	0.50
1:D:216:ARG:NH2	1:D:239:SER:OG	2.45	0.50
1:I:216:ARG:NE	1:I:236:HIS:O	2.44	0.50
1:G:251:LEU:HD23	1:G:283[A]:CYS:SG	2.50	0.50
1:A:238:GLU:HG3	1:A:246:GLU:HG3	1.93	0.50
1:E:331:ARG:NH1	6:E:524:HOH:O	2.45	0.49
1:E:261:ALA:O	1:E:331:ARG:NH2	2.46	0.49
1:H:216:ARG:HD2	1:H:236:HIS:O	2.13	0.48
1:H:238:GLU:HG3	1:H:246:GLU:CG	2.43	0.48
1:D:131:ILE:HD12	1:D:167:TYR:CZ	2.49	0.48
1:B:131:ILE:HD12	1:B:167:TYR:CZ	2.49	0.48
1:C:266:THR:CG2	1:C:337:LEU:HD21	2.43	0.48
1:B:144:ARG:HG2	1:B:170:TYR:OH	2.14	0.47
1:D:139:LEU:N	1:D:140:PRO:CD	2.78	0.47
1:D:214:MET:HB3	1:D:216:ARG:NH1	2.29	0.47
1:E:238:GLU:HG3	1:E:246:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:CYS:SG	1:F:345:VAL:HG22	2.54	0.46
1:F:233:MET:HE1	1:F:257:LYS:HG3	1.97	0.46
1:F:153:TYR:CD1	1:F:363:LEU:HD22	2.51	0.46
1:B:364:CYS:SG	1:B:366:LEU:HD11	2.56	0.45
1:A:139:LEU:N	1:A:140:PRO:CD	2.79	0.45
1:B:333:GLU:HB2	1:B:336:HIS:CG	2.51	0.45
1:G:248:ILE:HG23	1:G:283[A]:CYS:SG	2.57	0.45
1:H:277:ASP:N	1:H:277:ASP:OD1	2.50	0.45
1:B:226:GLY:O	1:F:179:THR:HG21	2.16	0.45
1:C:139:LEU:N	1:C:140:PRO:CD	2.79	0.45
1:F:149:CYS:SG	1:F:345:VAL:CG2	3.05	0.44
1:F:266:THR:HG23	1:F:337:LEU:HD21	1.99	0.44
1:H:238:GLU:HG3	1:H:246:GLU:HG3	1.97	0.44
1:B:266:THR:CG2	1:B:337:LEU:HD11	2.47	0.44
1:C:292:ASP:OD2	1:C:324:ARG:NH2	2.50	0.44
1:E:139:LEU:N	1:E:140:PRO:CD	2.81	0.44
1:B:241:ARG:NH1	1:B:277:ASP:OD2	2.50	0.44
1:F:296:PHE:CE1	1:F:339:PRO:HD2	2.53	0.44
1:B:238:GLU:HG3	1:B:246:GLU:HG3	2.00	0.43
1:E:165:PRO:HB2	1:E:166:PRO:HD3	2.00	0.43
1:H:339:PRO:HA	1:H:366:LEU:HD23	2.00	0.43
1:I:139:LEU:N	1:I:140:PRO:CD	2.81	0.43
1:E:351:ASP:N	1:E:351:ASP:OD1	2.50	0.43
1:I:239:SER:C	1:I:240:THR:HG23	2.39	0.43
1:A:158:VAL:HB	1:A:193:LEU:HB2	2.01	0.43
1:B:139:LEU:N	1:B:140:PRO:HD2	2.34	0.43
1:C:218:LEU:HD21	1:C:233:MET:HE3	2.01	0.43
1:E:277:ASP:C	1:E:278:GLN:HG2	2.38	0.43
1:G:165:PRO:HB2	1:G:166:PRO:HD3	2.01	0.43
1:I:168:CYS:O	1:I:172:LYS:HG2	2.19	0.43
1:G:139:LEU:N	1:G:140:PRO:CD	2.81	0.43
1:H:216:ARG:HD3	1:H:236:HIS:O	2.19	0.43
1:D:207:ILE:HD12	1:D:207:ILE:N	2.33	0.42
1:H:134:LEU:HD21	1:H:188:TYR:CD1	2.55	0.42
1:A:214:MET:HB3	1:A:216:ARG:NH1	2.34	0.42
1:E:238:GLU:HG3	1:E:246:GLU:HG3	2.01	0.42
1:B:286:LEU:HD12	1:B:286:LEU:N	2.34	0.42
1:H:139:LEU:N	1:H:140:PRO:CD	2.81	0.42
1:D:339:PRO:HA	1:D:366:LEU:HD23	2.01	0.42
1:I:207:ILE:HD12	1:I:207:ILE:N	2.34	0.42
1:B:238:GLU:HG3	1:B:246:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:ARG:HG3	1:I:225:LEU:CD1	2.50	0.42
1:A:339:PRO:HA	1:A:366:LEU:HD23	2.01	0.42
1:D:131:ILE:HD12	1:D:167:TYR:CE1	2.55	0.42
1:B:209:PHE:O	1:B:212:THR:HG22	2.20	0.41
1:E:139:LEU:HB3	1:E:140:PRO:HD3	2.02	0.41
1:F:214:MET:HB3	1:F:216:ARG:NH1	2.35	0.41
1:D:244:SER:OG	1:D:279:GLU:OE2	2.25	0.41
1:F:126:PHE:HA	1:F:155:PRO:HB2	2.03	0.41
1:F:134:LEU:HD21	1:F:188:TYR:CD1	2.56	0.41
1:G:218:LEU:HD11	1:G:233:MET:HE3	2.02	0.41
1:G:139:LEU:HB3	1:G:140:PRO:HD3	2.01	0.41
1:I:165:PRO:N	1:I:166:PRO:HD2	2.35	0.41
1:I:287:PRO:HG2	1:I:290:VAL:CG2	2.51	0.41
1:B:207:ILE:HD12	1:B:207:ILE:N	2.36	0.41
1:D:308:ASP:OD1	1:D:309:THR:N	2.54	0.41
1:E:289:ASN:OD1	1:E:289:ASN:N	2.52	0.41
1:D:184:ASN:HB2	1:D:189:PHE:HB3	2.03	0.41
1:D:261:ALA:HB3	1:D:331:ARG:NH2	2.35	0.41
1:F:165:PRO:N	1:F:166:PRO:HD2	2.36	0.41
1:H:348:GLU:N	1:H:348:GLU:OE1	2.54	0.41
1:B:216:ARG:HD2	1:B:236:HIS:O	2.20	0.41
1:E:123:THR:CG2	1:E:365:THR:HG23	2.49	0.41
1:C:216:ARG:HD2	1:C:236:HIS:O	2.21	0.40
1:A:315:LEU:HD13	1:A:358:ASP:HB3	2.02	0.40
1:C:269:PHE:CD1	1:C:269:PHE:C	2.94	0.40
1:E:277:ASP:O	1:E:278:GLN:CB	2.69	0.40
1:F:366:LEU:HD23	1:F:367:ASN:N	2.36	0.40
1:H:207:ILE:HD12	1:H:207:ILE:N	2.36	0.40
1:B:170:TYR:CE2	1:B:174:ARG:HG3	2.56	0.40
1:I:257:LYS:HD3	1:I:257:LYS:O	2.22	0.40
1:B:225:LEU:HD23	1:B:225:LEU:C	2.42	0.40
1:C:305:TYR:CD1	1:C:322:LYS:HB3	2.57	0.40
1:F:278:GLN:HB2	1:F:281:ILE:CG2	2.51	0.40
1:F:246:GLU:OE1	1:F:249:ARG:NH2	2.52	0.40

