Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:57 pm BST

PDB ID	:	2BQZ
Title	:	Crystal structure of a ternary complex of the human histone methyltransferase Pr-SET7 (also known as SET8)
Authors	:	Xiao, B.; Jing, C.; Kelly, G.; Walker, P.A.; Muskett, F.W.; Frenkiel, T.A.; Martin, S.R.; Sarma, K.; Reinberg, D.; Gamblin, S.J.; Wilson, J.R.
Deposited on	:	2005-04-28
Resolution	:	1.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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.
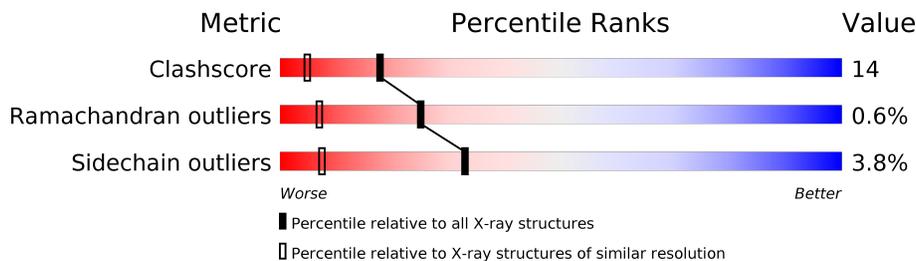
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	161	83% 16% •
1	E	161	78% 20% ••
2	B	10	30% 50% 20%
2	F	10	50% 30% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3437 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 SET8 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total 1290	C 805	N 229	O 250	S 6	0	0	0
1	E	161	Total 1290	C 805	N 229	O 250	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	PRO	ARG	conflict	UNP Q86W83
E	316	PRO	ARG	conflict	UNP Q86W83

- Molecule 2 is a protein called HISTONE H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total 97	C 59	N 23	O 15	0	0	0
2	F	10	Total 97	C 59	N 23	O 15	0	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

SAH
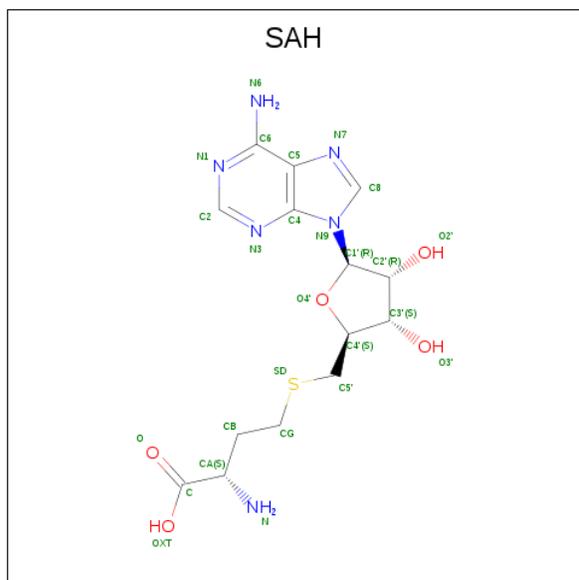
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	14	6	4	1		
3	E	1	Total	C	N	O	S	0	0
			25	14	6	4	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	29	Total	O	0	0
			29	29		
4	E	248	Total	O	0	0
			248	248		
4	F	18	Total	O	0	0
			18	18		

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 the various outlier classes 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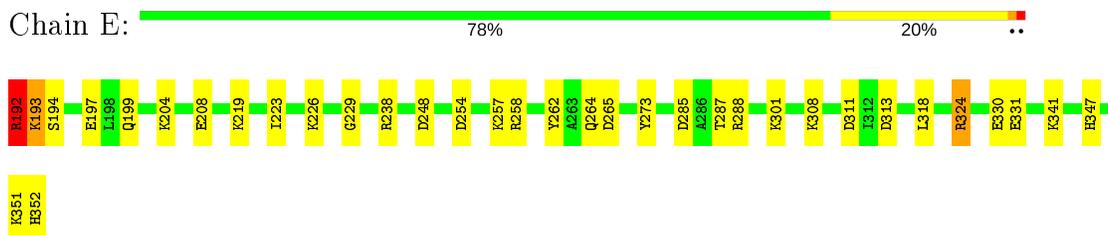 for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: SET8 PROTEIN

