



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 03:05 PM EDT

PDB ID : 6O65  
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](mailto: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>.

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

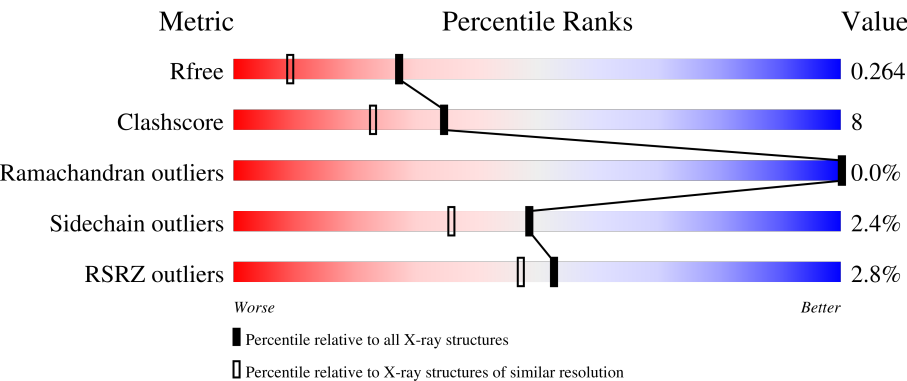
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 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 <sub>free</sub>	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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  $\geq 3$ , 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	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>78%15%• 5%</div></div>
1	B	304	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>76%20%• •</div></div>
1	C	304	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>79%17%•</div></div>
1	D	304	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>78%18%•</div></div>

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Mol	Chain	Length	Quality of chain
1	E	304	 2% 83% 12% 5%
1	F	304	 2% 84% 12% 4%
1	G	304	 2% 82% 13% 5%
1	H	304	 2% 81% 15% 4%

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 [i](#)

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

- # S4M

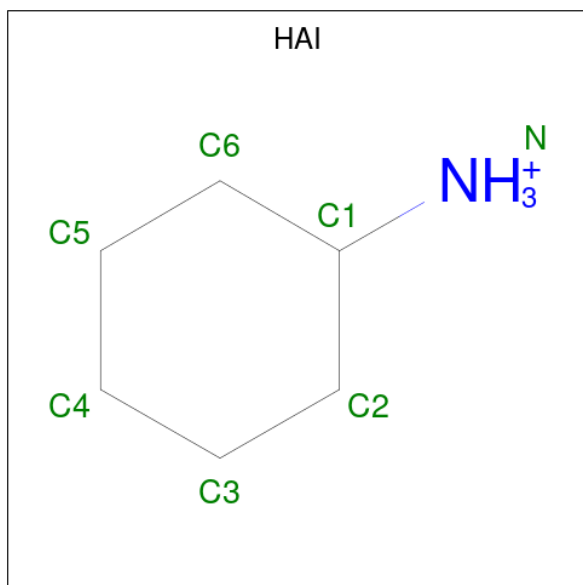
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 24	C 14	N 6	O 3	S 1	0	0
2	B	1	Total 24	C 14	N 6	O 3	S 1	0	0
2	C	1	Total 24	C 14	N 6	O 3	S 1	0	0
2	D	1	Total 24	C 14	N 6	O 3	S 1	0	0
2	E	1	Total 24	C 14	N 6	O 3	S 1	0	0



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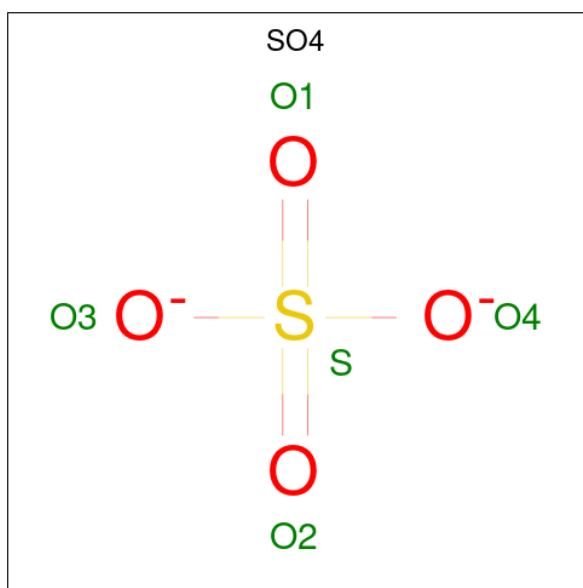
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	G	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	H	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is CYCLOHEXYLAMMONIUM ION (three-letter code: HAI) (formula:  $C_6H_{14}N$ ).



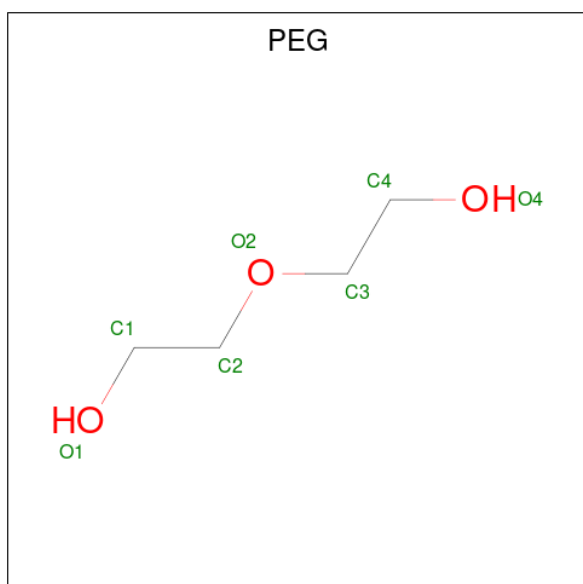
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			7	6	1		
3	B	1	Total	C	N	0	0
			7	6	1		
3	C	1	Total	C	N	0	0
			7	6	1		
3	D	1	Total	C	N	0	0
			7	6	1		
3	E	1	Total	C	N	0	0
			7	6	1		
3	F	1	Total	C	N	0	0
			7	6	1		
3	G	1	Total	C	N	0	0
			7	6	1		
3	H	1	Total	C	N	0	0
			7	6	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



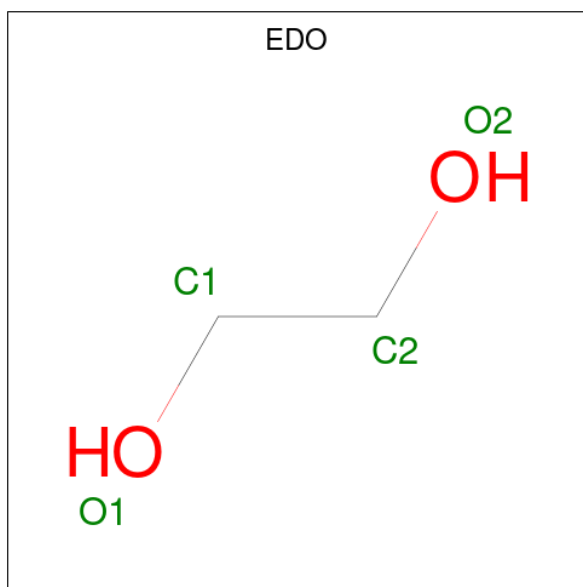
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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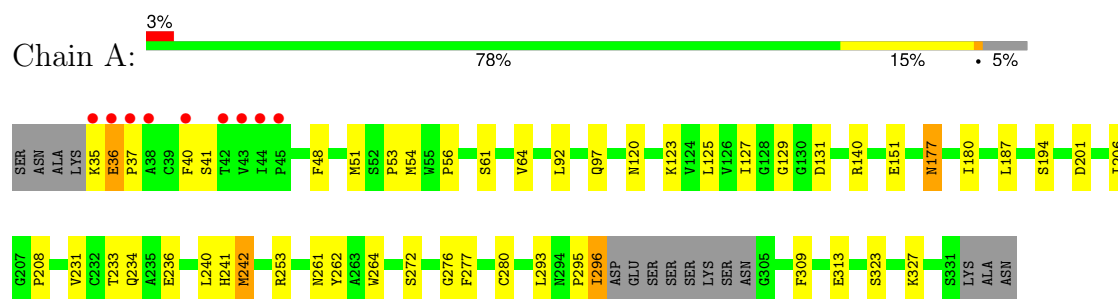
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	306	Total 306	O 306	0	0
7	H	309	Total 309	O 309	0	0