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	243/256 (95%)	236 (97%)	7 (3%)	0	100	100
1	B	248/256 (97%)	239 (96%)	9 (4%)	0	100	100
1	C	246/256 (96%)	238 (97%)	8 (3%)	0	100	100
1	D	233/256 (91%)	224 (96%)	9 (4%)	0	100	100
1	E	247/256 (96%)	239 (97%)	8 (3%)	0	100	100
1	F	240/256 (94%)	229 (95%)	11 (5%)	0	100	100
1	G	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
1	H	242/256 (94%)	233 (96%)	8 (3%)	1 (0%)	34	45
1	I	245/256 (96%)	233 (95%)	12 (5%)	0	100	100
All	All	2185/2304 (95%)	2105 (96%)	79 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	287	PRO

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	216/224 (96%)	212 (98%)	4 (2%)	57	71
1	B	219/224 (98%)	217 (99%)	2 (1%)	78	87
1	C	217/224 (97%)	212 (98%)	5 (2%)	50	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	210/224 (94%)	203 (97%)	7 (3%)	38	50
1	E	218/224 (97%)	215 (99%)	3 (1%)	67	78
1	F	213/224 (95%)	211 (99%)	2 (1%)	78	87
1	G	215/224 (96%)	213 (99%)	2 (1%)	78	87
1	H	216/224 (96%)	213 (99%)	3 (1%)	67	78
1	I	216/224 (96%)	213 (99%)	3 (1%)	67	78
All	All	1940/2016 (96%)	1909 (98%)	31 (2%)	62	76

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	THR
1	A	315	LEU
1	A	331	ARG
1	A	337	LEU
1	B	139	LEU
1	B	274	ASN
1	C	184	ASN
1	C	198	ARG
1	C	283	CYS
1	C	313	ASN
1	C	366	LEU
1	D	184	ASN
1	D	228	ASN
1	D	265	THR
1	D	282	LYS
1	D	283	CYS
1	D	331	ARG
1	D	351	ASP
1	E	215	MET
1	E	351	ASP
1	E	367	ASN
1	F	173	LYS
1	F	324	ARG
1	G	276	ARG
1	G	336	HIS
1	H	182	THR
1	H	336	HIS
1	H	369	VAL
1	I	184	ASN

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Mol	Chain	Res	Type
1	I	315	LEU
1	I	336	HIS

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

Mol	Chain	Res	Type
1	D	243	HIS
1	D	336	HIS
1	F	302	HIS
1	G	367	ASN
1	I	367	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](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\# Z > 2$
2	D5M	C	402	3	22,24,24	1.89	6 (27%)	24,36,36	1.42	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	F	401	3	4,4,4	0.92	0	6,6,6	0.42	0
2	D5M	H	401	3	22,24,24	1.88	6 (27%)	24,36,36	1.41	2 (8%)
2	D5M	E	401	3	22,24,24	1.89	6 (27%)	24,36,36	1.41	3 (12%)
2	D5M	D	402	3	22,24,24	1.88	6 (27%)	24,36,36	1.41	3 (12%)
2	D5M	B	401	3	22,24,24	1.89	6 (27%)	24,36,36	1.43	2 (8%)
2	D5M	A	401	3	22,24,24	1.91	6 (27%)	24,36,36	1.41	3 (12%)

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	C	402	3	-	0/6/22/22	0/3/3/3
2	D5M	H	401	3	-	0/6/22/22	0/3/3/3
2	D5M	E	401	3	-	0/6/22/22	0/3/3/3
2	D5M	D	402	3	-	0/6/22/22	0/3/3/3
2	D5M	B	401	3	-	0/6/22/22	0/3/3/3
2	D5M	A	401	3	-	0/6/22/22	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	D5M	C2-N3	4.39	1.39	1.32
2	H	401	D5M	C2-N3	4.38	1.39	1.32
2	C	402	D5M	C2-N3	4.37	1.39	1.32
2	B	401	D5M	C2-N3	4.35	1.39	1.32
2	A	401	D5M	C2-N3	4.32	1.39	1.32
2	D	402	D5M	C2-N3	4.26	1.39	1.32
2	A	401	D5M	O4'-C4'	-3.28	1.37	1.45
2	B	401	D5M	O4'-C4'	-3.22	1.37	1.45
2	E	401	D5M	O4'-C4'	-3.21	1.37	1.45
2	D	402	D5M	O4'-C4'	-3.17	1.37	1.45
2	H	401	D5M	O4'-C4'	-3.13	1.38	1.45
2	C	402	D5M	O4'-C4'	-3.05	1.38	1.45
2	A	401	D5M	C2-N1	2.94	1.39	1.33
2	C	402	D5M	C2-N1	2.91	1.39	1.33
2	D	402	D5M	C2-N1	2.91	1.39	1.33
2	H	401	D5M	C2-N1	2.88	1.39	1.33
2	E	401	D5M	C2-N1	2.86	1.39	1.33
2	B	401	D5M	C2-N1	2.82	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	D5M	O3'-C3'	-2.55	1.37	1.43
2	H	401	D5M	C6-N6	2.52	1.43	1.34
2	C	402	D5M	C6-N6	2.51	1.43	1.34
2	D	402	D5M	C6-N6	2.51	1.43	1.34
2	B	401	D5M	C6-N6	2.51	1.43	1.34
2	A	401	D5M	C6-N6	2.51	1.43	1.34
2	E	401	D5M	C6-N6	2.50	1.43	1.34
2	E	401	D5M	O3'-C3'	-2.46	1.38	1.43
2	A	401	D5M	O3'-C3'	-2.41	1.38	1.43
2	B	401	D5M	O3'-C3'	-2.40	1.38	1.43
2	D	402	D5M	O3'-C3'	-2.38	1.38	1.43
2	H	401	D5M	O3'-C3'	-2.34	1.38	1.43
2	B	401	D5M	C6-C5	-2.29	1.34	1.43
2	A	401	D5M	C6-C5	-2.25	1.34	1.43
2	C	402	D5M	C6-C5	-2.24	1.35	1.43
2	E	401	D5M	C6-C5	-2.24	1.35	1.43
2	D	402	D5M	C6-C5	-2.23	1.35	1.43
2	H	401	D5M	C6-C5	-2.22	1.35	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	D5M	N3-C2-N1	-5.31	120.38	128.68
2	E	401	D5M	N3-C2-N1	-5.29	120.40	128.68
2	A	401	D5M	N3-C2-N1	-5.25	120.48	128.68
2	B	401	D5M	N3-C2-N1	-5.23	120.50	128.68
2	H	401	D5M	N3-C2-N1	-5.18	120.58	128.68
2	D	402	D5M	N3-C2-N1	-5.07	120.75	128.68
2	B	401	D5M	O4'-C1'-C2'	2.25	110.50	106.25
2	D	402	D5M	C2'-C3'-C4'	2.15	107.25	102.76
2	E	401	D5M	C2'-C1'-N9	-2.14	109.34	114.27
2	A	401	D5M	C2'-C1'-N9	-2.11	109.40	114.27
2	H	401	D5M	C2'-C1'-N9	-2.09	109.45	114.27
2	D	402	D5M	C2'-C1'-N9	-2.08	109.46	114.27
2	E	401	D5M	O4'-C1'-C2'	2.06	110.14	106.25
2	A	401	D5M	C2'-C3'-C4'	2.01	106.95	102.76