Chain A:

83%   16%   ·

R192 E197 R203 K234 Q235 R238 F241 D248 D254 D265 Y273 L278 N291 L296 C305 Q306 D311 I312 D313 I319 L320 I321 A322 S323 R324 D325 R339 S340 K341 A342 H347 L350 K351 H352

• Molecule 1: SET8 PROTEIN

Chain E:

78%   20%   ··

R192 K193 S194 E197 L198 Q199 K204 E208 K219 I223 K226 G229 R238 D248 D254 K257 R258 Y262 A263 Q264 D265 Y273 D285 A286 T287 R288 K301 K308 D311 I312 D313 L318 R324 E330 E331 K341 H347

K351 H352

• Molecule 2: HISTONE H4

Chain B:

30%   50%   20%

R17 H18 R19 K20 V21 L22 R23 D24 N25 Y26

• Molecule 2: HISTONE H4

Chain F:

50%   30%   20%

R17 R23 D24 N25 Y26

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4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.18Å 46.32Å 52.00Å 64.74° 86.66° 90.61°	Depositor
Resolution (Å)	20.00 – 1.50	Depositor
% Data completeness (in resolution range)	94.0 (20.00-1.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.187 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3437	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

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: MLZ, 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	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.49	0/1312	0.87	8/1759 (0.5%)
1	E	0.53	0/1312	0.87	9/1759 (0.5%)
2	B	0.56	0/87	0.99	0/112
2	F	0.45	0/87	1.18	1/112 (0.9%)
All	All	0.51	0/2798	0.89	18/3742 (0.5%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	ARG	NE-CZ-NH2	9.47	125.03	120.30
1	E	193	LYS	N-CA-C	-9.29	85.91	111.00
1	E	192	ARG	CB-CA-C	-7.36	95.68	110.40
1	A	313	ASP	CB-CG-OD2	6.56	124.21	118.30
1	E	313	ASP	CB-CG-OD2	6.27	123.95	118.30
1	A	265	ASP	CB-CG-OD2	6.17	123.86	118.30
2	F	25	ASN	N-CA-C	6.09	127.45	111.00
1	A	311	ASP	CB-CG-OD2	5.89	123.60	118.30
1	E	324	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	248	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	254	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	324	ARG	CG-CD-NE	5.41	123.16	111.80
1	E	265	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	324	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	E	324	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	E	192	ARG	C-N-CA	-5.14	108.86	121.70
1	E	254	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	311	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1290	0	1272	26	1
1	E	1290	0	1272	34	1
2	B	97	0	97	11	0
2	F	97	0	97	7	0
3	A	25	0	19	0	0
3	E	25	0	19	0	0
4	A	318	0	0	14	1
4	B	29	0	0	9	0
4	E	248	0	0	10	0
4	F	18	0	0	0	0
All	All	3437	0	2776	76	2

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 14.