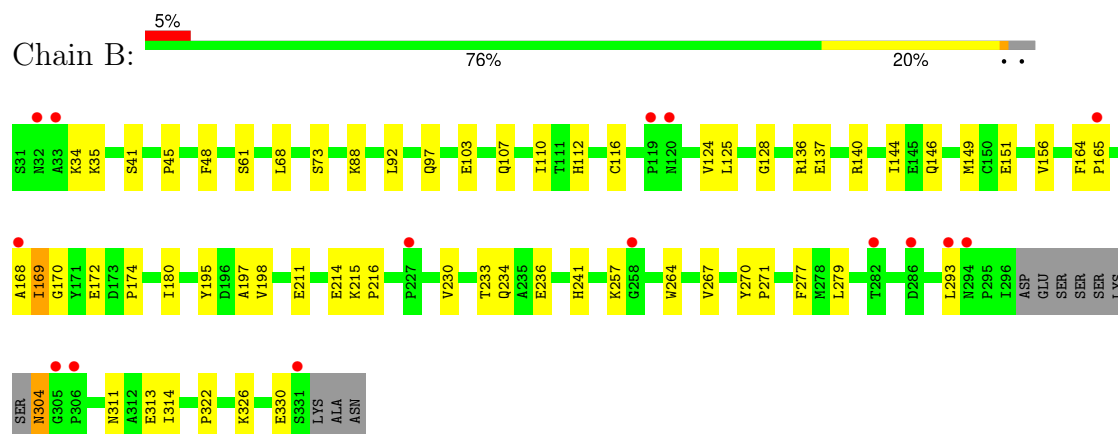
### 3 Residue-property plots [i](#)

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.

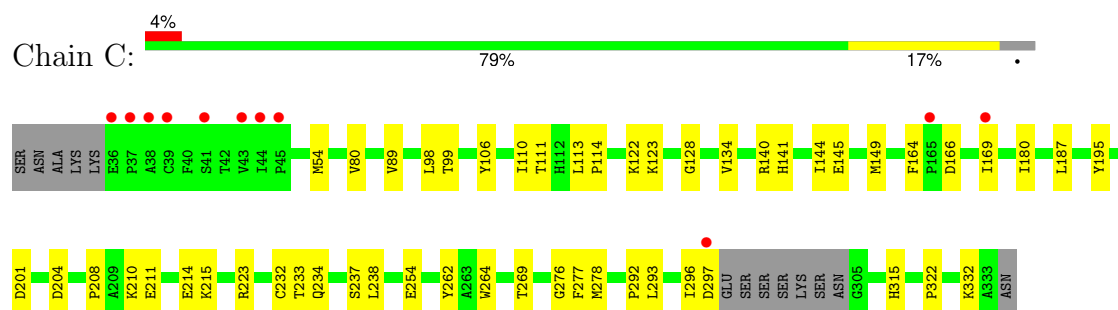
#### • Molecule 1: Spermidine synthase 1



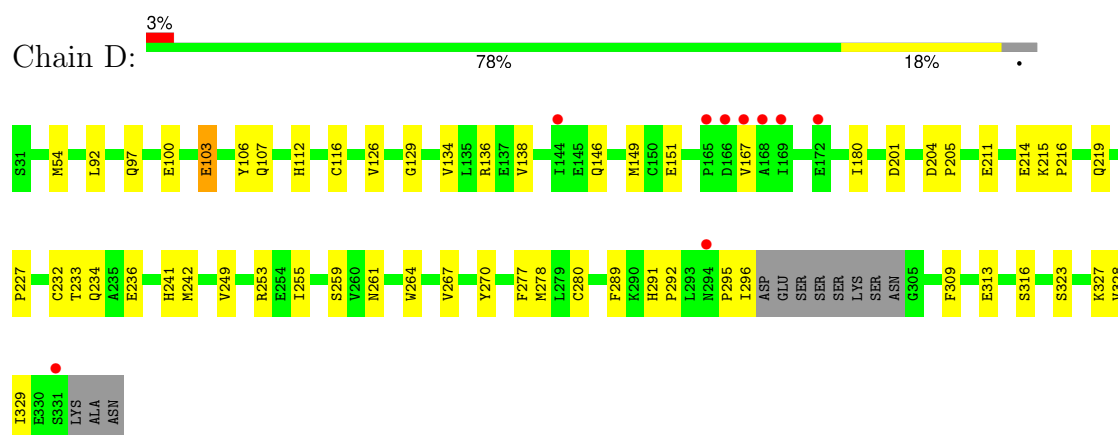
#### • Molecule 1: Spermidine synthase 1



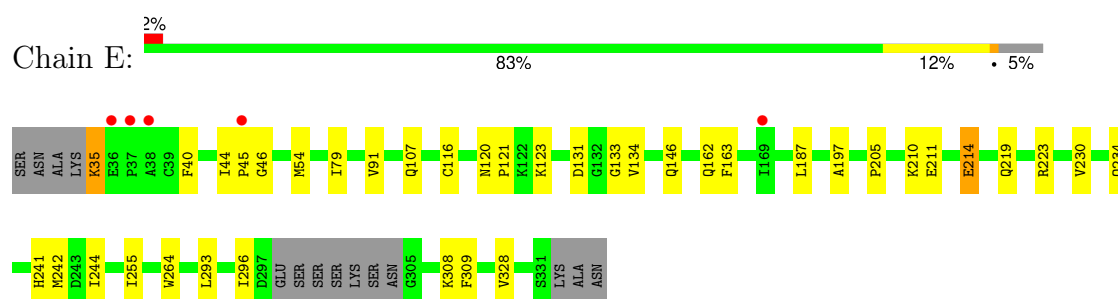
#### • Molecule 1: Spermidine synthase 1



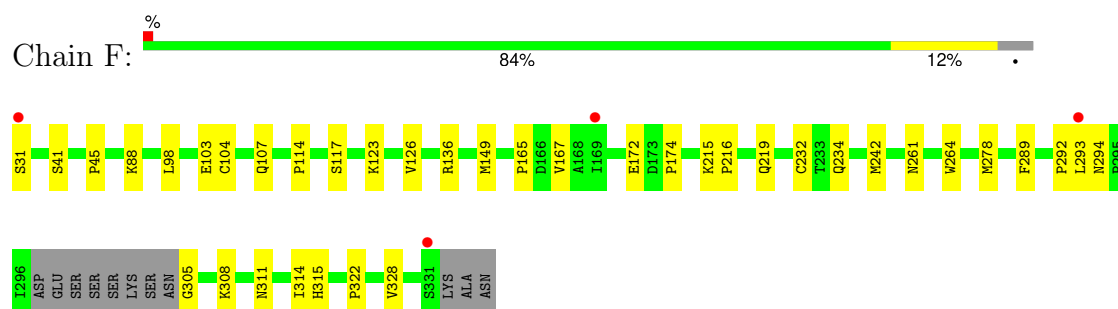
#### • Molecule 1: Spermidine synthase 1