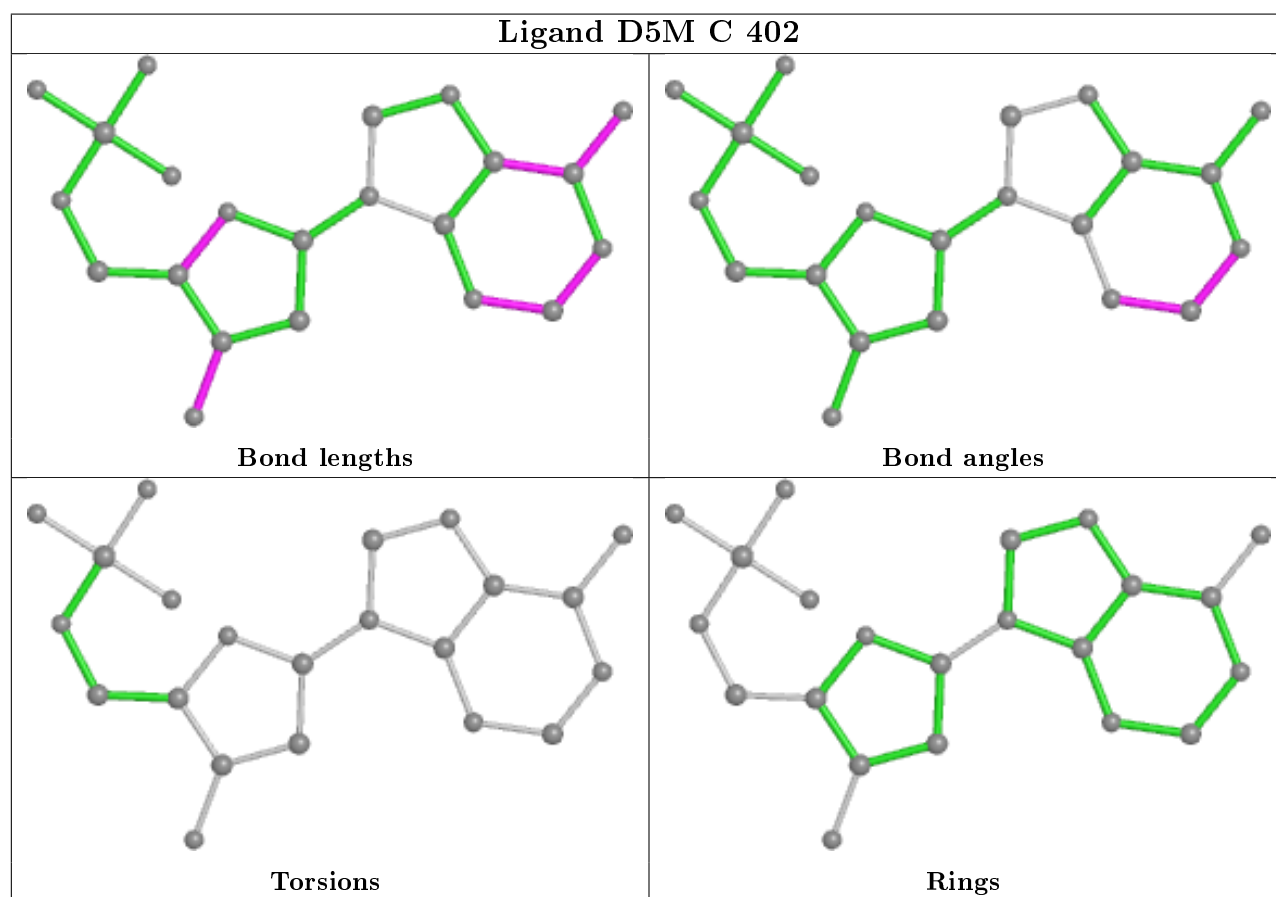
There are no chirality outliers.

