



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:32 AM UTC

PDB ID : 6O65 / pdb_00006o65
Title : Crystal Structure of Arabidopsis thaliana Spermidine Synthase isoform 1 (At-SPDS1) in complex with decarboxylated S-adenosylmethionine and cyclohexylamine
Authors : Sekula, B.; Dauter, Z.
Deposited on : 2019-03-05
Resolution : 1.80 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

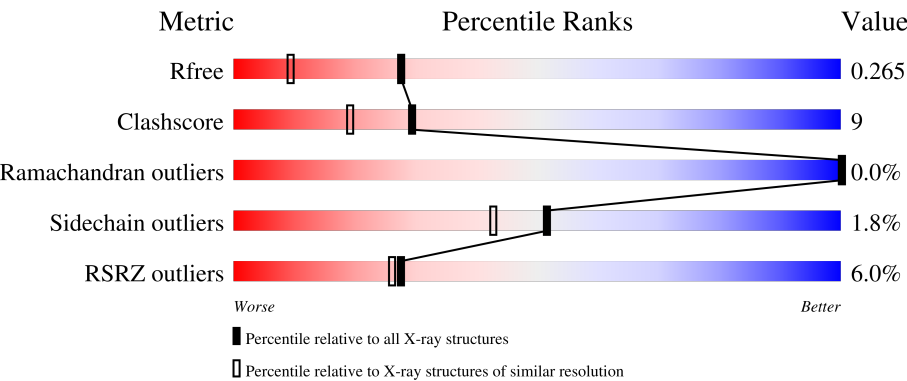
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	5% 78% 14% • 5%
1	B	304	10% 72% 22% • •
1	C	304	6% 74% 21% • •
1	D	304	10% 74% 22% • •

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Mol	Chain	Length	Quality of chain
1	E	304	
1	F	304	
1	G	304	
1	H	304	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	E	403	-	-	X	-
6	EDO	G	404	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20468 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	2	0
			2240	1444	361	420	15			
1	B	294	Total	C	N	O	S	0	0	0
			2265	1456	367	427	15			
1	C	291	Total	C	N	O	S	0	3	0
			2259	1454	362	428	15			
1	D	293	Total	C	N	O	S	0	3	0
			2274	1465	366	428	15			
1	E	290	Total	C	N	O	S	0	4	0
			2259	1457	361	426	15			
1	F	293	Total	C	N	O	S	0	1	0
			2262	1456	365	425	16			
1	G	289	Total	C	N	O	S	0	2	0
			2239	1446	359	419	15			
1	H	294	Total	C	N	O	S	0	2	0
			2277	1464	367	431	15			

There are 24 discrepancies between the modelled and reference sequences:

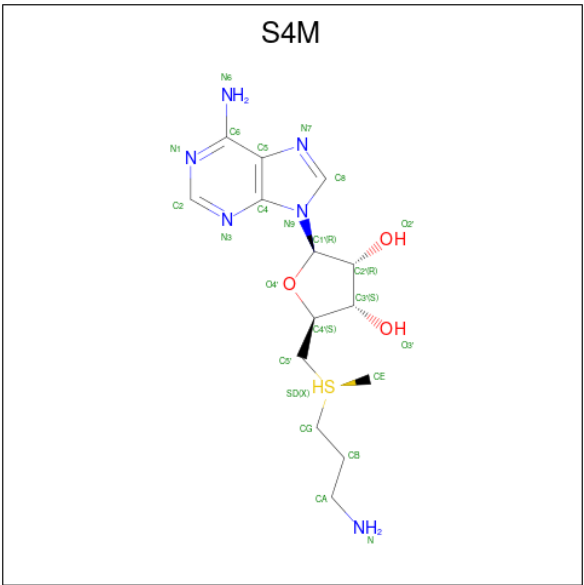
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	SER	-	expression tag	UNP Q9ZUB3
A	32	ASN	-	expression tag	UNP Q9ZUB3
A	33	ALA	-	expression tag	UNP Q9ZUB3
B	31	SER	-	expression tag	UNP Q9ZUB3
B	32	ASN	-	expression tag	UNP Q9ZUB3
B	33	ALA	-	expression tag	UNP Q9ZUB3
C	31	SER	-	expression tag	UNP Q9ZUB3
C	32	ASN	-	expression tag	UNP Q9ZUB3
C	33	ALA	-	expression tag	UNP Q9ZUB3
D	31	SER	-	expression tag	UNP Q9ZUB3
D	32	ASN	-	expression tag	UNP Q9ZUB3
D	33	ALA	-	expression tag	UNP Q9ZUB3
E	31	SER	-	expression tag	UNP Q9ZUB3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	32	ASN	-	expression tag	UNP Q9ZUB3
E	33	ALA	-	expression tag	UNP Q9ZUB3
F	31	SER	-	expression tag	UNP Q9ZUB3
F	32	ASN	-	expression tag	UNP Q9ZUB3
F	33	ALA	-	expression tag	UNP Q9ZUB3
G	31	SER	-	expression tag	UNP Q9ZUB3
G	32	ASN	-	expression tag	UNP Q9ZUB3
G	33	ALA	-	expression tag	UNP Q9ZUB3
H	31	SER	-	expression tag	UNP Q9ZUB3
H	32	ASN	-	expression tag	UNP Q9ZUB3
H	33	ALA	-	expression tag	UNP Q9ZUB3

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



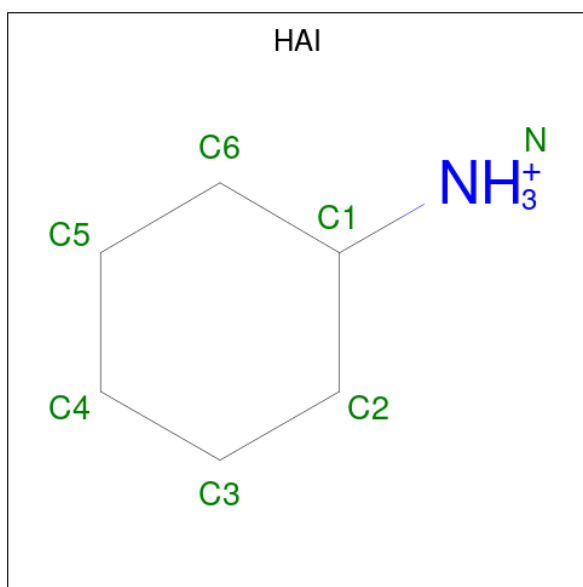
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	D	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	E	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

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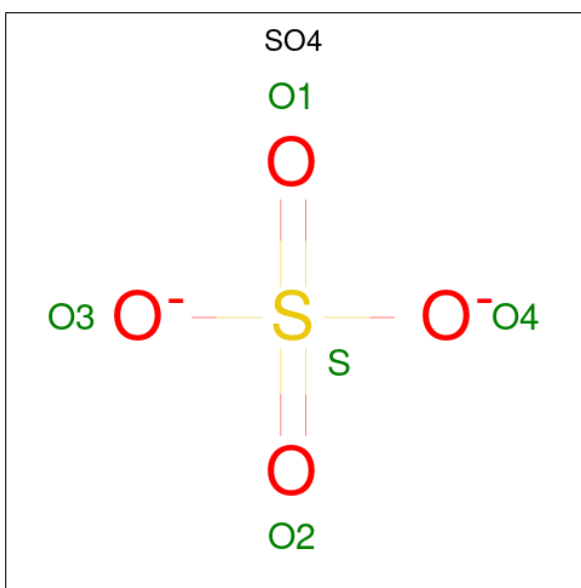
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	G	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	H	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is CYCLOHEXYLAMMONIUM ION (CCD ID: HAI) (formula: C₆H₁₄N).



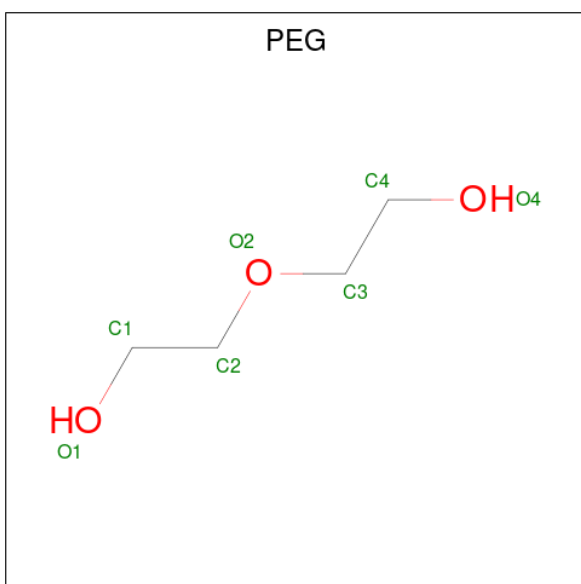
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			7	6	1		
3	B	1	Total	C	N	0	0
			7	6	1		
3	C	1	Total	C	N	0	0
			7	6	1		
3	D	1	Total	C	N	0	0
			7	6	1		
3	E	1	Total	C	N	0	0
			7	6	1		
3	F	1	Total	C	N	0	0
			7	6	1		
3	G	1	Total	C	N	0	0
			7	6	1		
3	H	1	Total	C	N	0	0
			7	6	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



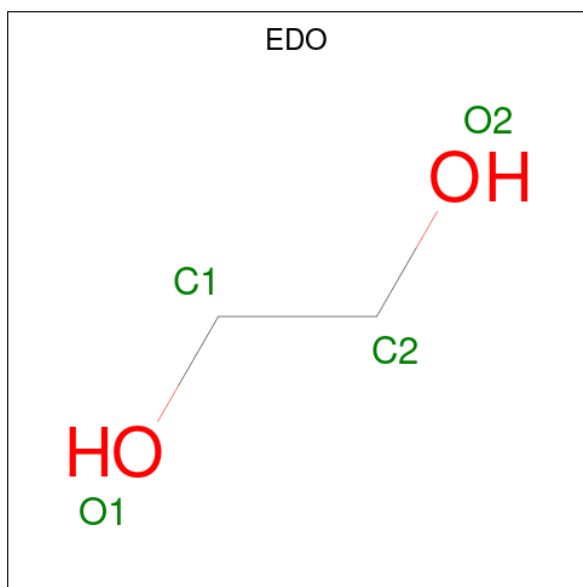
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	253	Total	O	0	0
			253	253		
7	B	240	Total	O	0	0
			240	240		
7	C	221	Total	O	0	0
			221	221		
7	D	233	Total	O	0	0
			233	233		
7	E	258	Total	O	0	0
			258	258		
7	F	283	Total	O	0	0
			283	283		

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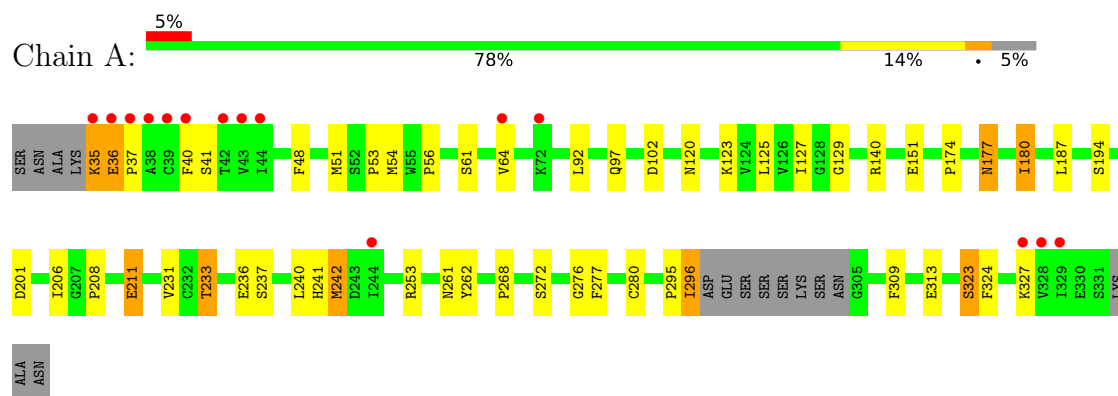
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	306	Total 306	O 306	0	0
7	H	309	Total 309	O 309	0	0

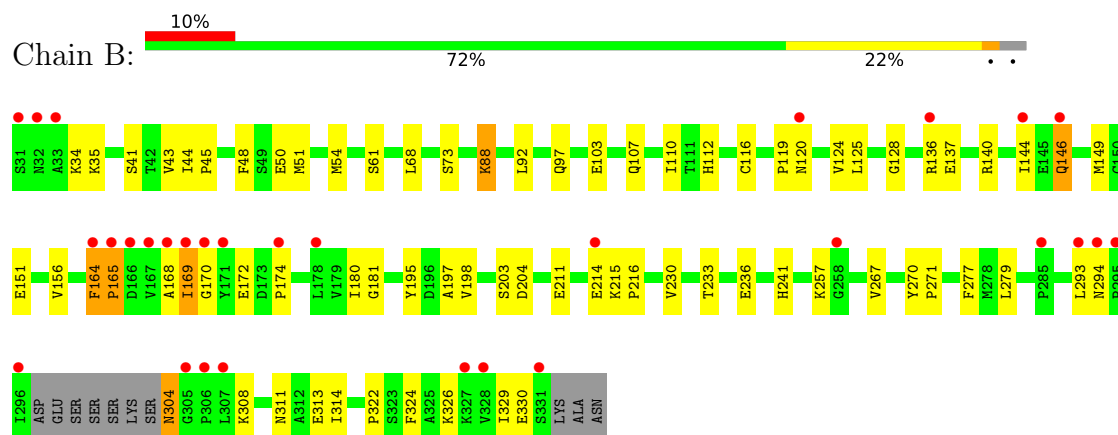
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