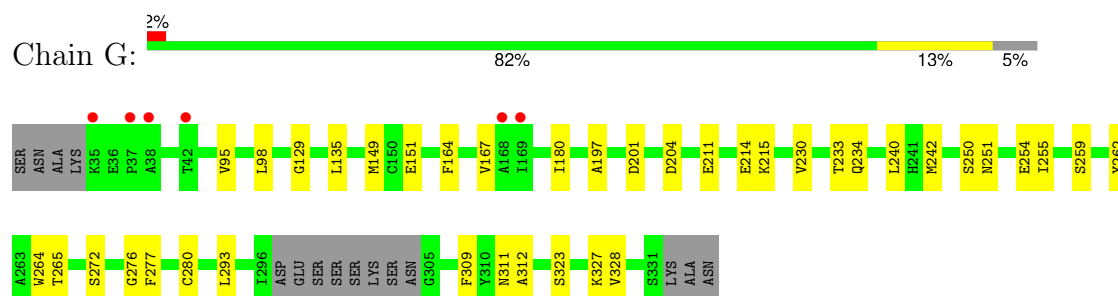
- Molecule 1: Spermidine synthase 1



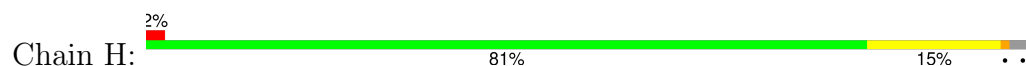
- Molecule 1: Spermidine synthase 1

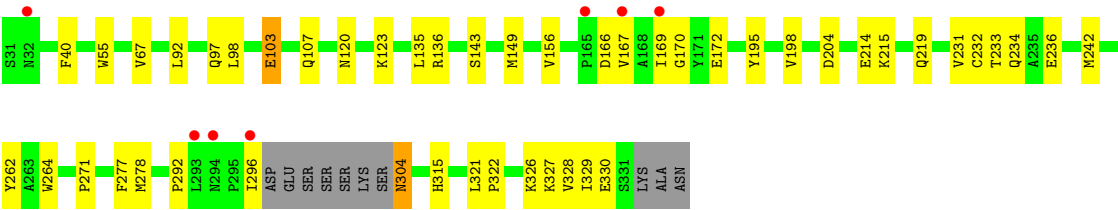


- Molecule 1: Spermidine synthase 1



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 81.7 (47.60-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.219 , 0.261 0.225 , 0.264	Depositor DCC
$R_{free}$ test set	1621 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtrriage
Anisotropy	0.451	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, HAI, S4M, SO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.86	0/2302	0.96	0/3126
1	B	0.85	0/2321	0.95	0/3152
1	C	0.87	0/2324	0.98	0/3157
1	D	0.90	0/2339	0.95	0/3176
1	E	0.99	0/2327	1.07	0/3160
1	F	1.01	0/2321	1.04	0/3151
1	G	1.01	0/2301	1.05	0/3126
1	H	1.03	0/2339	1.06	0/3176
All	All	0.94	0/18574	1.01	0/25224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2240	0	2218	35	0
1	B	2265	0	2234	43	0
1	C	2259	0	2226	32	0
1	D	2274	0	2253	43	0
1	E	2259	0	2237	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2262	0	2237	29	0
1	G	2239	0	2221	27	0
1	H	2277	0	2246	43	0
2	A	24	0	24	0	0
2	B	24	0	24	1	0
2	C	24	0	24	3	0
2	D	24	0	24	1	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	2	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	11	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	304	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 8.

All (304) 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: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:E:107:GLN:HE21	1:E:133:GLY:C	1.87	0.77
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: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:E:35:LYS:N	1:E:40:PHE:HB3	2.04	0.72
1:E:107:GLN:NE2	1:E:133:GLY:C	2.44	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
1:H:103:GLU:CD	1:H:107:GLN:NE2	2.46	0.69
1:H:215:LYS:HG2	1:H:219:GLN:NE2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:242:MET:HA	1:A:242:MET:HE3	1.74	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:E:242:MET:HE2	1:E:328:VAL:HG11	1.79	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
5:G:403:PEG:H21	7:G:621:HOH:O	2.00	0.62
1:B:304:ASN:ND2	7:B:504:HOH:O	2.33	0.61
1:G:242:MET:HE1	1:G:328:VAL:CG1	2.30	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: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
1:E:162:GLN:HG2	1:E:163:PHE:CE2	2.40	0.57
1:H:103:GLU:CD	1:H:107:GLN:HE22	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211[B]:GLU:HA	1:E:214:GLU:HG3	1.86	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: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:C:297:ASP:OD1	1:C:297:ASP:C	2.47	0.53
1:H:304:ASN:N	7:H:514:HOH:O	2.41	0.53
1:B:128:GLY:O	1:B:149:MET:HE3	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:197:ALA:HA	1:E:230:VAL:O	2.11	0.50
1:F:123:LYS:NZ	7:F:514:HOH:O	2.44	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:E:116:CYS:HG	1:E:296:ILE:HD12	1.79	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:G:242:MET:HE1	1:G:328:VAL:HG11	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:242:MET:HA	1:A:242:MET:HE2	1.97	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
2:F:401:S4M:HE1	2:F:401:S4M:HB1	1.83	0.46
1:A:295:PRO:HB3	7:A:592:HOH:O	2.16	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: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
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:F:103:GLU:HG3	1:F:104:CYS:N	2.33	0.44
1:C:106:TYR:CE1	2:C:401:S4M:HA2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
2:E:401:S4M:HE2	2:E:401:S4M:HB1	1.83	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211[A]:GLU:HA	1:E:211[A]:GLU:OE1	2.18	0.42
1:H:233:THR:O	1:H:277:PHE:HA	2.19	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: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:C:111:THR:C	1:C:114:PRO:HD2	2.41	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:D:242:MET:HE2	1:D:328:VAL:HG21	2.01	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: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
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
2:H:401:S4M:HE1	2:H:401:S4M:HB1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:GLY:HA2	1:G:201:ASP:OD2	2.21	0.41
1:C:128:GLY:O	1:C:149:MET:HE3	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 [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	287/304 (94%)	275 (96%)	11 (4%)	1 (0%)	41	27
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	239 (96%)	10 (4%)	31	16
1	B	251/260 (96%)	244 (97%)	7 (3%)	43	30
1	C	251/260 (96%)	246 (98%)	5 (2%)	55	44
1	D	253/260 (97%)	248 (98%)	5 (2%)	55	44
1	E	252/260 (97%)	244 (97%)	8 (3%)	39	25
1	F	251/260 (96%)	247 (98%)	4 (2%)	62	54
1	G	249/260 (96%)	243 (98%)	6 (2%)	49	36
1	H	253/260 (97%)	248 (98%)	5 (2%)	55	44
All	All	2009/2080 (97%)	1959 (98%)	50 (2%)	49	34

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	MET
1	A	131	ASP
1	A	177[A]	ASN
1	A	177[B]	ASN
1	A	187	LEU
1	A	234	GLN
1	A	242	MET

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Mol	Chain	Res	Type
1	A	264	TRP
1	A	293	LEU
1	A	296	ILE
1	B	34	LYS
1	B	103	GLU
1	B	169	ILE
1	B	234	GLN
1	B	264	TRP
1	B	293	LEU
1	B	304	ASN
1	C	187	LEU
1	C	234	GLN
1	C	237	SER
1	C	264	TRP
1	C	293	LEU
1	D	103[A]	GLU
1	D	103[B]	GLU
1	D	234	GLN
1	D	264	TRP
1	D	316	SER
1	E	35	LYS
1	E	131	ASP
1	E	187	LEU
1	E	214	GLU
1	E	234	GLN
1	E	264	TRP
1	E	293	LEU
1	E	308	LYS
1	F	98	LEU
1	F	234	GLN
1	F	264	TRP
1	F	294	ASN
1	G	98[A]	LEU
1	G	98[B]	LEU
1	G	234	GLN
1	G	264	TRP
1	G	265	THR
1	G	293	LEU
1	H	98	LEU
1	H	103	GLU
1	H	234	GLN
1	H	264	TRP

