



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:57 PM UTC

PDB ID : 2BH2 / pdb_00002bh2
Title : Crystal Structure of E. coli 5-methyluridine methyltransferase RumA in complex with ribosomal RNA substrate and S-adenosylhomocysteine.
Authors : Lee, T.T.; Agarwalla, S.; Stroud, R.M.
Deposited on : 2005-01-06
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

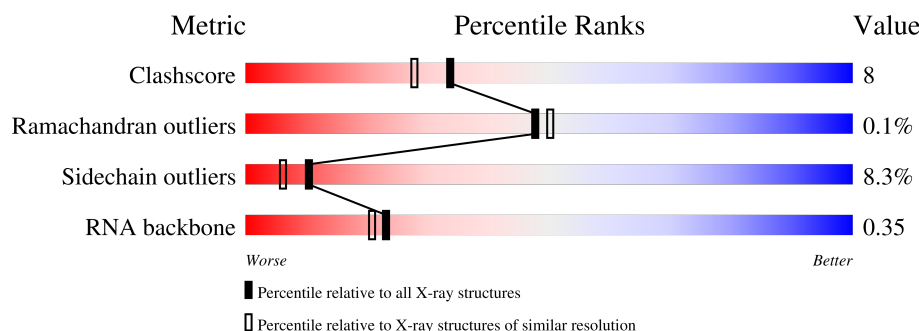
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RNA backbone	3983	1112 (2.50-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	76% 18% . .
1	B	433	74% 20% . .
2	C	37	46% 22% 8% 5% 19%
2	D	37	41% 22% 14% 5% 19%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8156 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.

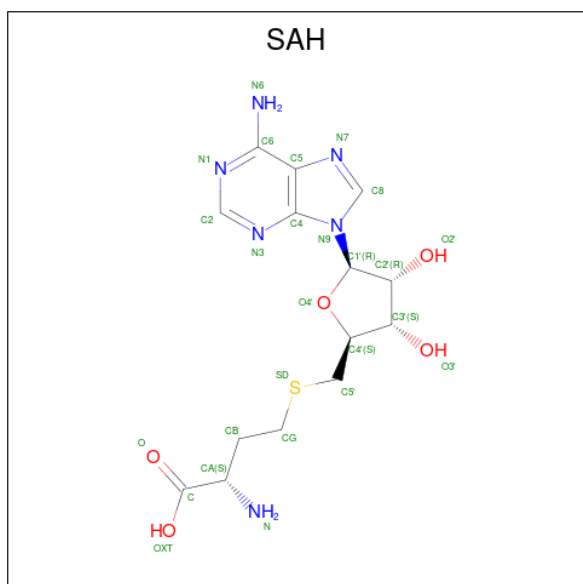
- Molecule 1 is a protein called 23S RRNA (URACIL-5-)-METHYLTRANSFERASE RUMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3245	2039	586	602	18			
1	B	416	Total	C	N	O	S	0	0	0
			3229	2029	583	599	18			

- Molecule 2 is a RNA chain called 23S RIBOSOMAL RNA 1932-1968.

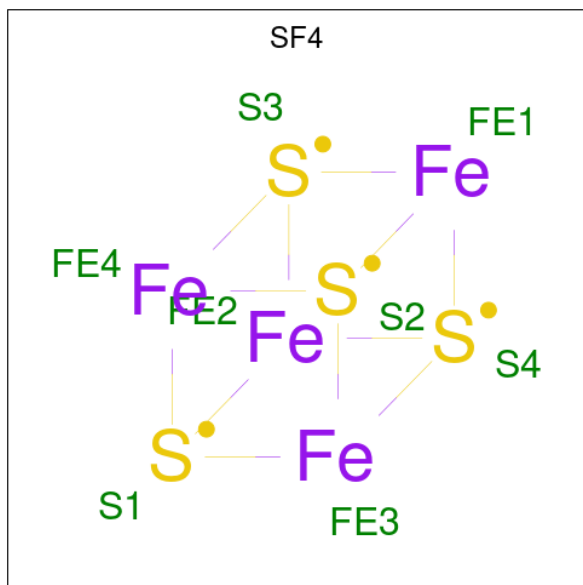
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	30	Total 637	C 286	F 1	N 112	O 209	P 29	0	0	0
2	D	30	Total 637	C 286	F 1	N 112	O 209	P 29	0	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is water.