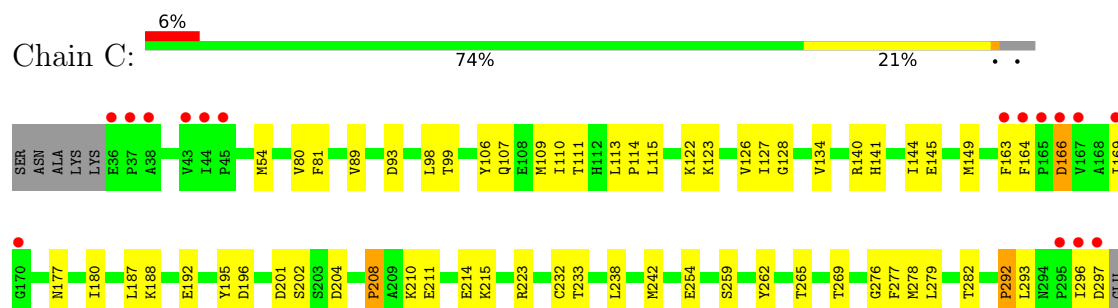
• Molecule 1: Spermidine synthase 1

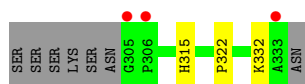


• Molecule 1: Spermidine synthase 1

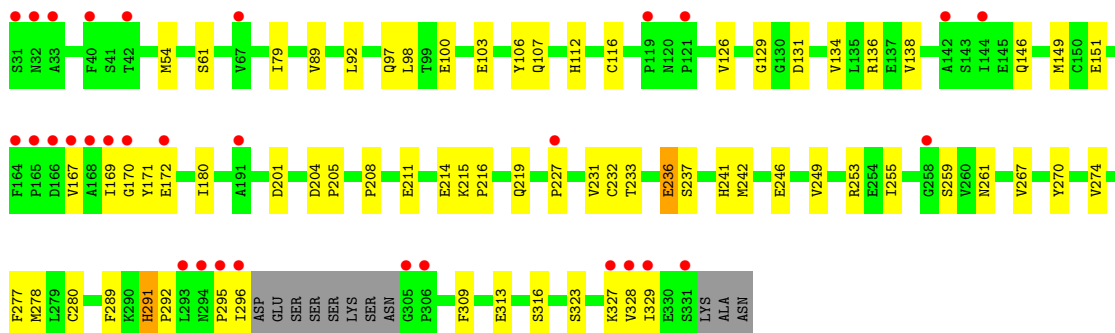
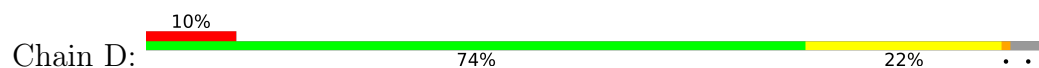


• Molecule 1: Spermidine synthase 1

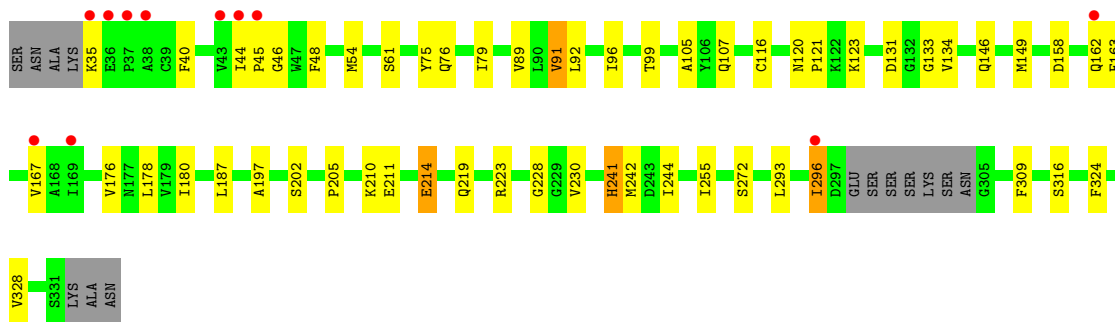
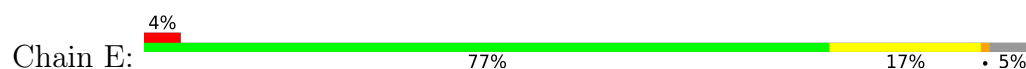




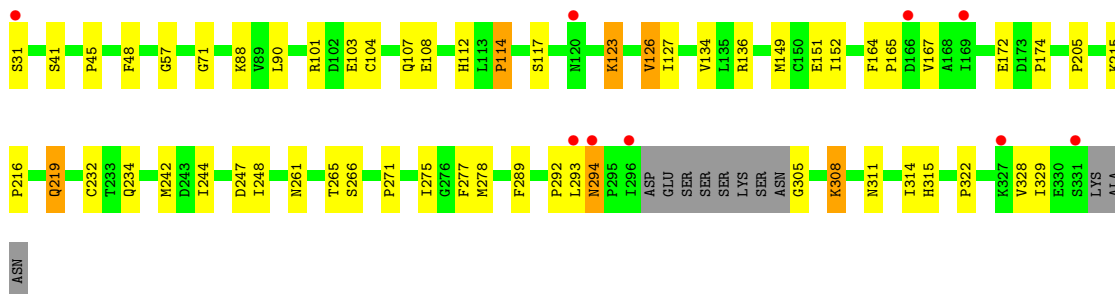
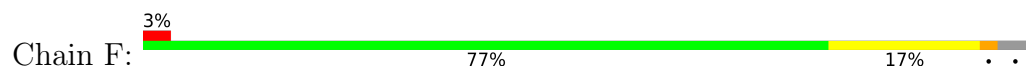
• Molecule 1: Spermidine synthase 1



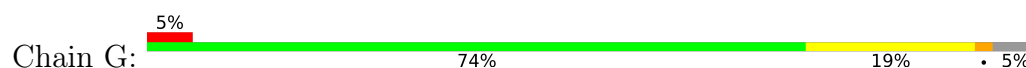
• Molecule 1: Spermidine synthase 1



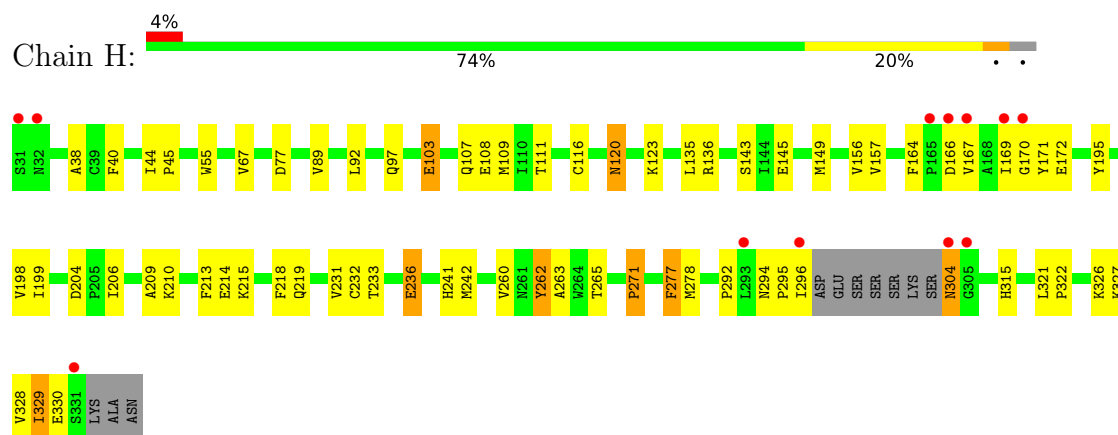
• Molecule 1: Spermidine synthase 1



• Molecule 1: Spermidine synthase 1



- Molecule 1: Spermidine synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.20Å 107.56Å 142.42Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	47.60 – 1.80 47.60 – 1.80	Depositor EDS
% Data completeness (in resolution range)	81.6 (47.60-1.80) 82.1 (47.60-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.219 , 0.261 0.225 , 0.265	Depositor DCC
R_{free} test set	1911 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtrriage
Anisotropy	0.451	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20468	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.56 % 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 4.2128e-04. 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: HAI, S4M, EDO, SO4, PEG

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	5/2302 (0.2%)	1.42	4/3126 (0.1%)
1	B	1.22	4/2321 (0.2%)	1.41	6/3152 (0.2%)
1	C	1.23	8/2324 (0.3%)	1.44	13/3157 (0.4%)
1	D	1.27	9/2339 (0.4%)	1.42	6/3176 (0.2%)
1	E	1.39	16/2327 (0.7%)	1.46	4/3160 (0.1%)
1	F	1.39	14/2321 (0.6%)	1.46	13/3151 (0.4%)
1	G	1.42	17/2301 (0.7%)	1.50	19/3126 (0.6%)
1	H	1.42	15/2339 (0.6%)	1.48	13/3176 (0.4%)
All	All	1.32	88/18574 (0.5%)	1.45	78/25224 (0.3%)

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	91	VAL	C-O	-8.03	1.15	1.24
1	G	181	GLY	C-O	-7.11	1.16	1.23
1	F	126	VAL	C-O	7.02	1.31	1.24
1	G	255[A]	ILE	C-O	6.87	1.31	1.23
1	G	255[B]	ILE	C-O	6.87	1.31	1.23
1	G	165	PRO	C-O	-6.84	1.15	1.23
1	E	176	VAL	C-O	-6.82	1.16	1.24
1	G	241	HIS	CE1-NE2	6.80	1.39	1.32
1	G	323	SER	C-O	-6.80	1.16	1.24
1	H	262	TYR	C-O	6.77	1.32	1.24
1	D	89	VAL	C-O	6.72	1.31	1.24
1	B	44	ILE	N-CA	6.70	1.51	1.45
1	G	50	GLU	C-O	-6.68	1.14	1.23
1	E	316	SER	C-O	6.63	1.31	1.24
1	H	206	ILE	C-O	6.57	1.31	1.23
1	F	244	ILE	C-O	6.52	1.31	1.24
1	E	180	ILE	C-O	6.49	1.31	1.24
1	E	241	HIS	CE1-NE2	6.47	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	205	PRO	C-O	-6.40	1.15	1.24
1	F	277	PHE	C-O	6.38	1.31	1.23
1	D	208	PRO	C-O	-6.37	1.15	1.24
1	G	174	PRO	C-O	-6.30	1.15	1.24
1	F	271	PRO	C-O	6.29	1.31	1.23
1	D	79	ILE	C-O	6.24	1.30	1.24
1	D	61	SER	C-O	6.18	1.31	1.24
1	A	233	THR	C-O	6.15	1.31	1.23
1	C	208	PRO	C-O	-6.14	1.16	1.24
1	F	248	ILE	C-O	6.13	1.31	1.24
1	H	89	VAL	C-O	6.06	1.30	1.24
1	H	236	GLU	C-O	6.06	1.31	1.24
1	H	199	ILE	C-O	6.04	1.30	1.24
1	H	109	MET	C-O	6.03	1.31	1.24
1	G	310	TYR	C-O	5.99	1.30	1.23
1	F	108	GLU	C-O	5.96	1.31	1.24
1	H	108	GLU	C-O	5.88	1.31	1.24
1	H	111	THR	C-O	5.86	1.31	1.23
1	H	271	PRO	C-O	5.86	1.31	1.23
1	E	89	VAL	C-O	5.86	1.30	1.24
1	E	96	ILE	C-O	5.80	1.30	1.24
1	E	92	LEU	C-O	5.79	1.30	1.24
1	B	203	SER	C-O	5.77	1.31	1.23
1	F	90	LEU	C-O	5.68	1.30	1.23
1	H	260	VAL	C-O	5.61	1.29	1.24
1	F	275	ILE	C-O	5.59	1.30	1.23
1	H	77	ASP	C-O	5.57	1.30	1.24
1	A	180	ILE	C-O	5.57	1.30	1.23
1	C	126	VAL	C-O	5.57	1.30	1.24
1	E	61	SER	C-O	5.52	1.30	1.23
1	F	152	ILE	C-O	5.50	1.31	1.24
1	D	231	VAL	C-O	5.48	1.29	1.24
1	E	149	MET	C-O	5.46	1.30	1.23
1	H	263	ALA	C-O	5.42	1.30	1.23
1	G	89	VAL	C-O	5.39	1.29	1.24
1	D	236	GLU	C-O	5.38	1.30	1.24
1	B	50	GLU	C-O	5.37	1.30	1.24
1	F	112	HIS	C-O	5.35	1.30	1.24
1	H	241	HIS	CE1-NE2	5.32	1.37	1.32
1	C	202	SER	C-O	-5.31	1.17	1.23
1	C	107[A]	GLN	C-O	5.30	1.30	1.24
1	C	107[B]	GLN	C-O	5.30	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	275	ILE	C-O	5.28	1.29	1.23
1	E	105	ALA	C-O	-5.22	1.18	1.24
1	D	237	SER	C-O	5.22	1.30	1.24
1	E	178	LEU	C-O	5.21	1.30	1.24
1	F	234	GLN	C-O	5.18	1.30	1.24
1	C	177	ASN	C-O	5.17	1.29	1.23
1	C	265	THR	C-O	5.17	1.29	1.23
1	D	246	GLU	C-O	5.13	1.29	1.24
1	E	272	SER	CA-CB	-5.11	1.48	1.54
1	G	238	LEU	C-O	-5.11	1.17	1.24
1	E	99	THR	C-O	-5.11	1.17	1.23
1	E	202	SER	CA-CB	-5.11	1.45	1.53
1	H	277	PHE	C-O	5.09	1.29	1.23
1	C	109	MET	C-O	5.08	1.30	1.24
1	G	191	ALA	C-O	5.08	1.30	1.23
1	A	237	SER	C-O	5.08	1.30	1.24
1	A	268	PRO	C-O	-5.07	1.17	1.24
1	G	63	LYS	C-O	5.05	1.30	1.23
1	A	174	PRO	C-O	-5.05	1.17	1.24
1	F	151	GLU	N-CA	5.05	1.52	1.46
1	E	48	PHE	C-O	5.04	1.30	1.24
1	H	213	PHE	C-O	5.03	1.30	1.23
1	B	181	GLY	C-O	5.03	1.29	1.24
1	G	233	THR	C-O	5.03	1.30	1.23
1	G	288	ASP	C-O	-5.02	1.17	1.23
1	F	57	GLY	C-O	5.02	1.31	1.23
1	F	71	GLY	C-O	5.02	1.28	1.23
1	D	274	VAL	C-O	5.01	1.29	1.23