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Mol	Chain	Res	Type
1	H	304	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	B	189	ASN
1	B	219	GLN
1	B	261	ASN
1	C	70	GLN
1	C	189	ASN
1	C	219	GLN
1	C	261	ASN
1	D	82	GLN
1	D	189	ASN
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	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 monosaccharides 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	$\# Z  > 2$
2	S4M	B	401	-	21,26,26	0.60	0	19,37,37	1.53	3 (15%)
2	S4M	D	401	-	21,26,26	0.72	0	19,37,37	1.32	1 (5%)
4	SO4	E	404	-	4,4,4	0.45	0	6,6,6	0.22	0
3	HAI	G	402	-	7,7,7	0.41	0	8,8,8	0.40	0
6	EDO	G	404	-	3,3,3	0.37	0	2,2,2	0.11	0
4	SO4	B	403	-	4,4,4	0.33	0	6,6,6	0.20	0
3	HAI	E	402	-	7,7,7	0.59	0	8,8,8	1.01	0
5	PEG	G	403	-	6,6,6	0.20	0	5,5,5	0.20	0
2	S4M	H	401	-	21,26,26	0.66	0	19,37,37	1.58	4 (21%)
3	HAI	A	402	-	7,7,7	0.53	0	8,8,8	0.75	0
2	S4M	F	401	-	21,26,26	0.73	0	19,37,37	1.36	2 (10%)
3	HAI	D	402	-	7,7,7	0.39	0	8,8,8	0.52	0
3	HAI	H	402	-	7,7,7	0.35	0	8,8,8	0.50	0
5	PEG	E	403	-	6,6,6	0.28	0	5,5,5	0.21	0
3	HAI	B	402	-	7,7,7	0.56	0	8,8,8	0.79	0
6	EDO	F	403	-	3,3,3	0.18	0	2,2,2	0.25	0
3	HAI	F	402	-	7,7,7	0.41	0	8,8,8	1.29	2 (25%)
2	S4M	G	401	-	21,26,26	0.74	1 (4%)	19,37,37	1.39	3 (15%)
4	SO4	G	405	-	4,4,4	0.45	0	6,6,6	0.22	0
3	HAI	C	402	-	7,7,7	0.37	0	8,8,8	1.35	2 (25%)
4	SO4	C	403	-	4,4,4	0.35	0	6,6,6	0.15	0
2	S4M	C	401	-	21,26,26	0.73	1 (4%)	19,37,37	1.25	2 (10%)
2	S4M	A	401	-	21,26,26	0.66	0	19,37,37	1.55	2 (10%)
2	S4M	E	401	-	21,26,26	0.65	0	19,37,37	1.42	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S4M	B	401	-	-	2/8/28/28	0/3/3/3
2	S4M	D	401	-	-	5/8/28/28	0/3/3/3
6	EDO	G	404	-	-	0/1/1/1	-
3	HAI	G	402	-	-	-	0/1/1/1
3	HAI	E	402	-	-	-	0/1/1/1
5	PEG	G	403	-	-	2/4/4/4	-
2	S4M	H	401	-	-	2/8/28/28	0/3/3/3
3	HAI	A	402	-	-	-	0/1/1/1
2	S4M	F	401	-	-	3/8/28/28	0/3/3/3
3	HAI	D	402	-	-	-	0/1/1/1
3	HAI	H	402	-	-	-	0/1/1/1
5	PEG	E	403	-	-	2/4/4/4	-
3	HAI	B	402	-	-	-	0/1/1/1
6	EDO	F	403	-	-	1/1/1/1	-
3	HAI	F	402	-	-	-	0/1/1/1
2	S4M	G	401	-	-	2/8/28/28	0/3/3/3
3	HAI	C	402	-	-	-	0/1/1/1
2	S4M	C	401	-	-	2/8/28/28	0/3/3/3
2	S4M	A	401	-	-	2/8/28/28	0/3/3/3
2	S4M	E	401	-	-	3/8/28/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	S4M	C8-N7	-2.14	1.30	1.34
2	G	401	S4M	C8-N7	-2.08	1.30	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	S4M	C4'-O4'-C1'	-5.88	104.54	109.92
2	B	401	S4M	C4'-O4'-C1'	-4.76	105.57	109.92
2	D	401	S4M	C4'-O4'-C1'	-4.74	105.59	109.92
2	G	401	S4M	C4'-O4'-C1'	-4.35	105.94	109.92
2	H	401	S4M	C4'-O4'-C1'	-4.17	106.11	109.92
2	E	401	S4M	C4'-O4'-C1'	-4.05	106.22	109.92
2	F	401	S4M	C4'-O4'-C1'	-3.45	106.77	109.92
2	F	401	S4M	O4'-C4'-C5'	2.95	116.34	108.88
2	C	401	S4M	C5-C6-N6	2.94	124.79	120.31
2	C	401	S4M	C4'-O4'-C1'	-2.92	107.25	109.92
2	B	401	S4M	O4'-C4'-C5'	2.91	116.24	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	S4M	O4'-C4'-C5'	2.88	116.15	108.88
2	H	401	S4M	C5-C6-N6	2.38	123.93	120.31
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	B	401	S4M	C5-C6-N6	2.19	123.65	120.31
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
2	A	401	S4M	C5-C6-N6	2.15	123.59	120.31
2	H	401	S4M	O4'-C1'-N9	2.12	111.56	108.75
2	G	401	S4M	C5-C6-N6	2.11	123.53	120.31
2	E	401	S4M	C5-C6-N6	2.10	123.51	120.31
3	F	402	HAI	C3-C2-C1	2.07	114.58	111.77

There are no chirality outliers.

All (26) 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	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

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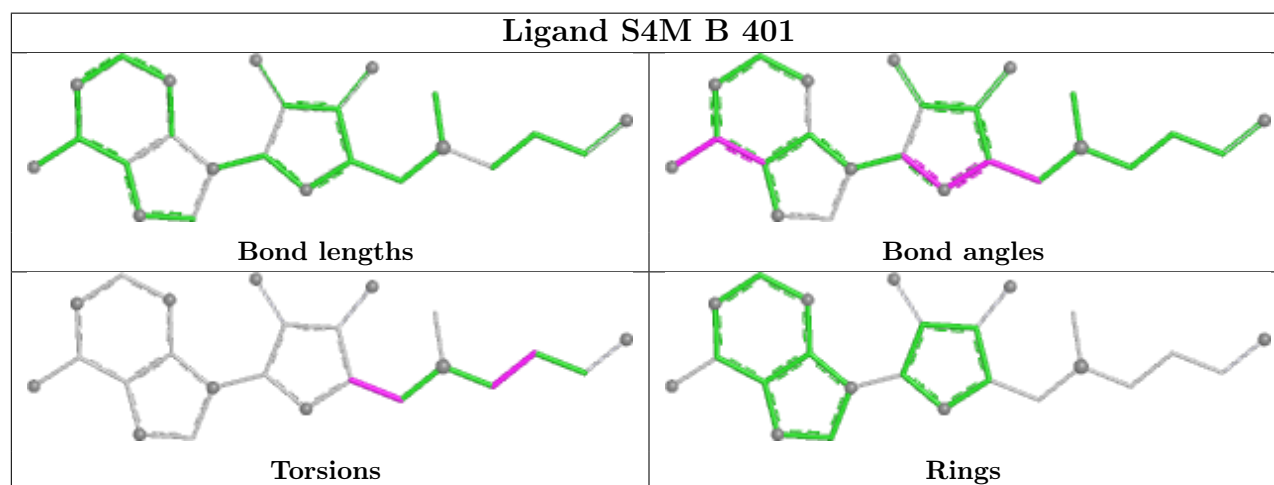
Mol	Chain	Res	Type	Atoms
2	D	401	S4M	CA-CB-CG-SD
2	H	401	S4M	CA-CB-CG-SD

