



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:11 PM UTC

PDB ID : 4YV0 / pdb_00004yv0
Title : Crystal structure of Trypanosoma cruzi spermidine synthase in complex with (2S)-N-methyl-N-phenyl-2,3-dihydro-1,4-benzodioxine- 2-carboxamid
Authors : Amano, Y.; Tateishi, Y.
Deposited on : 2015-03-19
Resolution : 1.95 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

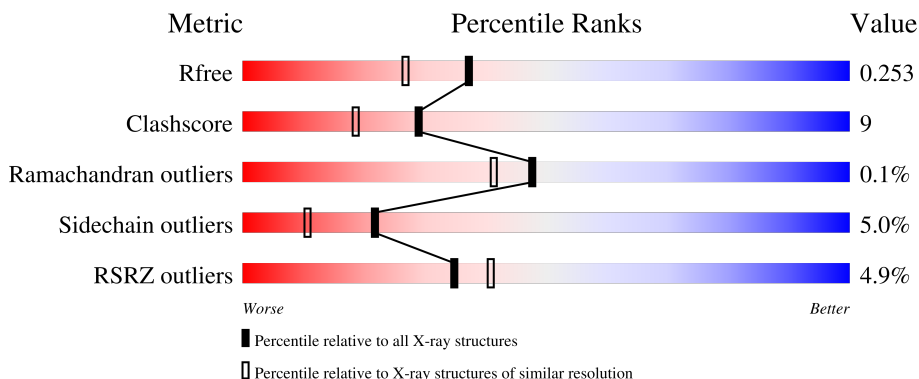
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	2% 72% 15% • 12%
1	B	304	6% 76% 17% • 5%
1	C	304	3% 73% 14% • 10%
1	D	304	7% 72% 19% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9249 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	269	Total	C	N	O	S	0	0	0
			2124	1350	364	396	14			
1	B	290	Total	C	N	O	S	0	0	0
			2281	1449	389	429	14			
1	C	273	Total	C	N	O	S	0	0	0
			2151	1366	368	403	14			
1	D	290	Total	C	N	O	S	0	0	0
			2281	1449	389	429	14			

There are 32 discrepancies between the modelled and reference sequences:

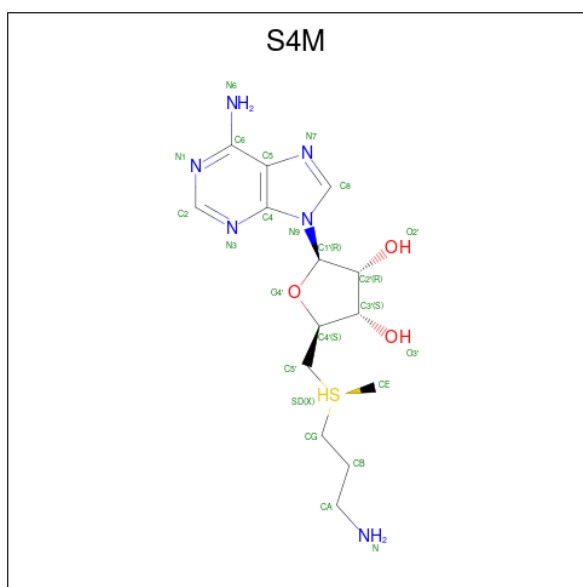
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73
A	0	HIS	-	expression tag	UNP Q4DA73
B	-7	MET	-	initiating methionine	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	-	initiating methionine	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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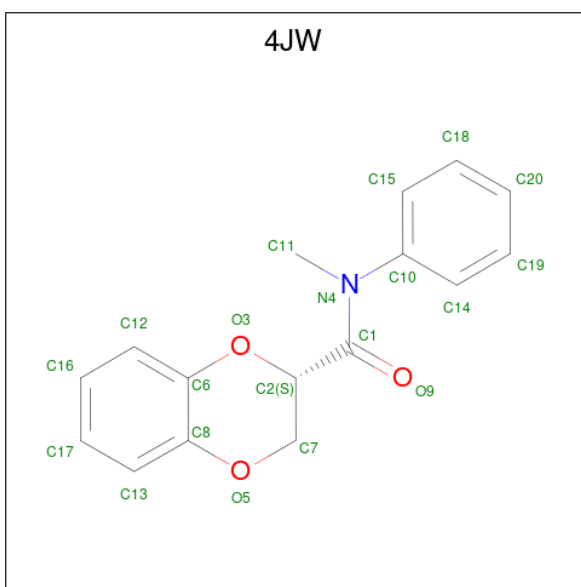
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	initiating methionine	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	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 (2S)-N-methyl-N-phenyl-2,3-dihydro-1,4-benzodioxine-2-carboxamide (CCD ID: 4JW) (formula: C₁₆H₁₅NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			20	16	1	3		
3	D	1	Total	C	N	O	0	0
			20	16	1	3		

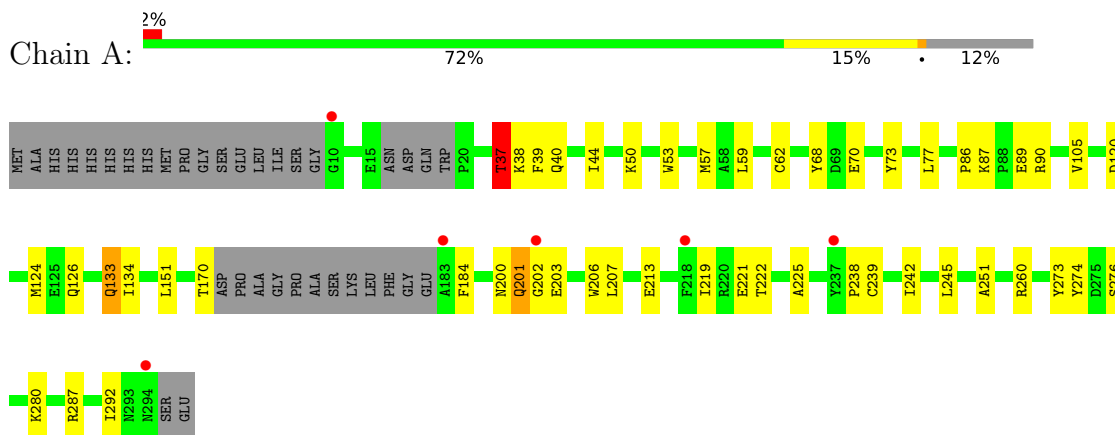
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	76	Total	O	0	0
			76	76		
4	C	77	Total	O	0	0
			77	77		
4	D	65	Total	O	0	0
			65	65		

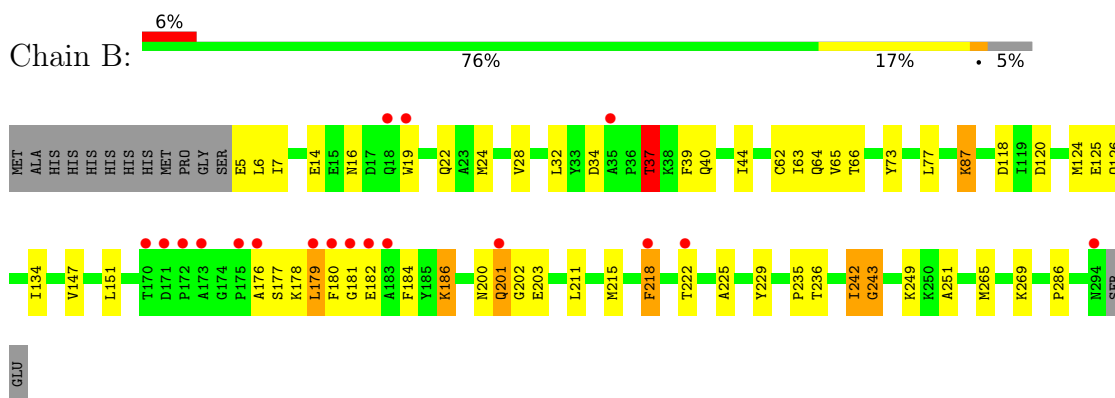
3 Residue-property plots [i](#)

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.