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	HIS	CB-CA-C	8.62	119.12	110.33
1	H	218	PHE	CA-C-O	-7.57	112.53	120.55
1	B	165	PRO	N-CA-C	7.33	123.96	113.47
1	H	120	ASN	O-C-N	-7.15	118.24	121.53
1	G	235	ALA	CA-C-O	-7.00	113.20	121.32
1	C	196	ASP	CA-CB-CG	-6.59	106.01	112.60
1	G	324	PHE	CA-CB-CG	6.56	120.36	113.80
1	F	265	THR	O-C-N	6.46	130.52	123.10
1	C	166	ASP	CA-CB-CG	6.39	118.99	112.60
1	G	223	ARG	CA-C-N	6.33	129.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	223	ARG	C-N-CA	6.33	129.39	120.28
1	G	158	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	188	LYS	N-CA-C	-6.18	104.65	111.82
1	H	265	THR	O-C-N	6.05	130.06	123.10
1	H	295	PRO	CB-CA-C	-6.03	103.90	111.56
1	H	164	PHE	CB-CA-C	6.03	117.09	110.15
1	G	318	ALA	N-CA-C	-6.00	105.82	113.01
1	B	164	PHE	CB-CA-C	5.98	116.53	109.47
1	H	171	TYR	N-CA-C	5.88	119.71	112.54
1	B	294	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	259	SER	CA-C-O	-5.85	114.31	120.80
1	G	138	VAL	N-CA-C	-5.82	104.68	110.62
1	G	235	ALA	O-C-N	5.82	129.69	121.83
1	F	205	PRO	CB-CA-C	-5.73	102.79	111.44
1	C	81	PHE	CA-CB-CG	5.72	119.52	113.80
1	G	234	GLN	CB-CA-C	5.59	118.65	110.26
1	H	116	CYS	N-CA-C	-5.58	106.23	113.16
1	F	101	ARG	CA-C-O	-5.55	114.66	120.55
1	C	93	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	291	HIS	CA-CB-CG	-5.52	108.28	113.80
1	H	44	ILE	CA-C-O	-5.51	116.09	119.51
1	H	157	VAL	N-CA-C	-5.51	105.13	110.42
1	G	110	ILE	CA-C-O	-5.48	114.55	120.47
1	G	169	ILE	CA-C-N	5.46	126.16	119.99
1	G	169	ILE	C-N-CA	5.46	126.16	119.99
1	G	169	ILE	CA-C-O	-5.45	115.39	121.17
1	D	169	ILE	CA-C-N	5.43	126.12	120.03
1	D	169	ILE	C-N-CA	5.43	126.12	120.03
1	G	254	GLU	CB-CG-CD	5.42	121.82	112.60
1	F	266	SER	CA-C-O	-5.42	114.42	120.54
1	C	282	THR	CA-CB-OG1	-5.41	101.49	109.60
1	G	306	PRO	CB-CA-C	-5.39	104.49	111.39
1	H	294	ASN	CA-CB-CG	5.37	117.97	112.60
1	D	172	GLU	CB-CA-C	5.35	118.96	109.65
1	G	75	TYR	CA-C-O	-5.35	113.28	119.64
1	G	112	HIS	CA-CB-CG	-5.33	108.47	113.80
1	B	43	VAL	CA-C-O	-5.32	115.50	120.34
1	F	247	ASP	CB-CA-C	-5.29	102.54	110.90
1	H	38	ALA	CA-C-O	-5.29	115.33	121.15
1	E	167	VAL	N-CA-C	-5.29	106.65	111.67
1	A	324	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	115	LEU	CA-C-O	-5.23	114.88	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	127	ILE	CA-C-N	5.22	126.32	120.42
1	F	127	ILE	C-N-CA	5.22	126.32	120.42
1	A	323	SER	CA-C-O	-5.22	115.08	120.92
1	C	127	ILE	CA-C-N	5.21	126.30	120.42
1	C	127	ILE	C-N-CA	5.21	126.30	120.42
1	H	45	PRO	CA-C-O	-5.19	115.82	121.27
1	H	145	GLU	CB-CG-CD	5.18	121.42	112.60
1	F	48	PHE	CA-C-O	-5.18	114.79	120.43
1	C	163	PHE	CB-CA-C	5.17	118.10	109.56
1	C	265	THR	O-C-N	5.17	128.69	123.26
1	E	228	GLY	N-CA-C	-5.16	108.15	115.43
1	F	164	PHE	CB-CA-C	-5.14	102.85	110.97
1	E	324	PHE	CA-CB-CG	5.13	118.93	113.80
1	C	292	PRO	CA-C-O	-5.12	115.89	121.27
1	F	114	PRO	CB-CA-C	-5.12	104.87	112.55
1	A	211	GLU	N-CA-C	-5.12	106.99	113.18
1	A	102	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	170	GLY	CA-C-O	-5.08	115.82	120.80
1	E	158	ASP	CA-C-O	-5.07	115.68	121.00
1	B	88	LYS	CB-CA-C	5.05	118.76	109.46
1	F	265	THR	CA-C-O	-5.04	116.05	121.45
1	G	164	PHE	CB-CA-C	5.04	115.59	109.85
1	B	308	LYS	N-CA-C	-5.03	107.31	113.50
1	F	134	VAL	CA-C-O	-5.03	115.72	120.95
1	F	219	GLN	CB-CG-CD	-5.03	104.05	112.60
1	G	213	PHE	CA-C-O	-5.02	113.47	119.35

