



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:47 AM GMT

PDB ID : 3C6M  
Title : Crystal structure of human spermine synthase in complex with spermine and 5-methylthioadenosine  
Authors : Min, J.; Wu, H.; Zeng, H.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Pegg, A.E.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-02-04  
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

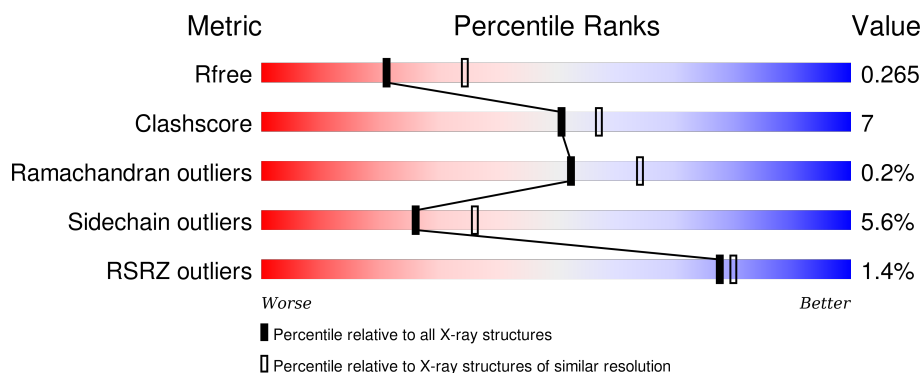
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	381	
1	B	381	
1	C	381	
1	D	381	

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
2	SPM	A	501	-	-	-	X
2	SPM	D	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10378 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 Spermine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2676	1714	436	509	17			
1	B	342	Total	C	N	O	S	0	0	0
			2719	1738	446	518	17			
1	C	291	Total	C	N	O	S	0	0	0
			2325	1490	379	440	16			
1	D	278	Total	C	N	O	S	0	0	0
			2222	1430	362	415	15			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	EXPRESSION TAG	UNP P52788
A	-13	GLY	-	EXPRESSION TAG	UNP P52788
A	-12	SER	-	EXPRESSION TAG	UNP P52788
A	-11	SER	-	EXPRESSION TAG	UNP P52788
A	-10	HIS	-	EXPRESSION TAG	UNP P52788
A	-9	HIS	-	EXPRESSION TAG	UNP P52788
A	-8	HIS	-	EXPRESSION TAG	UNP P52788
A	-7	HIS	-	EXPRESSION TAG	UNP P52788
A	-6	HIS	-	EXPRESSION TAG	UNP P52788
A	-5	HIS	-	EXPRESSION TAG	UNP P52788
A	-4	SER	-	EXPRESSION TAG	UNP P52788
A	-3	SER	-	EXPRESSION TAG	UNP P52788
A	-2	GLY	-	EXPRESSION TAG	UNP P52788
A	-1	LEU	-	EXPRESSION TAG	UNP P52788
A	0	VAL	-	EXPRESSION TAG	UNP P52788
A	1	PRO	-	EXPRESSION TAG	UNP P52788
A	2	ARG	-	EXPRESSION TAG	UNP P52788
A	3	GLY	-	EXPRESSION TAG	UNP P52788
A	4	SER	-	EXPRESSION TAG	UNP P52788
B	-14	MET	-	EXPRESSION TAG	UNP P52788
B	-13	GLY	-	EXPRESSION TAG	UNP P52788