All (76) 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:305:CYS:SG	4:A:2238:HOH:O	2.14	1.05
1:E:192:ARG:O	1:E:193:LYS:HB2	1.62	0.95
1:E:194:SER:H	1:E:197:GLU:HB3	1.49	0.78
1:E:223:ILE:HD12	1:E:229:GLY:HA3	1.65	0.76
1:E:192:ARG:O	1:E:193:LYS:C	2.23	0.74
1:E:192:ARG:O	1:E:193:LYS:CB	2.29	0.73
1:E:223:ILE:HD13	1:E:331:GLU:CD	2.09	0.72
1:E:248:ASP:OD2	1:E:258:ARG:NH1	2.23	0.70
2:F:25:ASN:O	2:F:26:TYR:HB2	1.93	0.68
4:E:2204:HOH:O	2:F:25:ASN:HA	1.93	0.67
1:A:350:LEU:HD21	4:B:2005:HOH:O	1.95	0.66
1:E:301:LYS:HE2	1:E:351:LYS:O	1.95	0.66
2:B:23:ARG:O	2:B:25:ASN:ND2	2.29	0.66
1:E:192:ARG:NH1	4:E:2002:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ASP:OD1	1:E:285:ASP:HB3	1.99	0.63
1:A:306:GLN:HG3	1:A:323:SER:HB3	1.79	0.63
1:A:291:ASN:HB2	4:A:2218:HOH:O	1.96	0.63
2:B:17:ARG:NH1	4:B:2001:HOH:O	2.32	0.62
1:A:296:LEU:HB2	4:A:2224:HOH:O	1.99	0.61
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.65	0.61
2:B:18:HIS:ND1	4:B:2005:HOH:O	2.31	0.60
1:E:324:ARG:NH2	1:E:330:GLU:OE2	2.29	0.60
1:A:324:ARG:HD2	1:A:325:ASP:O	2.03	0.59
1:A:238:ARG:NH1	1:A:238:ARG:HG3	2.18	0.58
1:E:223:ILE:CD1	1:E:229:GLY:HA3	2.30	0.58
1:A:339:ARG:NH1	4:A:2294:HOH:O	2.32	0.58
1:E:192:ARG:C	1:E:193:LYS:O	2.22	0.58
1:E:264:GLN:NE2	4:E:2105:HOH:O	2.36	0.58
1:A:347:HIS:HE2	2:B:17:ARG:N	2.02	0.57
1:A:319:ILE:HD12	1:A:321:ILE:HD11	1.86	0.57
1:E:223:ILE:HD13	1:E:331:GLU:OE2	2.05	0.57
1:E:199:GLN:O	1:E:199:GLN:HG3	2.05	0.56
1:A:203:ARG:NE	4:A:2021:HOH:O	2.39	0.55
1:E:257:LYS:HE2	4:E:2138:HOH:O	2.06	0.55
1:A:320:LEU:C	1:A:321:ILE:HD13	2.28	0.54
2:B:18:HIS:CG	4:B:2005:HOH:O	2.61	0.53
1:A:278:LEU:HB2	4:A:2184:HOH:O	2.09	0.53
1:E:347:HIS:HE2	2:F:17:ARG:N	2.07	0.52
1:A:203:ARG:NH2	4:A:2021:HOH:O	2.40	0.52
1:E:226:LYS:HE3	4:E:2043:HOH:O	2.09	0.52
1:E:193:LYS:HG3	4:E:2001:HOH:O	2.09	0.51
1:E:308:LYS:NZ	4:E:2201:HOH:O	2.43	0.51
1:A:296:LEU:HD12	4:A:2224:HOH:O	2.10	0.51
2:B:18:HIS:CE1	4:B:2005:HOH:O	2.63	0.50
2:F:25:ASN:CG	2:F:26:TYR:H	2.13	0.50
2:B:23:ARG:NH2	4:B:2012:HOH:O	2.45	0.49
2:F:23:ARG:HH11	2:F:23:ARG:HG2	1.77	0.49
1:A:241:PHE:HA	1:A:321:ILE:HD12	1.95	0.48
1:A:234:LYS:NZ	1:A:235:GLN:O	2.47	0.48
1:E:204:LYS:O	1:E:208:GLU:HG3	2.15	0.47
1:A:238:ARG:NH2	4:A:2075:HOH:O	2.48	0.46
1:E:287:THR:HG23	1:E:288:ARG:N	2.30	0.46
1:E:248:ASP:OD1	1:E:285:ASP:O	2.34	0.46
2:B:18:HIS:CD2	4:B:2004:HOH:O	2.69	0.46
1:A:324:ARG:HD3	4:A:2270:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ARG:HD2	4:E:2061:HOH:O	2.15	0.46
1:E:341:LYS:NZ	4:E:2235:HOH:O	2.20	0.45
1:A:341:LYS:HD3	4:A:2297:HOH:O	2.17	0.44
1:E:301:LYS:CE	1:E:351:LYS:O	2.65	0.44
1:A:320:LEU:O	1:A:321:ILE:HD13	2.18	0.43
1:E:262:TYR:OH	1:E:287:THR:HG21	2.19	0.43
1:E:262:TYR:CZ	1:E:287:THR:HG21	2.53	0.43
1:E:287:THR:CG2	1:E:288:ARG:N	2.81	0.43
1:A:350:LEU:HD11	4:B:2004:HOH:O	2.19	0.42
2:B:22:LEU:HD11	2:B:25:ASN:HD21	1.85	0.42
2:B:23:ARG:O	4:B:2011:HOH:O	2.21	0.42
2:F:25:ASN:CG	2:F:26:TYR:N	2.73	0.42
1:A:238:ARG:NE	4:A:2077:HOH:O	2.52	0.42
1:A:341:LYS:HD3	1:A:342:ALA:N	2.35	0.42
2:F:25:ASN:OD1	2:F:26:TYR:N	2.43	0.42
1:E:194:SER:H	1:E:197:GLU:CB	2.25	0.41
1:E:194:SER:O	1:E:197:GLU:HB3	2.21	0.41
1:E:192:ARG:HD3	4:E:2001:HOH:O	2.21	0.41
1:A:339:ARG:NH1	4:A:2293:HOH:O	2.42	0.41
4:A:2144:HOH:O	2:B:20:MLZ:HE2	2.21	0.41
1:E:223:ILE:CD1	1:E:331:GLU:OE2	2.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:OE2	1:E:238:ARG:NH2[1_455]	2.12	0.08
4:A:2167:HOH:O	4:A:2196:HOH:O[1_456]	2.14	0.06

