



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:53 AM UTC

PDB ID : 5Y4Q / pdb_00005y4q
Title : Crystal structure of Trypanosoma cruzi spermidine synthase in complex with
N-(4-methoxyphenyl)quinolin-4-amine
Authors : Amano, Y.; Tateishi, Y.
Deposited on : 2017-08-04
Resolution : 2.07 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

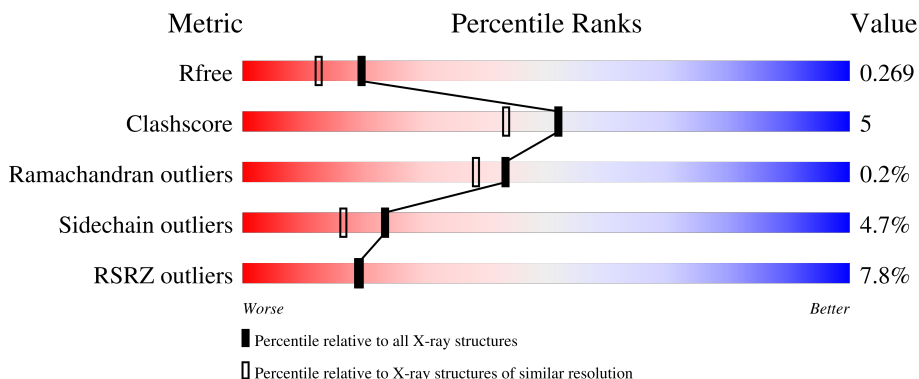
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	304	8% 74% 13% • 10%
1	B	304	9% 82% 9% • 8%
1	C	304	6% 77% 11% •• 11%
1	D	304	5% 78% 10% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8991 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 Spermidine synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2163	1374	371	404	14			
1	B	279	Total	C	N	O	S	0	0	0
			2209	1404	378	414	13			
1	C	272	Total	C	N	O	S	0	0	0
			2149	1363	369	403	14			
1	D	270	Total	C	N	O	S	0	0	0
			2140	1360	366	401	13			

There are 32 discrepancies between the modelled and reference sequences:

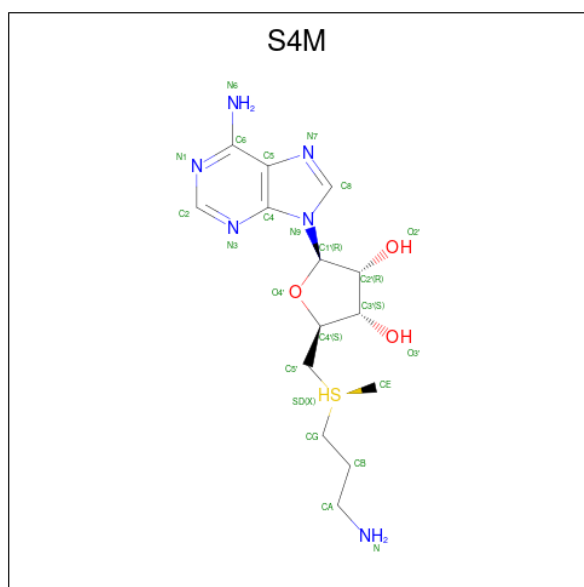
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73
A	0	HIS	-	expression tag	UNP Q4DA73
B	-7	MET	-	expression tag	UNP Q4DA73
B	-6	ALA	-	expression tag	UNP Q4DA73
B	-5	HIS	-	expression tag	UNP Q4DA73
B	-4	HIS	-	expression tag	UNP Q4DA73
B	-3	HIS	-	expression tag	UNP Q4DA73
B	-2	HIS	-	expression tag	UNP Q4DA73
B	-1	HIS	-	expression tag	UNP Q4DA73
B	0	HIS	-	expression tag	UNP Q4DA73
C	-7	MET	-	expression tag	UNP Q4DA73
C	-6	ALA	-	expression tag	UNP Q4DA73
C	-5	HIS	-	expression tag	UNP Q4DA73
C	-4	HIS	-	expression tag	UNP Q4DA73
C	-3	HIS	-	expression tag	UNP Q4DA73

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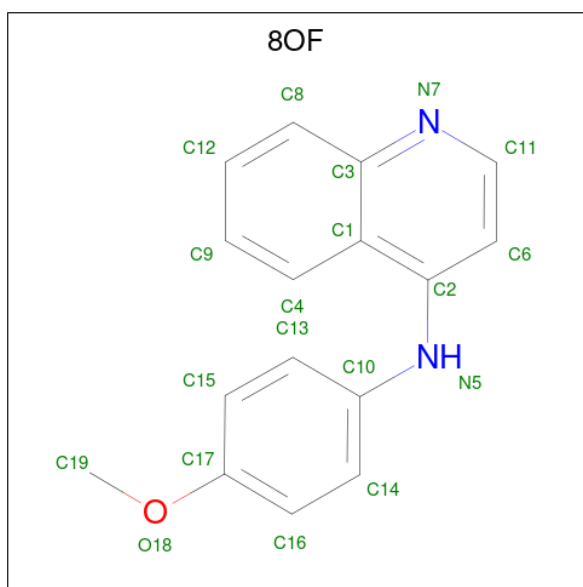
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	expression tag	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	UNP Q4DA73
D	-3	HIS	-	expression tag	UNP Q4DA73
D	-2	HIS	-	expression tag	UNP Q4DA73
D	-1	HIS	-	expression tag	UNP Q4DA73
D	0	HIS	-	expression tag	UNP Q4DA73

- Molecule 2 is 5'-[(S)-(3-AMINOPROPYL)(METHYL)-LAMBDA 4 -SULFANYL]-5'-DEOXYADENOSINE (CCD ID: S4M) (formula: C₁₄H₂₄N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	D	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is N-(4-methoxyphenyl)quinolin-4-amine (CCD ID: 8OF) (formula: C₁₆H₁₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	16	2	1		
3	B	1	Total	C	N	O	0	0
			19	16	2	1		
3	C	1	Total	C	N	O	0	0
			19	16	2	1		
3	D	1	Total	C	N	O	0	0
			19	16	2	1		

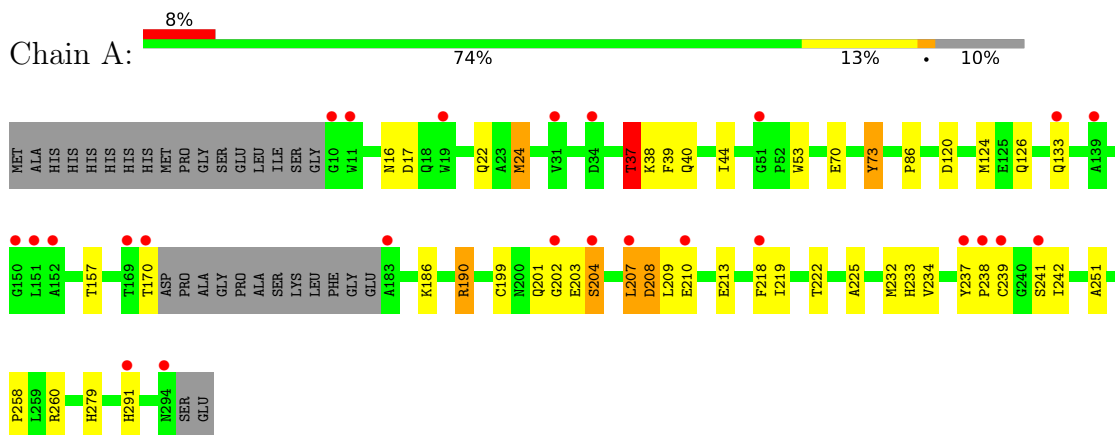
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	39	Total	O	0	0
			39	39		
4	C	52	Total	O	0	0
			52	52		
4	D	35	Total	O	0	0
			35	35		

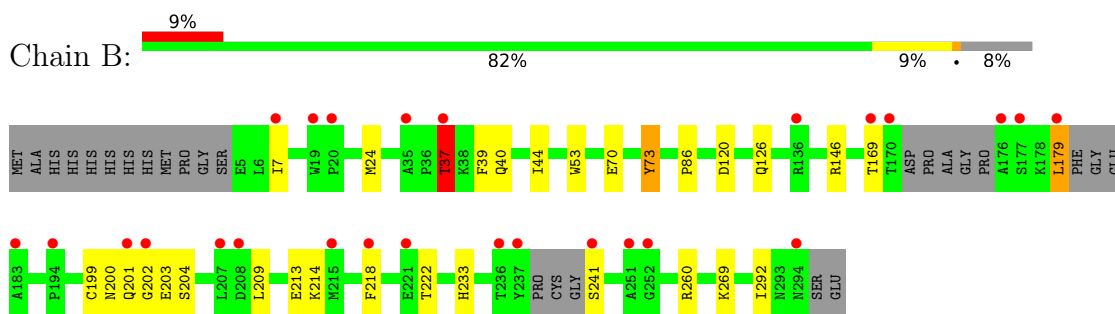
3 Residue-property plots [i](#)

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.