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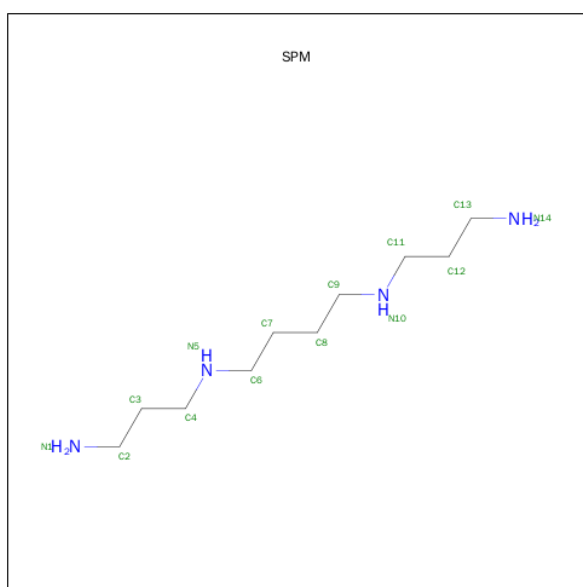
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	SER	-	EXPRESSION TAG	UNP P52788
B	-11	SER	-	EXPRESSION TAG	UNP P52788
B	-10	HIS	-	EXPRESSION TAG	UNP P52788
B	-9	HIS	-	EXPRESSION TAG	UNP P52788
B	-8	HIS	-	EXPRESSION TAG	UNP P52788
B	-7	HIS	-	EXPRESSION TAG	UNP P52788
B	-6	HIS	-	EXPRESSION TAG	UNP P52788
B	-5	HIS	-	EXPRESSION TAG	UNP P52788
B	-4	SER	-	EXPRESSION TAG	UNP P52788
B	-3	SER	-	EXPRESSION TAG	UNP P52788
B	-2	GLY	-	EXPRESSION TAG	UNP P52788
B	-1	LEU	-	EXPRESSION TAG	UNP P52788
B	0	VAL	-	EXPRESSION TAG	UNP P52788
B	1	PRO	-	EXPRESSION TAG	UNP P52788
B	2	ARG	-	EXPRESSION TAG	UNP P52788
B	3	GLY	-	EXPRESSION TAG	UNP P52788
B	4	SER	-	EXPRESSION TAG	UNP P52788
C	-14	MET	-	EXPRESSION TAG	UNP P52788
C	-13	GLY	-	EXPRESSION TAG	UNP P52788
C	-12	SER	-	EXPRESSION TAG	UNP P52788
C	-11	SER	-	EXPRESSION TAG	UNP P52788
C	-10	HIS	-	EXPRESSION TAG	UNP P52788
C	-9	HIS	-	EXPRESSION TAG	UNP P52788
C	-8	HIS	-	EXPRESSION TAG	UNP P52788
C	-7	HIS	-	EXPRESSION TAG	UNP P52788
C	-6	HIS	-	EXPRESSION TAG	UNP P52788
C	-5	HIS	-	EXPRESSION TAG	UNP P52788
C	-4	SER	-	EXPRESSION TAG	UNP P52788
C	-3	SER	-	EXPRESSION TAG	UNP P52788
C	-2	GLY	-	EXPRESSION TAG	UNP P52788
C	-1	LEU	-	EXPRESSION TAG	UNP P52788
C	0	VAL	-	EXPRESSION TAG	UNP P52788
C	1	PRO	-	EXPRESSION TAG	UNP P52788
C	2	ARG	-	EXPRESSION TAG	UNP P52788
C	3	GLY	-	EXPRESSION TAG	UNP P52788
C	4	SER	-	EXPRESSION TAG	UNP P52788
D	-14	MET	-	EXPRESSION TAG	UNP P52788
D	-13	GLY	-	EXPRESSION TAG	UNP P52788
D	-12	SER	-	EXPRESSION TAG	UNP P52788
D	-11	SER	-	EXPRESSION TAG	UNP P52788
D	-10	HIS	-	EXPRESSION TAG	UNP P52788
D	-9	HIS	-	EXPRESSION TAG	UNP P52788

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	EXPRESSION TAG	UNP P52788
D	-7	HIS	-	EXPRESSION TAG	UNP P52788
D	-6	HIS	-	EXPRESSION TAG	UNP P52788
D	-5	HIS	-	EXPRESSION TAG	UNP P52788
D	-4	SER	-	EXPRESSION TAG	UNP P52788
D	-3	SER	-	EXPRESSION TAG	UNP P52788
D	-2	GLY	-	EXPRESSION TAG	UNP P52788
D	-1	LEU	-	EXPRESSION TAG	UNP P52788
D	0	VAL	-	EXPRESSION TAG	UNP P52788
D	1	PRO	-	EXPRESSION TAG	UNP P52788
D	2	ARG	-	EXPRESSION TAG	UNP P52788
D	3	GLY	-	EXPRESSION TAG	UNP P52788
D	4	SER	-	EXPRESSION TAG	UNP P52788