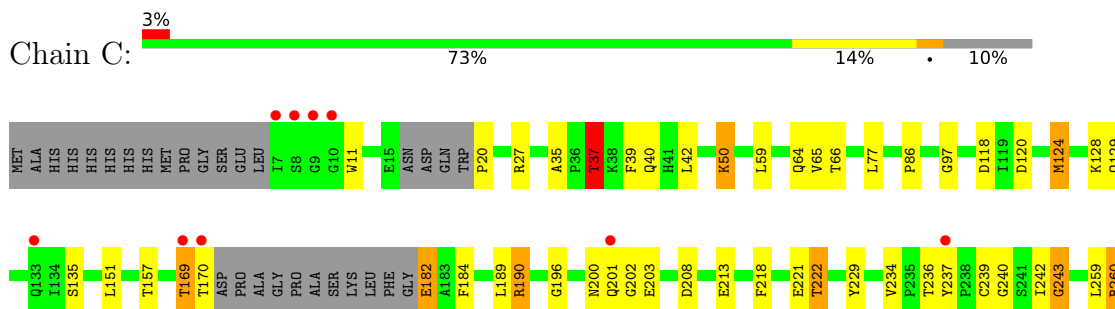
- Molecule 1: Spermidine synthase, putative

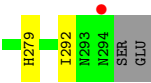


- Molecule 1: Spermidine synthase, putative

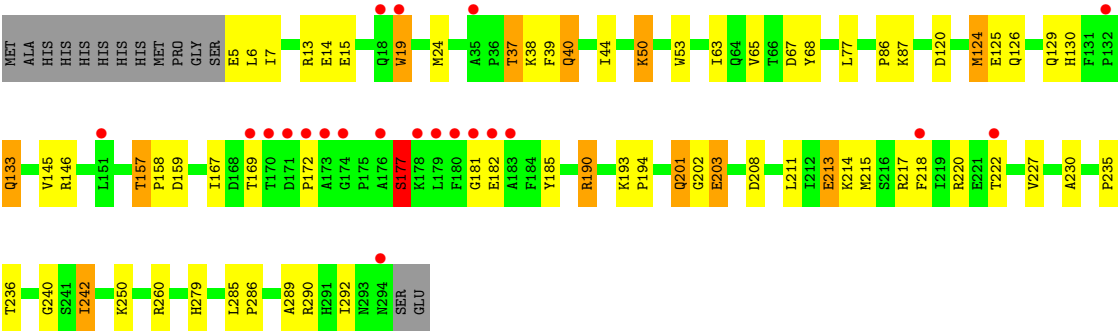


- Molecule 1: Spermidine synthase, putative





● Molecule 1: Spermidine synthase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.56Å 99.78Å 135.00Å 90.00° 90.64° 90.00°	Depositor
Resolution (Å)	29.41 – 1.95 29.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.41-1.95) 96.2 (29.41-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.208 , 0.253 0.208 , 0.253	Depositor DCC
R_{free} test set	4047 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9249	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 66.74 % 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 5.7553e-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: 4JW, S4M

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	1.23	2/2174 (0.1%)	1.17	3/2944 (0.1%)
1	B	1.26	0/2338	1.24	14/3172 (0.4%)
1	C	1.26	4/2201 (0.2%)	1.22	10/2980 (0.3%)
1	D	1.27	3/2338 (0.1%)	1.22	12/3172 (0.4%)
All	All	1.26	9/9051 (0.1%)	1.21	39/12268 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	ARG	CA-C	5.46	1.58	1.52
1	D	230	ALA	C-O	-5.43	1.17	1.24
1	C	243	GLY	C-O	5.42	1.29	1.23
1	D	279	HIS	CA-C	5.33	1.59	1.52
1	C	279	HIS	N-CA	5.29	1.52	1.46
1	A	62	CYS	N-CA	5.21	1.52	1.46
1	A	105	VAL	CA-C	5.17	1.59	1.52
1	D	158	PRO	CA-C	5.05	1.58	1.52
1	C	259	LEU	C-O	-5.04	1.18	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	ARG	NE-CZ-NH2	-8.45	111.59	119.20
1	C	190	ARG	NE-CZ-NH2	-8.21	111.81	119.20
1	C	190	ARG	CG-CD-NE	-7.08	96.42	112.00
1	B	182	GLU	N-CA-C	6.91	121.99	112.04
1	B	37	THR	N-CA-C	-6.80	99.40	109.81
1	C	189	LEU	CA-C-N	6.53	128.93	120.44
1	C	189	LEU	C-N-CA	6.53	128.93	120.44
1	C	37	THR	N-CA-C	-6.53	99.83	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	THR	CA-C-N	-6.44	112.90	120.11
1	D	157	THR	C-N-CA	-6.44	112.90	120.11
1	D	190	ARG	CG-CD-NE	-6.20	98.36	112.00
1	D	177	SER	N-CA-C	6.13	117.96	111.28
1	D	68	TYR	N-CA-C	6.08	117.98	111.36
1	D	67	ASP	N-CA-C	-5.98	104.77	111.28
1	B	177	SER	N-CA-C	5.87	117.76	111.36
1	C	35	ALA	CA-C-N	-5.87	114.56	120.31
1	C	35	ALA	C-N-CA	-5.87	114.56	120.31
1	D	227	VAL	N-CA-C	-5.78	100.35	108.27
1	B	242	ILE	CA-C-N	-5.77	114.64	122.03
1	B	242	ILE	C-N-CA	-5.77	114.64	122.03
1	C	196	GLY	N-CA-C	5.67	118.45	111.93
1	D	190	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	A	37	THR	N-CA-C	-5.61	101.87	109.95
1	D	242	ILE	CA-C-N	-5.60	114.86	122.03
1	D	242	ILE	C-N-CA	-5.60	114.86	122.03
1	B	181	GLY	N-CA-C	5.56	119.32	111.42
1	B	186	LYS	N-CA-C	-5.53	104.88	111.69
1	B	87	LYS	CA-C-N	-5.53	112.93	119.84
1	B	87	LYS	C-N-CA	-5.53	112.93	119.84
1	B	201	GLN	N-CA-C	-5.47	100.88	109.25
1	C	190	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	D	190	ARG	CD-NE-CZ	5.35	131.89	124.40
1	C	208	ASP	CB-CA-C	-5.33	102.87	111.18
1	B	134	ILE	N-CA-C	-5.32	107.24	111.81
1	A	274	TYR	N-CA-C	5.25	117.84	109.96
1	A	201	GLN	N-CA-C	-5.24	100.55	108.67
1	B	249	LYS	N-CA-C	-5.17	105.55	111.14
1	B	265	MET	N-CA-C	-5.09	102.77	110.50
1	B	243	GLY	N-CA-C	-5.03	103.62	111.12

There are no chirality outliers.

There are no planarity outliers.

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	2124	0	2087	37	0
1	B	2281	0	2230	39	0
1	C	2151	0	2112	45	0
1	D	2281	0	2230	40	0
2	A	24	0	24	1	0
2	B	24	0	24	1	0
2	C	24	0	24	4	0
2	D	24	0	24	1	0
3	B	20	0	15	0	0
3	D	20	0	15	0	0
4	A	58	0	0	3	0
4	B	76	0	0	1	0
4	C	77	0	0	0	0
4	D	65	0	0	2	0
All	All	9249	0	8785	155	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 9.