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	2240	0	2218	36	0
1	B	2265	0	2234	49	0
1	C	2259	0	2226	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2274	0	2253	45	0
1	E	2259	0	2237	50	0
1	F	2262	0	2237	30	0
1	G	2239	0	2221	27	0
1	H	2277	0	2246	44	0
2	A	24	0	24	0	0
2	B	24	0	24	2	0
2	C	24	0	24	3	0
2	D	24	0	24	2	0
2	E	24	0	24	1	0
2	F	24	0	24	1	0
2	G	24	0	24	0	0
2	H	24	0	24	1	0
3	A	7	0	14	0	0
3	B	7	0	14	0	0
3	C	7	0	14	0	0
3	D	7	0	14	1	0
3	E	7	0	14	0	0
3	F	7	0	14	0	0
3	G	7	0	14	0	0
3	H	7	0	14	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
5	E	7	0	10	10	0
5	G	7	0	10	2	0
6	F	4	0	6	0	0
6	G	4	0	6	8	0
7	A	253	0	0	7	0
7	B	240	0	0	12	0
7	C	221	0	0	4	0
7	D	233	0	0	5	0
7	E	258	0	0	5	0
7	F	283	0	0	13	0
7	G	306	0	0	6	0
7	H	309	0	0	12	0
All	All	20468	0	18208	315	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 (315) 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:E:35:LYS:HG3	1:E:46:GLY:H	1.01	1.12
1:E:107:GLN:NE2	1:E:133:GLY:HA3	1.63	1.10
1:H:136:ARG:HD3	1:H:169:ILE:HG23	1.38	1.05
1:E:35:LYS:HG3	1:E:46:GLY:N	1.73	1.01
1:E:107:GLN:HE21	1:E:133:GLY:HA3	1.19	1.00
1:E:107:GLN:HE21	1:E:133:GLY:CA	1.76	0.97
1:E:107:GLN:NE2	1:E:133:GLY:CA	2.30	0.95
6:G:404:EDO:H12	7:G:509:HOH:O	1.66	0.92
1:H:136:ARG:HD3	1:H:169:ILE:CG2	1.99	0.92
1:G:323:SER:O	1:G:327:LYS:HG3	1.69	0.91
1:E:244:ILE:HD11	5:E:403:PEG:H41	1.55	0.88
1:H:215:LYS:HG2	1:H:219:GLN:HE21	1.38	0.88
1:A:35:LYS:HD2	1:A:41:SER:O	1.75	0.87
1:E:54:MET:HB3	5:E:403:PEG:H11	1.55	0.86
1:H:136:ARG:CD	1:H:169:ILE:HG23	2.06	0.85
1:E:35:LYS:CG	1:E:46:GLY:H	1.88	0.85
1:D:103[A]:GLU:OE1	1:D:107[A]:GLN:NE2	2.11	0.83
1:C:106:TYR:O	1:C:110:ILE:HG22	1.79	0.82
1:E:107:GLN:HE21	1:E:133:GLY:C	1.87	0.81
1:G:311:ASN:HA	6:G:404:EDO:H11	1.63	0.80
1:E:242:MET:CE	1:E:328:VAL:HG11	2.12	0.80
1:A:36:GLU:HB2	1:A:37:PRO:HD3	1.64	0.79
1:E:116:CYS:SG	1:E:296:ILE:HD12	2.23	0.78
1:D:211:GLU:OE1	1:D:214:GLU:HG3	1.83	0.78
1:B:211:GLU:HG3	7:B:722:HOH:O	1.85	0.76
1:B:146:GLN:HG3	1:C:180:ILE:O	1.84	0.76
1:F:215:LYS:HG2	1:F:219:GLN:HE21	1.51	0.76
1:H:172:GLU:HB2	7:H:516:HOH:O	1.85	0.75
1:E:107:GLN:NE2	1:E:133:GLY:C	2.44	0.75
1:G:242:MET:CE	1:G:328:VAL:HG11	2.15	0.75
1:A:242:MET:HA	1:A:242:MET:CE	2.16	0.75
1:E:35:LYS:HD3	7:E:1843:HOH:O	1.86	0.73
1:F:165:PRO:HA	7:F:555:HOH:O	1.87	0.73
1:H:103:GLU:CD	1:H:107:GLN:NE2	2.46	0.73
1:E:35:LYS:N	1:E:40:PHE:HB3	2.04	0.72
1:A:242:MET:HA	1:A:242:MET:HE2	1.73	0.71
1:H:326:LYS:O	1:H:330:GLU:HG2	1.90	0.70
1:B:136:ARG:HD3	1:B:170:GLY:HA3	1.74	0.70
1:A:261:ASN:ND2	7:A:501:HOH:O	2.24	0.70
1:E:35:LYS:N	7:E:1602:HOH:O	2.23	0.69
1:F:31:SER:N	7:F:501:HOH:O	2.24	0.69
1:A:123:LYS:HE2	1:A:194:SER:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:LYS:HG2	1:H:219:GLN:NE2	2.07	0.69
1:A:120:ASN:ND2	7:A:503:HOH:O	2.25	0.68
1:F:308:LYS:HE3	7:F:698:HOH:O	1.94	0.68
1:H:215:LYS:CG	1:H:219:GLN:HE21	2.07	0.68
1:C:166:ASP:O	1:C:169:ILE:HG22	1.94	0.68
1:D:249:VAL:HG21	1:D:329:ILE:HD12	1.76	0.67
1:E:44:ILE:HG13	1:E:45:PRO:HD2	1.76	0.66
1:E:241:HIS:CE1	5:E:403:PEG:H12	2.30	0.66
1:B:128:GLY:O	1:B:149:MET:HE3	1.96	0.66
1:A:140:ARG:HB3	1:A:296:ILE:HD11	1.77	0.65
1:E:244:ILE:CD1	5:E:403:PEG:H41	2.27	0.65
1:G:311:ASN:CA	6:G:404:EDO:H11	2.26	0.64
1:A:35:LYS:HB2	7:A:601:HOH:O	1.97	0.64
1:B:233:THR:O	1:B:277:PHE:HA	1.97	0.64
1:A:36:GLU:HA	1:A:36:GLU:OE1	1.98	0.63
1:E:205:PRO:HD2	5:E:403:PEG:H22	1.80	0.63
1:B:211:GLU:OE1	1:B:214:GLU:HG3	1.99	0.63
1:D:112:HIS:CG	1:D:296:ILE:HD11	2.34	0.62
1:E:242:MET:HE2	1:E:328:VAL:HG11	1.82	0.62
5:G:403:PEG:H21	7:G:621:HOH:O	2.00	0.62
1:H:103:GLU:CD	1:H:107:GLN:HE22	2.08	0.62
1:B:304:ASN:ND2	7:B:504:HOH:O	2.33	0.61
1:H:103:GLU:OE1	1:H:167:VAL:HG22	2.01	0.61
1:E:116:CYS:SG	1:E:296:ILE:CD1	2.88	0.61
6:G:404:EDO:C1	7:G:509:HOH:O	2.35	0.61
1:F:136:ARG:HD2	7:F:515:HOH:O	1.99	0.61
1:D:129:GLY:HA2	1:D:201:ASP:OD2	2.00	0.61
1:E:107:GLN:NE2	1:E:134:VAL:N	2.49	0.60
1:E:241:HIS:NE2	5:E:403:PEG:H12	2.17	0.60
1:C:201:ASP:O	2:C:401:S4M:H5'2	2.02	0.59
1:D:313:GLU:HG3	7:D:648:HOH:O	2.03	0.59
1:H:169:ILE:HD13	7:H:758:HOH:O	2.01	0.59
1:F:136:ARG:NH2	7:F:506:HOH:O	2.36	0.58
1:E:242:MET:CE	1:E:328:VAL:CG1	2.81	0.58
1:A:231:VAL:HG12	1:A:280:CYS:HB2	1.85	0.58
1:C:223:ARG:NH1	7:C:503:HOH:O	2.35	0.58
1:G:242:MET:HE1	1:G:328:VAL:CG1	2.33	0.58
1:A:35:LYS:O	1:A:35:LYS:HG2	2.03	0.57
1:B:73:SER:HB2	7:B:633:HOH:O	2.03	0.57
1:D:136:ARG:HH11	1:D:167:VAL:HA	1.68	0.57
1:D:216:PRO:HA	1:D:219:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:GLN:HG2	1:E:163:PHE:CE2	2.40	0.57
1:E:211[B]:GLU:HA	1:E:214:GLU:HG3	1.86	0.57
1:C:297:ASP:OD1	1:C:297:ASP:C	2.47	0.57
1:D:242:MET:HE2	1:D:328:VAL:HG21	1.87	0.57
1:E:123:LYS:NZ	7:E:1607:HOH:O	2.37	0.57
1:E:211[A]:GLU:HA	1:E:214:GLU:HG3	1.85	0.57
1:B:313:GLU:HG3	7:B:606:HOH:O	2.05	0.56
1:D:131:ASP:OD2	2:D:401:S4M:HE2	2.06	0.56
1:D:323:SER:O	1:D:327:LYS:HG3	2.06	0.56
1:A:240:LEU:HD11	1:A:272:SER:HB3	1.86	0.56
1:H:107:GLN:HG3	7:H:526:HOH:O	2.05	0.56
1:D:249:VAL:HG21	1:D:329:ILE:CD1	2.35	0.56
1:C:214:GLU:OE2	1:C:214:GLU:HA	2.05	0.56
1:B:326:LYS:O	1:B:330:GLU:HG2	2.05	0.55
1:F:103:GLU:OE1	1:F:167:VAL:HG22	2.05	0.55
1:E:35:LYS:HB2	1:E:40:PHE:HD2	1.71	0.55
1:H:292:PRO:HB3	1:H:315:HIS:CE1	2.42	0.55
1:G:250:SER:O	1:G:254:GLU:HG3	2.06	0.55
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.22	0.55
1:F:88:LYS:HE2	7:F:632:HOH:O	2.06	0.55
1:E:54:MET:CB	5:E:403:PEG:H11	2.33	0.55
1:E:223:ARG:HD3	7:E:1629:HOH:O	2.06	0.55
1:B:215:LYS:HB3	1:B:216:PRO:HD3	1.89	0.55
1:E:210:LYS:HE3	1:E:211[A]:GLU:OE2	2.08	0.54
1:E:131:ASP:OD2	2:E:401:S4M:HE2	2.08	0.53
1:H:304:ASN:N	7:H:514:HOH:O	2.41	0.53
1:D:112:HIS:HB3	1:D:296:ILE:HD11	1.90	0.53
1:F:103:GLU:O	1:F:107:GLN:HG2	2.09	0.53
1:C:332:LYS:HD2	7:C:550:HOH:O	2.09	0.53
1:G:215:LYS:HE2	7:G:710:HOH:O	2.09	0.53
1:A:208:PRO:HD3	7:A:609:HOH:O	2.07	0.53
1:G:240:LEU:HD11	1:G:272:SER:HB3	1.90	0.53
1:D:215:LYS:HG3	1:D:255:ILE:HD11	1.90	0.53
1:D:227:PRO:HA	7:D:503:HOH:O	2.08	0.53
1:B:136:ARG:NH2	7:B:506:HOH:O	2.42	0.53
1:E:35:LYS:CG	1:E:46:GLY:N	2.60	0.52
1:H:136:ARG:CD	1:H:169:ILE:CG2	2.78	0.52
1:C:99:THR:HG21	1:C:269:THR:HG21	1.91	0.52
1:D:253:ARG:NH2	1:D:329:ILE:O	2.42	0.52
1:B:197:ALA:HA	1:B:230:VAL:O	2.09	0.52
1:B:41:SER:HB3	1:B:45:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:LYS:O	1:D:219:GLN:HG3	2.10	0.52
1:D:116:CYS:SG	1:D:296:ILE:HG13	2.51	0.51
1:G:95:VAL:HG11	1:G:204:ASP:OD2	2.10	0.51
1:G:211:GLU:OE1	1:G:211:GLU:HA	2.10	0.51
1:B:304:ASN:N	7:B:508:HOH:O	2.43	0.51
1:D:54:MET:SD	1:D:205:PRO:HD2	2.50	0.51
1:D:261:ASN:ND2	7:D:509:HOH:O	2.44	0.51
1:A:233:THR:O	1:A:277:PHE:HA	2.11	0.51
1:A:242:MET:HE2	1:A:242:MET:CA	2.39	0.50
1:E:197:ALA:HA	1:E:230:VAL:O	2.11	0.50
1:G:242:MET:HE1	1:G:328:VAL:HG11	1.87	0.50
1:F:123:LYS:NZ	7:F:514:HOH:O	2.44	0.50
1:C:128:GLY:O	1:C:149:MET:HE3	2.11	0.50
1:B:92:LEU:HD21	1:B:156:VAL:HG22	1.93	0.50
1:G:197:ALA:HA	1:G:230:VAL:O	2.12	0.50
1:H:103:GLU:OE1	1:H:107:GLN:NE2	2.45	0.49
1:B:107:GLN:NE2	7:B:504:HOH:O	2.45	0.49
1:D:215:LYS:CG	1:D:255:ILE:HD11	2.42	0.49
1:H:172:GLU:CB	7:H:516:HOH:O	2.55	0.49
1:D:267:VAL:HG11	1:D:270:TYR:CD2	2.47	0.49
1:B:110:ILE:HG13	1:B:277:PHE:CD1	2.48	0.48
1:E:244:ILE:CD1	5:E:403:PEG:C4	2.91	0.48
1:B:125:LEU:HB3	1:B:198:VAL:HG22	1.95	0.48
1:B:35:LYS:O	7:B:501:HOH:O	2.20	0.48
1:F:242:MET:CE	1:F:328:VAL:HG11	2.44	0.48
1:A:37:PRO:HB2	1:A:40:PHE:CD1	2.49	0.48
1:F:88:LYS:CE	7:F:632:HOH:O	2.61	0.48
1:F:261:ASN:HD22	1:F:289:PHE:HD2	1.62	0.48
1:G:323:SER:HB3	1:G:327:LYS:HE3	1.96	0.48
1:B:136:ARG:CD	1:B:170:GLY:HA3	2.41	0.47
1:B:279:LEU:N	1:B:279:LEU:HD22	2.29	0.47
1:H:169:ILE:CD1	7:H:758:HOH:O	2.59	0.47
1:G:242:MET:CE	1:G:328:VAL:CG1	2.87	0.47
1:G:312:ALA:H	6:G:404:EDO:C1	2.26	0.47
1:G:233:THR:O	1:G:277:PHE:HA	2.14	0.47
1:E:123:LYS:HE2	1:E:146:GLN:NE2	2.28	0.47
1:G:311:ASN:CB	6:G:404:EDO:H11	2.45	0.47
1:H:242:MET:CE	1:H:328:VAL:HG11	2.45	0.47
1:A:262:TYR:CZ	1:A:276:GLY:HA3	2.50	0.47
1:C:110:ILE:HB	1:C:277:PHE:CE1	2.50	0.47
1:F:215:LYS:O	1:F:219:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:403:PEG:H42	5:G:403:PEG:H22	1.54	0.47
1:H:136:ARG:HD3	1:H:169:ILE:HG22	1.90	0.47
1:B:267:VAL:HG11	1:B:270:TYR:CD2	2.50	0.47
1:F:219:GLN:NE2	7:F:522:HOH:O	2.47	0.47
1:B:68:LEU:CD1	1:B:88:LYS:HD3	2.45	0.47
1:H:262:TYR:HB3	1:H:329:ILE:HD13	1.97	0.47
1:D:146:GLN:OE1	7:D:501:HOH:O	2.20	0.46
1:H:135:LEU:HD11	1:H:149:MET:SD	2.55	0.46
1:C:111:THR:C	1:C:114:PRO:HD2	2.41	0.46
1:F:215:LYS:HB3	1:F:216:PRO:HD3	1.96	0.46
1:G:164:PHE:HB2	1:G:167:VAL:HG21	1.97	0.46
1:A:323:SER:O	1:A:327:LYS:HG3	2.16	0.46
1:B:92:LEU:HG	1:B:97:GLN:HG3	1.98	0.46
1:B:137:GLU:OE1	1:B:140:ARG:NE	2.44	0.46
1:B:168:ALA:O	7:B:502:HOH:O	2.20	0.46
1:C:122:LYS:HE2	1:C:145:GLU:OE2	2.15	0.46
1:E:255[A]:ILE:HD11	7:E:1755:HOH:O	2.14	0.46
1:H:55:TRP:CZ3	1:H:271:PRO:HG2	2.50	0.46
1:D:242:MET:CE	1:D:328:VAL:HG11	2.46	0.46
1:B:151:GLU:O	1:B:180:ILE:HA	2.16	0.46
1:A:295:PRO:HB3	7:A:592:HOH:O	2.16	0.45
1:B:51:MET:HE3	7:B:690:HOH:O	2.15	0.45
1:D:126:VAL:O	1:D:149:MET:HA	2.16	0.45
1:H:123:LYS:HE3	1:H:195:TYR:CE1	2.51	0.45
1:C:141:HIS:HB2	1:C:144:ILE:HG13	1.98	0.45
1:C:210:LYS:HE3	1:C:211[A]:GLU:OE2	2.17	0.45
1:F:305:GLY:N	7:F:506:HOH:O	2.48	0.45
1:D:291:HIS:HA	1:D:292:PRO:HD2	1.84	0.45
1:F:126:VAL:O	1:F:149:MET:HA	2.16	0.45
1:A:151:GLU:O	1:A:180:ILE:HA	2.16	0.45
1:H:214[A]:GLU:OE2	7:H:501:HOH:O	2.21	0.45
1:C:98:LEU:CD2	1:C:164:PHE:CE2	2.99	0.45
1:D:204:ASP:OD1	3:D:402:HAI:H1	2.16	0.45
1:E:35:LYS:HG3	1:E:46:GLY:CA	2.46	0.45
1:H:209:ALA:O	1:H:210:LYS:C	2.59	0.45
1:A:54:MET:HG3	1:A:206:ILE:HD12	1.97	0.45
1:H:327:LYS:HE3	7:H:644:HOH:O	2.16	0.45
1:A:48:PHE:O	1:A:61:SER:HA	2.17	0.44
1:B:97:GLN:O	2:B:401:S4M:HB2	2.16	0.44
1:C:292:PRO:HD3	1:C:315:HIS:CD2	2.52	0.44
1:G:151:GLU:O	1:G:180:ILE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:ASP:OD1	1:H:236:GLU:OE2	2.35	0.44
1:E:79:ILE:HB	1:E:91:VAL:HB	2.00	0.44
1:D:295:PRO:HB3	7:D:723:HOH:O	2.18	0.44
1:C:98:LEU:C	1:C:98:LEU:HD23	2.43	0.44
1:C:106:TYR:CE1	2:C:401:S4M:HA2	2.53	0.44
1:E:205:PRO:HG2	5:E:403:PEG:H42	2.00	0.44
1:C:208:PRO:HB2	2:C:401:S4M:N7	2.33	0.44
1:C:322:PRO:HB3	1:D:309:PHE:CD2	2.53	0.44
1:H:40:PHE:CZ	1:H:67:VAL:HG22	2.52	0.44
1:H:120:ASN:OD1	1:H:143:SER:HB2	2.18	0.44
1:G:262:TYR:OH	1:G:276:GLY:HA3	2.18	0.44
1:B:119:PRO:O	1:B:120:ASN:C	2.60	0.43
1:C:123:LYS:HG2	1:C:195:TYR:CD1	2.52	0.43
1:C:238:LEU:HG	7:C:581:HOH:O	2.18	0.43
1:D:116:CYS:SG	1:D:296:ILE:CG1	3.06	0.43
1:D:151:GLU:O	1:D:180:ILE:HA	2.17	0.43
1:E:219:GLN:HG2	1:E:255[A]:ILE:CD1	2.47	0.43
1:F:103:GLU:HG3	1:F:104:CYS:N	2.33	0.43
1:G:312:ALA:H	6:G:404:EDO:H11	1.82	0.43
1:A:92:LEU:HG	1:A:97:GLN:HG3	2.01	0.43
1:A:309:PHE:CD2	1:B:322:PRO:HB3	2.53	0.43
1:G:135:LEU:HD11	1:G:149:MET:SD	2.58	0.43
1:H:97:GLN:O	2:H:401:S4M:HB2	2.18	0.43
1:A:253:ARG:HG2	1:A:253:ARG:HH11	1.84	0.43
1:C:262:TYR:OH	1:C:276:GLY:HA3	2.17	0.43
1:G:309:PHE:CD2	1:H:322:PRO:HB3	2.54	0.43
1:B:124:VAL:CG2	1:B:144:ILE:HD12	2.47	0.43
1:B:271:PRO:HD3	7:B:590:HOH:O	2.18	0.43
1:C:140:ARG:HB3	1:C:296:ILE:HD11	2.00	0.43
1:D:92:LEU:HD12	1:D:97:GLN:HG3	2.00	0.43
1:F:293:LEU:C	1:F:294:ASN:CG	2.86	0.43
1:F:293:LEU:HD22	7:F:622:HOH:O	2.18	0.43
1:A:125:LEU:HD21	1:A:127:ILE:HD11	2.01	0.43
1:C:215:LYS:HE2	1:C:254:GLU:OE1	2.19	0.43
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.65	0.43
1:F:114:PRO:O	1:F:117:SER:HB2	2.18	0.43
1:F:292:PRO:HB3	1:F:315:HIS:CE1	2.54	0.43
6:G:404:EDO:C2	7:G:509:HOH:O	2.62	0.43
1:B:137:GLU:CD	1:B:140:ARG:HE	2.26	0.43
1:H:136:ARG:NH2	7:H:526:HOH:O	2.52	0.43
1:H:198:VAL:O	1:H:231:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HB2	7:B:703:HOH:O	2.19	0.42
1:B:257:LYS:HA	1:B:257:LYS:HD3	1.79	0.42
1:E:309:PHE:CD2	1:F:322:PRO:HB3	2.53	0.42
1:G:214:GLU:HG3	7:G:502:HOH:O	2.19	0.42
1:D:106:TYR:CE2	2:D:401:S4M:HA2	2.55	0.42
1:H:136:ARG:HG2	1:H:170:GLY:HA2	2.01	0.42
1:H:92:LEU:HD21	1:H:156:VAL:HG22	2.01	0.42
1:C:113:LEU:N	1:C:114:PRO:HD2	2.34	0.42
1:E:211[A]:GLU:HA	1:E:211[A]:GLU:OE1	2.18	0.42
1:A:242:MET:HA	1:A:242:MET:HE3	1.98	0.42
1:B:324:PHE:CD1	1:B:324:PHE:C	2.97	0.42
1:D:149:MET:HE1	1:D:171:TYR:OH	2.18	0.42
1:H:233:THR:O	1:H:277:PHE:HA	2.19	0.42
1:B:151:GLU:OE2	2:B:401:S4M:O3'	2.33	0.42
1:B:164:PHE:HA	1:B:165:PRO:HD3	1.87	0.42
1:C:54:MET:SD	1:C:204:ASP:HB3	2.60	0.42
1:C:134:VAL:HG23	7:C:512:HOH:O	2.19	0.42
1:D:112:HIS:CB	1:D:296:ILE:HD11	2.49	0.42
1:E:75:TYR:C	1:E:76:GLN:HG3	2.44	0.42
1:C:233:THR:O	1:C:277:PHE:HA	2.20	0.42
1:E:219:GLN:HG2	1:E:255[A]:ILE:HD12	2.02	0.42
1:A:53:PRO:O	1:A:56:PRO:HD3	2.20	0.42
1:B:169:ILE:HG22	1:B:170:GLY:N	2.35	0.42
1:A:129:GLY:HA2	1:A:201:ASP:OD2	2.19	0.42
1:H:166:ASP:HA	1:H:169:ILE:HG22	2.01	0.42
1:H:232:CYS:HA	1:H:278:MET:O	2.19	0.42
1:H:321:LEU:CD1	1:H:329:ILE:HD12	2.49	0.42
1:A:313:GLU:HG3	7:A:666:HOH:O	2.20	0.41
1:E:205:PRO:CD	5:E:403:PEG:H22	2.48	0.41
1:F:232:CYS:HA	1:F:278:MET:O	2.20	0.41
1:A:262:TYR:OH	1:A:276:GLY:HA3	2.20	0.41
1:B:48:PHE:O	1:B:61:SER:HA	2.21	0.41
1:D:112:HIS:O	1:D:116:CYS:HB2	2.20	0.41
1:D:236:GLU:HB3	1:D:241:HIS:ND1	2.35	0.41
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.55	0.41
1:E:120:ASN:N	1:E:121:PRO:CD	2.83	0.41
1:A:231:VAL:CG1	1:A:280:CYS:HB2	2.50	0.41
1:D:112:HIS:CG	1:D:296:ILE:CD1	3.02	0.41
1:B:54:MET:HE1	1:B:204:ASP:CB	2.51	0.41
1:D:232:CYS:HA	1:D:278:MET:O	2.20	0.41
1:D:259:SER:O	1:D:280:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:HB3	1:A:241:HIS:ND1	2.35	0.41
1:C:80:VAL:HA	1:C:89:VAL:O	2.20	0.41
1:F:41:SER:HB3	1:F:45:PRO:HA	2.02	0.41
1:F:311:ASN:H	1:F:314:ILE:HG22	1.85	0.41
1:D:134:VAL:O	1:D:138:VAL:HG23	2.21	0.41
1:D:233:THR:O	1:D:277:PHE:HA	2.20	0.41
1:F:172:GLU:HA	7:F:733:HOH:O	2.21	0.41
1:A:40:PHE:CE2	1:A:64:VAL:HG21	2.56	0.41
1:A:177[B]:ASN:ND2	7:A:518:HOH:O	2.50	0.41
1:B:112:HIS:O	1:B:116:CYS:HB2	2.21	0.41
1:B:169:ILE:O	1:B:172:GLU:HB2	2.21	0.41
2:F:401:S4M:HE2	2:F:401:S4M:HB1	1.95	0.41
1:G:129:GLY:HA2	1:G:201:ASP:OD2	2.21	0.41
1:C:262:TYR:CZ	1:C:276:GLY:HA3	2.56	0.41
1:D:100:GLU:HA	1:D:103[B]:GLU:OE1	2.21	0.41
1:D:103[B]:GLU:OE2	1:D:167:VAL:HG22	2.21	0.41
1:H:296:ILE:HG21	7:H:760:HOH:O	2.21	0.41
1:H:326:LYS:HG3	7:H:703:HOH:O	2.21	0.41
1:B:311:ASN:OD1	1:B:314:ILE:HG22	2.21	0.40
1:C:232:CYS:HA	1:C:278:MET:O	2.21	0.40
1:F:103:GLU:OE1	1:F:167:VAL:CG2	2.69	0.40
1:G:251:ASN:O	1:G:255[A]:ILE:HG12	2.21	0.40
1:F:174:PRO:HG2	7:F:720:HOH:O	2.20	0.40
1:G:259:SER:O	1:G:280:CYS:HA	2.21	0.40
1:H:219:GLN:NE2	7:H:518:HOH:O	2.46	0.40
1:B:124:VAL:HG21	1:B:144:ILE:HD12	2.02	0.40
1:E:35:LYS:N	1:E:40:PHE:CB	2.80	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	287/304 (94%)	275 (96%)	11 (4%)	1 (0%)	36	25
1	B	290/304 (95%)	277 (96%)	13 (4%)	0	100	100
1	C	290/304 (95%)	280 (97%)	10 (3%)	0	100	100
1	D	292/304 (96%)	279 (96%)	13 (4%)	0	100	100
1	E	290/304 (95%)	278 (96%)	12 (4%)	0	100	100
1	F	290/304 (95%)	278 (96%)	12 (4%)	0	100	100
1	G	287/304 (94%)	278 (97%)	9 (3%)	0	100	100
1	H	292/304 (96%)	282 (97%)	10 (3%)	0	100	100
All	All	2318/2432 (95%)	2227 (96%)	90 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	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	249/260 (96%)	241 (97%)	8 (3%)	34	22
1	B	251/260 (96%)	244 (97%)	7 (3%)	38	26
1	C	251/260 (96%)	246 (98%)	5 (2%)	48	38
1	D	253/260 (97%)	250 (99%)	3 (1%)	63	57
1	E	252/260 (97%)	248 (98%)	4 (2%)	55	47
1	F	251/260 (96%)	247 (98%)	4 (2%)	55	47
1	G	249/260 (96%)	245 (98%)	4 (2%)	55	47
1	H	253/260 (97%)	250 (99%)	3 (1%)	63	57
All	All	2009/2080 (97%)	1971 (98%)	38 (2%)	51	41