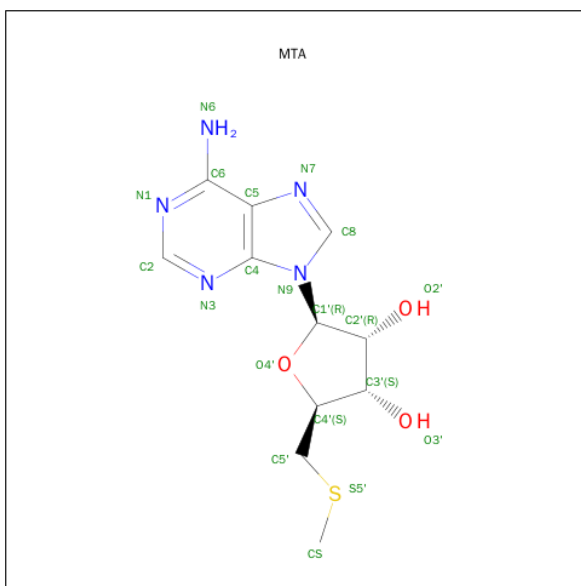
- Molecule 2 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			14	10	4		
2	B	1	Total	C	N	0	0
			14	10	4		
2	C	1	Total	C	N	0	0
			14	10	4		
2	D	1	Total	C	N	0	0
			14	10	4		

- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA)

(formula: C<sub>11</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	100	Total	O	0	0
			100	100		
4	C	67	Total	O	0	0
			67	67		
4	D	58	Total	O	0	0
			58	58		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

73% 14% 12%

MTT GLY SER SER HIS HIS HIS HIS SER SER GLY S4 R5 H6 F11 M12 L13 G14 A1A LYS GLY D16 S28 I29 F30 Q31 E32 N35 A36 E37 S38 V39 H40 T41 W42 Q43 D44 H45 G46 Y47 Y51 T52 N60 Y64 V69

D72 L73 Q74 S75 S76 ASP GLY ASP ASP ALA GLN LYS GLU GLU ILE D87 S88 K92 N97 S101 GLN ASP SER THR GLY ARG V108 R130 I136 D137 H154 D167 V168 H169 T190 I208 K214 Q223 I226 K233 R234 T235 R236 V240 L241 T242

G246 Y249 I253 K265 D276 A279 V280 P281 T284 SER PRO GLU GLU ASP SER T291 Q315 V319 L325 E329 Y351 L352 E353 L354 W355 A354 LYS PRO

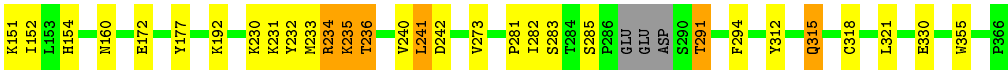
[illegible]

Chain C:

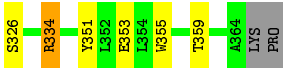
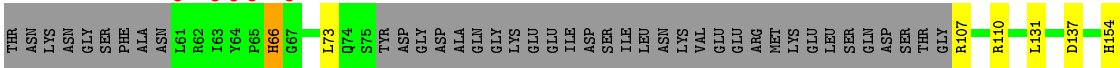
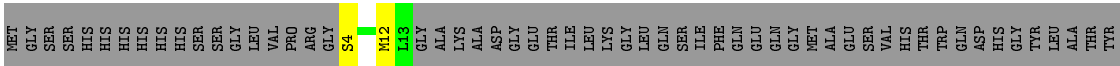
Sequence logo for Chain C. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A bar chart at the top shows the percentage of each amino acid in the sequence: MET (1%), GLY (65%), SER (9%), HIS (24%), and others (0%).