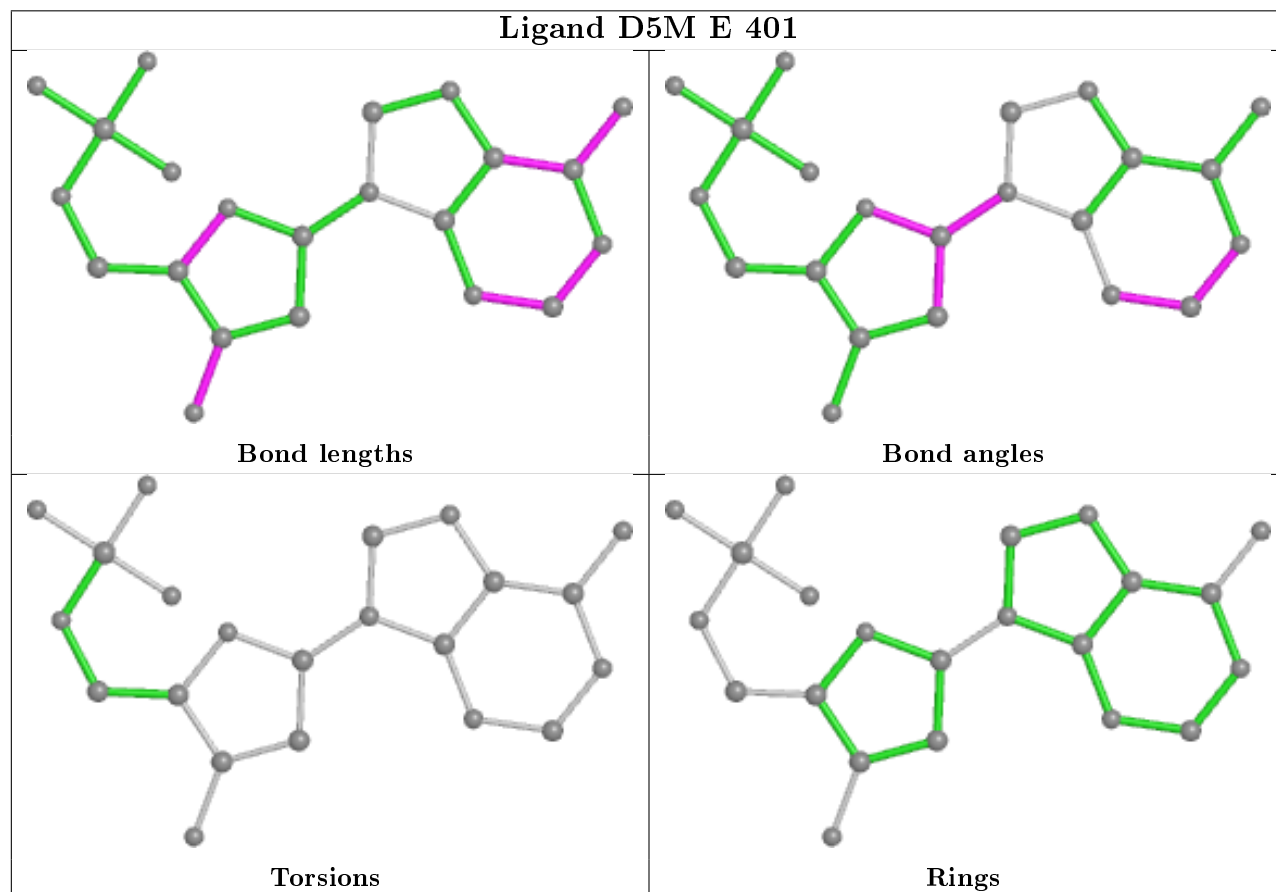
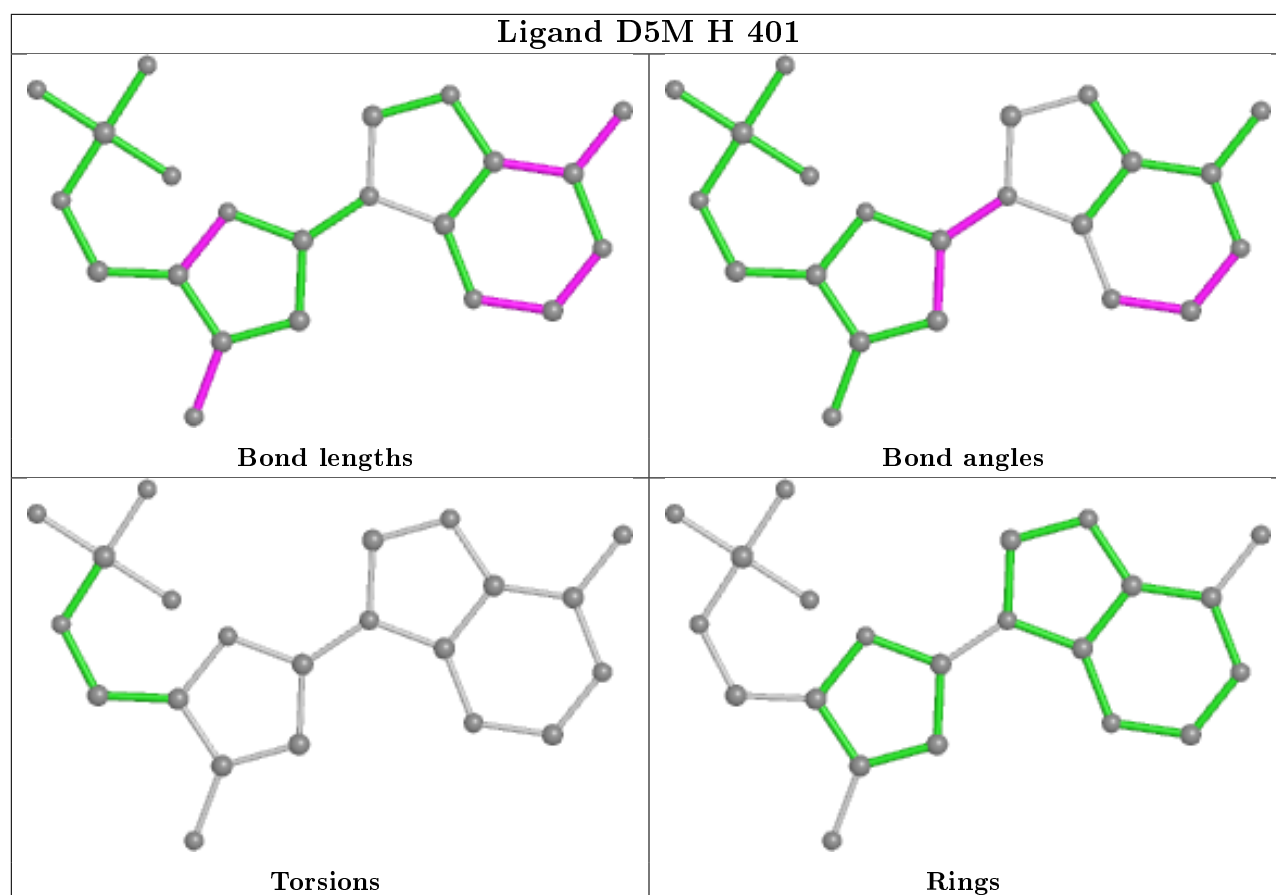
There are no torsion outliers.