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	51	MET
1	A	177[A]	ASN
1	A	177[B]	ASN
1	A	187	LEU
1	A	211	GLU
1	A	242	MET
1	A	296	ILE
1	B	34	LYS
1	B	103	GLU
1	B	146	GLN
1	B	169	ILE
1	B	293	LEU
1	B	304	ASN
1	B	329	ILE
1	C	187	LEU
1	C	192	GLU
1	C	242	MET
1	C	279	LEU
1	C	293	LEU
1	D	98[A]	LEU
1	D	98[B]	LEU
1	D	316	SER
1	E	187	LEU
1	E	214	GLU
1	E	293	LEU
1	E	296	ILE
1	F	123	LYS
1	F	294	ASN
1	F	308	LYS
1	F	329	ILE
1	G	35	LYS
1	G	98[A]	LEU
1	G	98[B]	LEU
1	G	265	THR
1	H	103	GLU
1	H	304	ASN
1	H	329	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	219	GLN
1	B	189	ASN
1	B	219	GLN
1	C	70	GLN
1	C	97	GLN
1	C	189	ASN
1	C	219	GLN
1	D	82	GLN
1	D	219	GLN
1	D	261	ASN
1	E	70	GLN
1	E	107	GLN
1	F	189	ASN
1	F	219	GLN
1	F	261	ASN
1	G	189	ASN
1	H	76	GLN
1	H	97	GLN
1	H	107	GLN
1	H	189	ASN
1	H	219	GLN
1	H	261	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 ⓘ