All (155) 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:HG22	1:A:40:GLN:H	1.19	1.04
1:C:37:THR:HG21	1:C:120:ASP:OD2	1.60	1.01
1:A:37:THR:HG21	1:A:120:ASP:OD2	1.65	0.97
1:D:37:THR:HG22	1:D:39:PHE:H	1.27	0.96
1:A:37:THR:CG2	1:A:39:PHE:H	1.79	0.95
1:D:203:GLU:HG3	1:D:211:LEU:HD23	1.49	0.95
1:B:37:THR:HG21	1:B:120:ASP:OD2	1.66	0.95
1:C:37:THR:CG2	1:C:39:PHE:H	1.81	0.92
1:A:37:THR:HG23	1:A:39:PHE:H	1.33	0.91
1:B:202:GLY:O	1:B:203:GLU:HB2	1.70	0.91
1:B:37:THR:HG22	1:B:40:GLN:H	1.34	0.91
1:C:37:THR:HG22	1:C:40:GLN:H	1.39	0.86
1:C:37:THR:HG22	1:C:39:PHE:H	1.40	0.84
1:D:37:THR:CG2	1:D:39:PHE:H	1.91	0.83
1:D:37:THR:HG21	1:D:120:ASP:OD2	1.78	0.83
1:C:118:ASP:HB3	1:C:124:MET:HE1	1.60	0.81
1:D:37:THR:HG22	1:D:39:PHE:N	1.96	0.80
1:A:37:THR:HG22	1:A:40:GLN:N	1.97	0.80
1:B:203:GLU:HG3	1:B:211:LEU:HD23	1.68	0.74
1:D:202:GLY:O	1:D:203:GLU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:NH2	4:A:401:HOH:O	2.22	0.71
1:A:219:ILE:O	1:A:222:THR:HG22	1.91	0.71
1:C:37:THR:HG23	1:C:39:PHE:H	1.57	0.69
1:A:239:CYS:HB3	1:B:235:PRO:HB3	1.74	0.68
1:B:218:PHE:O	1:B:222:THR:HG23	1.93	0.68
1:C:239:CYS:HB3	1:D:235:PRO:HB3	1.76	0.67
1:C:169:THR:O	1:C:201:GLN:OE1	2.12	0.67
1:A:213:GLU:HG3	1:A:292:ILE:HD11	1.77	0.66
1:B:37:THR:CG2	1:B:39:PHE:H	2.09	0.66
1:B:64:GLN:OE1	2:B:301:S4M:HG1	1.95	0.66
1:C:202:GLY:O	1:C:203:GLU:HB2	1.94	0.65
1:C:97:GLY:HA3	1:C:124:MET:HE2	1.77	0.65
1:D:14:GLU:HG2	1:D:19:TRP:HH2	1.62	0.65
1:C:97:GLY:CA	1:C:124:MET:HE2	2.27	0.65
1:A:37:THR:HG22	1:A:39:PHE:H	1.60	0.65
1:A:50:LYS:HE2	4:A:458:HOH:O	1.96	0.64
1:C:218:PHE:O	1:C:222:THR:HG23	1.97	0.64
1:D:172:PRO:O	1:D:177:SER:HB2	1.97	0.64
1:D:133:GLN:HB2	4:D:442:HOH:O	1.97	0.63
1:C:37:THR:HG22	1:C:39:PHE:N	2.13	0.61
1:A:207:LEU:HD11	1:A:238:PRO:HB2	1.83	0.61
1:D:213:GLU:HG3	1:D:217:ARG:HH12	1.65	0.60
1:B:14:GLU:OE2	1:B:62:CYS:HA	2.00	0.60
1:C:213:GLU:HG2	1:C:292:ILE:CD1	2.31	0.60
1:C:59:LEU:HD12	2:C:301:S4M:HE3	1.83	0.59
1:D:37:THR:HB	1:D:40:GLN:O	2.03	0.58
1:D:289:ALA:O	1:D:292:ILE:HG12	2.03	0.58
1:B:37:THR:HG22	1:B:39:PHE:H	1.69	0.57
1:A:87:LYS:HE2	1:A:89:GLU:OE1	2.04	0.56
1:B:229:TYR:CZ	1:B:243:GLY:HA3	2.41	0.56
1:D:157:THR:O	1:D:190:ARG:NH2	2.34	0.56
1:D:202:GLY:O	1:D:203:GLU:CB	2.52	0.56
1:A:202:GLY:O	1:A:203:GLU:HB2	2.05	0.56
1:D:201:GLN:OE1	1:D:242:ILE:HD11	2.06	0.56
1:C:200:ASN:OD1	1:C:200:ASN:C	2.48	0.55
1:C:118:ASP:HB3	1:C:124:MET:CE	2.34	0.55
1:D:182:GLU:HG3	1:D:218:PHE:CD1	2.42	0.54
1:C:240:GLY:HA3	1:D:240:GLY:HA3	1.90	0.53
1:B:44:ILE:CD1	1:B:126:GLN:HB3	2.38	0.53
1:A:287:ARG:NH1	4:A:403:HOH:O	2.42	0.53
1:B:176:ALA:HA	1:B:179:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:GLU:HG2	1:D:214:LYS:N	2.25	0.52
1:C:213:GLU:CG	1:C:292:ILE:HD11	2.39	0.52
1:D:44:ILE:CD1	1:D:126:GLN:HB3	2.40	0.52
1:A:201:GLN:NE2	1:A:242:ILE:HD11	2.25	0.51
1:C:59:LEU:CD1	2:C:301:S4M:HE3	2.41	0.51
1:B:24:MET:HE3	1:B:63:ILE:HD12	1.93	0.50
1:C:213:GLU:HG2	1:C:292:ILE:HD11	1.93	0.50
1:C:66:THR:HG21	1:C:236:THR:HG21	1.92	0.50
1:C:37:THR:HG22	1:C:40:GLN:N	2.16	0.50
1:C:50:LYS:N	1:C:50:LYS:HD3	2.27	0.50
1:C:64:GLN:HB3	2:C:301:S4M:HB2	1.93	0.50
1:C:218:PHE:O	1:C:222:THR:CG2	2.60	0.49
1:C:202:GLY:O	1:C:203:GLU:CB	2.58	0.49
1:D:37:THR:HG23	1:D:38:LYS:N	2.28	0.49
1:D:181:GLY:O	1:D:185:TYR:HD2	1.94	0.49
1:A:37:THR:HG23	1:A:38:LYS:N	2.27	0.49
1:C:229:TYR:CZ	1:C:243:GLY:HA3	2.48	0.48
1:D:13:ARG:NE	1:D:15:GLU:OE2	2.38	0.48
1:B:14:GLU:OE2	1:B:63:ILE:N	2.38	0.48
1:A:225:ALA:HB1	1:A:251:ALA:HA	1.96	0.48
1:C:11:TRP:CE2	1:C:27:ARG:HG3	2.48	0.48
1:A:40:GLN:HG3	1:A:59:LEU:HD22	1.95	0.48
1:B:202:GLY:O	1:B:203:GLU:CB	2.42	0.48