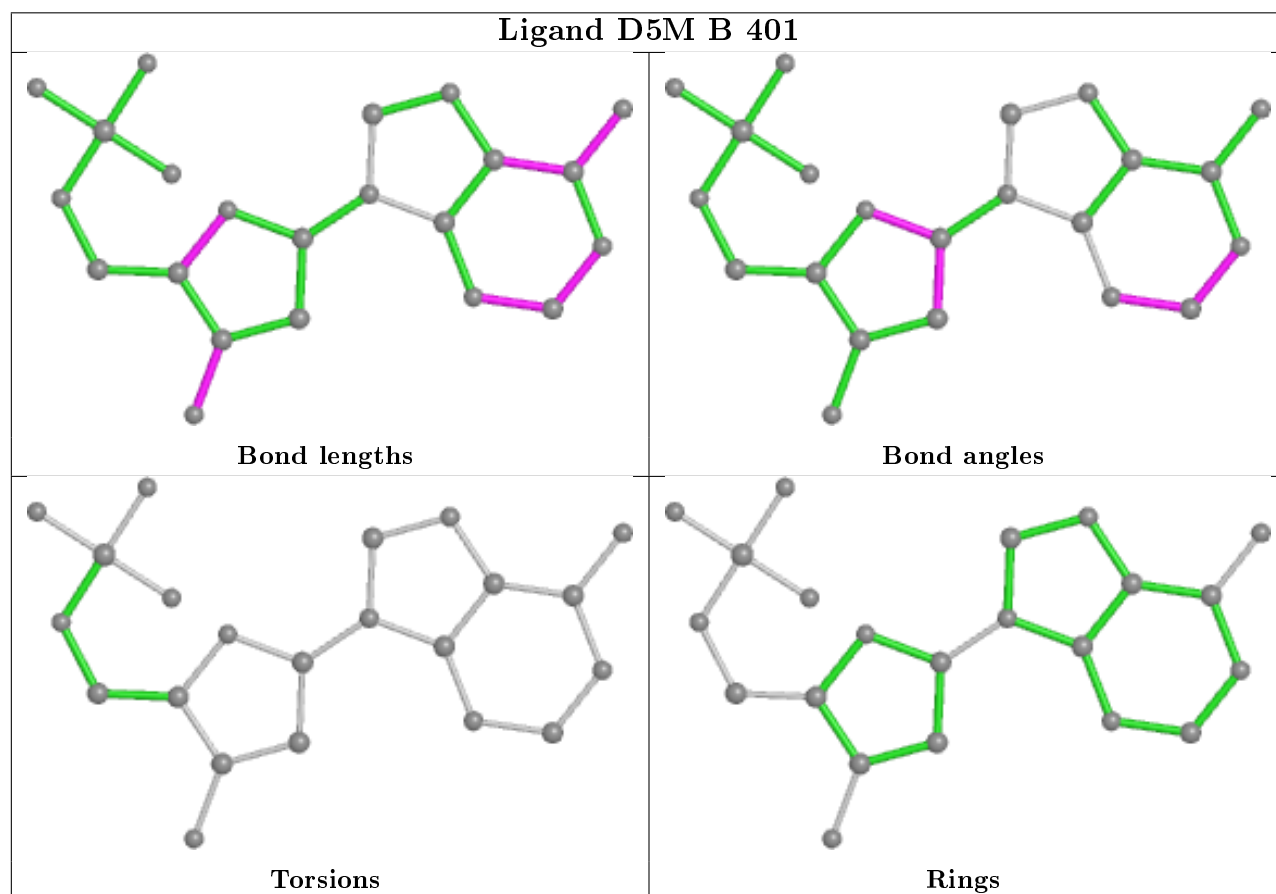
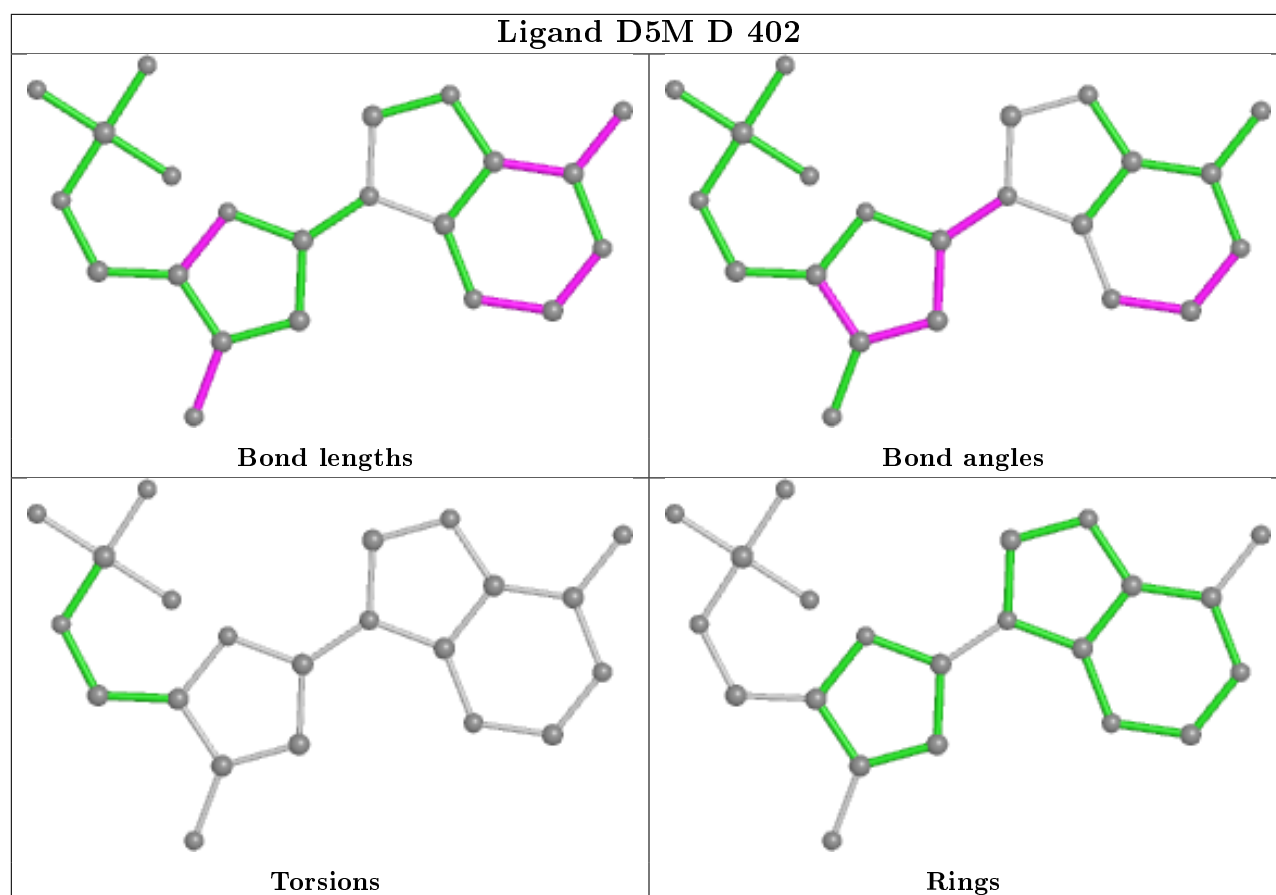
There are no ring outliers.