24 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	$\# Z > 2$
3	HAI	F	402	-	7,7,7	0.41	0	8,8,8	1.29	2 (25%)
2	S4M	E	401	-	25,26,26	0.32	0	33,37,37	0.88	2 (6%)
6	EDO	F	403	-	3,3,3	0.18	0	2,2,2	0.25	0
3	HAI	G	402	-	7,7,7	0.41	0	8,8,8	0.40	0
4	SO4	B	403	-	4,4,4	0.33	0	6,6,6	0.20	0
3	HAI	H	402	-	7,7,7	0.35	0	8,8,8	0.50	0
2	S4M	G	401	-	25,26,26	0.39	0	33,37,37	0.82	2 (6%)
6	EDO	G	404	-	3,3,3	0.37	0	2,2,2	0.11	0
3	HAI	E	402	-	7,7,7	0.59	0	8,8,8	1.01	0
2	S4M	C	401	-	25,26,26	0.38	0	33,37,37	0.70	0
4	SO4	G	405	-	4,4,4	0.45	0	6,6,6	0.22	0
2	S4M	F	401	-	25,26,26	0.35	0	33,37,37	0.83	1 (3%)
5	PEG	E	403	-	6,6,6	0.28	0	5,5,5	0.21	0
5	PEG	G	403	-	6,6,6	0.20	0	5,5,5	0.20	0
3	HAI	C	402	-	7,7,7	0.37	0	8,8,8	1.35	2 (25%)
3	HAI	A	402	-	7,7,7	0.53	0	8,8,8	0.75	0
2	S4M	H	401	-	25,26,26	0.31	0	33,37,37	0.92	1 (3%)
2	S4M	A	401	-	25,26,26	0.36	0	33,37,37	0.70	1 (3%)
3	HAI	B	402	-	7,7,7	0.56	0	8,8,8	0.79	0
4	SO4	C	403	-	4,4,4	0.35	0	6,6,6	0.15	0
2	S4M	B	401	-	25,26,26	0.25	0	33,37,37	0.84	1 (3%)
2	S4M	D	401	-	25,26,26	0.42	0	33,37,37	0.73	0
3	HAI	D	402	-	7,7,7	0.39	0	8,8,8	0.52	0
4	SO4	E	404	-	4,4,4	0.45	0	6,6,6	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HAI	F	402	-	-	-	0/1/1/1
2	S4M	E	401	-	-	3/12/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	F	403	-	-	1/1/1/1	-
3	HAI	G	402	-	-	-	0/1/1/1
2	S4M	G	401	-	-	2/12/28/28	0/3/3/3
3	HAI	H	402	-	-	-	0/1/1/1
6	EDO	G	404	-	-	0/1/1/1	-
3	HAI	E	402	-	-	-	0/1/1/1
2	S4M	C	401	-	-	3/12/28/28	0/3/3/3
2	S4M	F	401	-	-	4/12/28/28	0/3/3/3
5	PEG	E	403	-	-	2/4/4/4	-
5	PEG	G	403	-	-	2/4/4/4	-
3	HAI	C	402	-	-	-	0/1/1/1
3	HAI	A	402	-	-	-	0/1/1/1
2	S4M	H	401	-	-	2/12/28/28	0/3/3/3
2	S4M	A	401	-	-	2/12/28/28	0/3/3/3
3	HAI	B	402	-	-	-	0/1/1/1
2	S4M	B	401	-	-	2/12/28/28	0/3/3/3
2	S4M	D	401	-	-	6/12/28/28	0/3/3/3
3	HAI	D	402	-	-	-	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	S4M	O4'-C4'-C5'	2.95	116.34	108.88
2	B	401	S4M	O4'-C4'-C5'	2.91	116.24	108.88
2	H	401	S4M	O4'-C4'-C5'	2.88	116.15	108.88
2	G	401	S4M	O2'-C2'-C1'	2.49	118.67	110.10
2	E	401	S4M	O2'-C2'-C1'	2.34	118.15	110.10
3	F	402	HAI	C6-C1-C2	2.31	112.64	110.29
2	G	401	S4M	O4'-C4'-C5'	2.29	114.67	108.88
2	E	401	S4M	O4'-C4'-C5'	2.27	114.61	108.88
2	A	401	S4M	C4'-O4'-C1'	-2.23	104.54	109.47
3	C	402	HAI	C5-C6-C1	2.19	114.73	111.77
3	C	402	HAI	C6-C1-C2	2.16	112.48	110.29
3	F	402	HAI	C3-C2-C1	2.07	114.58	111.77

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	S4M	CA-CB-CG-SD
2	A	401	S4M	C4'-C5'-SD-CE
2	B	401	S4M	CA-CB-CG-SD
2	C	401	S4M	CA-CB-CG-SD
2	D	401	S4M	C4'-C5'-SD-CE
2	E	401	S4M	CA-CB-CG-SD
2	E	401	S4M	O4'-C4'-C5'-SD
2	E	401	S4M	C3'-C4'-C5'-SD
2	F	401	S4M	CA-CB-CG-SD
2	F	401	S4M	O4'-C4'-C5'-SD
2	G	401	S4M	CA-CB-CG-SD
2	G	401	S4M	O4'-C4'-C5'-SD
2	H	401	S4M	O4'-C4'-C5'-SD
5	G	403	PEG	C4-C3-O2-C2
5	G	403	PEG	O2-C3-C4-O4
5	E	403	PEG	O2-C3-C4-O4
2	C	401	S4M	C2'-C1'-N9-C8
2	B	401	S4M	O4'-C4'-C5'-SD
2	C	401	S4M	O4'-C4'-C5'-SD
2	D	401	S4M	O4'-C4'-C5'-SD
2	D	401	S4M	C3'-C4'-C5'-SD
2	F	401	S4M	C3'-C4'-C5'-SD
6	F	403	EDO	O1-C1-C2-O2
2	D	401	S4M	N-CA-CB-CG
5	E	403	PEG	C4-C3-O2-C2
2	D	401	S4M	CA-CB-CG-SD
2	H	401	S4M	CA-CB-CG-SD
2	D	401	S4M	C2'-C1'-N9-C8
2	F	401	S4M	C2'-C1'-N9-C8

There are no ring outliers.

10 monomers are involved in 31 short contacts:

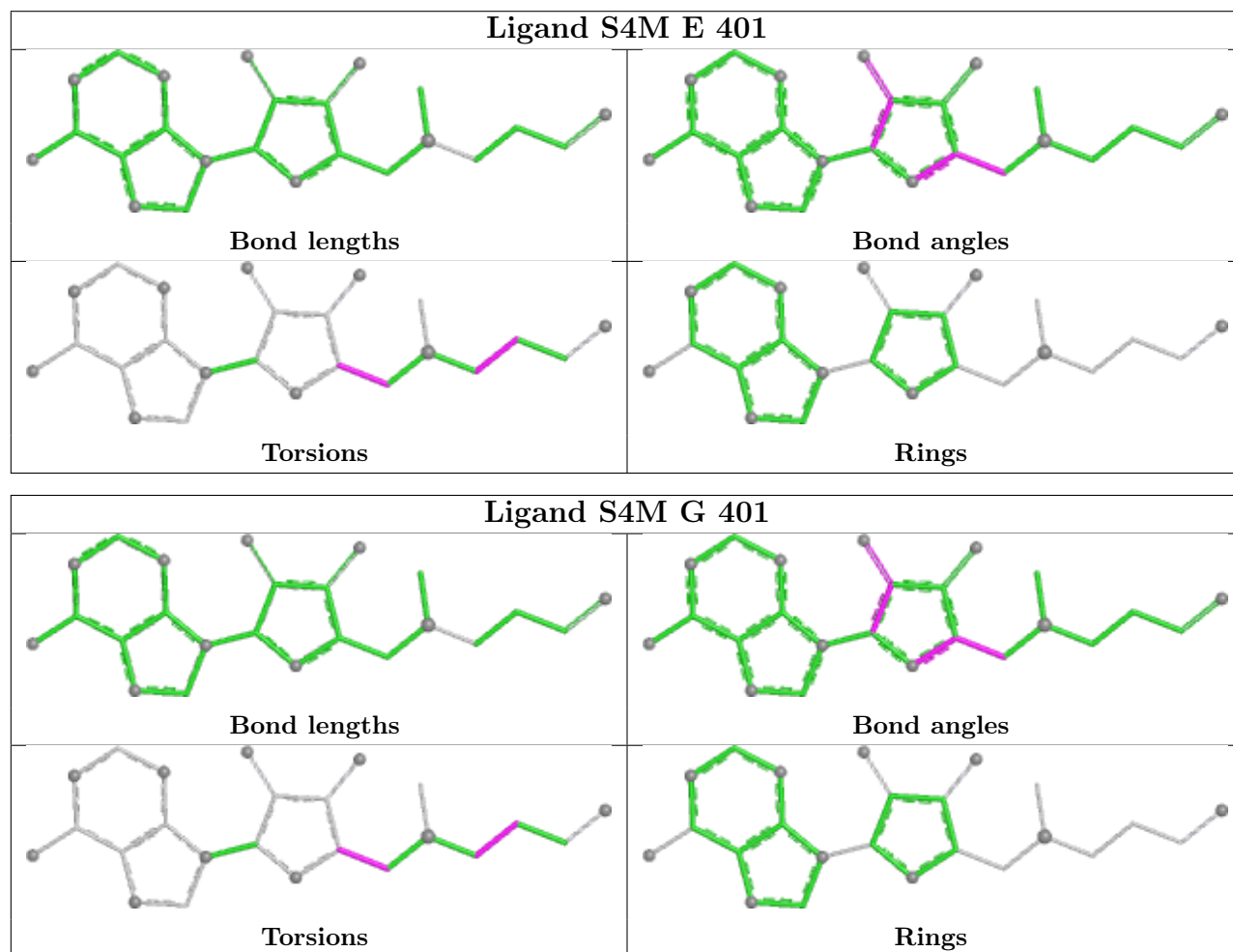
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	S4M	1	0
6	G	404	EDO	8	0
2	C	401	S4M	3	0
2	F	401	S4M	1	0
5	E	403	PEG	10	0
5	G	403	PEG	2	0
2	H	401	S4M	1	0
2	B	401	S4M	2	0
2	D	401	S4M	2	0

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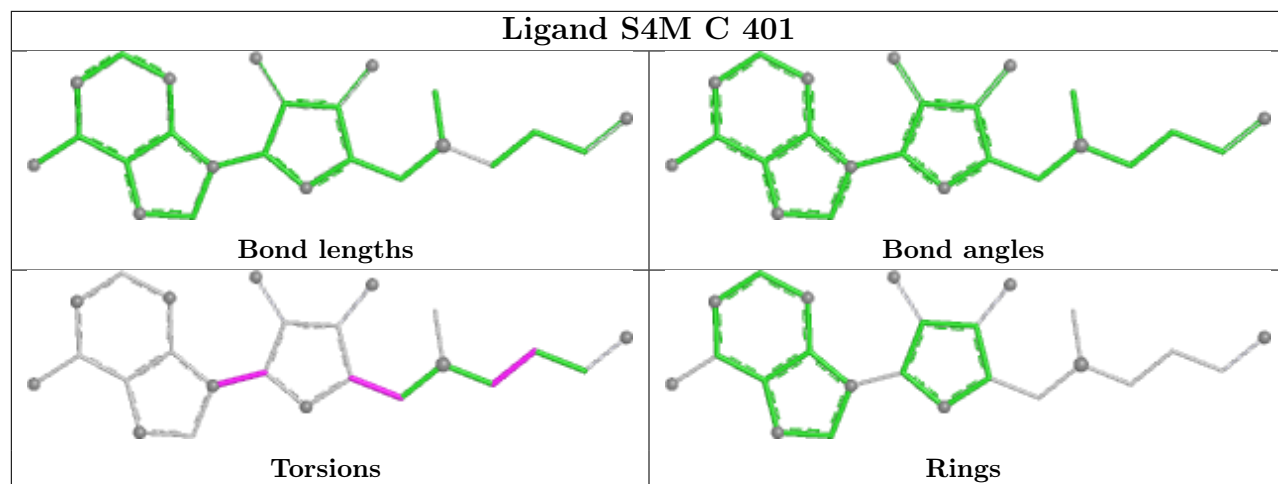
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	HAI	1	0

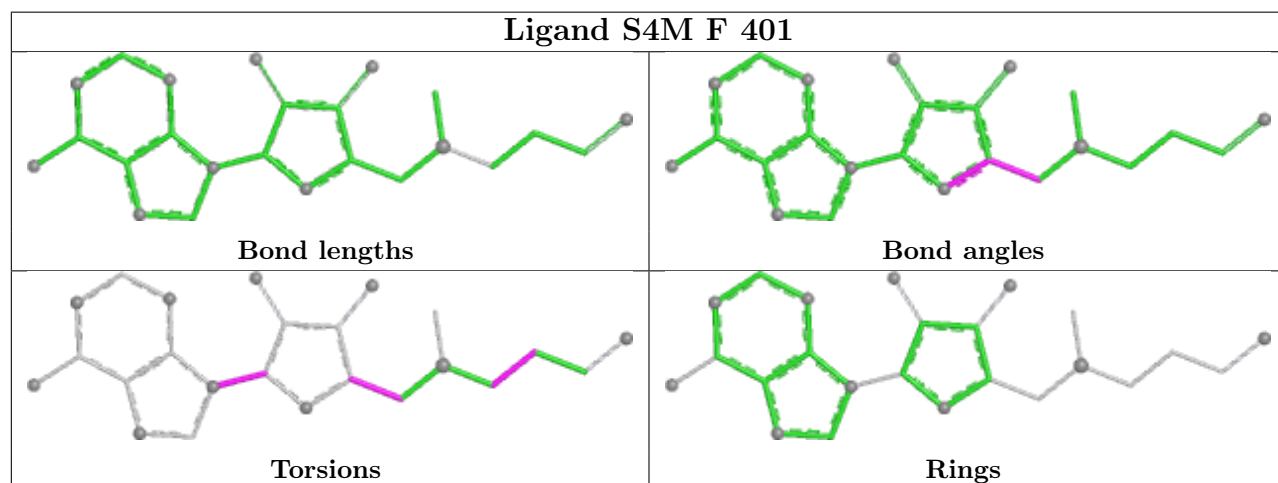
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