1:A:213:GLU:HG3	1:A:292:ILE:CD1	2.43	0.48
1:D:86:PRO:O	1:D:260:ARG:HD3	2.14	0.48
1:A:151:LEU:HD12	1:A:184:PHE:HB2	1.94	0.47
1:D:146:ARG:HG3	4:D:402:HOH:O	2.13	0.47
1:B:6:LEU:O	1:B:7:ILE:HD13	2.14	0.47
1:A:273:TYR:CD1	1:B:286:PRO:HB3	2.49	0.47
1:B:37:THR:HG23	1:B:39:PHE:H	1.78	0.47
1:B:37:THR:CG2	1:B:120:ASP:OD2	2.51	0.47
1:A:206:TRP:CD2	1:B:235:PRO:HG3	2.50	0.47
1:D:37:THR:CG2	1:D:38:LYS:N	2.75	0.47
1:D:167:ILE:HG22	1:D:169:THR:HG23	1.97	0.47
1:B:6:LEU:HD22	1:B:28:VAL:HG21	1.96	0.46
1:C:151:LEU:CD1	1:C:184:PHE:HB2	2.45	0.46
1:A:287:ARG:HH11	1:A:287:ARG:HG2	1.80	0.46
1:B:179:LEU:HA	1:B:184:PHE:CD2	2.51	0.46
1:D:129:GLN:HG2	1:D:130:HIS:NE2	2.30	0.46
1:A:37:THR:CG2	1:A:39:PHE:N	2.63	0.46
1:B:178:LYS:C	1:B:180:PHE:H	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LEU:O	1:D:215:MET:HG3	2.17	0.45
1:A:133:GLN:H	1:A:133:GLN:HG2	1.45	0.45
1:B:66:THR:HG21	1:B:236:THR:HG21	1.99	0.45
1:A:200:ASN:HD21	1:A:245:LEU:HD12	1.81	0.45
1:C:86:PRO:O	1:C:260:ARG:HD3	2.17	0.45
1:A:86:PRO:O	1:A:260:ARG:HD3	2.17	0.44
1:A:44:ILE:CD1	1:A:126:GLN:HB3	2.47	0.44
1:A:70:GLU:HG2	1:A:134:ILE:HD11	1.98	0.44
1:A:273:TYR:CE1	1:B:286:PRO:HG3	2.53	0.44
1:C:213:GLU:CG	1:C:292:ILE:CD1	2.95	0.44
1:D:14:GLU:HG2	1:D:19:TRP:CH2	2.48	0.44
1:B:218:PHE:C	1:B:218:PHE:CD1	2.96	0.44
2:C:301:S4M:HE2	2:C:301:S4M:HB1	1.88	0.43
1:A:200:ASN:OD1	1:A:200:ASN:C	2.61	0.43
1:C:213:GLU:HG2	1:C:292:ILE:HD13	2.00	0.43
1:B:16:ASN:HB3	1:B:19:TRP:CE2	2.54	0.43
1:D:37:THR:HG22	1:D:40:GLN:H	1.83	0.43
1:C:20:PRO:HG2	1:D:50:LYS:CB	2.49	0.43
1:B:32:LEU:HD12	1:B:44:ILE:HG22	2.01	0.43
1:D:203:GLU:HB3	1:D:208:ASP:HB2	2.00	0.43
1:B:22:GLN:NE2	4:B:406:HOH:O	2.52	0.43
1:A:276:SER:O	1:A:280:LYS:HG3	2.19	0.43
1:A:73:TYR:CE2	2:A:301:S4M:HA2	2.54	0.42
1:B:24:MET:HE3	1:B:63:ILE:CD1	2.49	0.42
1:A:44:ILE:HD11	1:A:57:MET:HE2	2.01	0.42
1:A:37:THR:HG22	1:A:39:PHE:N	2.29	0.42
1:A:53:TRP:CZ3	1:A:68:TYR:HD2	2.36	0.42
1:B:211:LEU:O	1:B:215:MET:HG3	2.18	0.42
1:B:73:TYR:OH	1:B:201:GLN:HG2	2.20	0.42
2:D:301:S4M:HE2	2:D:301:S4M:HB1	1.76	0.42
1:C:213:GLU:HG3	1:C:292:ILE:HD11	2.01	0.42
1:C:20:PRO:HG2	1:D:50:LYS:HB2	2.02	0.41
1:B:118:ASP:O	1:B:147:VAL:HA	2.20	0.41
1:C:97:GLY:HA2	1:C:124:MET:HE2	2.00	0.41
1:B:200:ASN:OD1	1:B:200:ASN:C	2.63	0.41
1:B:269:LYS:HE3	1:B:269:LYS:HB3	1.90	0.41
1:B:203:GLU:HG3	1:B:211:LEU:CD2	2.43	0.41
1:C:64:GLN:C	1:C:65:VAL:HG23	2.45	0.41
1:D:24:MET:HE3	1:D:63:ILE:HD12	2.02	0.41
1:B:225:ALA:HB1	1:B:251:ALA:HA	2.03	0.41
1:D:218:PHE:CD1	1:D:218:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:VAL:HG11	1:C:237:TYR:CD2	2.56	0.41
1:D:124:MET:HE3	1:D:145:VAL:CG1	2.51	0.41
1:D:193:LYS:HB3	1:D:194:PRO:HD2	2.02	0.41
1:C:151:LEU:HD11	1:C:184:PHE:HB2	2.03	0.40
1:C:157:THR:O	1:C:190:ARG:NH2	2.27	0.40
1:C:182:GLU:HA	1:C:218:PHE:HZ	1.85	0.40
1:B:5:GLU:N	1:B:34:ASP:OD2	2.54	0.40
1:C:42:LEU:HD13	1:C:59:LEU:HD21	2.02	0.40
1:D:53:TRP:CZ3	1:D:236:THR:HG23	2.55	0.40
1:C:37:THR:CG2	1:C:40:GLN:H	2.22	0.40
1:D:285:LEU:O	1:D:286:PRO:C	2.62	0.40
1:C:128:LYS:HA	1:C:135:SER:OG	2.21	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	263/304 (86%)	253 (96%)	10 (4%)	0	100	100
1	B	288/304 (95%)	276 (96%)	12 (4%)	0	100	100
1	C	267/304 (88%)	257 (96%)	10 (4%)	0	100	100
1	D	288/304 (95%)	276 (96%)	11 (4%)	1 (0%)	36	28
All	All	1106/1216 (91%)	1062 (96%)	43 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	203	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/262 (89%)	228 (97%)	6 (3%)	40	33
1	B	250/262 (95%)	239 (96%)	11 (4%)	25	15
1	C	237/262 (90%)	226 (95%)	11 (5%)	24	13
1	D	250/262 (95%)	229 (92%)	21 (8%)	10	3
All	All	971/1048 (93%)	922 (95%)	49 (5%)	22	11