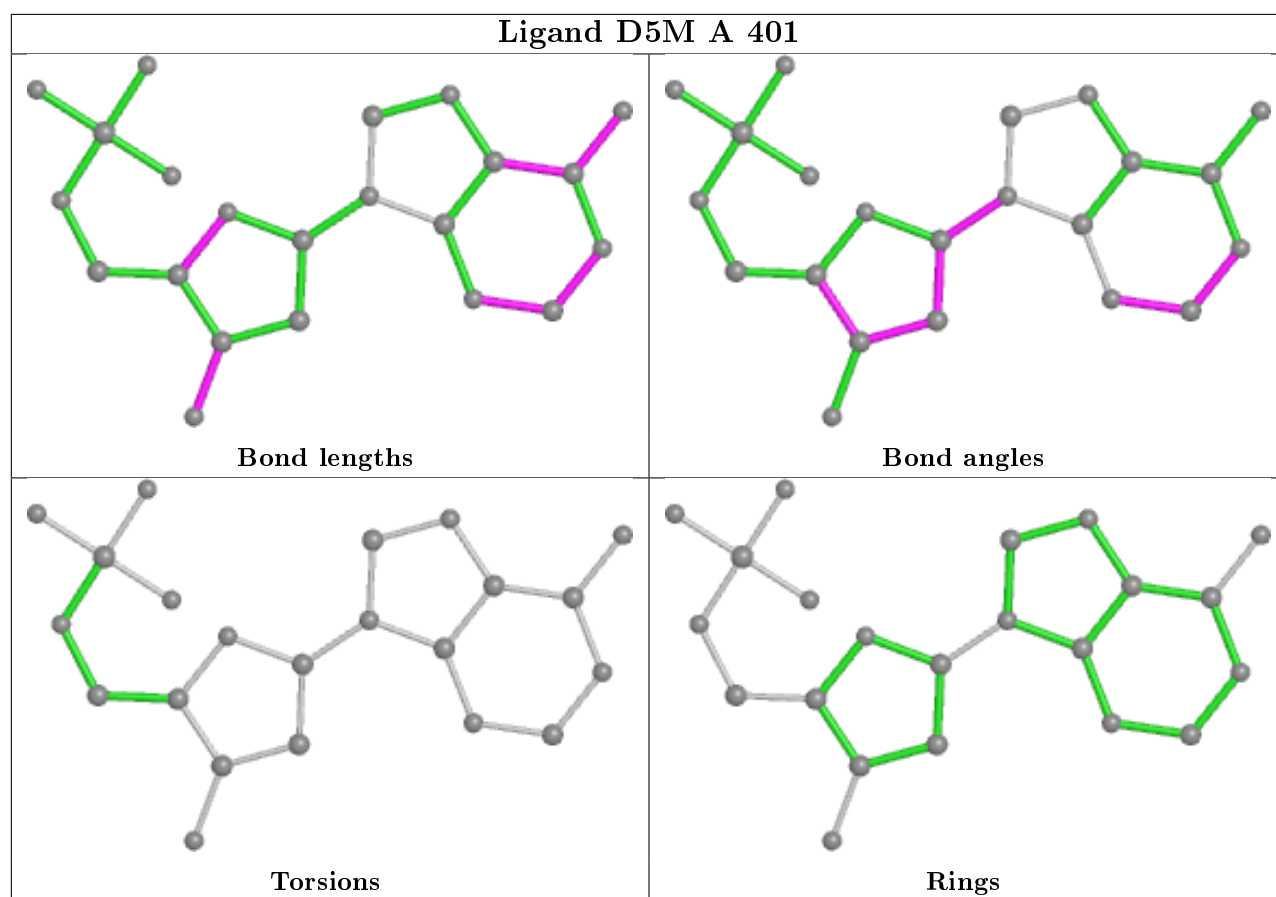
No monomer is involved in short contacts.

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.









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	246/256 (96%)	-0.04	1 (0%) 92 96	24, 39, 74, 104	0
1	B	249/256 (97%)	0.10	4 (1%) 72 78	26, 51, 91, 139	0
1	C	248/256 (96%)	-0.06	4 (1%) 72 78	22, 36, 68, 96	0
1	D	238/256 (92%)	0.10	8 (3%) 45 54	27, 44, 82, 117	0
1	E	249/256 (97%)	0.08	3 (1%) 79 84	27, 44, 79, 98	0
1	F	244/256 (95%)	0.74	31 (12%) 3 5	38, 72, 111, 145	0
1	G	243/256 (94%)	-0.04	1 (0%) 92 96	25, 42, 77, 105	0
1	H	244/256 (95%)	0.16	12 (4%) 29 37	28, 51, 89, 122	0
1	I	246/256 (96%)	0.08	8 (3%) 46 56	25, 51, 102, 134	0
All	All	2207/2304 (95%)	0.12	72 (3%) 46 56	22, 46, 92, 145	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	243	HIS	5.6
1	F	298	GLY	5.0
1	F	306	THR	5.0
1	F	297	LEU	4.9
1	F	294	TRP	4.8
1	D	309	THR	4.8
1	D	311	ALA	4.0
1	F	300	PRO	4.0
1	F	281	ILE	3.9
1	F	366	LEU	3.7
1	H	317	ILE	3.7
1	F	242	GLU	3.7
1	C	319	ALA	3.6
1	F	337	LEU	3.5
1	B	321	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	305	TYR	3.4
1	F	241	ARG	3.4
1	F	277	ASP	3.4
1	F	285	GLY	3.4
1	I	337	LEU	3.3
1	F	303	CYS	3.3
1	F	301	LYS	3.1
1	F	304	GLN	3.1
1	E	122	SER	2.9
1	H	321	TYR	2.9
1	I	334	GLU	2.9
1	B	242	GLU	2.9
1	E	278	GLN	2.9
1	F	336	HIS	2.8
1	F	278	GLN	2.8
1	F	296	PHE	2.8
1	F	280	VAL	2.7
1	H	315	LEU	2.7
1	F	340	GLN	2.7
1	F	321	TYR	2.7
1	F	123	THR	2.6
1	C	321	TYR	2.6
1	B	282	LYS	2.6
1	F	341	SER	2.6
1	D	308	ASP	2.6
1	I	225	LEU	2.6
1	H	320	ALA	2.5
1	D	312	ASN	2.5
1	D	310	LYS	2.4
1	H	241	ARG	2.4
1	I	123	THR	2.4
1	E	277	ASP	2.3
1	H	288	ASP	2.3
1	D	122	SER	2.3
1	H	184	ASN	2.3
1	G	262	PRO	2.3
1	I	226	GLY	2.3
1	F	124	ILE	2.3
1	I	366	LEU	2.3
1	A	335	GLY	2.2
1	F	325	PHE	2.2
1	I	241	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	277	ASP	2.2
1	D	215	MET	2.2
1	H	332	ALA	2.2
1	C	320	ALA	2.2
1	D	351	ASP	2.2
1	I	338	ILE	2.2
1	H	318	PRO	2.2
1	H	316	ARG	2.1
1	F	240	THR	2.1
1	C	317	ILE	2.1
1	B	368	VAL	2.1
1	F	134	LEU	2.0
1	F	302	HIS	2.0
1	F	322	LYS	2.0
1	H	278	GLN	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 carbohydrates 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.