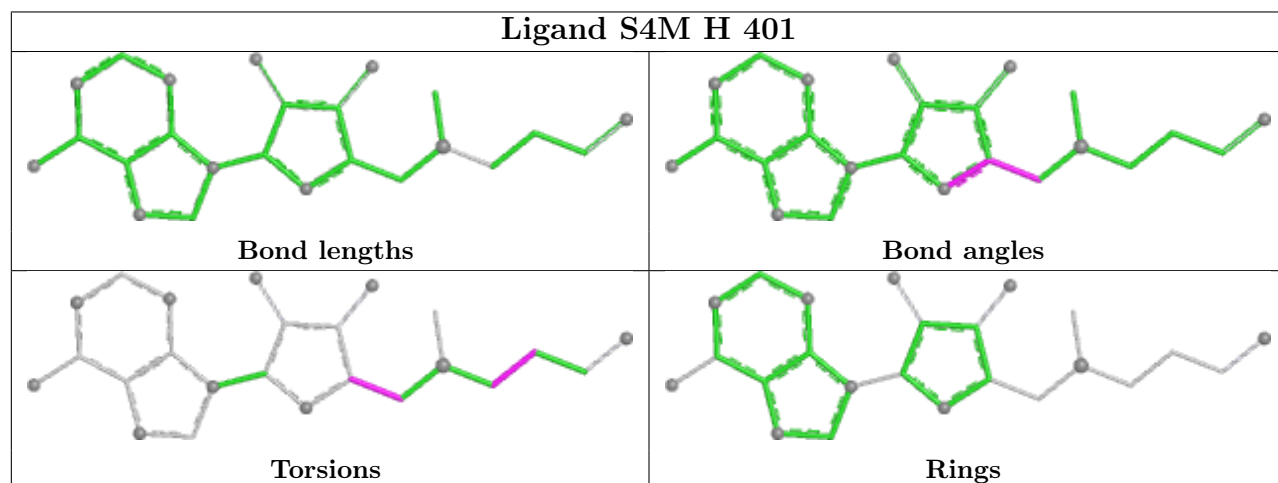
Ligand S4M C 401

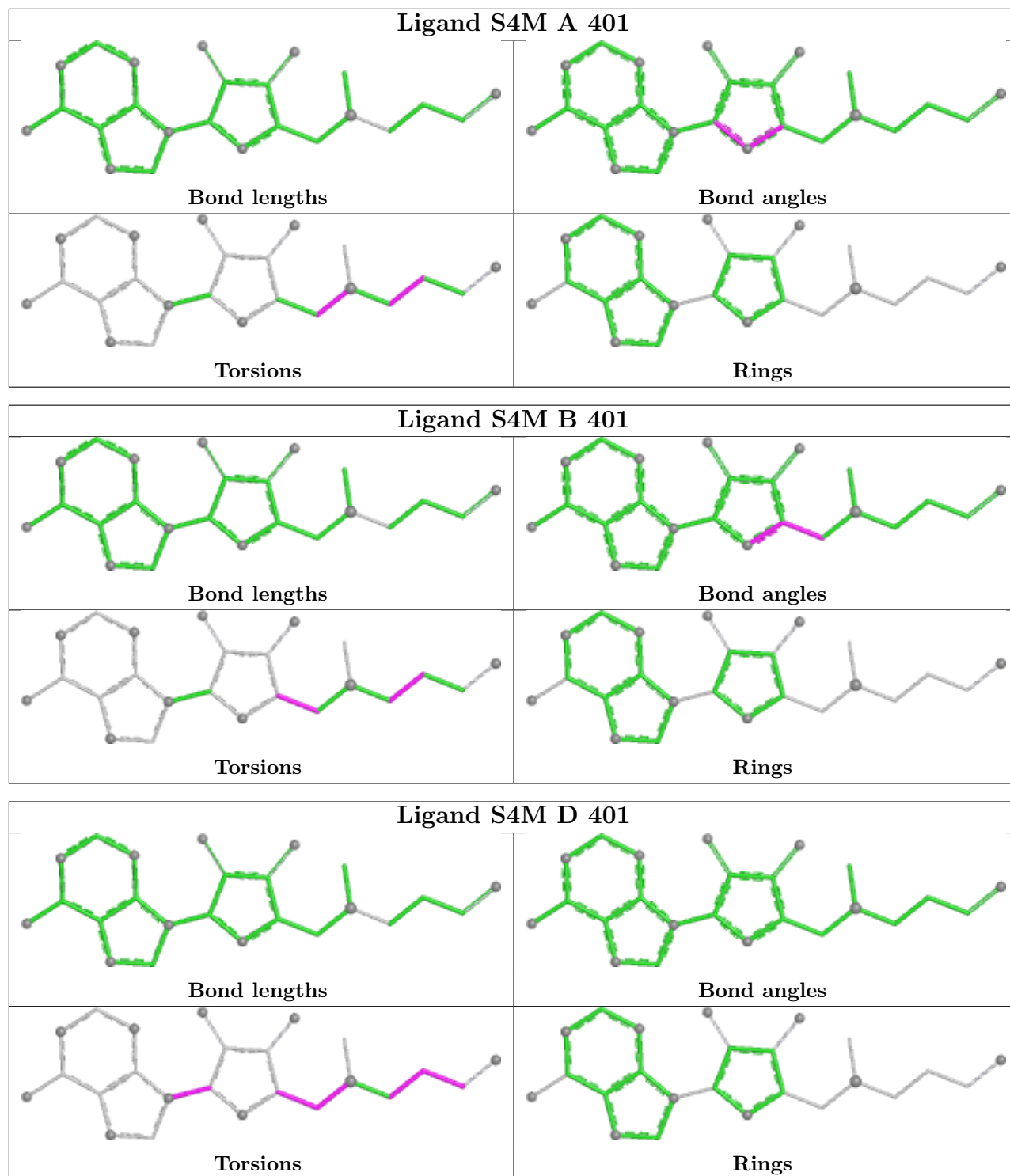


Ligand S4M F 401



Ligand S4M H 401





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	289/304 (95%)	0.47	15 (5%)	33	31	11, 18, 35, 64	2 (0%)
1	B	294/304 (96%)	0.86	30 (10%)	12	10	14, 23, 42, 55	0
1	C	291/304 (95%)	0.62	19 (6%)	25	23	9, 21, 39, 60	3 (1%)
1	D	293/304 (96%)	0.85	31 (10%)	11	9	9, 22, 41, 58	3 (1%)
1	E	290/304 (95%)	0.11	11 (3%)	44	44	7, 12, 32, 54	4 (1%)
1	F	293/304 (96%)	0.19	9 (3%)	51	51	7, 13, 28, 50	1 (0%)
1	G	289/304 (95%)	0.15	14 (4%)	35	34	7, 12, 31, 51	2 (0%)
1	H	294/304 (96%)	0.18	12 (4%)	41	41	8, 12, 27, 44	2 (0%)
All	All	2333/2432 (95%)	0.43	141 (6%)	27	26	7, 17, 37, 64	17 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	ILE	6.7
1	B	165	PRO	5.4
1	H	167	VAL	5.3
1	D	167	VAL	5.1
1	G	37	PRO	4.9
1	C	169	ILE	4.9
1	D	331	SER	4.8
1	B	167	VAL	4.7
1	H	293	LEU	4.7
1	A	38	ALA	4.5
1	B	296	ILE	4.4
1	G	38	ALA	4.4
1	C	43	VAL	4.3
1	D	293	LEU	4.3
1	C	166	ASP	4.1
1	F	31	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	32	ASN	4.0
1	B	295	PRO	4.0
1	A	44	ILE	3.9
1	B	166	ASP	3.8
1	D	305	GLY	3.8
1	D	165	PRO	3.7
1	D	295	PRO	3.7
1	D	166	ASP	3.7
1	D	296	ILE	3.6
1	H	169	ILE	3.6
1	C	165	PRO	3.6
1	D	32	ASN	3.6
1	H	32	ASN	3.6
1	A	72	LYS	3.5
1	F	293	LEU	3.5
1	A	35	LYS	3.5
1	B	293	LEU	3.5
1	D	294	ASN	3.4
1	B	328	VAL	3.2
1	G	169	ILE	3.2
1	H	296	ILE	3.2
1	A	42	THR	3.2
1	C	44	ILE	3.1
1	G	44	ILE	3.1
1	A	37	PRO	3.1
1	C	37	PRO	3.1
1	D	172	GLU	3.1
1	H	304	ASN	3.1
1	E	167	VAL	3.0
1	G	43	VAL	3.0
1	D	142	ALA	3.0
1	A	64	VAL	3.0
1	H	31	SER	3.0
1	A	328	VAL	2.9
1	H	166	ASP	2.9
1	C	170	GLY	2.9
1	G	305	GLY	2.9
1	B	306	PRO	2.9
1	B	33	ALA	2.9
1	B	169	ILE	2.9
1	F	331	SER	2.9
1	A	36	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	328	VAL	2.8
1	H	165	PRO	2.8
1	G	40	PHE	2.8
1	E	169	ILE	2.8
1	H	170	GLY	2.8
1	D	168	ALA	2.8
1	E	43	VAL	2.8
1	F	166	ASP	2.8
1	D	33	ALA	2.8
1	B	258	GLY	2.8
1	B	31	SER	2.7
1	E	38	ALA	2.7
1	E	296	ILE	2.7
1	E	37	PRO	2.7
1	D	227	PRO	2.7
1	B	331	SER	2.7
1	G	167	VAL	2.7
1	B	171	TYR	2.6
1	B	327	LYS	2.6
1	F	294	ASN	2.6
1	D	329	ILE	2.6
1	A	43	VAL	2.6
1	C	296	ILE	2.6
1	G	168	ALA	2.6
1	B	164	PHE	2.5
1	E	35	LYS	2.5
1	B	168	ALA	2.5
1	C	38	ALA	2.5
1	F	296	ILE	2.5
1	D	67	VAL	2.5
1	A	39	CYS	2.4
1	D	327	LYS	2.4
1	B	174	PRO	2.4
1	C	167	VAL	2.4
1	D	258	GLY	2.4
1	A	40	PHE	2.4
1	B	170	GLY	2.4
1	C	305	GLY	2.4
1	B	144	ILE	2.4
1	E	162	GLN	2.4
1	C	36	GLU	2.3
1	D	144	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	305	GLY	2.3
1	C	297	ASP	2.3
1	B	136	ARG	2.2
1	B	285	PRO	2.2
1	C	45	PRO	2.2
1	C	164	PHE	2.2
1	D	191	ALA	2.2
1	G	35	LYS	2.2
1	G	39	CYS	2.2
1	G	42	THR	2.2
1	C	333	ALA	2.2
1	E	44	ILE	2.2
1	G	166	ASP	2.2
1	E	36	GLU	2.2
1	B	178	LEU	2.2
1	H	305	GLY	2.2
1	D	121	PRO	2.2
1	D	306	PRO	2.2
1	F	327	LYS	2.2
1	A	329	ILE	2.1
1	H	331	SER	2.1
1	D	119	PRO	2.1
1	E	45	PRO	2.1
1	G	165	PRO	2.1
1	B	120	ASN	2.1
1	B	146	GLN	2.1
1	D	40	PHE	2.1
1	D	164	PHE	2.1
1	A	244	ILE	2.1
1	D	31	SER	2.1
1	B	214	GLU	2.1
1	D	170	GLY	2.1
1	A	327	LYS	2.0
1	D	42	THR	2.0
1	B	307	LEU	2.0
1	C	163	PHE	2.0
1	F	169	ILE	2.0
1	B	294	ASN	2.0
1	F	120	ASN	2.0
1	C	295	PRO	2.0
1	C	306	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