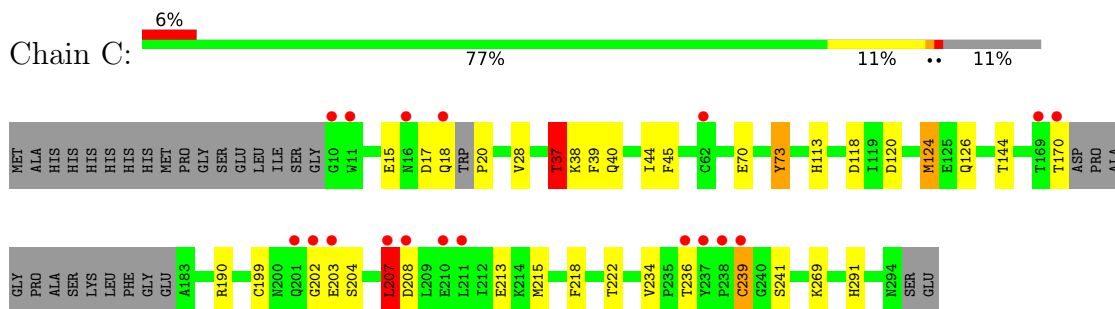
- Molecule 1: Spermidine synthase, putative



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ALA	SER	ALA	ALA	MET
LYS	LYS	HIS	HIS	ALA
LEU	LEU	HIS	HIS	ALA
PHE	PHE	HIS	HIS	ALA
GLY	GLY	HIS	HIS	ALA
GLU	GLU	HIS	HIS	ALA
ALA	ALA	HIS	HIS	ALA
F184	F184	MET	MET	MET
F194	F194	PRO	PRO	GLY
C199	C199	SER	SER	GLY
N200	N200	E5	E5	E5
Q201	Q201	L6	L6	L6
G202	G202	I7	I7	I7
E203	E203	S8	S8	S8
S204	S204	G9	G9	G9
L207	L207	N16	N16	N16
L211	L211	D17	D17	D17
T212	T212	GLN	GLN	TRP
E213	E213	P20	P20	P20
K214	K214	G21	G21	Q22
M215	M215	Q22	Q22	Q22
F218	F218	T37	T37	T37
E221	E221	K38	K38	K38
T236	T236	F39	F39	F39
Y237	Y237	Q40	Q40	Q40
PRO	PRO	W53	W53	W53
CYS	CYS	E70	E70	E70
GLY	GLY	Y73	Y73	Y73
SER	SER	P86	P86	P86
I242	I242	D118	D118	D118
K250	K250	T119	T119	T119
A251	A251	D120	D120	D120
R260	R260	G121	G121	G121
K269	K269	M124	M124	M124
L285	L285	Q133	Q133	Q133
P286	P286	R136	R136	R136
R290	R290	P141	P141	P141
H291	H291	R142	R142	R142
I292	I292	W293	W293	W293
N293	N293	T169	T169	T169
N294	N294	THR	THR	THR
SER	SER	ASP	ASP	ASP
GLU	GLU	PRO	PRO	PRO
		ALA	ALA	ALA
		GLY	GLY	GLY
		PRO	PRO	PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.98Å 99.67Å 134.50Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 50.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.07) 99.0 (50.00-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.241 , 0.269 0.241 , 0.269	Depositor DCC
R_{free} test set	3524 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8991	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0643e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S4M, 8OF

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	0.92	0/2216	1.07	10/3005 (0.3%)
1	B	0.90	0/2259	1.02	1/3058 (0.0%)
1	C	0.93	0/2199	1.06	6/2978 (0.2%)
1	D	0.89	0/2188	1.01	4/2960 (0.1%)
All	All	0.91	0/8862	1.04	21/12001 (0.2%)

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

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ARG	NE-CZ-NH2	-10.05	110.15	119.20
1	A	190	ARG	NE-CZ-NH2	-8.89	111.20	119.20
1	C	37	THR	N-CA-C	-8.03	98.39	109.95
1	C	190	ARG	NE-CZ-NH1	7.67	129.17	121.50
1	A	37	THR	N-CA-C	-7.24	99.27	109.69
1	C	190	ARG	CD-NE-CZ	6.66	133.72	124.40
1	A	190	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	C	190	ARG	CG-CD-NE	-6.06	98.66	112.00
1	A	190	ARG	CD-NE-CZ	5.79	132.51	124.40
1	A	190	ARG	CG-CD-NE	-5.76	99.34	112.00
1	B	37	THR	N-CA-C	-5.67	101.78	109.95
1	D	53	TRP	N-CA-C	5.67	118.40	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	THR	N-CA-C	-5.45	102.10	109.95
1	A	53	TRP	N-CA-C	5.41	118.09	111.82
1	A	237	TYR	CA-C-N	5.39	125.06	119.56
1	A	237	TYR	C-N-CA	5.39	125.06	119.56
1	C	207	LEU	N-CA-C	5.25	117.08	111.36
1	D	9	GLY	N-CA-C	-5.23	108.47	114.69
1	A	219	ILE	N-CA-C	5.13	115.34	110.42
1	A	204	SER	N-CA-C	5.00	117.76	109.46
1	D	142	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2163	0	2115	31	0
1	B	2209	0	2168	21	0
1	C	2149	0	2105	24	0
1	D	2140	0	2100	17	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	0	0
2	D	24	0	24	0	0
3	A	19	0	0	1	0
3	B	19	0	0	0	0
3	C	19	0	0	1	0
3	D	19	0	0	0	0
4	A	32	0	0	2	0
4	B	39	0	0	0	0
4	C	52	0	0	1	0
4	D	35	0	0	0	0
All	All	8991	0	8584	88	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 5.