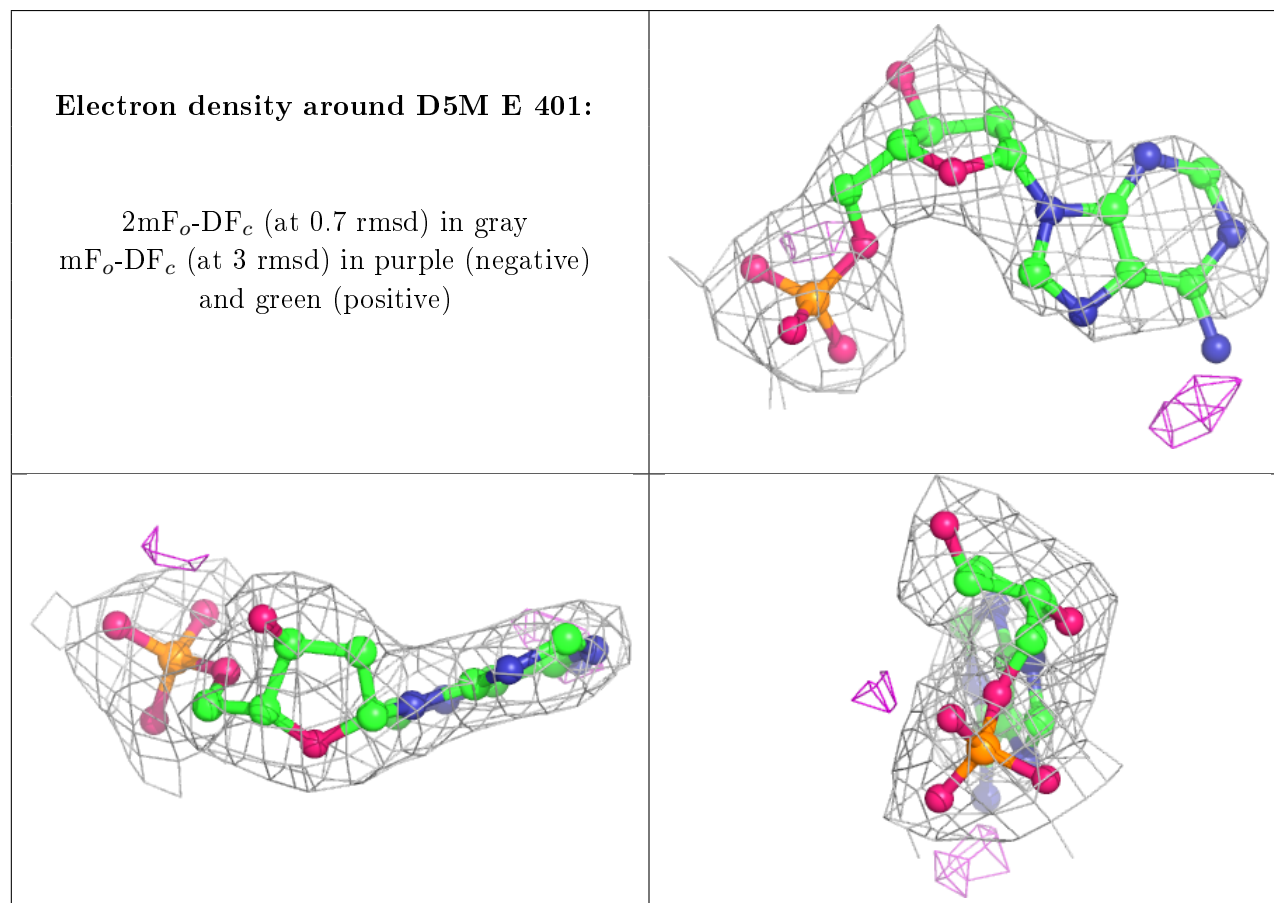
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	I	402	1/1	0.73	0.10	55,55,55,55	0
3	MG	G	401	1/1	0.92	0.12	50,50,50,50	0
3	MG	F	402	1/1	0.92	0.07	69,69,69,69	0
3	MG	D	403	1/1	0.92	0.05	48,48,48,48	0
2	D5M	E	401	22/22	0.95	0.18	39,70,80,82	0
4	CL	D	401	1/1	0.95	0.08	74,74,74,74	0
2	D5M	B	401	22/22	0.95	0.21	45,93,112,114	0
4	CL	I	401	1/1	0.95	0.12	68,68,68,68	0

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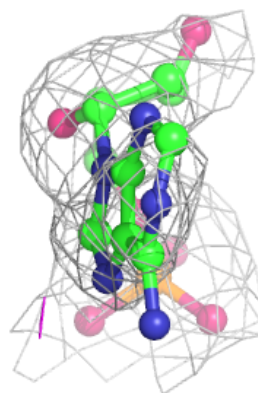
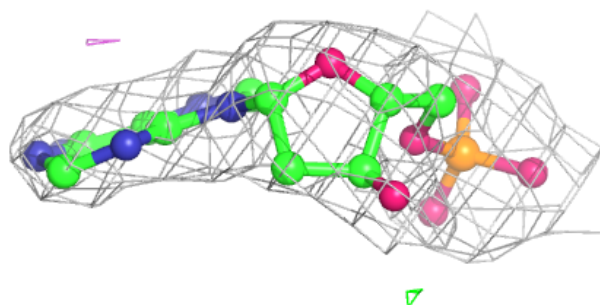
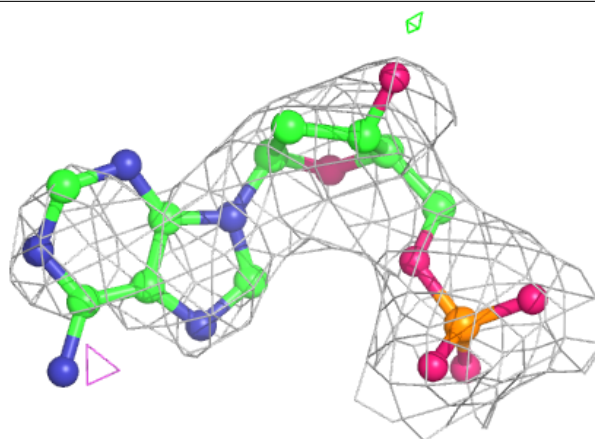
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	D5M	H	401	22/22	0.96	0.23	41,75,89,90	0
2	D5M	D	402	22/22	0.97	0.20	41,66,68,70	0
2	D5M	C	402	22/22	0.97	0.20	30,55,57,57	0
2	D5M	A	401	22/22	0.97	0.18	34,86,103,104	0
3	MG	H	402	1/1	0.97	0.06	40,40,40,40	0
3	MG	C	403	1/1	0.98	0.07	32,32,32,32	0
5	PO4	F	401	5/5	0.98	0.11	67,67,67,68	0
3	MG	B	402	1/1	0.98	0.03	47,47,47,47	0
4	CL	C	401	1/1	0.99	0.09	49,49,49,49	0
3	MG	E	402	1/1	0.99	0.05	38,38,38,38	0
3	MG	A	402	1/1	0.99	0.05	36,36,36,36	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.