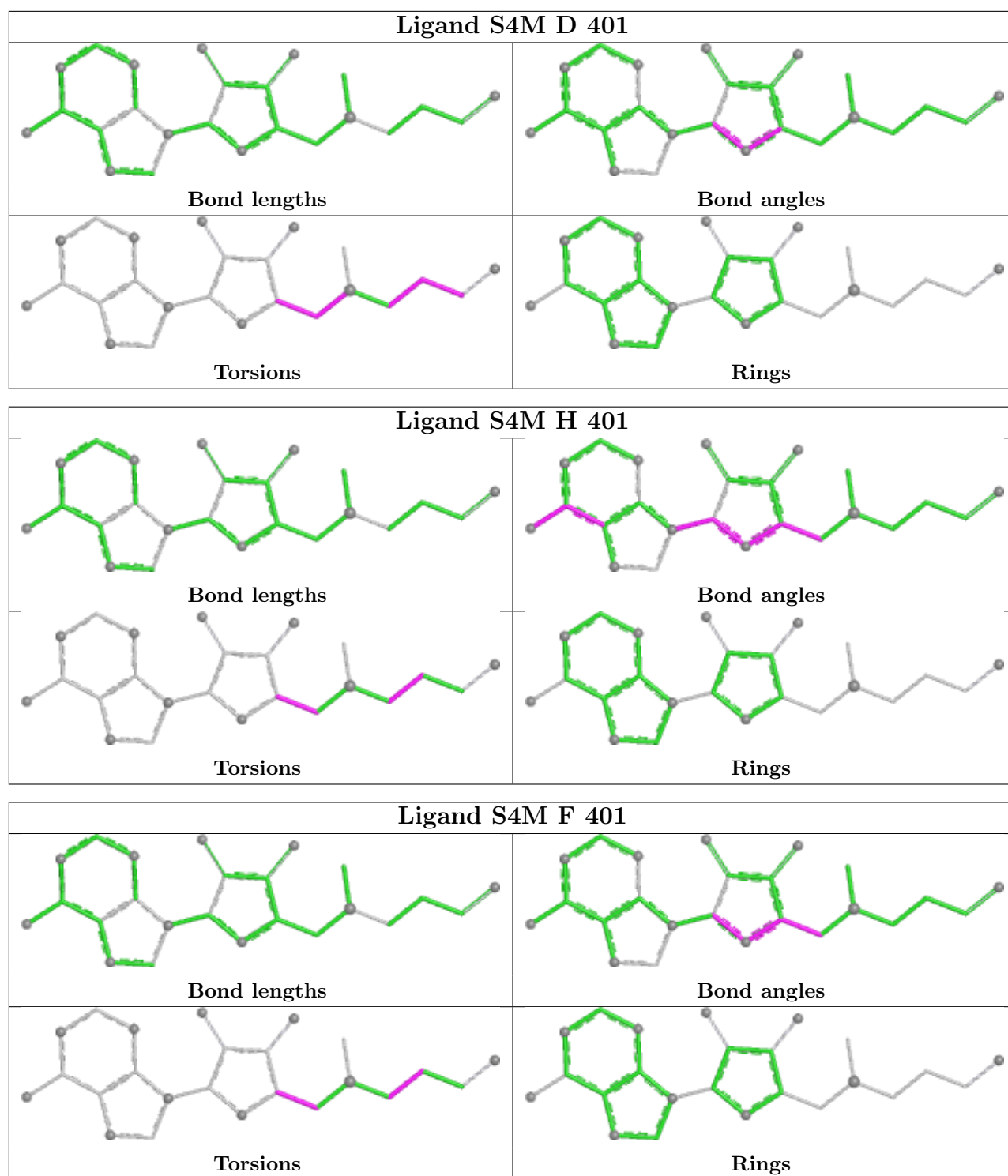
There are no ring outliers.

10 monomers are involved in 30 short contacts:

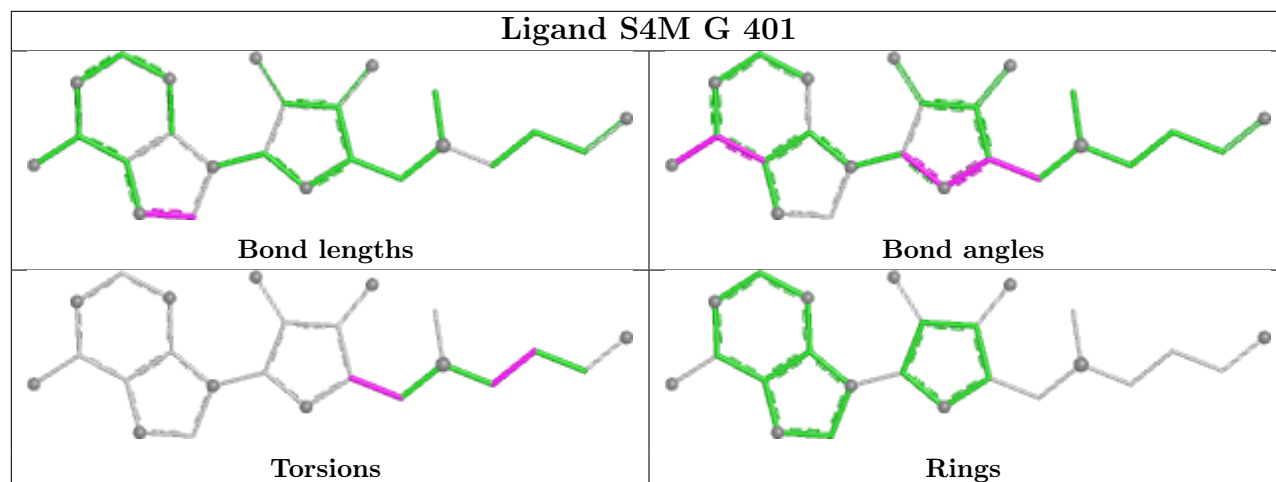
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	S4M	1	0
2	D	401	S4M	1	0
6	G	404	EDO	8	0
5	G	403	PEG	2	0
2	H	401	S4M	2	0
2	F	401	S4M	1	0
3	D	402	HAI	1	0
5	E	403	PEG	10	0
2	C	401	S4M	3	0
2	E	401	S4M	1	0

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.

