



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:55 PM BST

PDB ID : 3J6Q
EMDB ID: : EMD-5926
Title : Identification of the active sites in the methyltransferases of a transcribing dsRNA virus
Authors : Zhu, B.; Yang, C.; Liu, H.; Cheng, L.; Song, F.; Zeng, S.; Huang, X.; Ji, G.; Zhu, P.
Deposited on : 2014-03-20
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

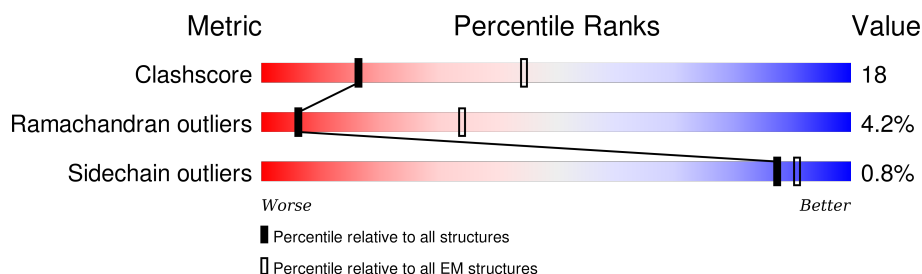
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1058	80% 16% .
1	B	1058	80% 16% .
1	C	1058	80% 16% .
1	D	1058	81% 16% .
1	E	1058	81% 16% .

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
1	GPL	B	234	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAH	A	1101	-	-	X	-
2	SAH	A	1102	-	-	X	-
2	SAH	B	1101	-	-	X	-
2	SAH	B	1102	-	-	X	-
2	SAH	C	1101	-	-	X	-
2	SAH	C	1102	-	-	X	-
2	SAH	D	1101	-	-	X	-
2	SAH	D	1102	-	-	X	-
2	SAH	E	1101	-	-	X	-
2	SAH	E	1102	-	-	X	-

2 Entry composition [i](#)

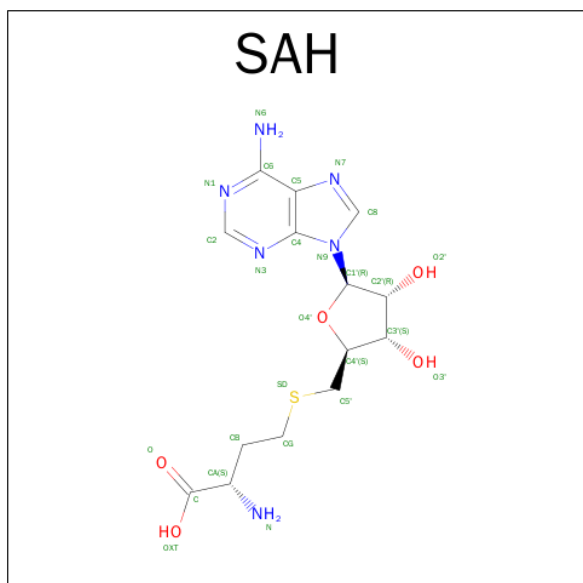
There are 2 unique types of molecules in this entry. The entry contains 42575 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Structural protein VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	B	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	C	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	D	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	E	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			52	28	12	10	2	