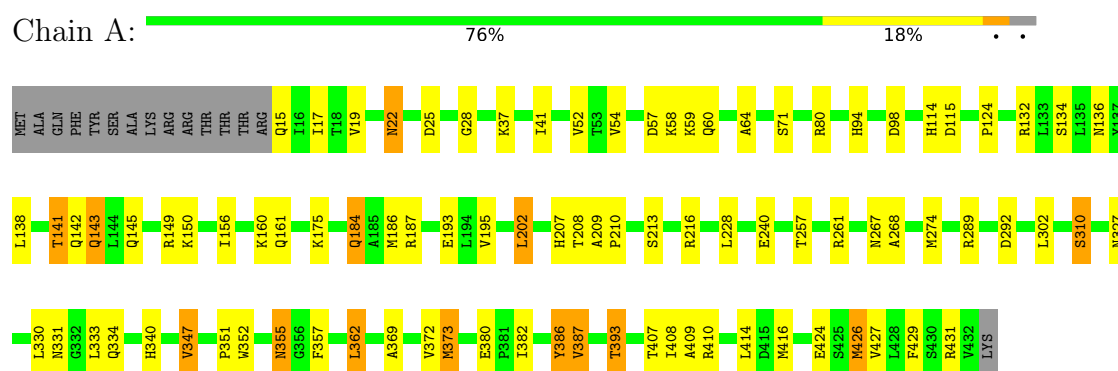
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		
5	B	142	Total	O	0	0
			142	142		
5	C	23	Total	O	0	0
			23	23		
5	D	32	Total	O	0	0
			32	32		

3 Residue-property plots

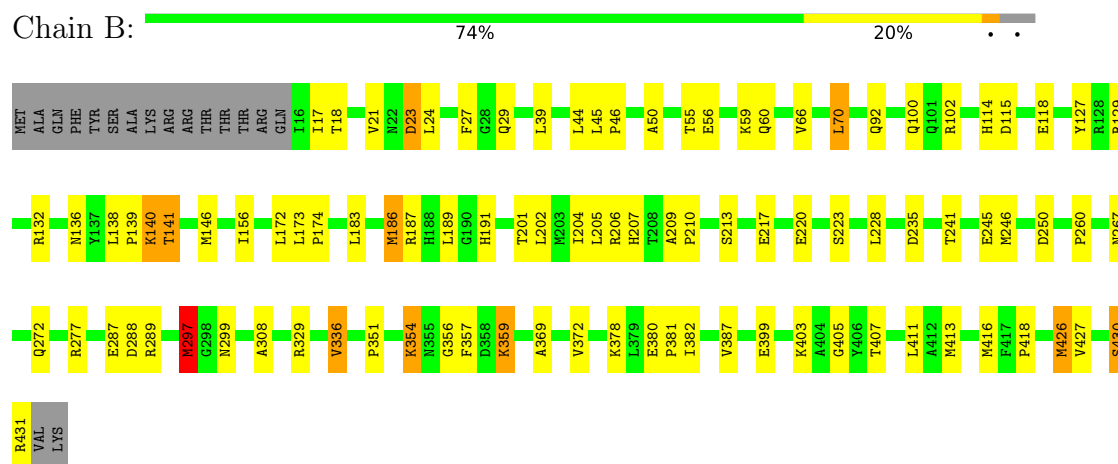
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

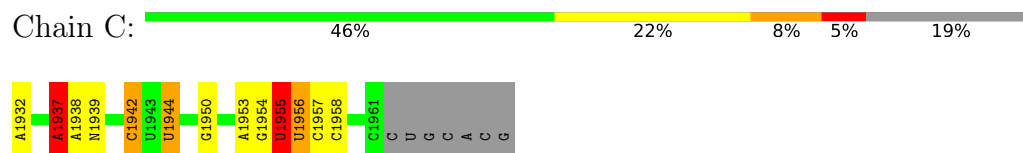
• Molecule 1: 23S rRNA (URACIL-5-)-METHYLTRANSFERASE RUMA



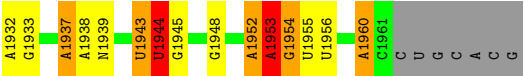
• Molecule 1: 23S rRNA (URACIL-5-)-METHYLTRANSFERASE RUMA