All (88) 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:37:THR:HG21	1:A:120:ASP:OD2	1.57	1.05
1:B:37:THR:HG21	1:B:120:ASP:OD2	1.56	1.03
1:C:37:THR:HG21	1:C:120:ASP:OD2	1.61	1.00
1:D:37:THR:HG21	1:D:120:ASP:OD2	1.70	0.91
1:C:37:THR:HG22	1:C:39:PHE:H	1.38	0.86
1:C:236:THR:HG21	1:D:22:GLN:HE22	1.42	0.84
1:A:37:THR:HG22	1:A:39:PHE:H	1.45	0.81
1:A:37:THR:CG2	1:A:39:PHE:H	1.97	0.78
1:B:37:THR:HG22	1:B:39:PHE:H	1.48	0.78
1:D:37:THR:HG22	1:D:39:PHE:H	1.52	0.75
1:C:18:GLN:O	1:C:20:PRO:HD3	1.89	0.73
1:A:37:THR:HG22	1:A:40:GLN:H	1.53	0.72
1:B:37:THR:HG22	1:B:40:GLN:H	1.55	0.71
1:C:37:THR:CG2	1:C:39:PHE:H	2.03	0.70
1:A:234:VAL:HG12	4:A:405:HOH:O	1.91	0.69
1:A:204:SER:O	1:A:208:ASP:HB3	1.92	0.69
1:A:86:PRO:O	1:A:260:ARG:HD3	1.93	0.68
1:D:37:THR:HG22	1:D:40:GLN:H	1.58	0.68
1:B:37:THR:CG2	1:B:39:PHE:H	2.07	0.67
1:A:218:PHE:O	1:A:222:THR:HG23	1.95	0.67
1:C:37:THR:HG22	1:C:40:GLN:H	1.60	0.67
1:D:37:THR:CG2	1:D:39:PHE:H	2.08	0.67
1:B:169:THR:HG21	1:B:179:LEU:HD23	1.78	0.65
1:D:121:GLY:HA2	1:D:124:MET:HE3	1.82	0.62
1:C:37:THR:HB	1:C:40:GLN:O	2.00	0.62
1:C:207:LEU:HG	1:C:239:CYS:O	2.00	0.61
1:D:86:PRO:O	1:D:260:ARG:HD3	2.02	0.60
1:D:70:GLU:HA	1:D:73:TYR:CZ	2.37	0.59
1:C:234:VAL:HG12	4:C:406:HOH:O	2.03	0.58
1:D:202:GLY:O	1:D:203:GLU:HB2	2.05	0.57
1:A:37:THR:HG22	1:A:39:PHE:N	2.17	0.57
1:C:70:GLU:HA	1:C:73:TYR:CZ	2.40	0.57
1:A:24:MET:HG2	1:B:24:MET:HE2	1.86	0.56
1:B:70:GLU:HA	1:B:73:TYR:CZ	2.41	0.56
1:A:186:LYS:HG3	1:A:222:THR:HB	1.88	0.56
1:A:234:VAL:CG1	4:A:405:HOH:O	2.52	0.56
1:C:204:SER:HB2	1:C:241:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:HG3	1:A:242:ILE:HG23	1.87	0.55
1:C:37:THR:HG22	1:C:39:PHE:N	2.16	0.55
1:C:218:PHE:O	1:C:222:THR:HG23	2.08	0.54
1:D:37:THR:HB	1:D:40:GLN:O	2.08	0.54
1:C:213:GLU:OE2	1:C:291:HIS:CD2	2.61	0.53
1:A:204:SER:HB2	1:A:241:SER:H	1.73	0.53
1:B:86:PRO:O	1:B:260:ARG:HD3	2.09	0.53
1:A:24:MET:HG3	1:A:238:PRO:HG3	1.92	0.52
1:A:157:THR:O	1:A:190:ARG:NH2	2.28	0.52
1:A:70:GLU:HA	1:A:73:TYR:CZ	2.45	0.52
1:A:233:HIS:CE1	1:B:233:HIS:CE1	2.99	0.50
1:D:213:GLU:HG2	1:D:292:ILE:HD11	1.92	0.50
1:A:24:MET:HG2	1:B:24:MET:CE	2.42	0.49
1:D:200:ASN:OD1	1:D:200:ASN:C	2.55	0.49
1:A:44:ILE:CD1	1:A:126:GLN:HB3	2.43	0.49
1:B:204:SER:HB2	1:B:241:SER:O	2.13	0.49
1:A:207:LEU:C	1:A:209:LEU:H	2.20	0.49
1:D:118:ASP:HB3	1:D:124:MET:HE2	1.95	0.49
1:A:202:GLY:O	1:A:203:GLU:HB2	2.14	0.48
1:A:22:GLN:NE2	1:B:53:TRP:HE1	2.11	0.48
1:C:203:GLU:HB3	1:C:208:ASP:OD1	2.14	0.48
1:A:44:ILE:HD12	1:A:126:GLN:HB3	1.96	0.47
1:D:213:GLU:HG2	1:D:292:ILE:CD1	2.46	0.46
1:B:213:GLU:HG2	1:B:292:ILE:CD1	2.46	0.46
1:B:213:GLU:HG2	1:B:292:ILE:HD11	1.97	0.46
1:A:37:THR:HB	1:A:40:GLN:O	2.16	0.46
1:B:202:GLY:O	1:B:203:GLU:HB2	2.16	0.46
1:B:37:THR:HB	1:B:40:GLN:O	2.16	0.45
1:D:37:THR:HG22	1:D:39:PHE:N	2.26	0.45
1:B:37:THR:CG2	1:B:120:ASP:OD2	2.47	0.45
1:A:213:GLU:OE1	1:A:291:HIS:HD2	2.00	0.45
1:B:37:THR:HG22	1:B:39:PHE:N	2.25	0.44
1:B:209:LEU:O	1:B:213:GLU:HG3	2.18	0.43
1:C:202:GLY:O	1:C:203:GLU:HB2	2.19	0.43
1:D:285:LEU:O	1:D:286:PRO:C	2.60	0.43
1:B:200:ASN:OD1	1:B:200:ASN:C	2.62	0.42
1:A:225:ALA:HB1	1:A:251:ALA:HA	2.01	0.42
1:C:28:VAL:HG13	1:C:45:PHE:HB2	2.01	0.42
1:A:38:LYS:HE3	1:A:39:PHE:CZ	2.55	0.42
1:C:120:ASP:O	1:C:124:MET:HE3	2.20	0.41
1:A:37:THR:HG23	1:A:38:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:HIS:HE1	1:C:144:THR:OG1	2.03	0.41
1:C:204:SER:HB2	1:C:241:SER:O	2.21	0.41
1:A:73:TYR:CD1	3:A:302:8OF:C15	3.04	0.41
1:B:44:ILE:CD1	1:B:126:GLN:HB3	2.50	0.41
1:C:118:ASP:HB3	1:C:124:MET:CE	2.51	0.41
1:A:258:PRO:HG3	1:A:279:HIS:CG	2.56	0.41
1:C:37:THR:HG23	1:C:38:LYS:N	2.36	0.41
1:D:203:GLU:HG3	1:D:211:LEU:HD23	2.02	0.40
1:C:73:TYR:CD1	3:C:302:8OF:C15	3.05	0.40
1:C:44:ILE:CD1	1:C:126:GLN:HB3	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	269/304 (88%)	259 (96%)	8 (3%)	2 (1%)	18	10
1	B	271/304 (89%)	262 (97%)	9 (3%)	0	100	100
1	C	266/304 (88%)	258 (97%)	8 (3%)	0	100	100
1	D	262/304 (86%)	252 (96%)	10 (4%)	0	100	100
All	All	1068/1216 (88%)	1031 (96%)	35 (3%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	A	207	LEU

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	238/262 (91%)	226 (95%)	12 (5%)	22	14
1	B	243/262 (93%)	232 (96%)	11 (4%)	24	18
1	C	237/262 (90%)	227 (96%)	10 (4%)	26	20
1	D	236/262 (90%)	224 (95%)	12 (5%)	21	14
All	All	954/1048 (91%)	909 (95%)	45 (5%)	23	16

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	17	ASP
1	A	24	MET
1	A	37	THR
1	A	73	TYR
1	A	124	MET
1	A	133	GLN
1	A	170	THR
1	A	199	CYS
1	A	201	GLN
1	A	210	GLU
1	A	239	CYS
1	B	7	ILE
1	B	37	THR
1	B	73	TYR
1	B	146	ARG
1	B	179	LEU
1	B	199	CYS
1	B	201	GLN
1	B	214	LYS
1	B	218	PHE
1	B	222	THR
1	B	269	LYS
1	C	17	ASP

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Mol	Chain	Res	Type
1	C	37	THR
1	C	73	TYR
1	C	124	MET
1	C	170	THR
1	C	199	CYS
1	C	207	LEU
1	C	215	MET
1	C	239	CYS
1	C	269	LYS
1	D	7	ILE
1	D	16	ASN
1	D	37	THR
1	D	73	TYR
1	D	133	GLN
1	D	136	ARG
1	D	199	CYS
1	D	204	SER
1	D	214	LYS
1	D	250	LYS
1	D	269	LYS
1	D	290	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	129	GLN
1	A	130	HIS
1	A	233	HIS
1	A	291	HIS
1	B	22	GLN
1	B	64	GLN
1	B	113	HIS
1	B	126	GLN
1	B	129	GLN
1	B	130	HIS
1	B	233	HIS
1	C	113	HIS
1	C	126	GLN
1	C	129	GLN
1	C	130	HIS
1	D	22	GLN

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Mol	Chain	Res	Type
1	D	64	GLN
1	D	113	HIS
1	D	129	GLN
1	D	201	GLN