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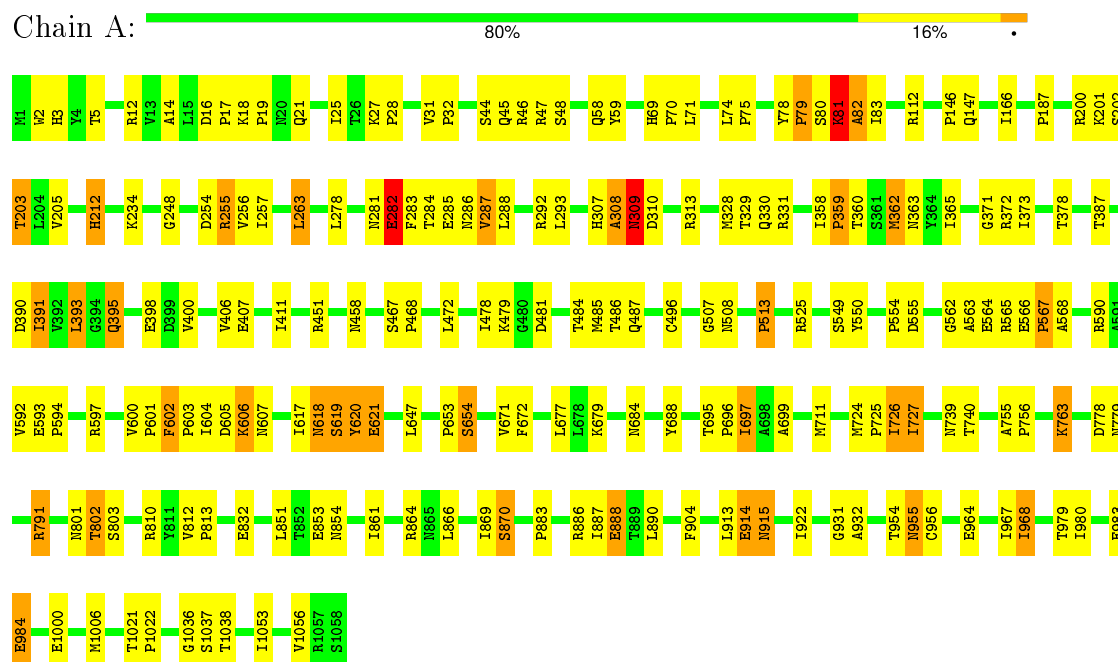
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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	B	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	B	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	C	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	C	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	D	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	D	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	E	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	E	1	Total	C	N	O	S	0
			52	28	12	10	2	

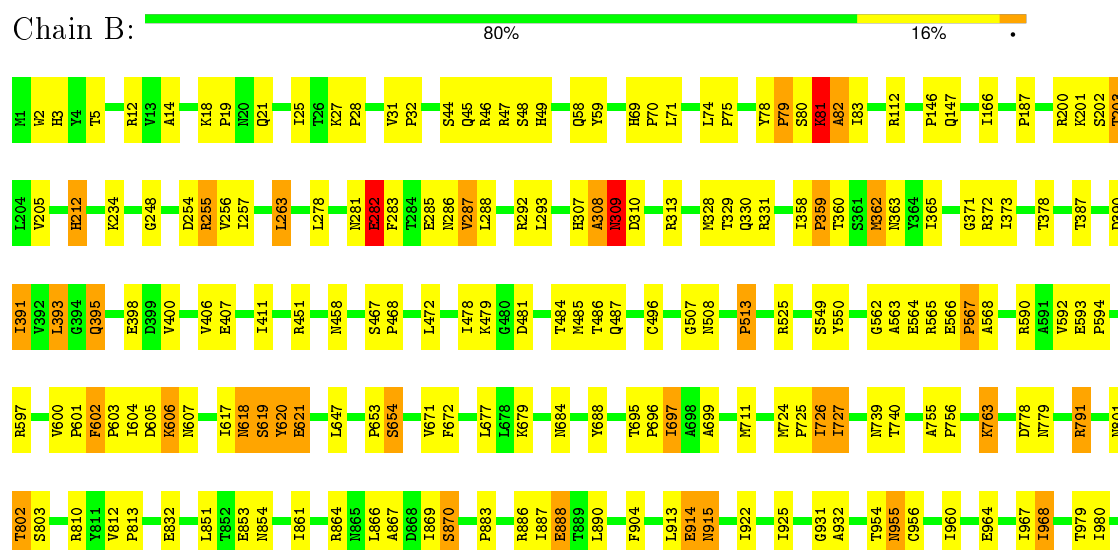
3 Residue-property plots

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. 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. 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: Structural protein VP3