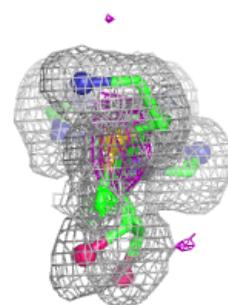
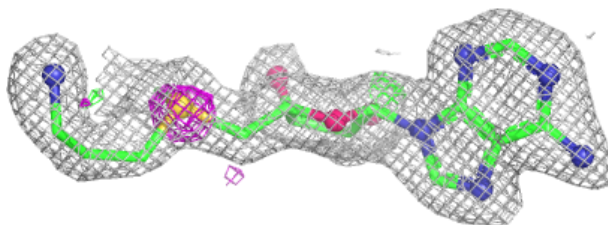
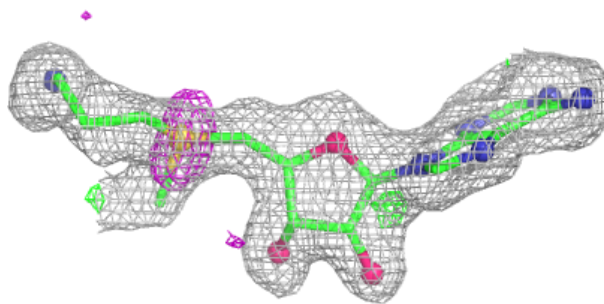
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	E	403	7/7	0.81	0.21	22,24,30,31	0
3	HAI	B	402	7/7	0.86	0.12	17,19,19,19	0
3	HAI	A	402	7/7	0.87	0.10	17,18,18,19	0
3	HAI	H	402	7/7	0.89	0.10	9,9,9,10	0
5	PEG	G	403	7/7	0.89	0.13	34,36,38,40	0
2	S4M	D	401	24/24	0.90	0.10	15,18,25,28	0
2	S4M	F	401	24/24	0.90	0.09	9,10,10,11	0
3	HAI	D	402	7/7	0.90	0.10	14,15,15,15	0
3	HAI	C	402	7/7	0.91	0.10	17,18,18,18	0
2	S4M	C	401	24/24	0.91	0.10	14,20,25,27	0
3	HAI	E	402	7/7	0.91	0.08	9,9,10,10	0
6	EDO	F	403	4/4	0.91	0.09	27,29,29,32	0
6	EDO	G	404	4/4	0.91	0.12	23,24,26,31	0
3	HAI	F	402	7/7	0.92	0.09	9,9,9,10	0
2	S4M	H	401	24/24	0.92	0.08	9,10,10,11	0
2	S4M	B	401	24/24	0.92	0.09	14,17,23,26	0
2	S4M	G	401	24/24	0.93	0.08	9,11,11,11	0
2	S4M	E	401	24/24	0.93	0.08	10,11,11,11	0
3	HAI	G	402	7/7	0.93	0.08	9,9,10,10	0
2	S4M	A	401	24/24	0.93	0.09	14,16,21,23	0
4	SO4	C	403	5/5	0.94	0.11	29,37,38,40	0
4	SO4	B	403	5/5	0.95	0.08	27,29,33,34	0
4	SO4	G	405	5/5	0.96	0.10	23,27,28,34	0
4	SO4	E	404	5/5	0.97	0.10	22,26,32,34	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.

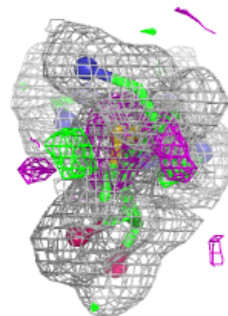
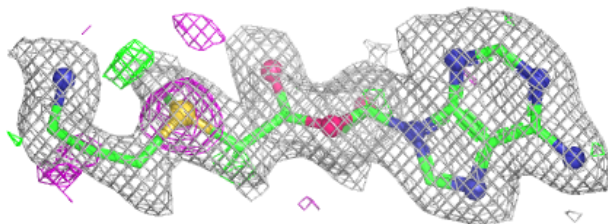
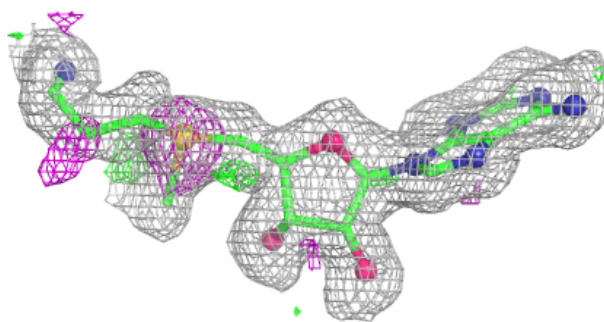
Electron density around S4M D 401:

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



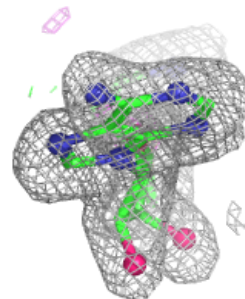
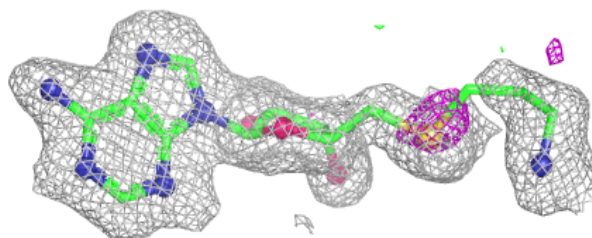
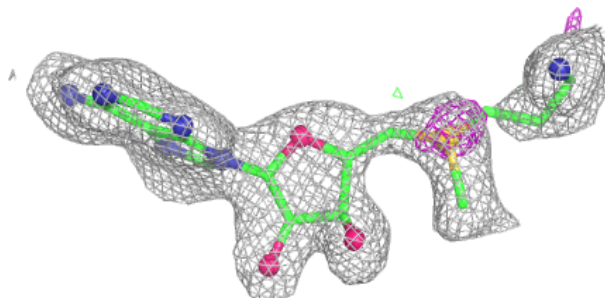
Electron density around S4M F 401:

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

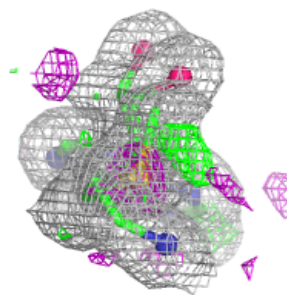
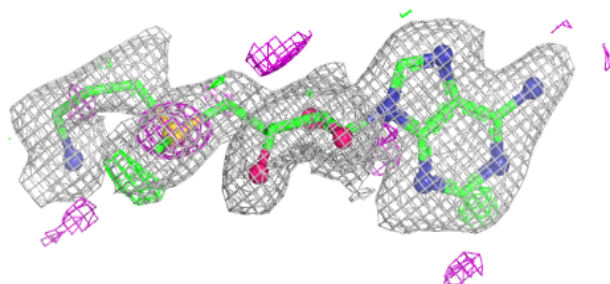
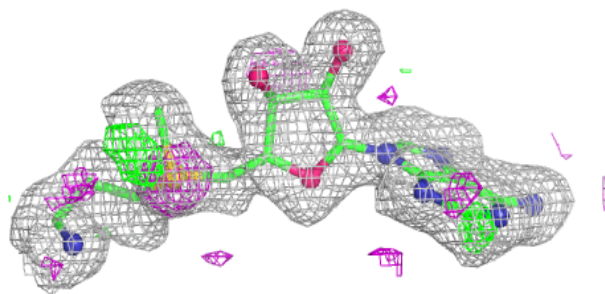


Electron density around S4M C 401:

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

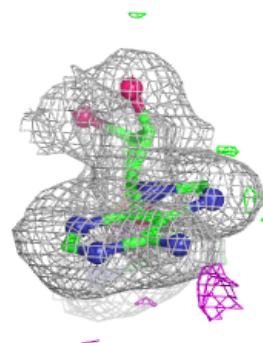
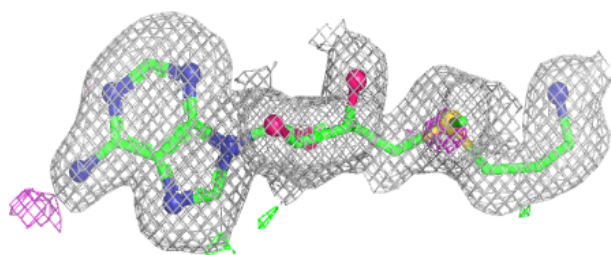
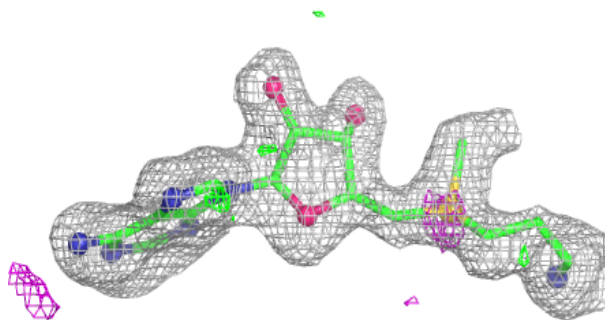
**Electron density around S4M H 401:**

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

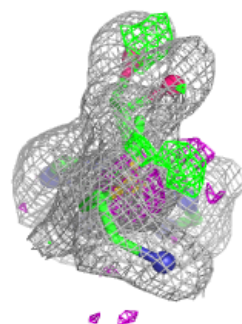
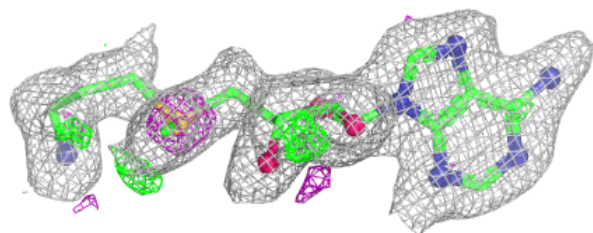
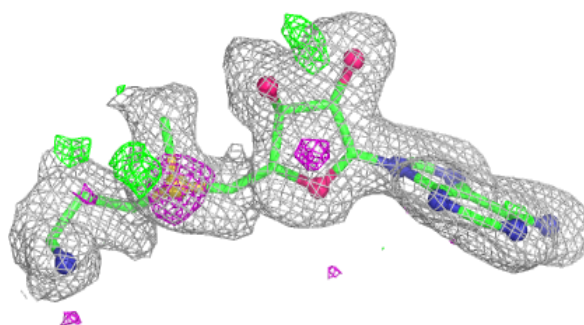


Electron density around S4M B 401:

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

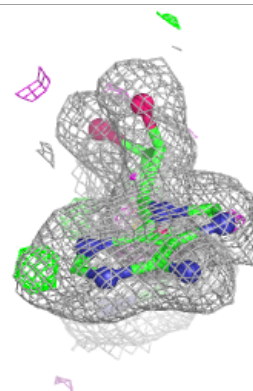
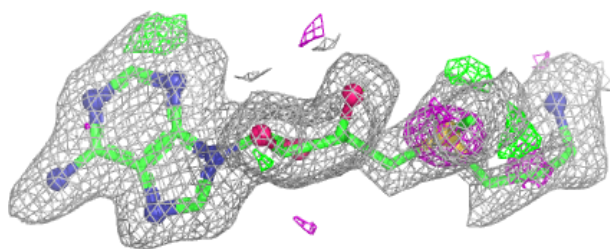
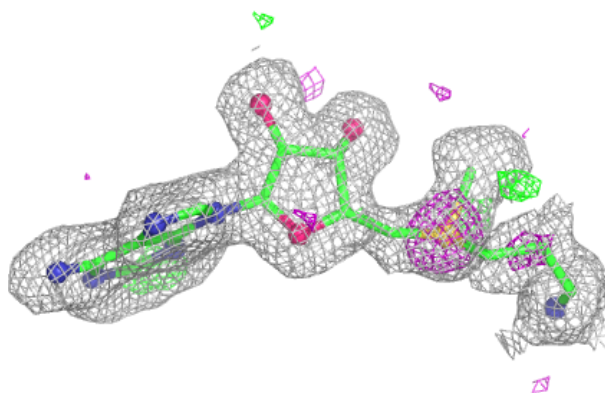
**Electron density around S4M G 401:**

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

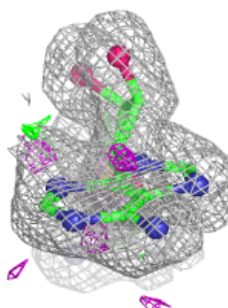
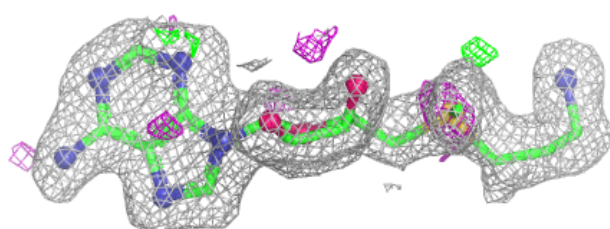
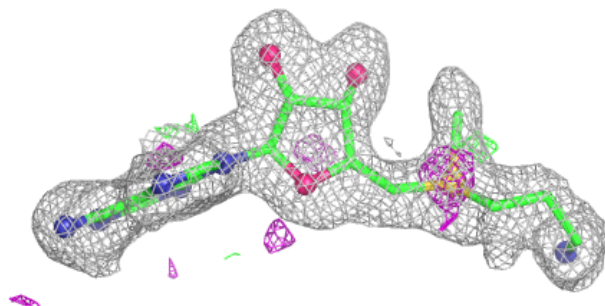


Electron density around S4M E 401:

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

**Electron density around S4M 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.