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 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	$\# Z > 2$
2	S4M	B	301	-	25,26,26	0.57	0	33,37,37	1.19	4 (12%)
3	8OF	A	302	-	21,21,21	1.06	1 (4%)	28,28,28	2.80	9 (32%)
3	8OF	D	302	-	21,21,21	1.01	0	28,28,28	2.03	6 (21%)
3	8OF	C	302	-	21,21,21	1.11	4 (19%)	28,28,28	2.34	6 (21%)
3	8OF	B	302	-	21,21,21	1.01	2 (9%)	28,28,28	1.78	4 (14%)
2	S4M	A	301	-	25,26,26	0.69	1 (4%)	33,37,37	1.16	1 (3%)
2	S4M	D	301	-	25,26,26	0.64	1 (4%)	33,37,37	1.14	3 (9%)
2	S4M	C	301	-	25,26,26	0.63	1 (4%)	33,37,37	0.92	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S4M	B	301	-	-	4/12/28/28	0/3/3/3
3	8OF	A	302	-	-	0/6/6/6	0/3/3/3
3	8OF	D	302	-	-	1/6/6/6	0/3/3/3
3	8OF	C	302	-	-	2/6/6/6	0/3/3/3
3	8OF	B	302	-	-	4/6/6/6	0/3/3/3
2	S4M	A	301	-	-	5/12/28/28	0/3/3/3
2	S4M	D	301	-	-	4/12/28/28	0/3/3/3
2	S4M	C	301	-	-	4/12/28/28	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	S4M	C6-N6	2.47	1.40	1.34
2	C	301	S4M	C6-N6	2.35	1.40	1.34
3	C	302	8OF	C3-N7	-2.31	1.33	1.37
3	C	302	8OF	C4-C1	-2.26	1.37	1.42
3	A	302	8OF	C3-N7	-2.15	1.33	1.37
3	B	302	8OF	C2-C1	-2.14	1.38	1.43
2	D	301	S4M	C6-N6	2.13	1.39	1.34
3	B	302	8OF	C8-C3	-2.13	1.38	1.41
3	C	302	8OF	C8-C3	-2.12	1.38	1.41
3	C	302	8OF	C2-C1	-2.08	1.38	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	8OF	C1-C2-N5	9.07	134.49	118.83
3	C	302	8OF	C1-C2-N5	7.17	131.22	118.83
3	A	302	8OF	C6-C2-N5	-6.92	105.96	123.47
3	A	302	8OF	C10-N5-C2	5.81	139.05	126.36
3	C	302	8OF	C6-C2-N5	-5.44	109.70	123.47
3	D	302	8OF	C1-C2-N5	4.88	127.27	118.83
3	C	302	8OF	C10-N5-C2	4.79	136.81	126.36
3	B	302	8OF	C19-O18-C17	-4.64	107.54	117.50
3	D	302	8OF	C19-O18-C17	-4.54	107.77	117.50
3	D	302	8OF	C6-C2-N5	-4.22	112.80	123.47
3	B	302	8OF	C1-C2-N5	4.07	125.86	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	8OF	C10-N5-C2	3.99	135.07	126.36
2	A	301	S4M	CG-SD-C5'	-3.93	93.83	103.43
3	C	302	8OF	C19-O18-C17	-3.76	109.44	117.50
3	B	302	8OF	C6-C2-N5	-3.46	114.71	123.47
3	B	302	8OF	C10-N5-C2	3.39	133.76	126.36
2	D	301	S4M	CG-SD-C5'	-3.39	95.15	103.43
3	A	302	8OF	C13-C10-N5	-2.80	111.13	120.61
2	B	301	S4M	O4'-C1'-N9	2.78	113.43	108.09
3	A	302	8OF	C6-C11-N7	-2.57	120.77	124.60
3	D	302	8OF	C13-C10-N5	-2.49	112.19	120.61
2	C	301	S4M	O4'-C1'-N9	2.43	112.75	108.09
2	B	301	S4M	CG-SD-C5'	-2.33	97.75	103.43
3	A	302	8OF	C2-C1-C3	-2.31	116.53	118.01
3	A	302	8OF	C14-C10-N5	2.30	128.41	120.61
3	A	302	8OF	C19-O18-C17	-2.24	112.69	117.50
3	C	302	8OF	C13-C10-N5	-2.20	113.17	120.61
3	C	302	8OF	C12-C9-C4	2.15	123.28	120.40
3	A	302	8OF	C11-C6-C2	2.14	120.64	119.61
2	D	301	S4M	O3'-C3'-C4'	-2.13	104.97	111.08
2	B	301	S4M	C4-N9-C8	2.11	107.96	105.74
2	D	301	S4M	O4'-C4'-C5'	2.07	114.12	108.88
2	B	301	S4M	C2'-C3'-C4'	2.03	106.54	102.61
3	D	302	8OF	C6-C11-N7	-2.03	121.58	124.60

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	S4M	CB-CG-SD-CE
2	A	301	S4M	O4'-C4'-C5'-SD
2	A	301	S4M	C3'-C4'-C5'-SD
2	B	301	S4M	O4'-C4'-C5'-SD
2	B	301	S4M	C3'-C4'-C5'-SD
2	C	301	S4M	CA-CB-CG-SD
2	C	301	S4M	O4'-C4'-C5'-SD
2	C	301	S4M	C3'-C4'-C5'-SD
2	D	301	S4M	O4'-C4'-C5'-SD
2	D	301	S4M	C3'-C4'-C5'-SD
3	B	302	8OF	C16-C17-O18-C19
3	C	302	8OF	C16-C17-O18-C19
3	C	302	8OF	C15-C17-O18-C19
3	B	302	8OF	C15-C17-O18-C19

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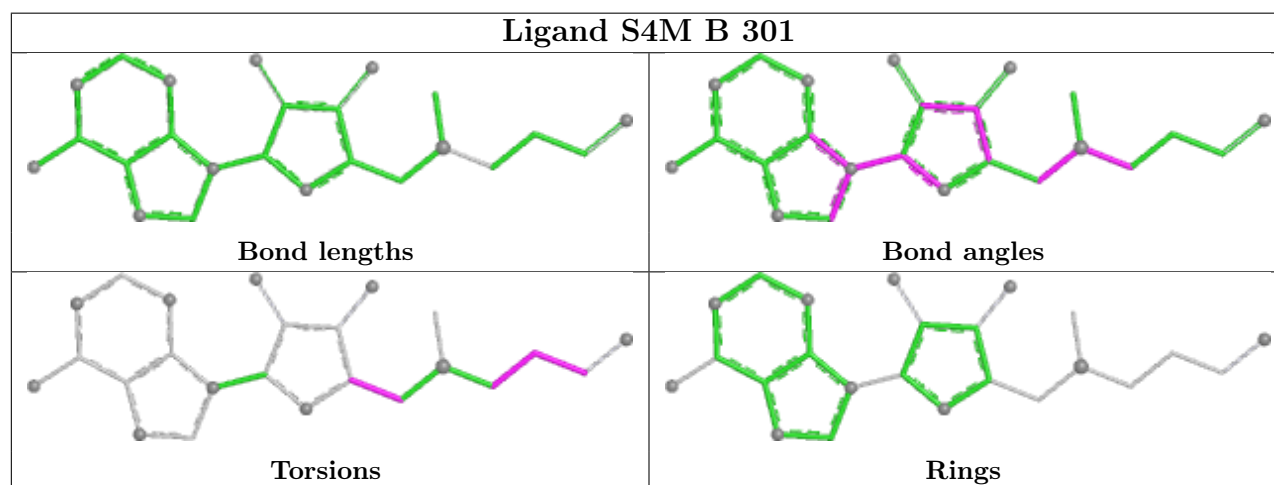
Mol	Chain	Res	Type	Atoms
2	B	301	S4M	N-CA-CB-CG
2	D	301	S4M	N-CA-CB-CG
3	B	302	8OF	C6-C2-N5-C10
2	A	301	S4M	N-CA-CB-CG
2	A	301	S4M	CB-CG-SD-C5'
3	D	302	8OF	C6-C2-N5-C10
3	B	302	8OF	C1-C2-N5-C10
2	B	301	S4M	CA-CB-CG-SD
2	D	301	S4M	CA-CB-CG-SD
2	C	301	S4M	CB-CG-SD-C5'

There are no ring outliers.