Position	Amino Acid	Information Content (bits)
1	THR	0.00
2	TYR	0.00
3	THR	0.00
4	ASN	0.00
5	LYS	0.00
6	ASN	0.00
7	GLY	0.00
8	GLY	0.00
9	PHE	0.00
10	ALA	0.00
11	ASN	0.00
12	LEU	0.00
13	ARG	0.00
14	ILE	0.00
15	TYR	0.00
16	PRO	0.00
17	GLY	0.00
18	HIS	0.00
19	GLY	0.00
20	L68	0.00
21	V69	0.00
22	L70	0.00
23	L71	0.00
24	D72	0.00
25	L73	0.00
26	Q74	0.00
27	S75	0.00
28	TYR	0.00
29	ASP	0.00
30	GLY	0.00
31	ASP	0.00
32	GLY	0.00
33	GLU	0.00
34	ALA	0.00
35	THR	0.00
36	Q81	0.00
37	E85	0.00
38	I86	0.00
39	D87	0.00
40	S88	0.00
41	I89	0.00
42	K92	0.00
43	V93	0.00
44	K98	0.00
45	GLU	0.00
46	LEU	0.00
47	GLN	0.00
48	ASP	0.00
49	ASP	0.00
50	SER	0.00
51	THR	0.00
52	GLY	0.00
53	R107	0.00
54	P112	0.00
55	P113	0.00
56	L131	0.00
57	Y141	0.00





• Molecule 1: Spermine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.26 Å 88.26 Å 197.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.65 – 2.45 33.06 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (35.65-2.45) 97.1 (33.06-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.209 , 0.271 0.206 , 0.265	Depositor DCC
$R_{free}$ test set	3045 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 8.5	EDS
Estimated twinning fraction	0.045 for -h,-k,l 0.069 for h,-h-k,-l 0.135 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 61243 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: MTA, SPM

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	0.62	0/2724	0.71	1/3677 (0.0%)
1	B	0.62	0/2766	0.71	0/3731
1	C	0.65	0/2363	0.71	0/3186
1	D	0.61	0/2262	0.71	1/3056 (0.0%)
All	All	0.63	0/10115	0.71	2/13650 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	234	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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	2676	0	2671	39	0
1	B	2719	0	2719	38	0
1	C	2325	0	2356	30	0
1	D	2222	0	2249	37	0
2	A	14	0	26	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	26	1	0
2	C	14	0	26	1	0
2	D	14	0	26	7	0
3	A	20	0	15	0	0
3	B	20	0	15	0	0
3	C	20	0	15	2	0
3	D	20	0	15	1	0
4	A	75	0	0	6	0
4	B	100	0	0	6	0
4	C	67	0	0	1	0
4	D	58	0	0	3	0
All	All	10378	0	10159	139	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 7.

The worst 5 of 139 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:D:334:ARG:HH11	1:D:334:ARG:HG2	1.19	1.04
1:A:44:ASP:HB2	4:A:562:HOH:O	1.56	1.03
1:A:12:MET:HG2	4:B:581:HOH:O	1.61	0.98
1:C:315:GLN:HE21	1:C:355:TRP:HE1	1.21	0.88
1:A:137:ASP:OD1	1:A:154:HIS:HD2	1.57	0.87

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	326/381 (86%)	312 (96%)	13 (4%)	1 (0%)	46 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	332/381 (87%)	319 (96%)	13 (4%)	0	100	100
1	C	281/381 (74%)	268 (95%)	13 (5%)	0	100	100
1	D	270/381 (71%)	252 (93%)	16 (6%)	2 (1%)	26	32
All	All	1209/1524 (79%)	1151 (95%)	55 (4%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	D	66	HIS
1	D	200	GLY

### 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	296/333 (89%)	277 (94%)	19 (6%)	22	29
1	B	301/333 (90%)	285 (95%)	16 (5%)	28	39
1	C	261/333 (78%)	249 (95%)	12 (5%)	33	46
1	D	248/333 (74%)	233 (94%)	15 (6%)	24	33
All	All	1106/1332 (83%)	1044 (94%)	62 (6%)	26	36