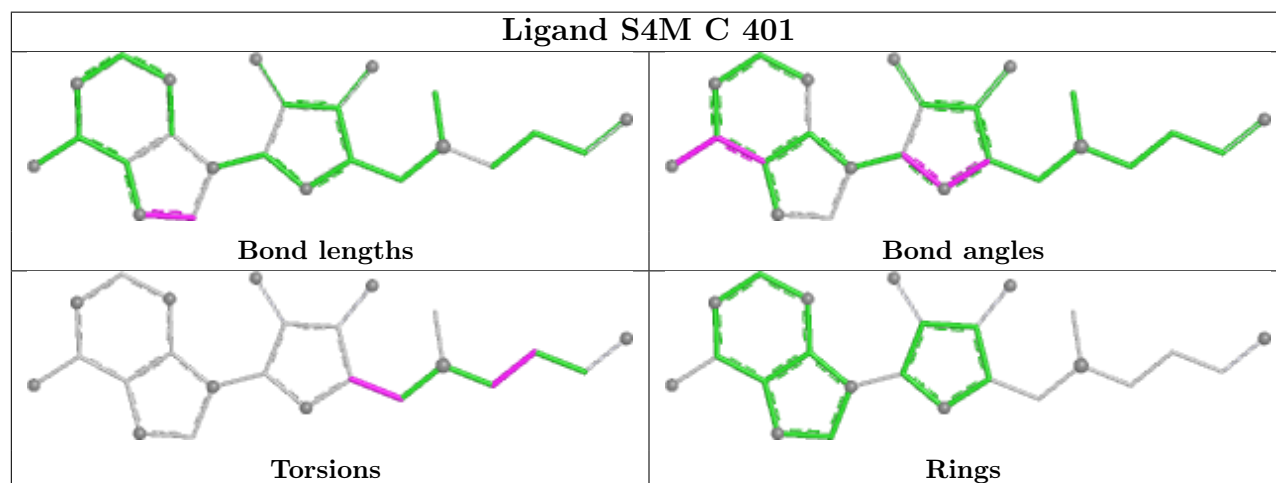




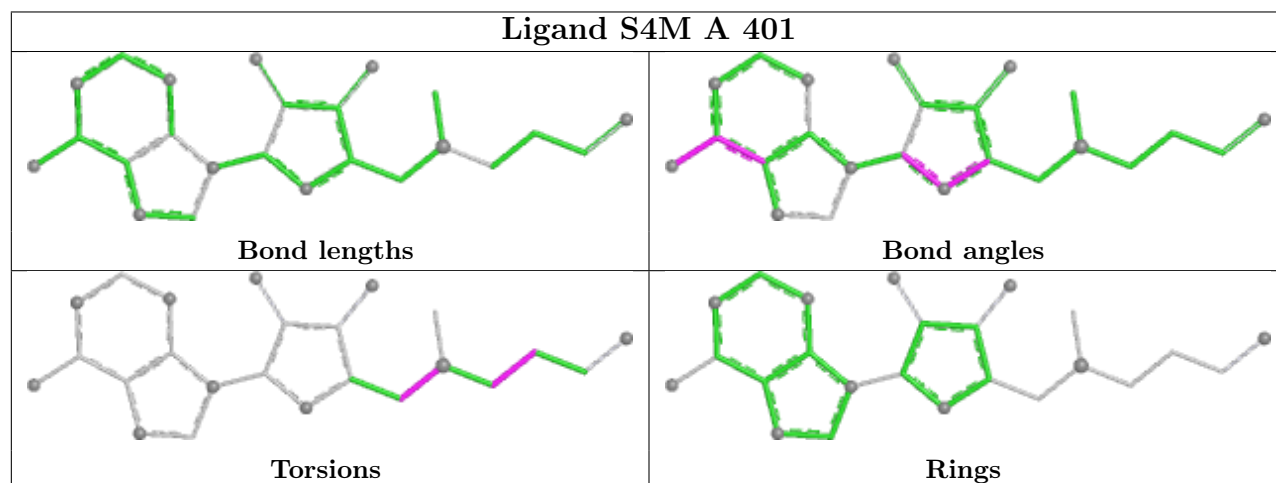
## Ligand S4M G 401



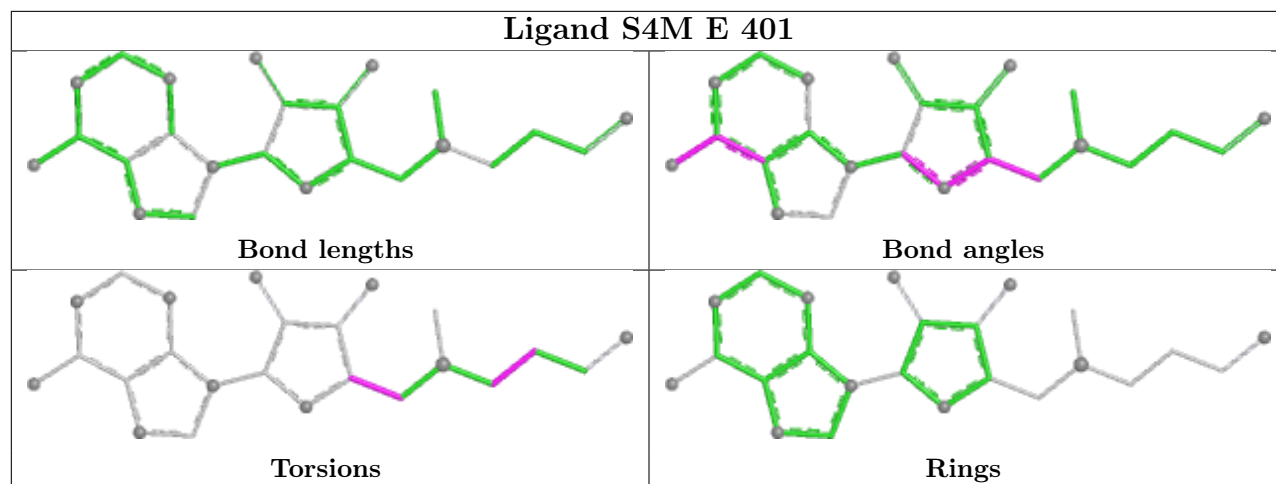
## Ligand S4M C 401



## Ligand S4M A 401







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	289/304 (95%)	0.09	9 (3%)	49	43	13, 19, 35, 64	0
1	B	294/304 (96%)	0.35	15 (5%)	28	22	14, 23, 42, 55	0
1	C	291/304 (95%)	0.18	11 (3%)	40	35	13, 21, 39, 60	0
1	D	293/304 (96%)	0.27	9 (3%)	49	43	14, 22, 41, 58	0
1	E	290/304 (95%)	0.09	5 (1%)	70	66	9, 12, 32, 54	0
1	F	293/304 (96%)	0.06	4 (1%)	75	72	10, 13, 28, 50	0
1	G	289/304 (95%)	0.13	6 (2%)	63	59	9, 12, 31, 51	0
1	H	294/304 (96%)	0.14	7 (2%)	59	54	10, 12, 27, 44	0
All	All	2333/2432 (95%)	0.16	66 (2%)	53	47	9, 17, 37, 64	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	ILE	5.7
1	D	331	SER	5.0
1	A	36	GLU	4.8
1	B	32	ASN	4.8
1	C	37	PRO	4.5
1	G	37	PRO	4.4
1	H	293	LEU	4.2
1	D	172	GLU	3.9
1	D	167	VAL	3.8
1	C	36	GLU	3.6
1	C	169	ILE	3.5
1	H	167	VAL	3.5
1	G	169	ILE	3.5
1	C	38	ALA	3.4
1	F	331	SER	3.3
1	A	35	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	44	ILE	3.2
1	E	37	PRO	3.1
1	A	42	THR	3.1
1	G	38	ALA	3.0
1	A	37	PRO	3.0
1	D	166	ASP	3.0
1	B	33	ALA	2.9
1	C	43	VAL	2.9
1	A	38	ALA	2.8
1	A	44	ILE	2.8
1	G	35	LYS	2.8
1	C	45	PRO	2.8
1	D	165	PRO	2.7
1	B	293	LEU	2.7
1	B	306	PRO	2.6
1	D	168	ALA	2.6
1	A	43	VAL	2.6
1	H	165	PRO	2.6
1	H	169	ILE	2.6
1	B	258	GLY	2.5
1	F	293	LEU	2.4
1	B	305	GLY	2.4
1	B	120	ASN	2.4
1	G	168	ALA	2.4
1	B	119	PRO	2.4
1	B	165	PRO	2.4
1	C	297	ASP	2.3
1	E	36	GLU	2.3
1	E	38	ALA	2.3
1	B	227	PRO	2.3
1	B	168	ALA	2.2
1	B	282	THR	2.2
1	E	169	ILE	2.2
1	B	294	ASN	2.2
1	E	45	PRO	2.2
1	B	331	SER	2.1
1	B	286	ASP	2.1
1	H	296	ILE	2.1
1	F	169	ILE	2.1
1	D	294	ASN	2.1
1	D	144	ILE	2.1
1	H	32	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	40	PHE	2.0
1	C	165	PRO	2.0
1	C	39	CYS	2.0
1	F	31	SER	2.0
1	A	45	PRO	2.0
1	H	294	ASN	2.0
1	C	41	SER	2.0
1	G	42	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HAI	B	402	7/7	0.79	0.17	17,19,19,19	0
5	PEG	E	403	7/7	0.86	0.21	22,24,30,31	0
3	HAI	H	402	7/7	0.89	0.15	9,9,9,10	0
3	HAI	A	402	7/7	0.89	0.14	17,18,18,19	0
2	S4M	B	401	24/24	0.90	0.11	14,17,23,26	0
2	S4M	C	401	24/24	0.90	0.12	14,20,25,27	0
3	HAI	E	402	7/7	0.91	0.13	9,9,10,10	0
2	S4M	A	401	24/24	0.91	0.11	14,16,21,23	0
2	S4M	D	401	24/24	0.91	0.12	15,18,25,28	0
3	HAI	D	402	7/7	0.92	0.12	14,15,15,15	0
2	S4M	H	401	24/24	0.93	0.12	9,10,10,11	0
3	HAI	C	402	7/7	0.93	0.10	17,18,18,18	0
2	S4M	F	401	24/24	0.93	0.12	9,10,10,11	0
5	PEG	G	403	7/7	0.93	0.11	34,36,38,40	0
6	EDO	G	404	4/4	0.93	0.15	23,24,26,31	0