• Molecule 1: Structural protein VP3



M1006	T802	R597	S202	H1
T1021	S803	V600	I203	H2
P1022	R810	F601	L204	H3
G1036	V811	P602	V205	V4
S1037	P813	P603	H212	T5
T1038	E832	D605	K234	
I1053	L851	M607	G248	R12
V1056	T852	I617	D254	V13
R1057	E853	M618	R255	A14
S1058	M854	S619	V256	L15
	I861	Y620	I257	D16
	R864	E621	L263	P17
	M865	L647	L278	K18
	L866	P653	M281	P19
	I869	S654	F283	P20
	S870	V671	T284	Q21
	P883	F672	E285	
	R886	L677	M286	I25
	I887	L678	V287	T26
	E888	K679	L288	K27
	T889	M684	R292	V31
	L890	T484	L293	P32
	F904	M485	H307	S44
	L913	T486	A308	Q45
	E914	Q487	R309	R46
	M915	C496	D310	R47
	I922	G507	R313	S48
	G931	M508	M328	Q58
	A932	P513	T329	I59
	T954	R525	Q330	H69
M955	P725	S549	R331	P70
C956	I726	Y550	I358	L71
E964	I727	G562	P359	L74
I967	M739	A563	T360	P75
I968	T740	E564	I83	Y78
T979	A755	R565	S361	P79
I980	P756	E566	M362	S80
	K763	P567	N363	R81
	D778	A568	I364	A82
	M779	R590	G371	P84
E983	R791	A591	R372	R112
E984	M801	V592	I373	P146
E1000		E593	T378	Q147
		P594	T387	I166
				P187
				R200
				K201

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	30000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	EMAN	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

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: GPL, SAH

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.61	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	B	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	C	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	D	0.62	3/8615 (0.0%)	0.54	2/11731 (0.0%)
1	E	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
All	All	0.62	15/43075 (0.0%)	0.55	10/58655 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
All	All	0	25

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	513	PRO	N-CD	6.56	1.57	1.47
1	D	513	PRO	N-CD	6.55	1.57	1.47
1	B	513	PRO	N-CD	6.54	1.57	1.47
1	A	513	PRO	N-CD	6.54	1.57	1.47
1	C	513	PRO	N-CD	6.47	1.56	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	79	PRO	CA-N-CD	-5.23	104.17	111.50
1	C	79	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	79	PRO	CA-N-CD	-5.22	104.19	111.50
1	D	79	PRO	CA-N-CD	-5.21	104.20	111.50
1	B	79	PRO	CA-N-CD	-5.19	104.23	111.50

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	ALA	Peptide
1	A	309	ASN	Peptide
1	A	362	MET	Peptide
1	A	71	LEU	Peptide
1	A	81	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8463	0	8411	385	0
1	B	8463	0	8411	400	0
1	C	8463	0	8411	390	0
1	D	8463	0	8411	385	0
1	E	8463	0	8411	385	0
2	A	52	0	38	28	0
2	B	52	0	38	29	0
2	C	52	0	38	29	0
2	D	52	0	38	28	0
2	E	52	0	38	29	0
All	All	42575	0	42245	1567	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 18.

The worst 5 of 1567 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLN:CG	1:B:112:ARG:NH2	1.75	1.48
1:B:395:GLN:CG	1:C:112:ARG:NH2	1.77	1.48
1:C:395:GLN:CG	1:D:112:ARG:NH2	1.74	1.46
1:A:112:ARG:NH2	1:E:395:GLN:CG	1.74	1.45
1:D:395:GLN:CG	1:E:112:ARG:NH2	1.76	1.45

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 PDB entries followed by that with respect to all EM entries.

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	1055/1058 (100%)	889 (84%)	122 (12%)	44 (4%)	3	36
1	B	1055/1058 (100%)	889 (84%)	122 (12%)	44 (4%)	3	36
1	C	1055/1058 (100%)	887 (84%)	123 (12%)	45 (4%)	3	35
1	D	1055/1058 (100%)	887 (84%)	124 (12%)	44 (4%)	3	36
1	E	1055/1058 (100%)	887 (84%)	124 (12%)	44 (4%)	3	36
All	All	5275/5290 (100%)	4439 (84%)	615 (12%)	221 (4%)	6	36

5 of 221 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	282	GLU
1	A	287	VAL
1	A	309	ASN
1	A	330	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	942/942 (100%)	934 (99%)	8 (1%)	86	94
1	B	942/942 (100%)	934 (99%)	8 (1%)	86	94
1	C	942/942 (100%)	934 (99%)	8 (1%)	86	94
1	D	942/942 (100%)	934 (99%)	8 (1%)	86	94
1	E	942/942 (100%)	934 (99%)	8 (1%)	86	94
All	All	4710/4710 (100%)	4670 (99%)	40 (1%)	87	94