• Molecule 2: 23S RIBOSOMAL RNA 1932-1968



• Molecule 2: 23S RIBOSOMAL RNA 1932-1968



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.06 Å 63.54 Å 112.02 Å 90.00° 125.15° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15	Depositor
% Data completeness (in resolution range)	99.6 (50.00-2.15)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.174 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: SF4, SAH, FMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.20	4/3306 (0.1%)	1.10	6/4480 (0.1%)
1	B	1.23	6/3290 (0.2%)	1.09	4/4458 (0.1%)
2	C	1.02	2/687 (0.3%)	1.58	13/1069 (1.2%)
2	D	1.10	1/687 (0.1%)	1.70	22/1069 (2.1%)
All	All	1.19	13/7970 (0.2%)	1.22	45/11076 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	MET	SD-CE	-21.62	1.25	1.79
1	A	373	MET	SD-CE	-15.58	1.40	1.79
1	A	426	MET	SD-CE	-11.89	1.49	1.79
1	A	268	ALA	CA-CB	7.58	1.65	1.53
1	B	413	MET	SD-CE	-6.51	1.63	1.79
2	D	1939	FMU	O3'-P	6.05	1.62	1.56
2	C	1956	U	C1'-N1	5.82	1.56	1.47
1	B	426	MET	SD-CE	-5.70	1.65	1.79
1	B	45	LEU	C-O	-5.46	1.18	1.24
1	A	387	VAL	CA-CB	-5.44	1.47	1.54
1	B	359	LYS	CE-NZ	-5.23	1.33	1.49
1	B	308	ALA	CA-CB	-5.10	1.45	1.53
2	C	1958	C	C3'-O3'	5.06	1.49	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1952	A	C2'-C3'-O3'	14.72	131.57	109.50
2	D	1943	U	C3'-C2'-O2'	-9.84	95.94	110.70
2	C	1955	U	C5'-C4'-C3'	9.04	129.56	116.00
2	D	1952	A	P-O3'-C3'	7.99	132.19	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1937	A	N9-C1'-C2'	7.96	123.94	112.00
2	D	1943	U	N1-C1'-C2'	7.59	123.38	112.00
2	D	1952	A	C4'-C3'-O3'	-7.50	98.16	109.40
2	C	1955	U	N1-C1'-C2'	7.31	122.97	112.00
2	D	1943	U	C2'-C3'-O3'	-7.02	103.17	113.70
2	D	1937	A	O4'-C4'-C3'	-6.99	97.01	104.00
2	D	1956	U	O4'-C1'-N1	6.83	118.44	108.20
1	A	57	ASP	N-CA-C	6.78	120.51	111.30
2	D	1955	U	N1-C1'-C2'	6.77	122.15	112.00
2	C	1955	U	C4'-C3'-C2'	-6.67	95.92	102.60
1	B	336	VAL	CB-CA-C	-6.58	100.73	110.33
2	C	1957	C	C3'-C2'-O2'	6.25	120.07	110.70
2	D	1937	A	C1'-O4'-C4'	-6.23	103.67	109.90
1	B	92	GLN	N-CA-C	5.99	118.62	110.06
2	C	1956	U	N1-C1'-C2'	-5.92	105.11	114.00
2	D	1943	U	P-O3'-C3'	-5.89	111.36	120.20
2	D	1944	U	C3'-C2'-O2'	5.83	119.44	110.70
1	A	228	LEU	CB-CA-C	-5.82	99.92	109.53
2	D	1944	U	O4'-C1'-C2'	-5.82	101.78	107.60
1	A	28	GLY	N-CA-C	5.72	123.25	115.30
2	C	1950	G	O3'-P-O5'	-5.59	95.61	104.00
2	D	1944	U	O4'-C1'-N1	5.58	116.88	108.50
2	D	1932	A	O4'-C1'-N9	5.57	116.85	108.50
2	D	1933	G	C1'-C2'-O2'	5.56	116.74	108.40
2	C	1956	U	O4'-C1'-N1	5.51	116.47	108.20
1	A	143	GLN	N-CA-C	5.46	118.38	109.59
1	A	94	HIS	N-CA-C	5.36	119.45	113.01
1	B	141	THR	N-CA-C	-5.32	99.47	110.80
2	C	1942	C	N1-C1'-C2'	5.29	119.93	112.00
2	C	1955	U	O5'-C5'-C4'	5.29	119.43	111.50
2	D	1960	A	C4'-C3'-C2'	5.28	107.88	102.60
2	D	1937	A	C4'-C3'-O3'	-5.24	105.14	113.00
2	D	1953	A	O5'-C5'-C4'	5.20	119.50	111.70
2	C	1953	A	O4'-C1'-C2'	-5.20	100.60	105.80
1	B	100	GLN	N-CA-C	-5.11	105.62	111.14
2	C	1944	U	O3'-P-O5'	-5.10	96.35	104.00
2	C	1955	U	C5'-C4'-O4'	-5.09	102.16	109.80