*Continued on next page...*

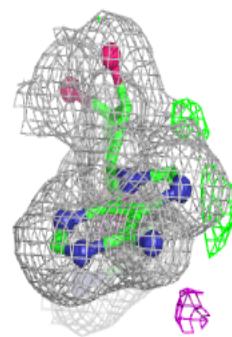
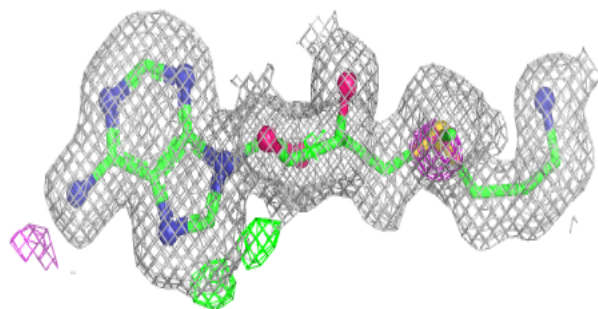
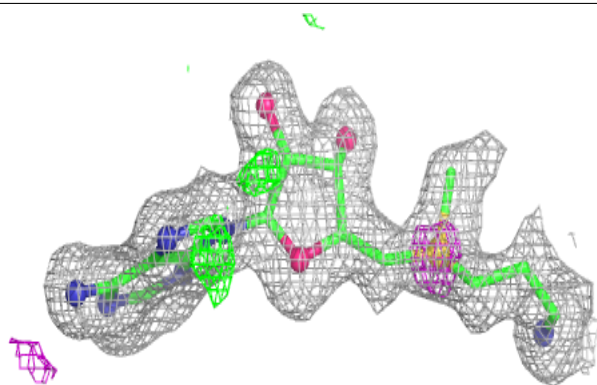
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HAI	F	402	7/7	0.94	0.12	9,9,9,10	0
3	HAI	G	402	7/7	0.94	0.14	9,9,10,10	0
6	EDO	F	403	4/4	0.94	0.08	27,29,29,32	0
2	S4M	E	401	24/24	0.94	0.10	10,11,11,11	0
2	S4M	G	401	24/24	0.95	0.10	9,11,11,11	0
4	SO4	B	403	5/5	0.96	0.12	27,29,33,34	0
4	SO4	C	403	5/5	0.96	0.16	29,37,38,40	0
4	SO4	E	404	5/5	0.97	0.15	22,26,32,34	0
4	SO4	G	405	5/5	0.98	0.09	23,27,28,34	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.

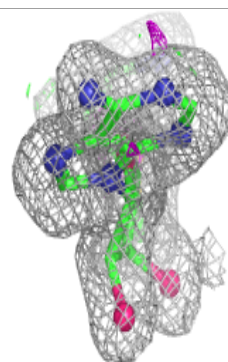
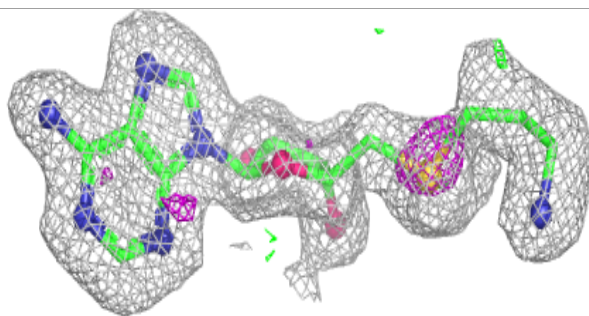
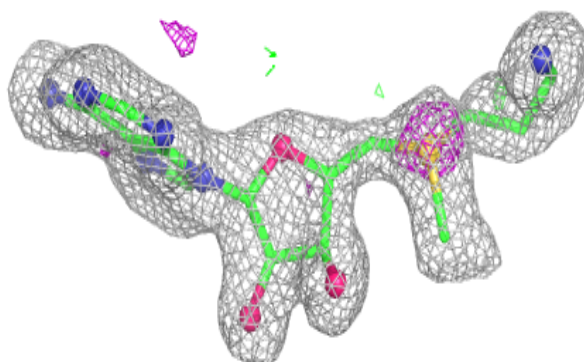
**Electron density around S4M B 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

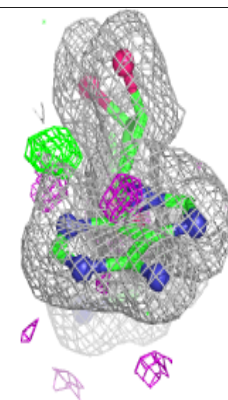
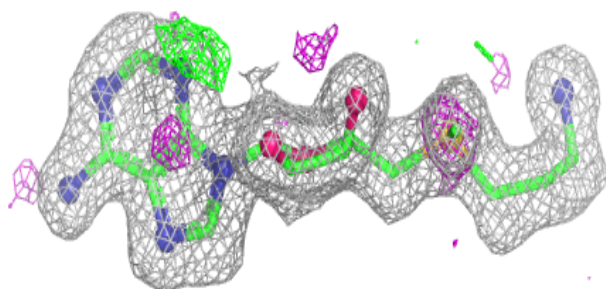
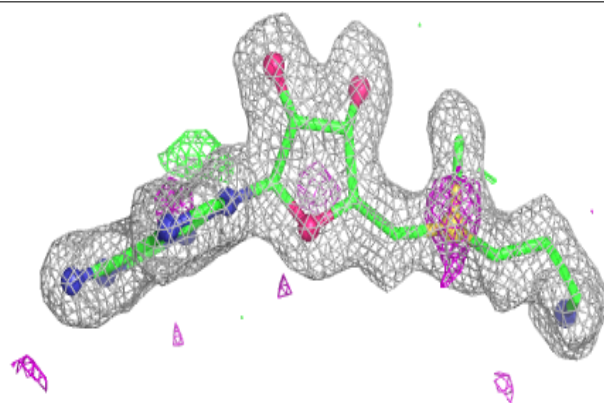


**Electron density around S4M C 401:**

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

**Electron density around S4M A 401:**

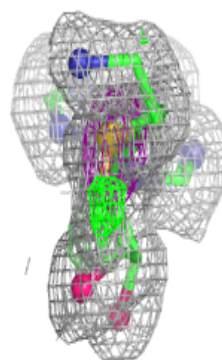
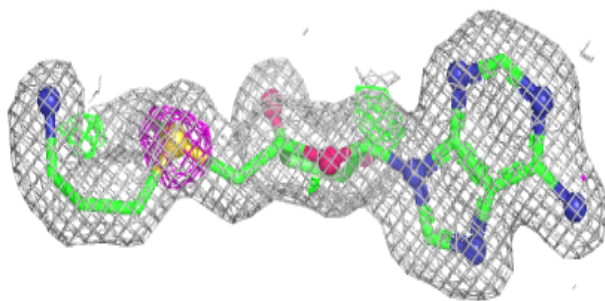
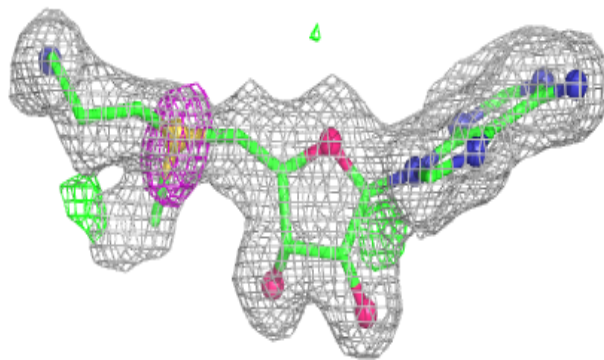
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



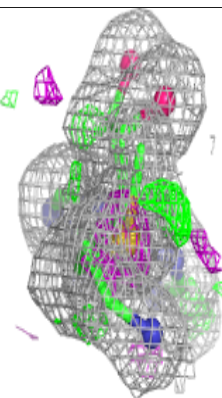
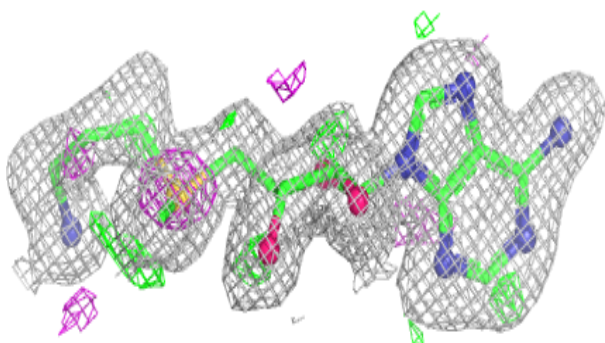
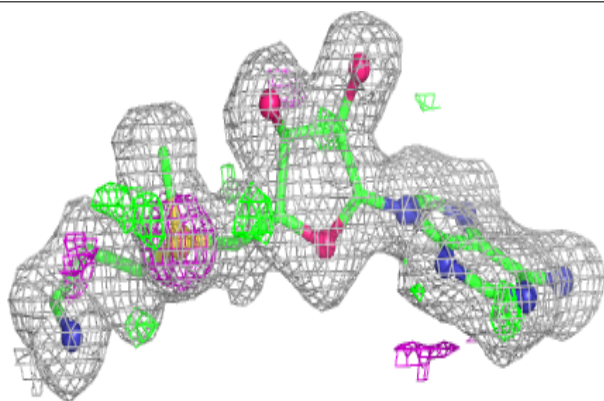