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	77	LEU
1	A	124	MET
1	A	133	GLN
1	A	170	THR
1	A	221	GLU
1	B	37	THR
1	B	65	VAL
1	B	77	LEU
1	B	87	LYS
1	B	124	MET
1	B	125	GLU
1	B	151	LEU
1	B	179	LEU
1	B	186	LYS
1	B	218	PHE
1	B	242	ILE
1	C	37	THR
1	C	50	LYS
1	C	77	LEU
1	C	124	MET
1	C	129	GLN
1	C	169	THR
1	C	170	THR

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Mol	Chain	Res	Type
1	C	182	GLU
1	C	221	GLU
1	C	222	THR
1	C	242	ILE
1	D	5	GLU
1	D	6	LEU
1	D	7	ILE
1	D	19	TRP
1	D	37	THR
1	D	40	GLN
1	D	50	LYS
1	D	65	VAL
1	D	77	LEU
1	D	87	LYS
1	D	124	MET
1	D	125	GLU
1	D	133	GLN
1	D	159	ASP
1	D	177	SER
1	D	201	GLN
1	D	213	GLU
1	D	220	ARG
1	D	222	THR
1	D	250	LYS
1	D	290	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	233	HIS
1	B	22	GLN
1	B	113	HIS
1	B	129	GLN
1	B	228	GLN
1	C	22	GLN
1	C	113	HIS
1	C	201	GLN
1	D	22	GLN
1	D	126	GLN
1	D	160	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	A	301	-	25,26,26	0.77	1 (4%)	33,37,37	1.29	3 (9%)
3	4JW	D	302	-	22,22,22	1.25	2 (9%)	25,30,30	1.35	1 (4%)
2	S4M	D	301	-	25,26,26	0.81	1 (4%)	33,37,37	1.46	6 (18%)
2	S4M	C	301	-	25,26,26	0.68	0	33,37,37	1.15	4 (12%)
2	S4M	B	301	-	25,26,26	0.52	0	33,37,37	1.28	3 (9%)
3	4JW	B	302	-	22,22,22	0.99	1 (4%)	25,30,30	1.29	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	S4M	A	301	-	-	5/12/28/28	0/3/3/3
3	4JW	D	302	-	-	0/11/21/21	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S4M	D	301	-	-	4/12/28/28	0/3/3/3
2	S4M	C	301	-	-	4/12/28/28	0/3/3/3
2	S4M	B	301	-	-	3/12/28/28	0/3/3/3
3	4JW	B	302	-	-	0/11/21/21	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	4JW	C1-N4	3.99	1.41	1.35
3	B	302	4JW	C1-N4	3.17	1.40	1.35
3	D	302	4JW	O5-C8	2.76	1.40	1.37
2	D	301	S4M	C6-N6	2.50	1.40	1.34
2	A	301	S4M	C6-N6	2.34	1.40	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	4JW	C7-O5-C8	-4.74	105.82	115.29
2	A	301	S4M	CG-SD-C5'	-4.33	92.85	103.43
2	B	301	S4M	O4'-C1'-C2'	-3.53	99.07	106.62
2	D	301	S4M	CG-SD-C5'	-3.28	95.40	103.43
3	B	302	4JW	O9-C1-N4	3.26	125.60	121.48
2	B	301	S4M	O4'-C1'-N9	3.21	114.25	108.09
2	B	301	S4M	CG-SD-C5'	-3.10	95.85	103.43
2	C	301	S4M	N9-C8-N7	-2.91	109.81	113.94
3	B	302	4JW	C7-O5-C8	-2.82	109.66	115.29
2	D	301	S4M	O4'-C1'-N9	2.59	113.07	108.09
2	D	301	S4M	C4'-O4'-C1'	-2.49	103.97	109.47
3	B	302	4JW	O5-C8-C6	-2.49	119.80	122.02
2	D	301	S4M	N6-C6-N1	2.47	123.89	118.38
2	A	301	S4M	C4'-O4'-C1'	-2.44	104.07	109.47
2	C	301	S4M	O4'-C1'-C2'	-2.37	101.55	106.62
2	C	301	S4M	C4-N9-C8	2.36	108.21	105.74
2	D	301	S4M	C5-C6-N6	-2.29	117.61	123.29
2	D	301	S4M	O4'-C4'-C5'	2.21	114.45	108.88
2	A	301	S4M	O4'-C1'-N9	2.15	112.22	108.09
2	C	301	S4M	C5-N7-C8	2.12	106.78	103.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	S4M	CA-CB-CG-SD
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	CA-CB-CG-SD
2	D	301	S4M	O4'-C4'-C5'-SD
2	D	301	S4M	C3'-C4'-C5'-SD
2	C	301	S4M	N-CA-CB-CG
2	A	301	S4M	N-CA-CB-CG
2	B	301	S4M	N-CA-CB-CG
2	A	301	S4M	CB-CG-SD-C5'
2	D	301	S4M	CB-CG-SD-C5'

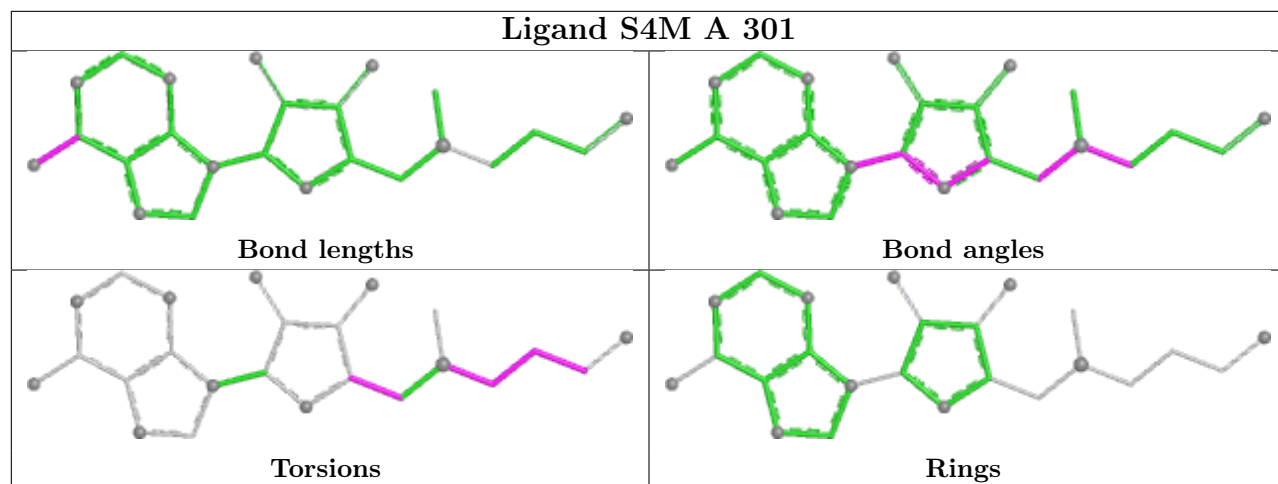
There are no ring outliers.

4 monomers are involved in 7 short contacts:

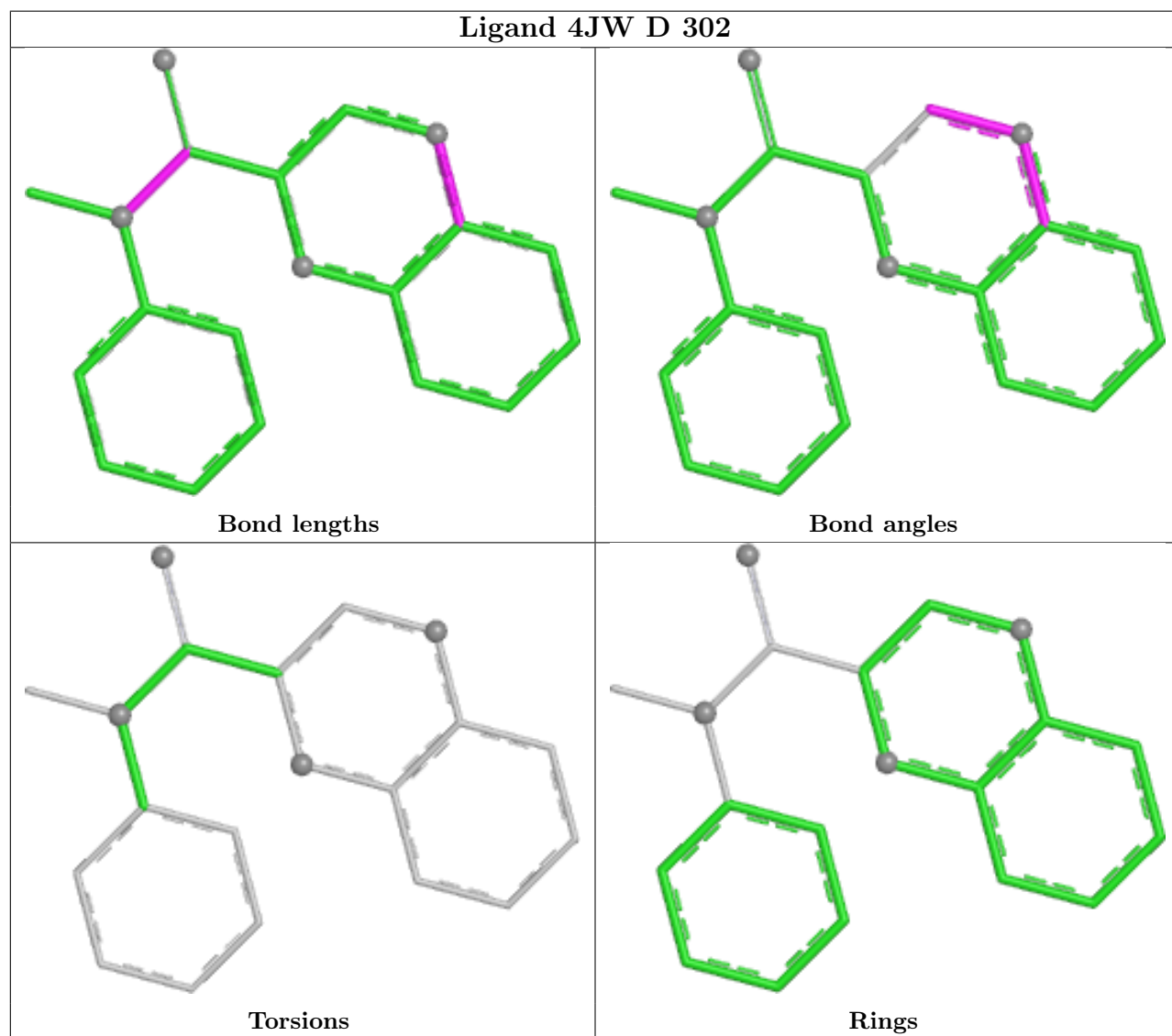
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	S4M	1	0
2	D	301	S4M	1	0
2	C	301	S4M	4	0
2	B	301	S4M	1	0