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	481	ASP
1	C	791	ARG
1	E	620	TYR
1	C	620	TYR
1	C	1006	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	GLN
1	E	45	GLN
1	D	21	GLN
1	B	21	GLN
1	C	45	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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
1	GPL	A	234	1	28,34,35	2.80	4 (14%)	30,49,51	1.79	6 (20%)
1	GPL	B	234	1	28,34,35	2.80	4 (14%)	30,49,51	1.79	6 (20%)
1	GPL	C	234	1	28,34,35	2.81	4 (14%)	30,49,51	1.78	6 (20%)
1	GPL	D	234	1	28,34,35	2.79	4 (14%)	30,49,51	1.78	6 (20%)
1	GPL	E	234	1	28,34,35	2.81	4 (14%)	30,49,51	1.78	6 (20%)

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
1	GPL	A	234	1	-	0/14/37/39	0/3/3/3
1	GPL	B	234	1	-	0/14/37/39	0/3/3/3
1	GPL	C	234	1	-	0/14/37/39	0/3/3/3
1	GPL	D	234	1	-	0/14/37/39	0/3/3/3
1	GPL	E	234	1	-	0/14/37/39	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	234	GPL	P-O1P	2.04	1.48	1.46
1	D	234	GPL	P-O1P	2.07	1.48	1.46
1	A	234	GPL	P-O1P	2.08	1.48	1.46
1	C	234	GPL	P-O1P	2.16	1.48	1.46
1	B	234	GPL	P-O1P	2.18	1.48	1.46

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	GPL	C5-C6-N1	-4.29	117.91	123.52
1	E	234	GPL	C5-C6-N1	-4.26	117.95	123.52
1	C	234	GPL	C5-C6-N1	-4.26	117.96	123.52
1	D	234	GPL	C5-C6-N1	-4.25	117.96	123.52
1	A	234	GPL	C5-C6-N1	-4.20	118.03	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	GPL	8	0
1	B	234	GPL	9	0
1	C	234	GPL	8	0
1	D	234	GPL	8	0
1	E	234	GPL	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	SAH	A	1101	-	22,28,28	1.12	2 (9%)	18,40,40	1.86	1 (5%)
2	SAH	A	1102	-	22,28,28	1.11	2 (9%)	18,40,40	2.01	2 (11%)
2	SAH	B	1101	-	22,28,28	1.11	2 (9%)	18,40,40	1.87	1 (5%)
2	SAH	B	1102	-	22,28,28	1.10	2 (9%)	18,40,40	1.98	2 (11%)
2	SAH	C	1101	-	22,28,28	1.12	2 (9%)	18,40,40	1.88	1 (5%)
2	SAH	C	1102	-	22,28,28	1.09	2 (9%)	18,40,40	1.97	1 (5%)
2	SAH	D	1101	-	22,28,28	1.12	2 (9%)	18,40,40	1.86	1 (5%)
2	SAH	D	1102	-	22,28,28	1.11	2 (9%)	18,40,40	1.99	1 (5%)
2	SAH	E	1101	-	22,28,28	1.11	2 (9%)	18,40,40	1.85	1 (5%)
2	SAH	E	1102	-	22,28,28	1.11	2 (9%)	18,40,40	1.98	1 (5%)

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	SAH	A	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	A	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	B	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	B	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	C	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	C	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	D	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	D	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	E	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	E	1102	-	-	0/7/31/31	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	SAH	C5'-SD	-2.45	1.76	1.81
2	E	1102	SAH	C5'-SD	-2.43	1.76	1.81
2	B	1102	SAH	C5'-SD	-2.41	1.76	1.81
2	D	1102	SAH	C5'-SD	-2.41	1.76	1.81
2	C	1102	SAH	C5'-SD	-2.41	1.76	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1102	SAH	N3-C2-N1	-6.95	123.41	128.87
2	D	1102	SAH	N3-C2-N1	-6.87	123.47	128.87
2	E	1102	SAH	N3-C2-N1	-6.83	123.50	128.87
2	B	1102	SAH	N3-C2-N1	-6.82	123.52	128.87
2	C	1102	SAH	N3-C2-N1	-6.81	123.52	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 143 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	SAH	14	0
2	A	1102	SAH	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	SAH	14	0
2	B	1102	SAH	15	0
2	C	1101	SAH	15	0
2	C	1102	SAH	14	0
2	D	1101	SAH	14	0
2	D	1102	SAH	14	0
2	E	1101	SAH	14	0
2	E	1102	SAH	15	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.