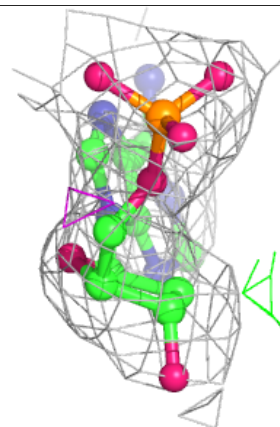
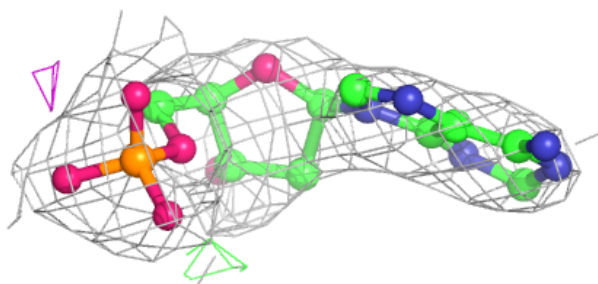
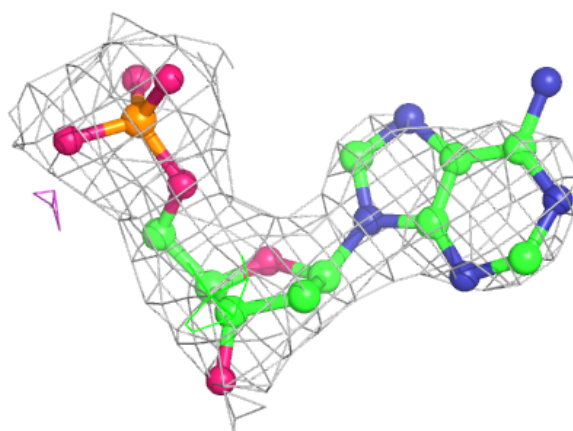
Electron density around D5M B 401:

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

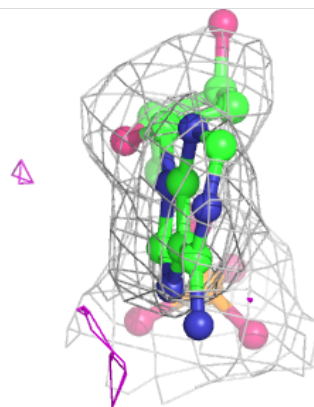
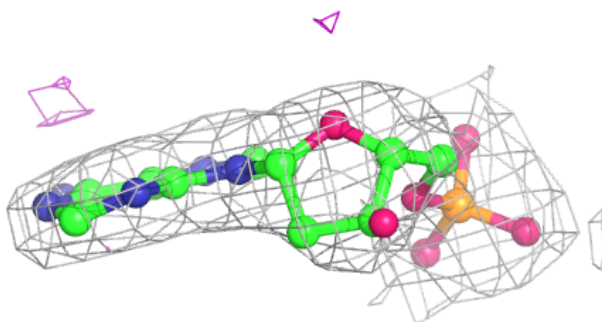
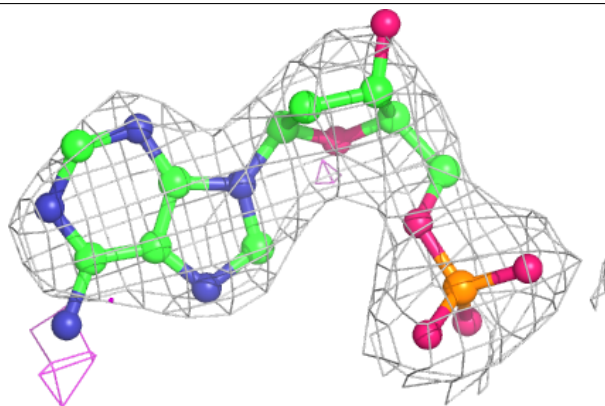


Electron density around D5M H 401:

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

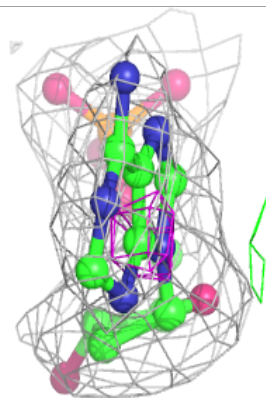
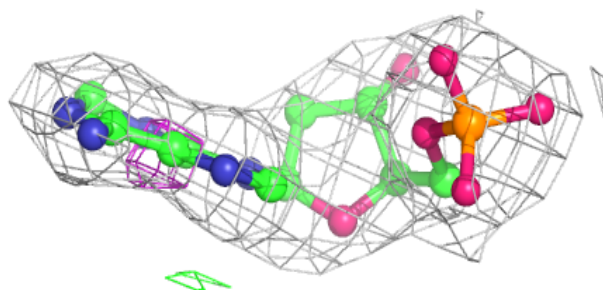
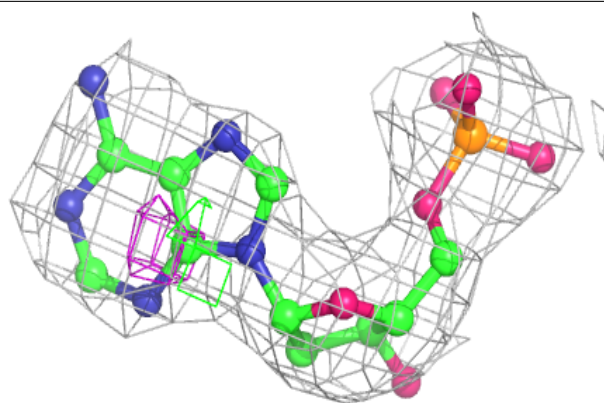
**Electron density around D5M D 402:**

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

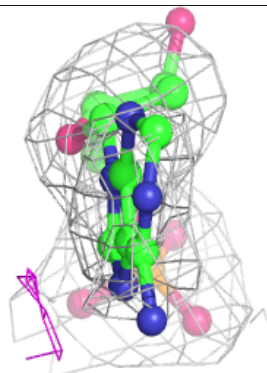
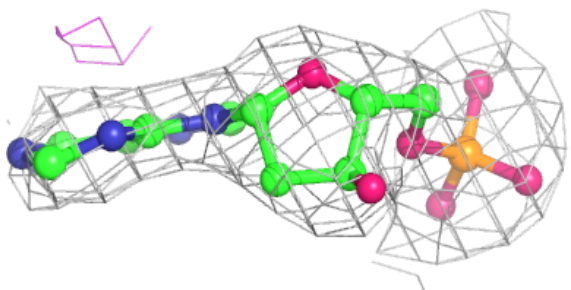
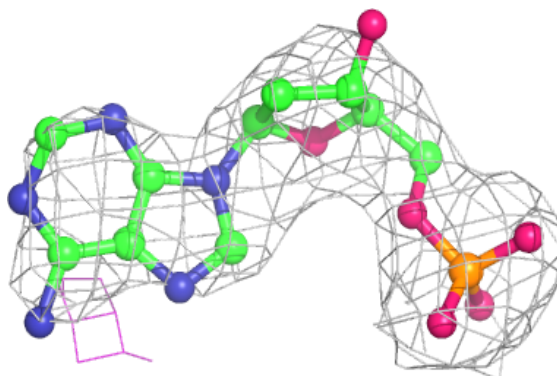


Electron density around D5M C 402:

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

**Electron density around D5M A 401:**

$2mF_o-DF_c$ (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.