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	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
1	E	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	B	7/10 (70%)	4 (57%)	2 (29%)	1 (14%)	0	0
2	F	7/10 (70%)	4 (57%)	2 (29%)	1 (14%)	0	0
All	All	332/342 (97%)	318 (96%)	12 (4%)	2 (1%)	25	7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	24	ASP
2	B	24	ASP

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 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	137/137 (100%)	134 (98%)	3 (2%)	52	22
1	E	137/137 (100%)	132 (96%)	5 (4%)	35	8
2	B	9/9 (100%)	7 (78%)	2 (22%)	1	0
2	F	9/9 (100%)	8 (89%)	1 (11%)	6	0
All	All	292/292 (100%)	281 (96%)	11 (4%)	33	7

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ARG
1	A	273	TYR
1	A	341	LYS
2	B	24	ASP
2	B	25	ASN
1	E	192	ARG
1	E	219	LYS
1	E	273	TYR
1	E	318	LEU

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Mol	Chain	Res	Type
1	E	352	HIS
2	F	26	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
1	E	276	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)

2 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	$\#|Z| > 2$
2	MLZ	B	20	2	8,9,10	0.77	0	4,9,11	1.88	3 (75%)
2	MLZ	F	20	2	8,9,10	0.79	0	4,9,11	1.74	1 (25%)

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	MLZ	B	20	2	-	1/7/8/10	-
2	MLZ	F	20	2	-	0/7/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	20	MLZ	CM-NZ-CE	2.77	119.97	111.95
2	B	20	MLZ	CM-NZ-CE	2.30	118.58	111.95
2	B	20	MLZ	CD-CE-NZ	2.15	119.81	112.05
2	B	20	MLZ	CG-CD-CE	-2.05	103.86	113.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	20	MLZ	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	20	MLZ	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	SAH	E	1354	-	23,27,28	1.14	2 (8%)	20,38,40	1.33	3 (15%)
3	SAH	A	1354	-	23,27,28	1.10	2 (8%)	20,38,40	1.48	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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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	SAH	E	1354	-	-	2/8/29/31	0/3/3/3
3	SAH	A	1354	-	-	2/8/29/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1354	SAH	C2-N3	3.68	1.38	1.32
3	A	1354	SAH	C2-N3	3.43	1.37	1.32
3	A	1354	SAH	C2-N1	2.44	1.38	1.33
3	E	1354	SAH	C2-N1	2.23	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1354	SAH	N3-C2-N1	-3.85	122.66	128.68
3	A	1354	SAH	N3-C2-N1	-3.77	122.79	128.68
3	A	1354	SAH	C5-C6-N6	2.53	124.19	120.35
3	E	1354	SAH	C5-C6-N6	2.50	124.16	120.35
3	E	1354	SAH	C5-C6-N1	-2.13	115.53	120.35
3	A	1354	SAH	C2-N1-C6	2.12	122.38	118.75
3	A	1354	SAH	C5-C6-N1	-2.06	115.68	120.35