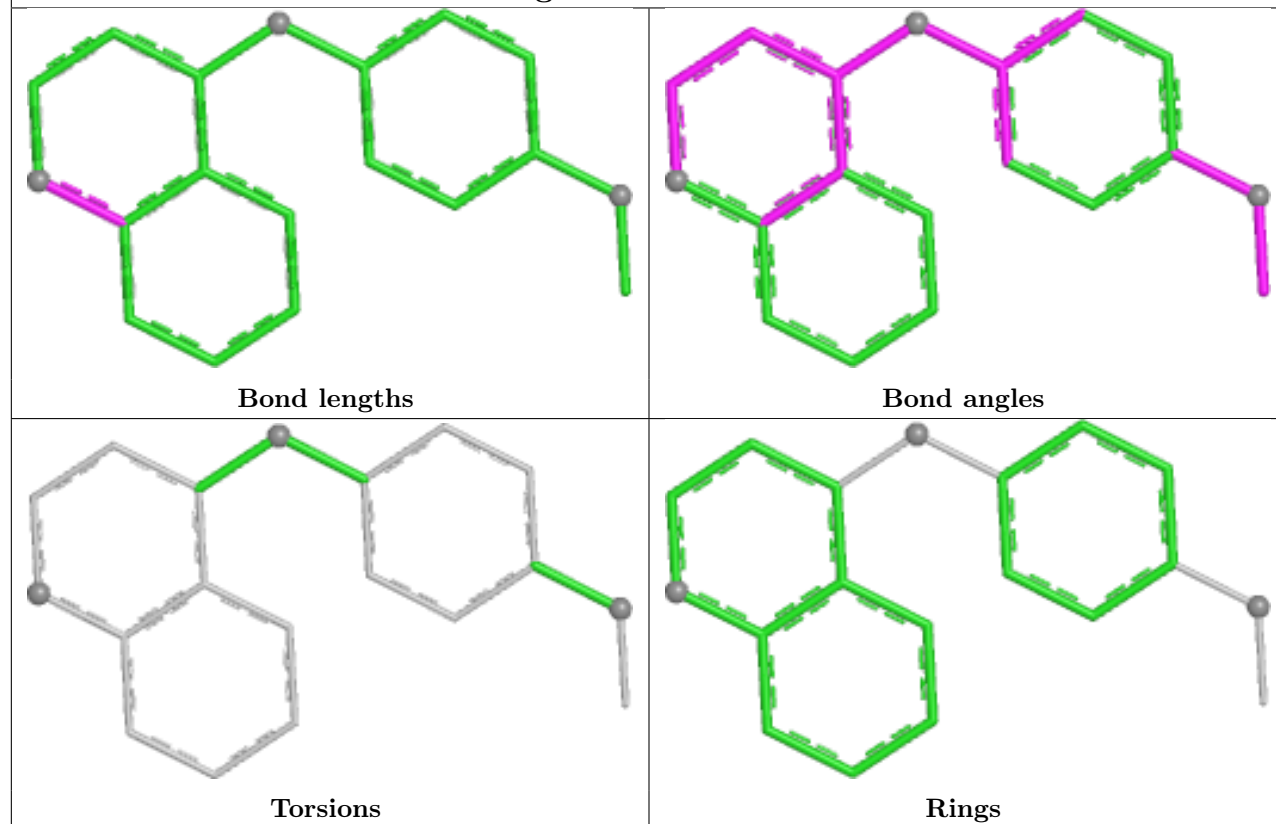
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	8OF	1	0
3	C	302	8OF	1	0

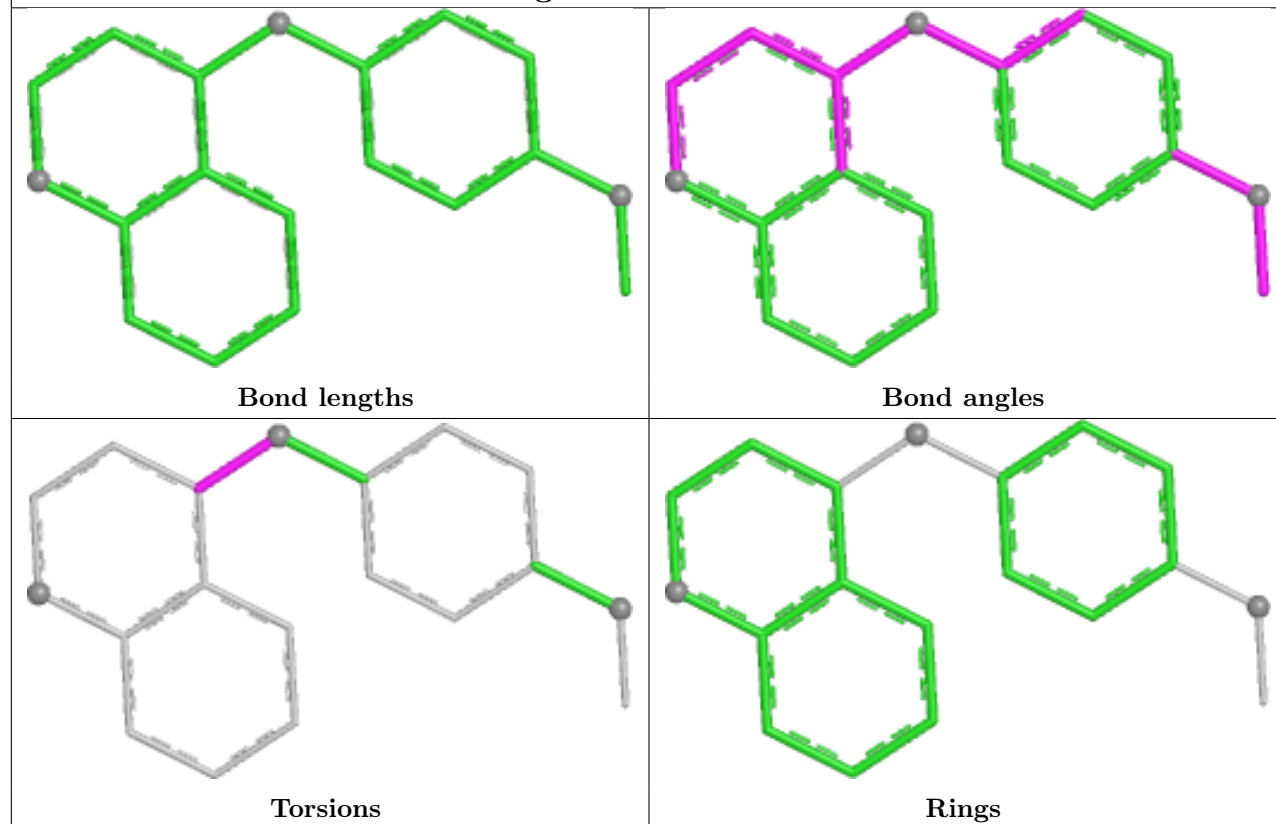
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