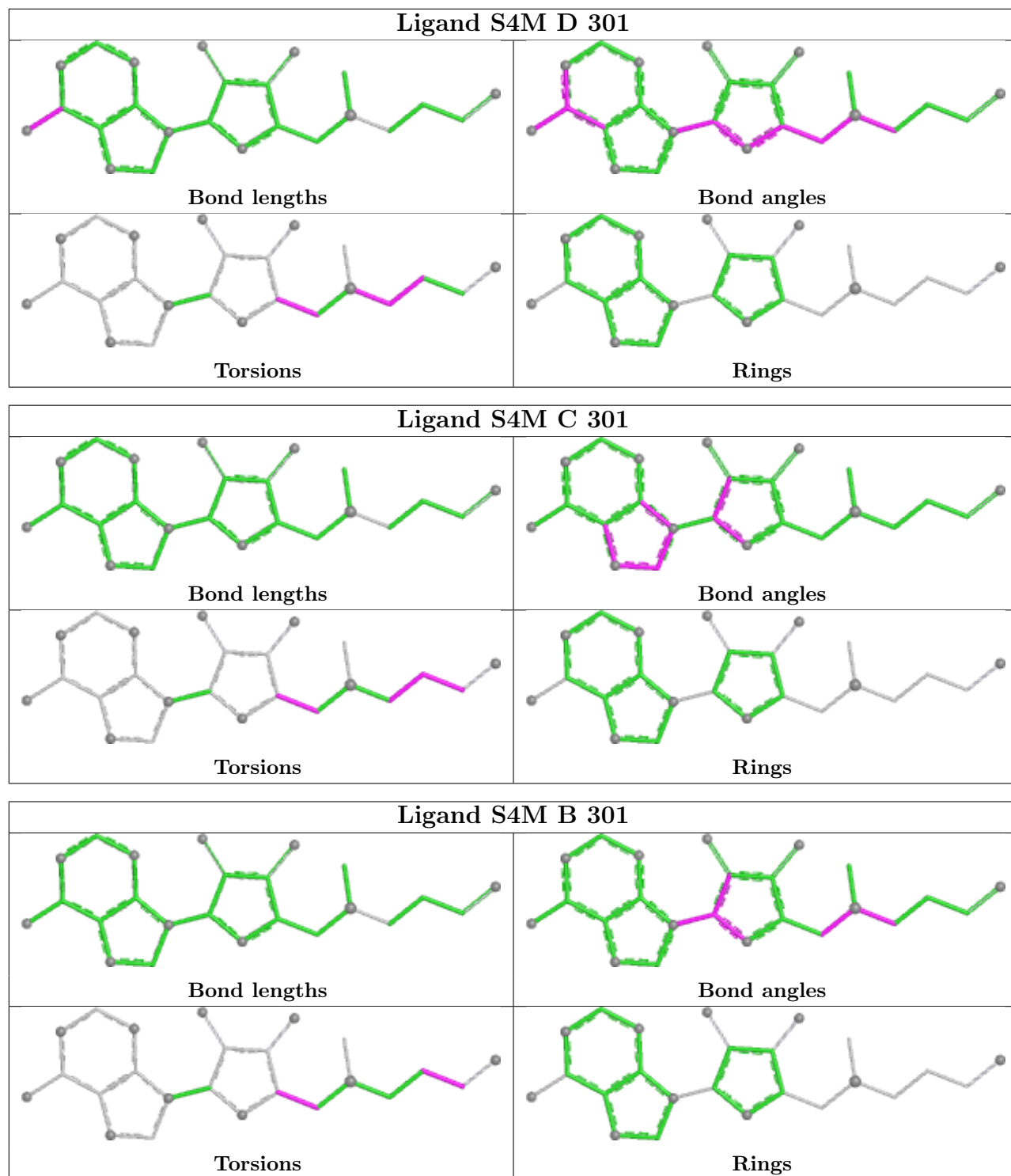
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