There are no chirality outliers.
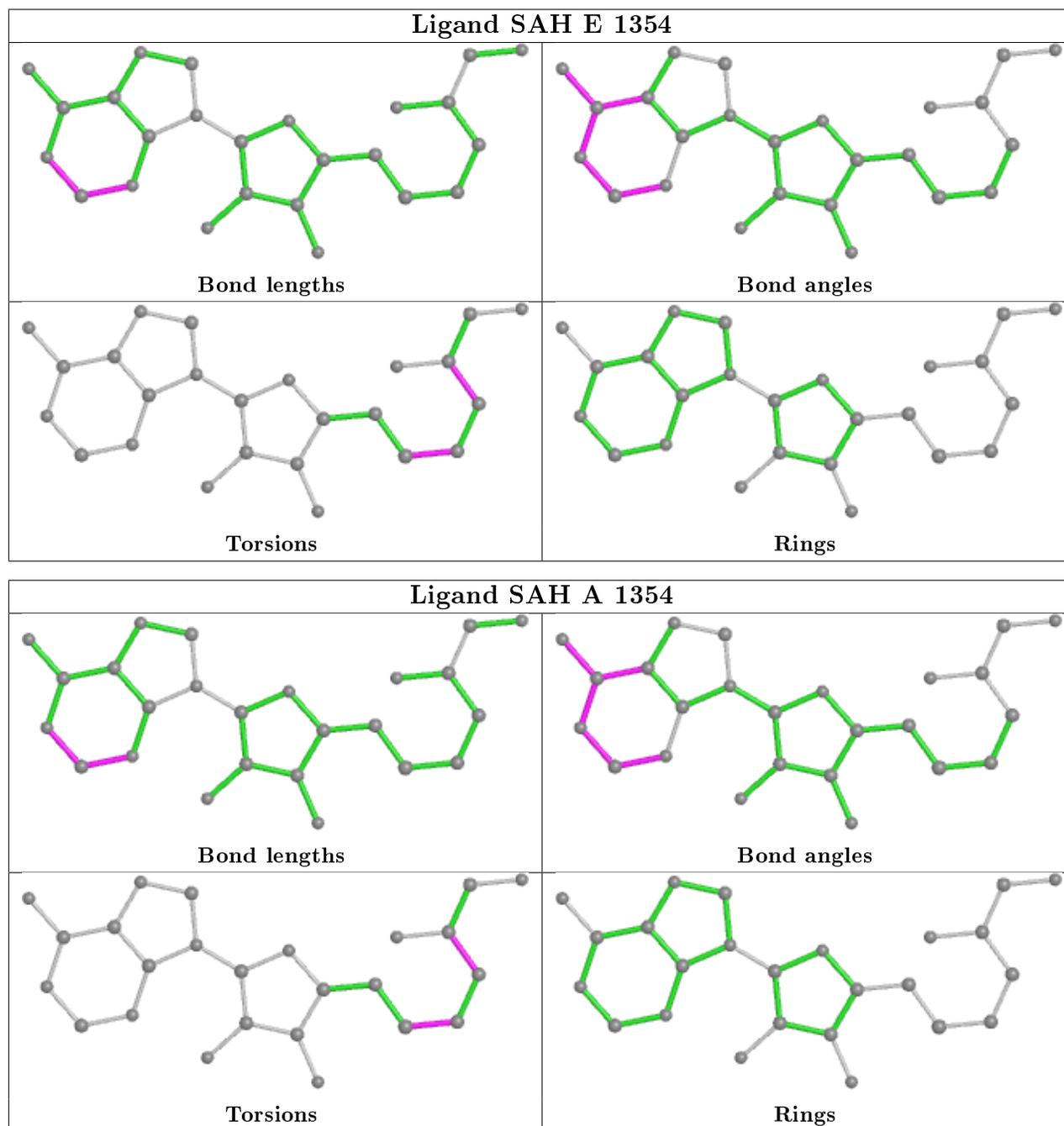
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1354	SAH	C-CA-CB-CG
3	A	1354	SAH	C-CA-CB-CG
3	A	1354	SAH	CB-CG-SD-C5'
3	E	1354	SAH	CB-CG-SD-C5'

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 SAH E 1354

Bond lengths — Bond angles — Torsions — Rings

Ligand SAH A 1354

Bond lengths — Bond angles — Torsions — Rings

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.