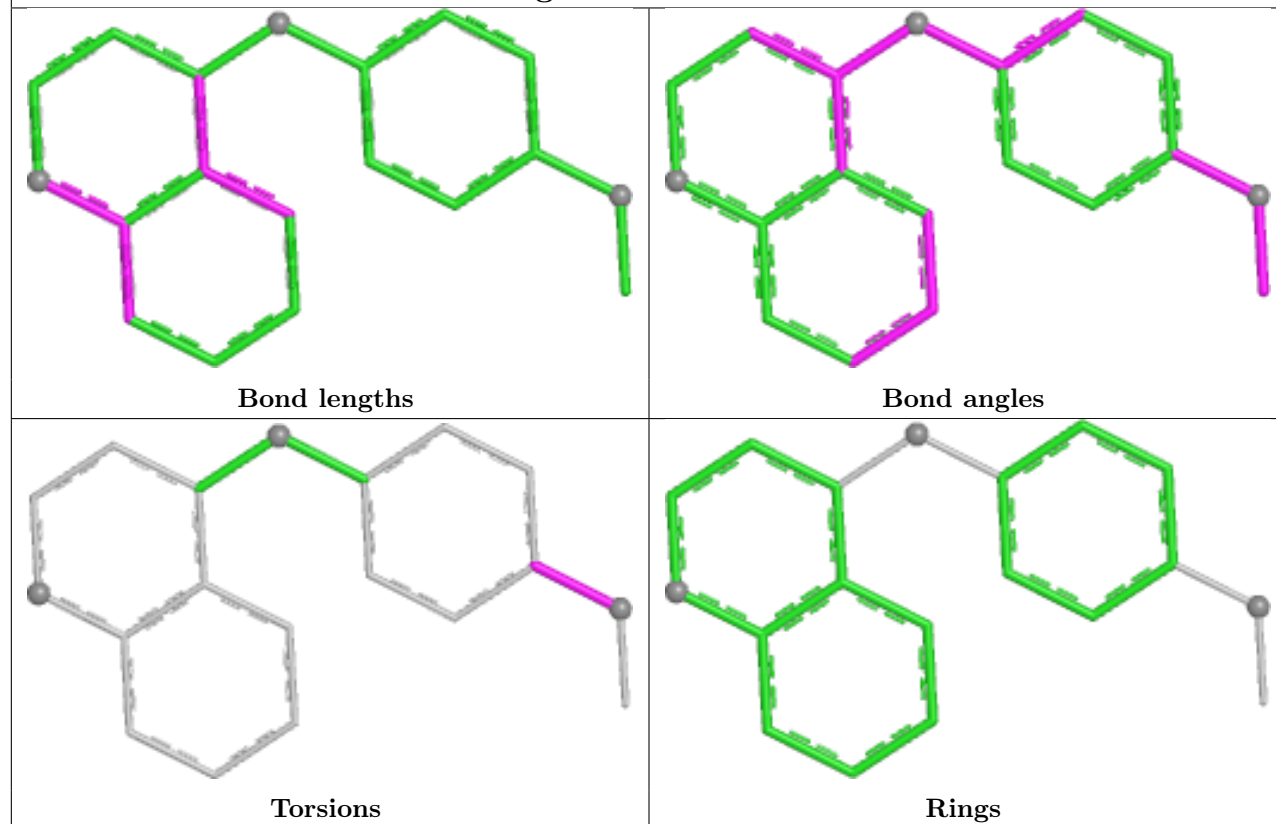
Ligand 8OF A 302



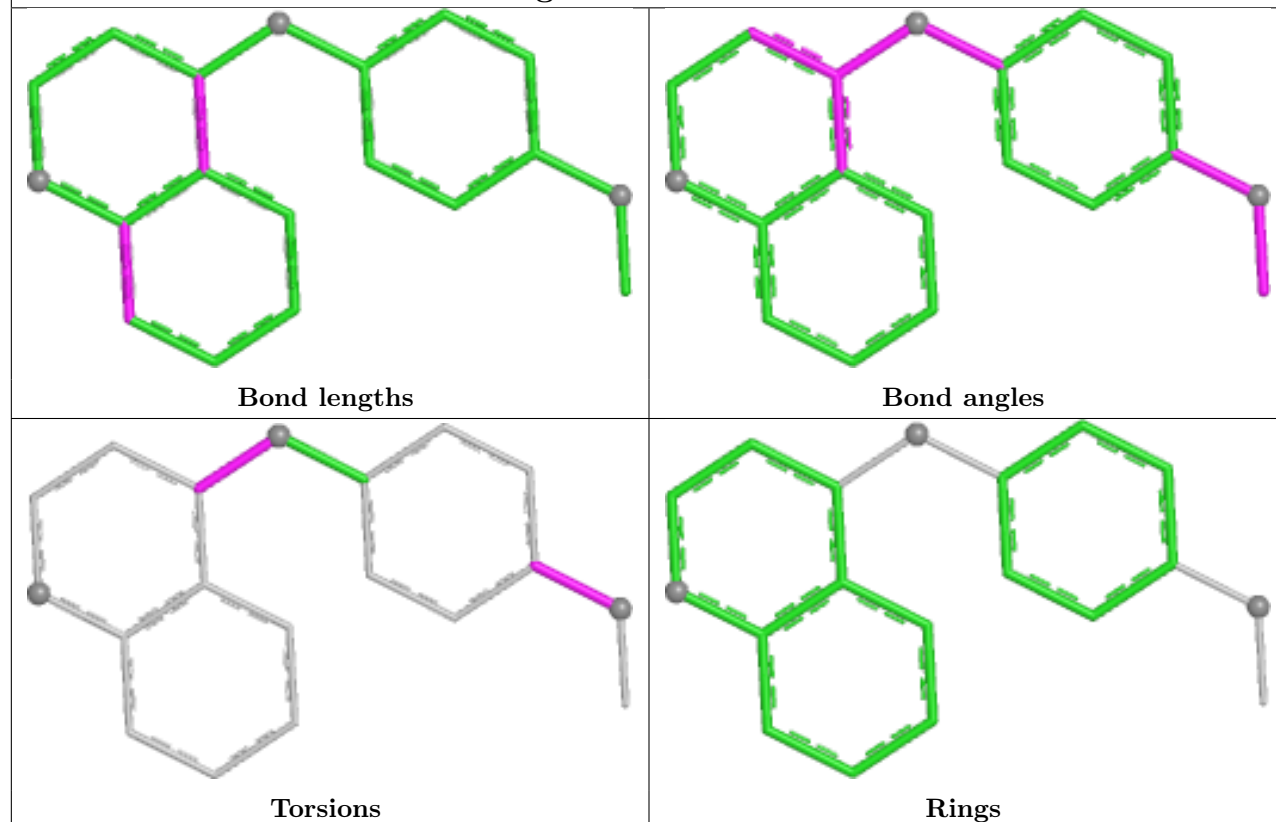
Ligand 8OF D 302

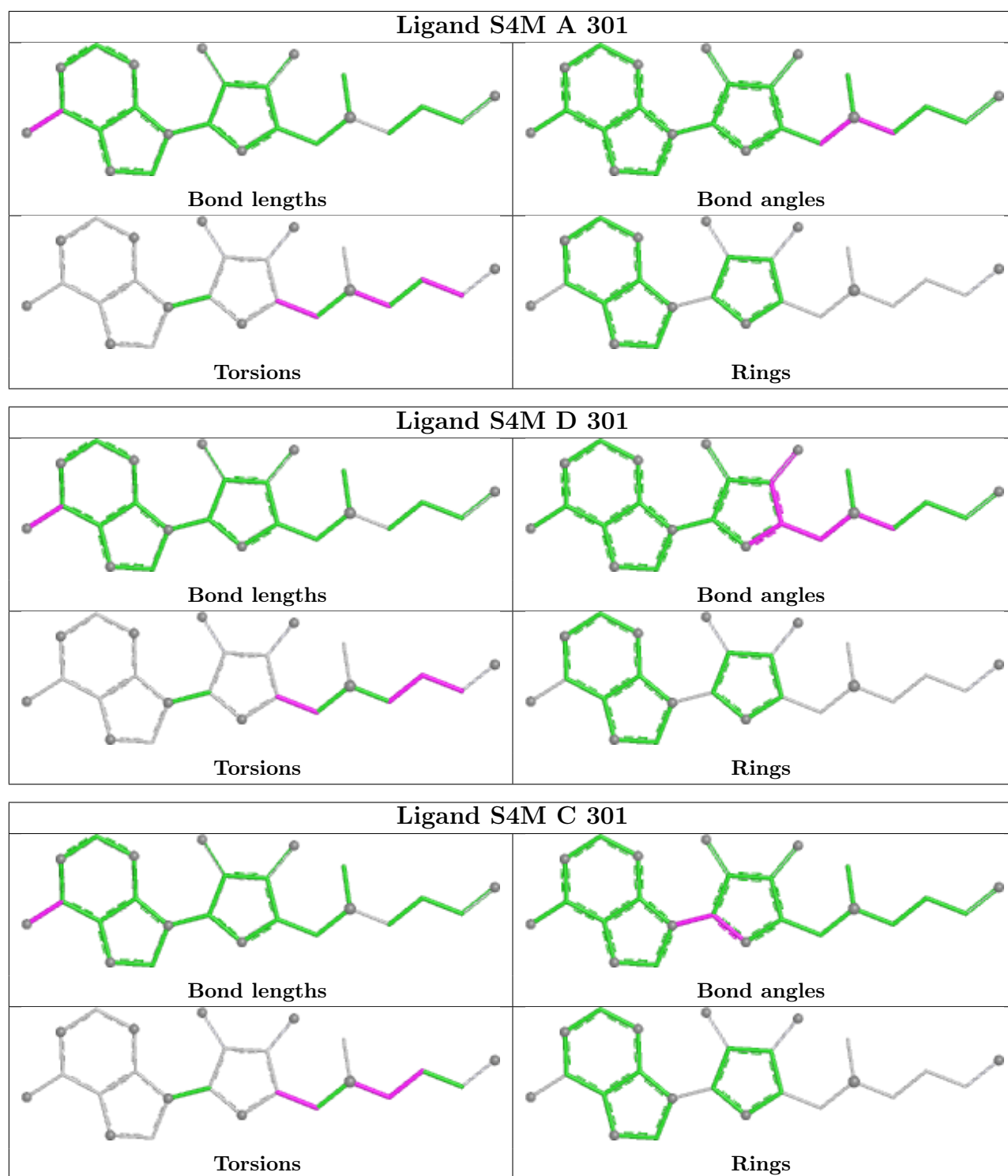


Ligand 8OF C 302



Ligand 8OF B 302





5.7 Other polymers [i](#)

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, 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	273/304 (89%)	0.79	25 (9%) 14 15	22, 35, 56, 73	0
1	B	279/304 (91%)	0.68	26 (9%) 14 14	21, 35, 59, 73	0
1	C	272/304 (89%)	0.57	18 (6%) 24 24	20, 32, 55, 81	0
1	D	270/304 (88%)	0.54	16 (5%) 28 28	19, 34, 51, 77	0
All	All	1094/1216 (89%)	0.65	85 (7%) 19 19	19, 34, 56, 81	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	5.5
1	A	19	TRP	4.8
1	A	183	ALA	4.8
1	D	236	THR	4.5
1	D	218	PHE	4.2
1	C	207	LEU	4.2
1	B	241	SER	4.2
1	C	239	CYS	4.2
1	B	176	ALA	4.1
1	A	239	CYS	4.1
1	C	11	TRP	3.9
1	D	17	ASP	3.8
1	C	238	PRO	3.8
1	C	170	THR	3.7
1	D	20	PRO	3.6
1	B	218	PHE	3.5
1	C	10	GLY	3.5
1	C	18	GLN	3.4
1	A	11	TRP	3.3
1	B	237	TYR	3.2
1	C	202	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	202	GLY	3.2
1	B	294	ASN	3.1
1	C	203	GLU	3.1
1	B	170	THR	3.0
1	D	202	GLY	3.0
1	B	19	TRP	3.0
1	D	237	TYR	3.0
1	A	10	GLY	3.0
1	D	251	ALA	2.9
1	C	169	THR	2.9
1	A	152	ALA	2.9
1	D	207	LEU	2.9
1	A	170	THR	2.9
1	D	141	PRO	2.8
1	A	139	ALA	2.8
1	A	207	LEU	2.8
1	A	31	VAL	2.8
1	B	236	THR	2.8
1	D	242	ILE	2.8
1	A	210	GLU	2.7
1	D	169	THR	2.7
1	A	51	GLY	2.7