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	THR
1	B	365	LYS
1	D	284	THR
1	B	296	ARG
1	C	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	C	81	GLN
1	D	169	ASN
1	B	169	ASN
1	B	315	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MTA	A	401	-	17,22,22	1.28	2 (11%)	17,32,32	3.54	7 (41%)
2	SPM	A	501	-	13,13,13	0.66	0	12,12,12	1.84	4 (33%)
3	MTA	B	401	-	17,22,22	1.26	2 (11%)	17,32,32	3.26	7 (41%)
2	SPM	B	501	-	13,13,13	0.44	0	12,12,12	0.95	0
3	MTA	C	401	-	17,22,22	1.21	1 (5%)	17,32,32	3.27	9 (52%)
2	SPM	C	501	-	13,13,13	0.30	0	12,12,12	0.93	0
3	MTA	D	401	-	17,22,22	1.15	2 (11%)	17,32,32	3.93	9 (52%)
2	SPM	D	501	-	13,13,13	0.35	0	12,12,12	1.22	2 (16%)

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	MTA	A	401	-	-	0/3/23/23	0/3/3/3
2	SPM	A	501	-	-	0/11/11/11	0/0/0/0
3	MTA	B	401	-	-	0/3/23/23	0/3/3/3
2	SPM	B	501	-	-	0/11/11/11	0/0/0/0
3	MTA	C	401	-	-	0/3/23/23	0/3/3/3
2	SPM	C	501	-	-	0/11/11/11	0/0/0/0
3	MTA	D	401	-	-	0/3/23/23	0/3/3/3
2	SPM	D	501	-	-	0/11/11/11	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MTA	C5'-S5'	-3.63	1.76	1.80
3	D	401	MTA	C5'-S5'	-3.03	1.77	1.80
3	A	401	MTA	C2-N3	2.20	1.36	1.32
3	B	401	MTA	C5-C4	2.68	1.46	1.40
3	D	401	MTA	C5-C4	2.85	1.46	1.40

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	MTA	CS-S5'-C5'	-12.07	81.60	101.21
3	A	401	MTA	CS-S5'-C5'	-10.16	84.69	101.21
3	B	401	MTA	N3-C2-N1	-9.83	121.37	128.89
3	C	401	MTA	CS-S5'-C5'	-8.12	88.02	101.21
3	D	401	MTA	N3-C2-N1	-7.74	122.97	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SPM	6	0
2	B	501	SPM	1	0
3	C	401	MTA	2	0
2	C	501	SPM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	MTA	1	0
2	D	501	SPM	7	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	336/381 (88%)	-0.20	4 (1%) 81 83	11, 26, 63, 69	0
1	B	342/381 (89%)	-0.28	4 (1%) 81 83	7, 22, 50, 58	0
1	C	291/381 (76%)	-0.28	5 (1%) 73 75	13, 25, 71, 78	0
1	D	278/381 (72%)	-0.20	5 (1%) 71 74	14, 29, 64, 80	0
All	All	1247/1524 (81%)	-0.24	18 (1%) 78 80	7, 26, 61, 80	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	65	PRO	5.0
1	C	86	ILE	4.6
1	D	67	GLY	3.6
1	D	64	TYR	3.6
1	A	30	PHE	3.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SPM	A	501	14/14	0.90	0.18	5.95	6,13,20,20	0
2	SPM	D	501	14/14	0.91	0.16	2.93	17,22,27,27	0
2	SPM	B	501	14/14	0.97	0.13	1.88	9,14,17,17	0
2	SPM	C	501	14/14	0.96	0.14	1.06	13,17,19,20	0
3	MTA	C	401	20/20	0.98	0.12	-0.36	17,19,21,21	0
3	MTA	B	401	20/20	0.99	0.11	-0.43	9,14,17,18	0
3	MTA	A	401	20/20	0.98	0.11	-0.56	16,21,22,23	0
3	MTA	D	401	20/20	0.98	0.11	-0.60	19,23,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.