**Electron density around S4M D 401:**

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

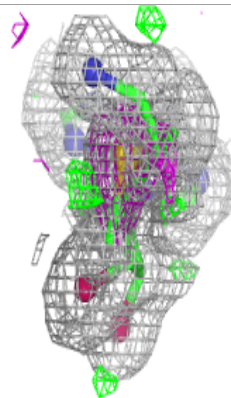
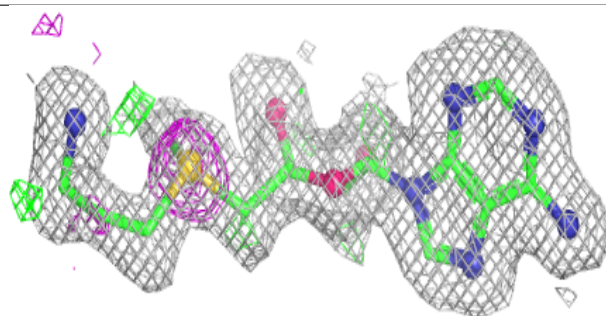
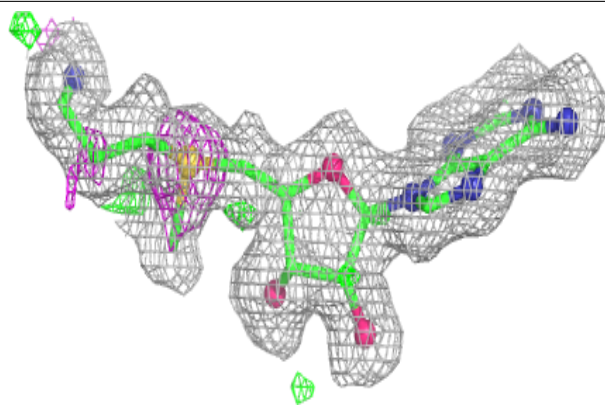
**Electron density around S4M H 401:**

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

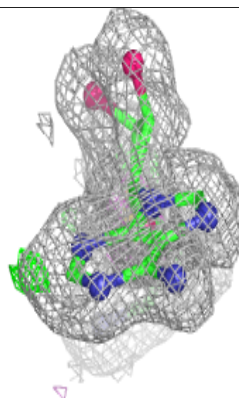
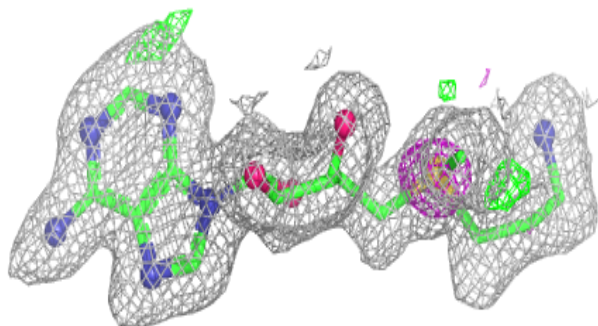
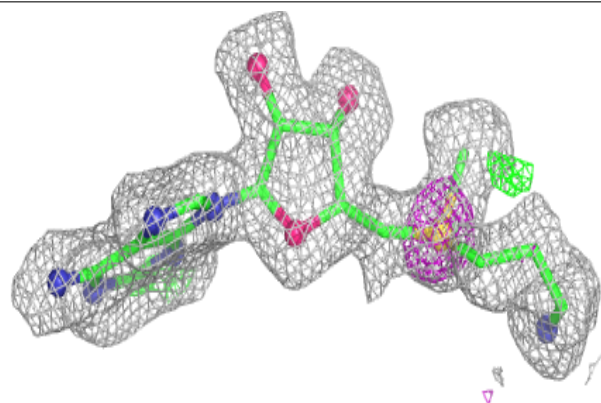


**Electron density around S4M F 401:**

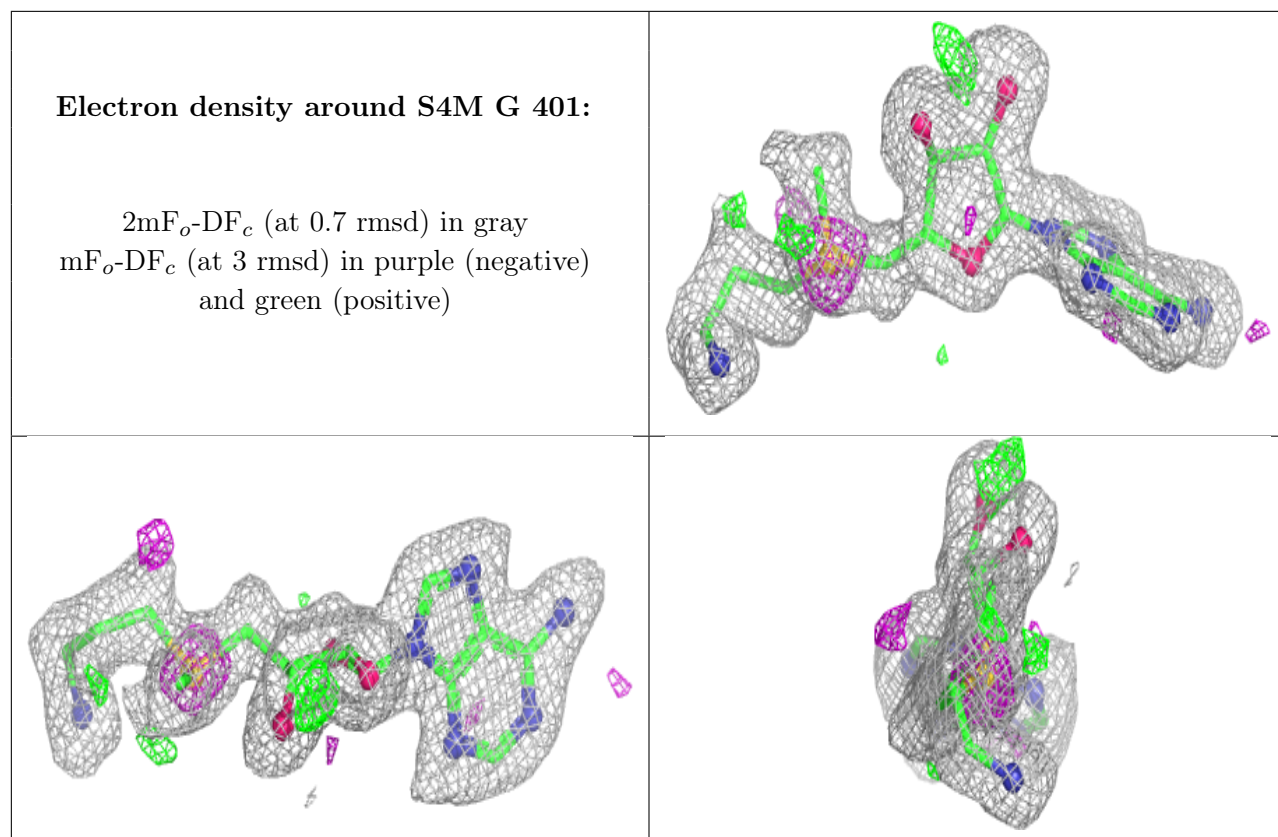
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.