1	B	35	ALA	2.7
1	B	20	PRO	2.7
1	A	241	SER	2.6
1	B	177	SER	2.6
1	D	194	PRO	2.6
1	B	207	LEU	2.6
1	C	211	LEU	2.5
1	A	294	ASN	2.5
1	B	7	ILE	2.5
1	B	37	THR	2.4
1	B	194	PRO	2.4
1	C	201	GLN	2.4
1	C	236	THR	2.4
1	A	34	ASP	2.3
1	B	136	ARG	2.3
1	A	291	HIS	2.3
1	D	221	GLU	2.3
1	A	202	GLY	2.3
1	B	215	MET	2.3
1	D	201	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	16	ASN	2.3
1	B	179	LEU	2.3
1	B	252	GLY	2.3
1	A	238	PRO	2.3
1	C	237	TYR	2.3
1	B	221	GLU	2.2
1	A	169	THR	2.2
1	A	218	PHE	2.2
1	B	251	ALA	2.2
1	C	210	GLU	2.2
1	C	62	CYS	2.2
1	A	150	GLY	2.1
1	D	215	MET	2.1
1	C	208	ASP	2.1
1	A	133	GLN	2.1
1	A	204	SER	2.1
1	B	208	ASP	2.1
1	B	169	THR	2.1
1	D	136	ARG	2.1
1	A	237	TYR	2.1
1	B	201	GLN	2.0
1	A	151	LEU	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(Å ²)	Q<0.9
3	8OF	B	302	19/19	0.78	0.19	70,72,75,75	0

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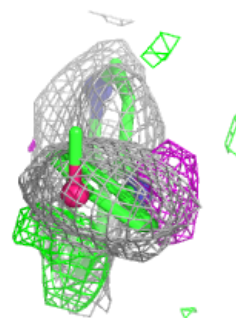
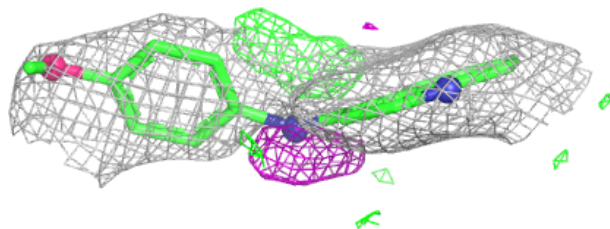
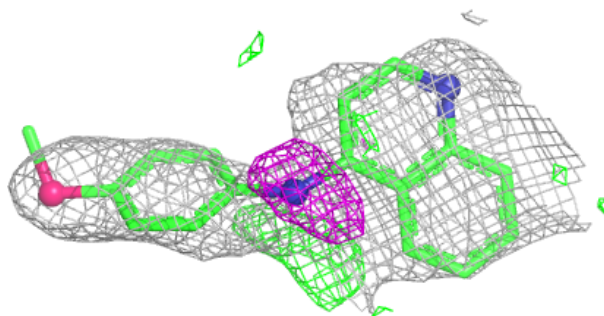
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	8OF	D	302	19/19	0.78	0.18	66,69,71,73	0
3	8OF	C	302	19/19	0.80	0.16	53,55,57,58	0
3	8OF	A	302	19/19	0.83	0.14	50,53,57,58	0
2	S4M	B	301	24/24	0.86	0.11	37,43,57,65	0
2	S4M	D	301	24/24	0.86	0.12	40,44,55,58	0
2	S4M	A	301	24/24	0.86	0.13	39,43,52,56	0
2	S4M	C	301	24/24	0.88	0.12	39,43,58,66	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.