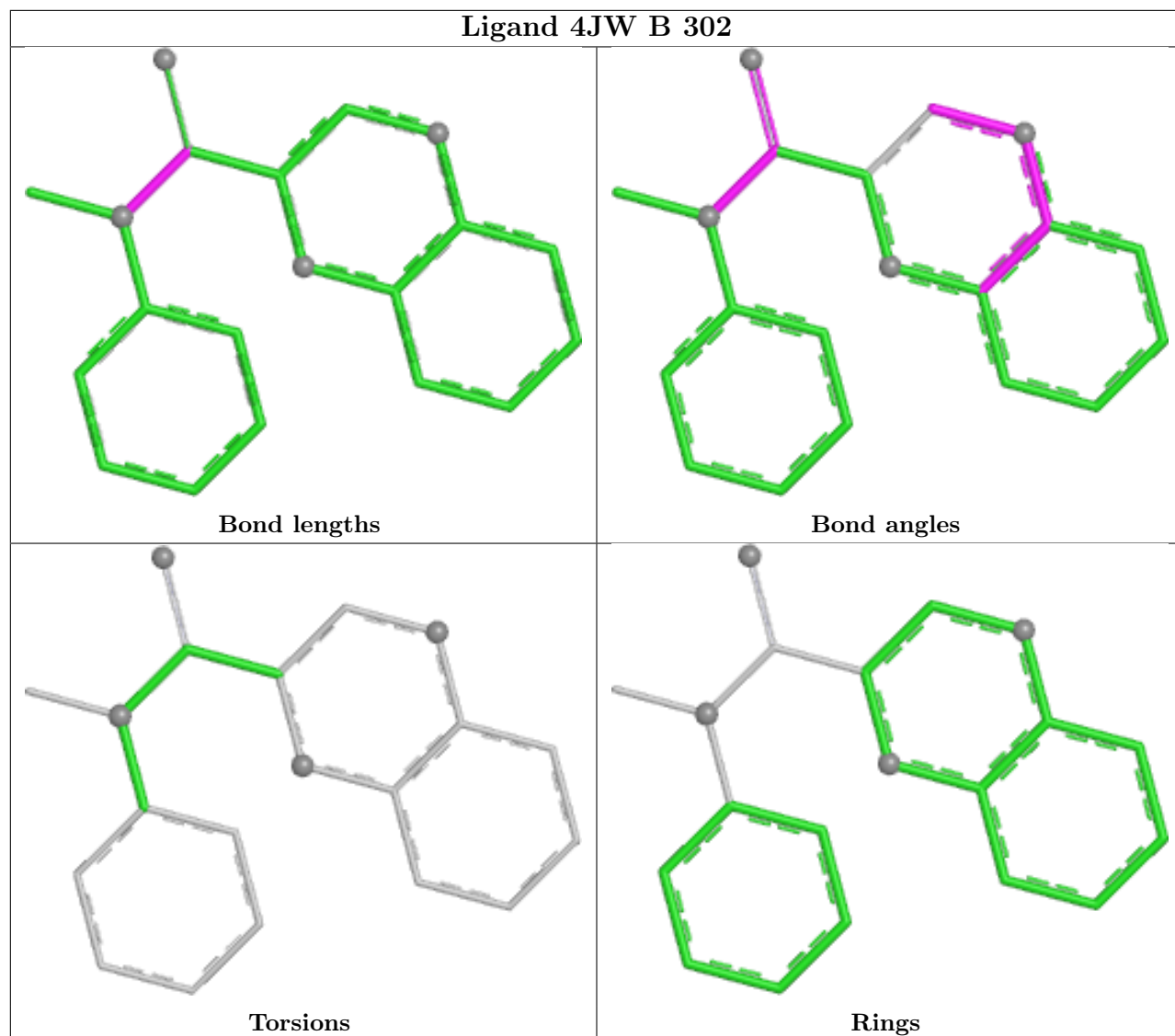
Ligand S4M A 301



Ligand 4JW D 302







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	269/304 (88%)	0.25	6 (2%) 62 69	14, 27, 44, 57	0
1	B	290/304 (95%)	0.34	18 (6%) 26 31	15, 27, 58, 85	0
1	C	273/304 (89%)	0.17	10 (3%) 45 52	12, 26, 45, 67	0
1	D	290/304 (95%)	0.36	21 (7%) 21 25	16, 27, 53, 73	0
All	All	1122/1216 (92%)	0.28	55 (4%) 35 41	12, 27, 49, 85	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	ILE	6.2
1	D	183	ALA	6.0
1	D	181	GLY	6.0
1	B	181	GLY	5.8
1	B	173	ALA	4.5
1	D	218	PHE	4.4
1	B	180	PHE	4.4
1	C	9	GLY	4.2
1	B	172	PRO	3.9
1	B	218	PHE	3.7
1	A	183	ALA	3.7
1	A	218	PHE	3.6
1	D	179	LEU	3.6
1	B	19	TRP	3.5
1	D	176	ALA	3.5
1	D	182	GLU	3.4
1	B	176	ALA	3.4
1	B	175	PRO	3.4
1	D	173	ALA	3.4
1	B	183	ALA	3.3
1	B	170	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	10	GLY	3.0
1	B	179	LEU	3.0
1	C	170	THR	3.0
1	D	170	THR	2.9
1	C	169	THR	2.8
1	D	18	GLN	2.8
1	A	202	GLY	2.8
1	C	10	GLY	2.8
1	A	237	TYR	2.7
1	C	8	SER	2.7
1	D	180	PHE	2.7
1	B	18	GLN	2.7
1	D	171	ASP	2.7
1	A	294	ASN	2.7
1	D	172	PRO	2.5
1	B	35	ALA	2.5
1	D	222	THR	2.5
1	D	132	PRO	2.5
1	C	237	TYR	2.5
1	B	294	ASN	2.5
1	B	182	GLU	2.5
1	B	171	ASP	2.4
1	C	294	ASN	2.4
1	D	19	TRP	2.3
1	B	222	THR	2.3
1	D	151	LEU	2.3
1	B	201	GLN	2.2
1	C	201	GLN	2.2
1	D	174	GLY	2.2
1	D	178	LYS	2.2
1	D	294	ASN	2.1
1	D	35	ALA	2.1
1	C	133	GLN	2.1
1	D	169	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

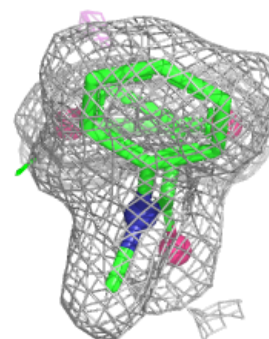
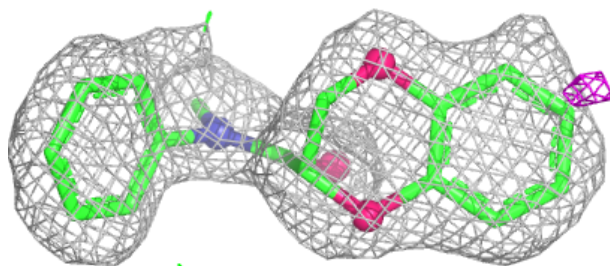
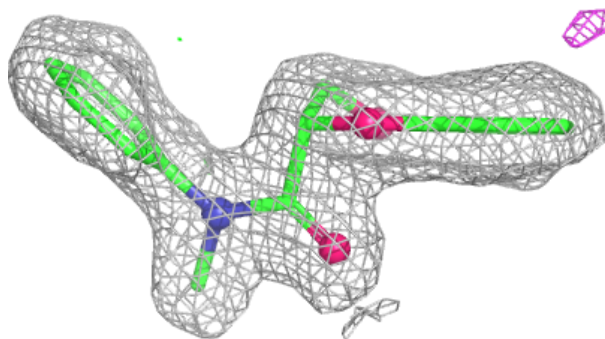
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	4JW	B	302	20/20	0.90	0.09	28,35,37,38	0
2	S4M	B	301	24/24	0.91	0.09	26,28,37,44	0
2	S4M	D	301	24/24	0.92	0.09	24,30,47,57	0
2	S4M	C	301	24/24	0.92	0.09	25,29,45,55	0
3	4JW	D	302	20/20	0.92	0.08	26,31,34,34	0
2	S4M	A	301	24/24	0.93	0.08	23,26,33,43	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.

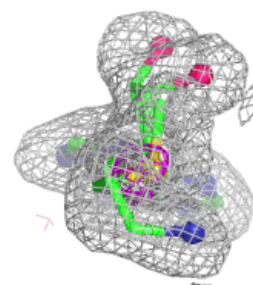
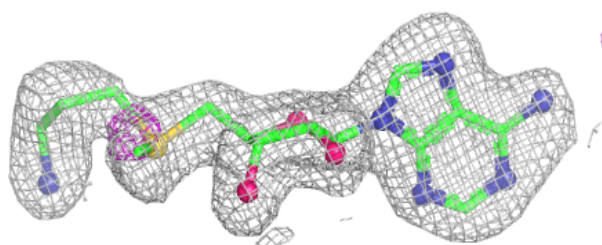
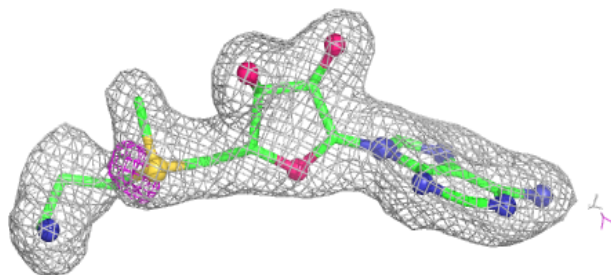
Electron density around 4JW B 302:

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

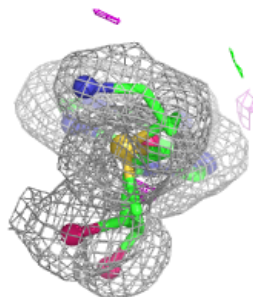
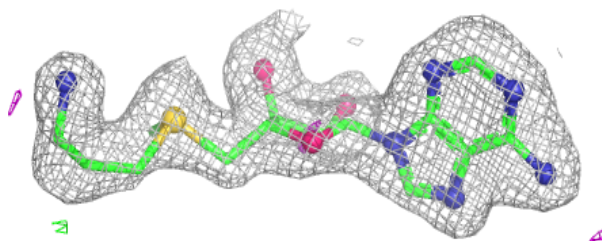
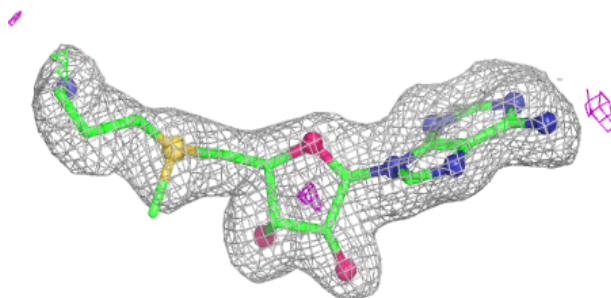


Electron density around S4M B 301:

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

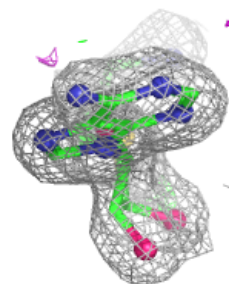
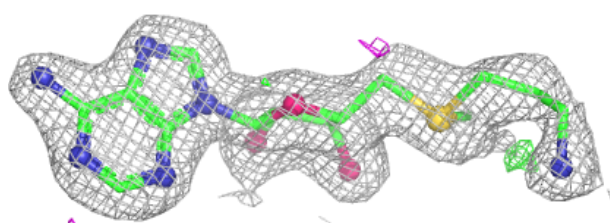
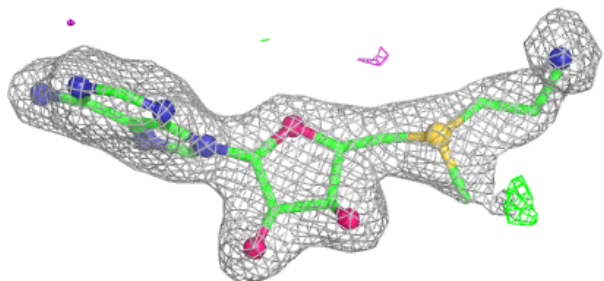
**Electron density around S4M D 301:**

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

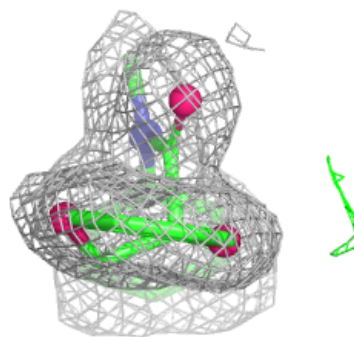
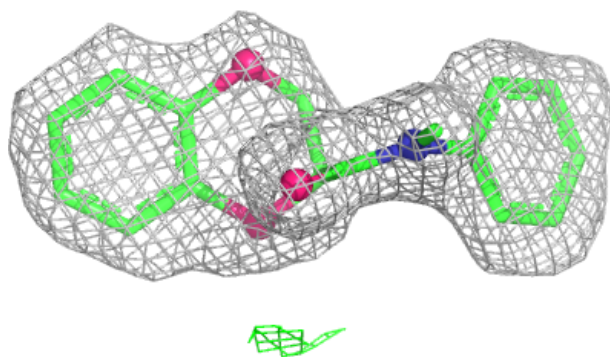
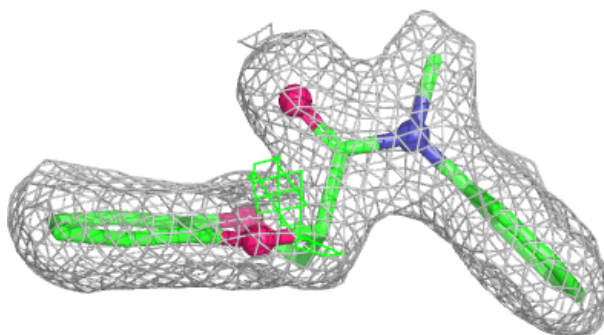


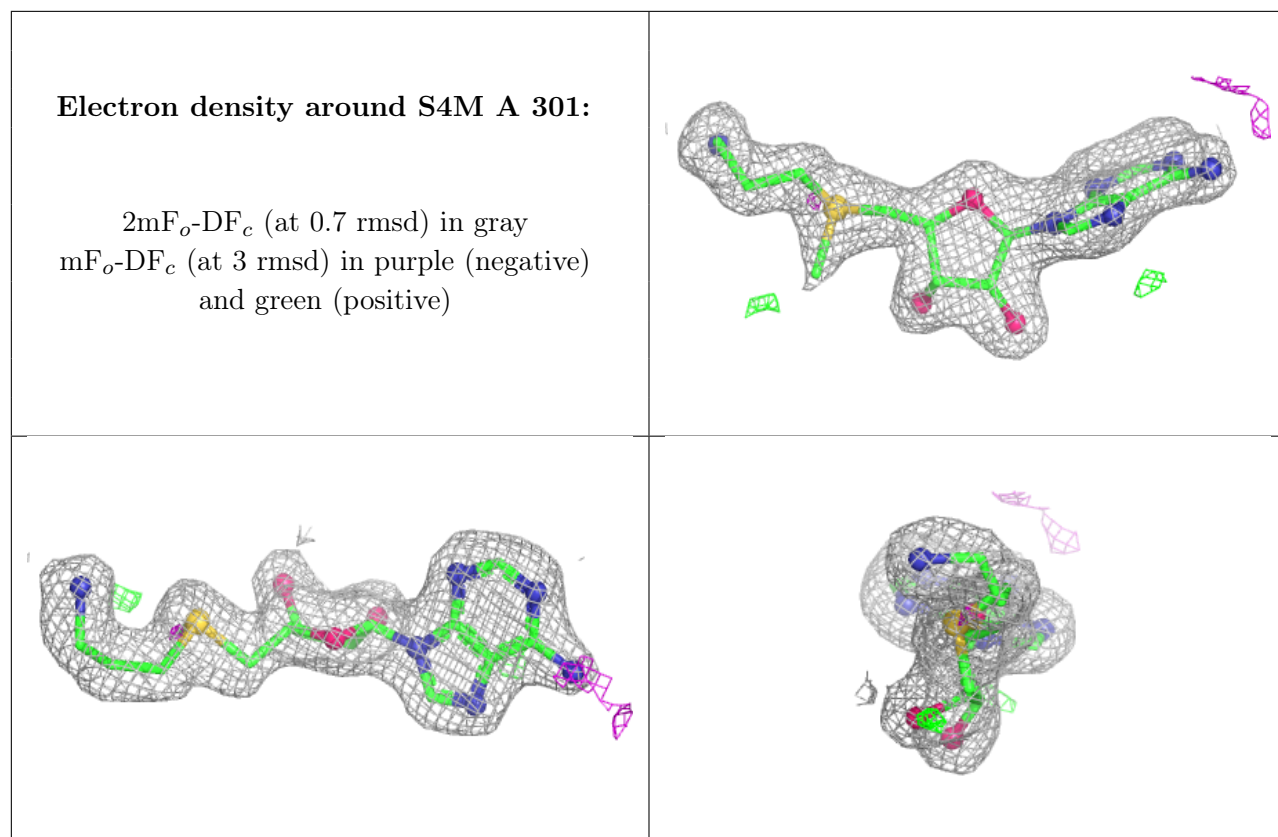
Electron density around S4M C 301:

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

**Electron density around 4JW 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.