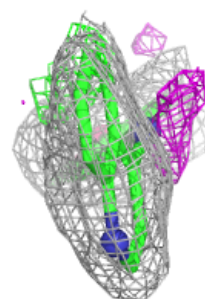
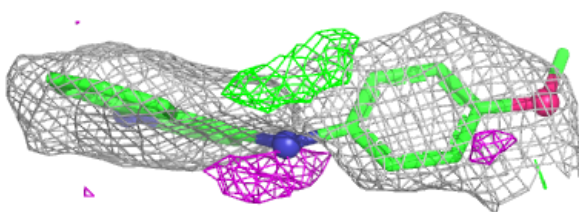
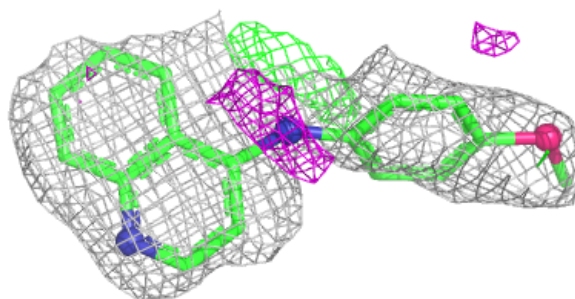
Electron density around 8OF B 302:

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

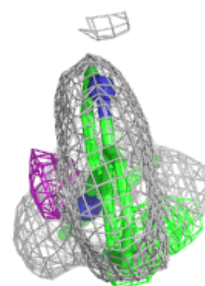
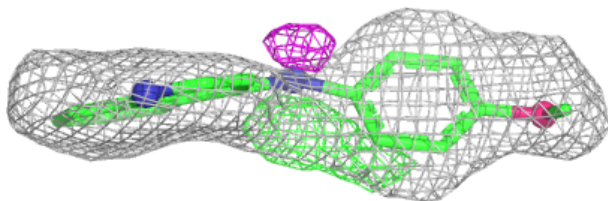
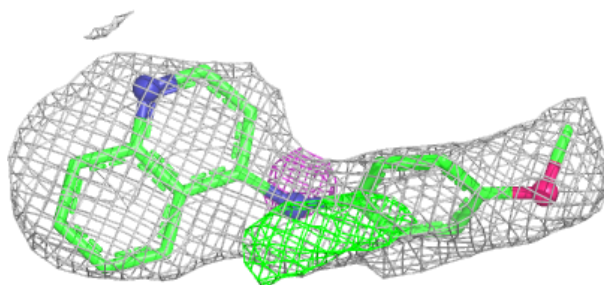


Electron density around 8OF D 302:

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

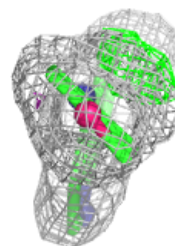
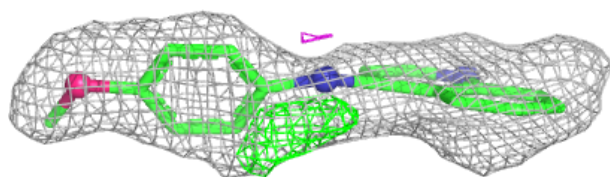
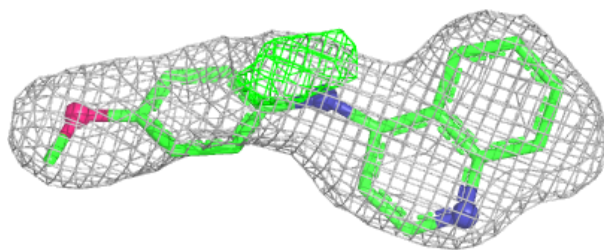
**Electron density around 8OF C 302:**

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

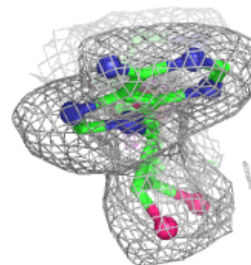
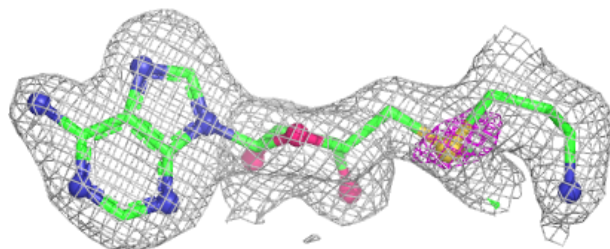
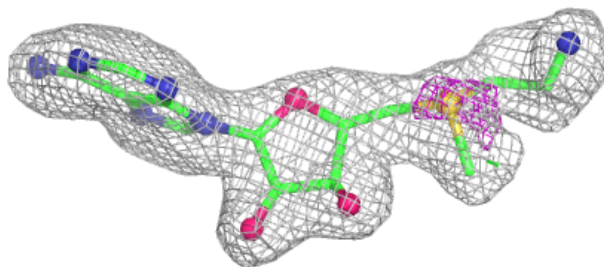


Electron density around 8OF A 302:

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

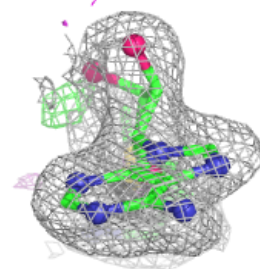
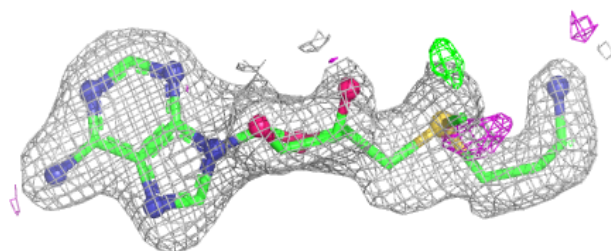
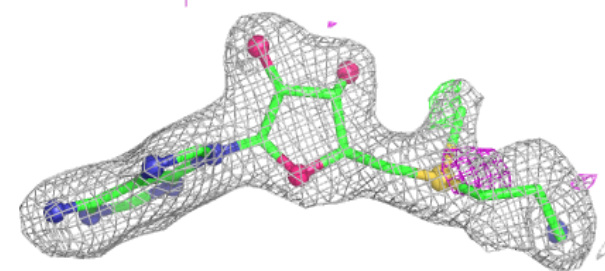
**Electron density around S4M B 301:**

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

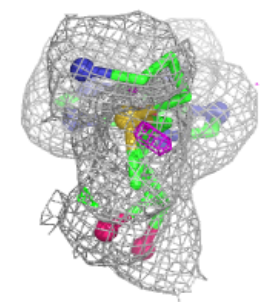
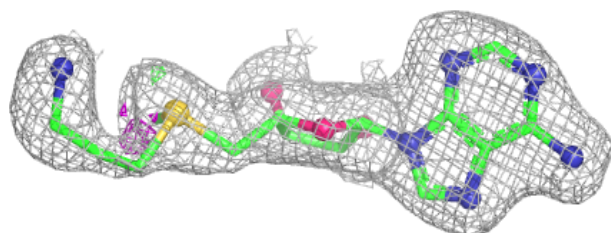
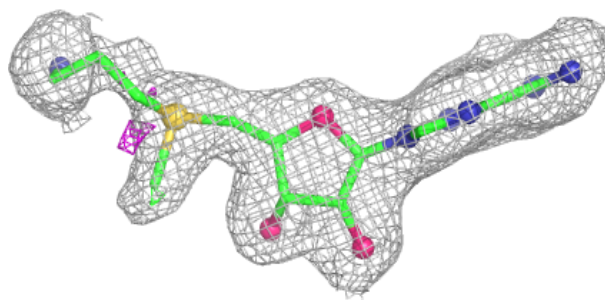


Electron density around S4M D 301:

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

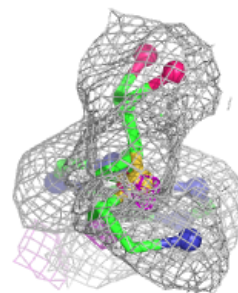
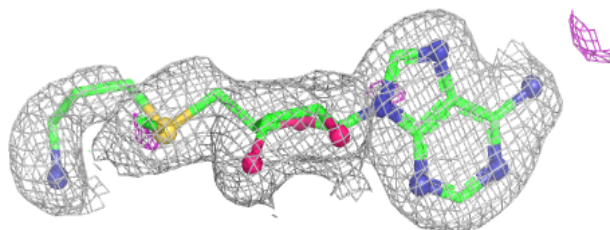
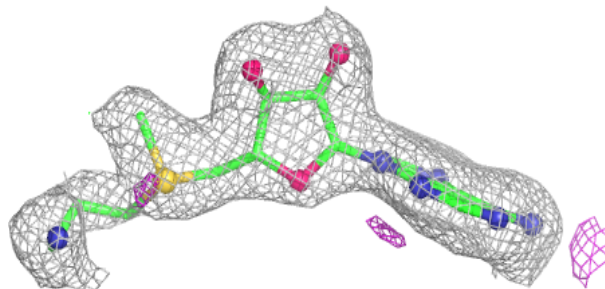
**Electron density around S4M A 301:**

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



Electron density around S4M 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.