1	A	54	VAL	N-CA-C	5.07	115.39	107.99
2	D	1948	G	C4'-C3'-C2'	-5.07	97.53	102.60
2	D	1952	A	OP1-P-O3'	-5.07	92.80	108.00
2	D	1952	A	C3'-C2'-O2'	5.06	122.19	114.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3245	0	3268	51	0
1	B	3229	0	3251	59	0
2	C	637	0	326	6	0
2	D	637	0	326	4	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	143	0	0	10	0
5	B	142	0	0	6	0
5	C	23	0	0	1	0
5	D	32	0	0	0	0
All	All	8156	0	7209	115	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 (115) 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)
2:C:1937:A:N6	5:C:2003:HOH:O	2.01	0.94
1:B:217:GLU:HG2	5:B:2064:HOH:O	1.70	0.91
1:B:288:ASP:OD2	1:B:359:LYS:HE3	1.73	0.88
1:B:288:ASP:OD2	1:B:359:LYS:CE	2.23	0.86
2:C:1955:U:OP2	2:C:1956:U:H5	1.66	0.78
1:A:355:ASN:HA	5:A:2115:HOH:O	1.85	0.75
1:A:292:ASP:OD1	5:A:2090:HOH:O	2.04	0.74
1:B:209:ALA:HB1	1:B:210:PRO:HD2	1.72	0.71
1:A:136:ASN:ND2	1:A:145:GLN:OE1	2.22	0.71
1:A:193:GLU:OE1	1:A:261:ARG:NH1	2.25	0.70
1:A:340:HIS:HD2	1:B:235:ASP:OD2	1.77	0.68
1:B:430:SER:O	1:B:431:ARG:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:HB3	5:B:2002:HOH:O	1.97	0.65
1:A:149:ARG:HD3	1:A:156:ILE:HD13	1.78	0.65
1:A:310:SER:HB2	5:A:2092:HOH:O	1.99	0.63
1:A:52:VAL:HG22	1:A:64:ALA:HB1	1.81	0.62
1:B:140:LYS:C	1:B:141:THR:O	2.38	0.62
1:A:393:THR:CG2	5:A:2124:HOH:O	2.47	0.62
1:A:59:LYS:HG2	1:A:60:GLN:HG2	1.81	0.62
1:B:351:PRO:O	1:B:354:LYS:NZ	2.24	0.61
1:B:191:HIS:ND1	1:B:206:ARG:HB3	2.16	0.61
1:A:138:LEU:O	1:A:141:THR:O	2.18	0.60
1:B:191:HIS:CE1	1:B:206:ARG:CB	2.86	0.59
1:A:267:ASN:HB3	1:A:416:MET:SD	2.43	0.58
1:B:289:ARG:HG2	1:B:357:PHE:CD1	2.39	0.58
1:A:132:ARG:NH1	2:C:1942:C:O2	2.34	0.57
1:B:183:LEU:O	1:B:186:MET:HG3	2.04	0.57
1:A:351:PRO:HB2	5:A:2114:HOH:O	2.03	0.57
1:A:302:LEU:HD23	1:A:333:LEU:HD12	1.85	0.57
1:B:387:VAL:HG22	1:B:426:MET:HG3	1.85	0.57
1:B:399:GLU:HB3	1:B:403:LYS:NZ	2.19	0.57
1:A:134:SER:HB2	1:A:156:ILE:HD12	1.87	0.56
1:A:393:THR:HG23	5:A:2124:HOH:O	2.03	0.56
1:A:331:ASN:ND2	5:A:2101:HOH:O	2.40	0.55
1:B:356:GLY:HA2	5:B:2119:HOH:O	2.06	0.54
1:A:210:PRO:HG3	1:B:351:PRO:HG3	1.90	0.54
1:A:289:ARG:HG2	1:A:357:PHE:CD1	2.42	0.54
1:A:427:VAL:HG13	1:A:429:PHE:CE2	2.43	0.54
1:A:184:GLN:HE21	1:A:184:GLN:HA	1.72	0.53
1:A:59:LYS:HE3	1:A:60:GLN:HE21	1.73	0.53
1:B:132:ARG:CG	1:B:191:HIS:HD2	2.21	0.53
1:A:387:VAL:HG22	1:A:426:MET:HE2	1.90	0.52
1:B:209:ALA:HB1	1:B:210:PRO:CD	2.39	0.52
1:B:132:ARG:HD2	1:B:191:HIS:CD2	2.45	0.52
1:B:207:HIS:HD2	1:B:209:ALA:O	1.93	0.51
1:A:369:ALA:HB3	1:A:373:MET:HE3	1.94	0.50
1:A:257:THR:HG22	1:A:327:ASN:OD1	2.12	0.50
1:B:297:MET:HE1	1:B:299:ASN:HB2	1.92	0.50
1:B:405:GLY:O	1:B:431:ARG:HG2	2.11	0.50
1:B:411:LEU:HD13	1:B:427:VAL:HG22	1.93	0.50
1:B:201:THR:HG22	1:B:228:LEU:CD1	2.42	0.50
1:B:202:LEU:C	1:B:202:LEU:HD12	2.36	0.50
1:B:267:ASN:HB3	1:B:416:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1955:U:OP2	2:C:1956:U:C5	2.57	0.49
1:A:22:ASN:HD22	1:A:22:ASN:C	2.20	0.49
1:B:132:ARG:HG3	1:B:191:HIS:HD2	1.78	0.48
1:A:114:HIS:CD2	1:A:408:ILE:CG2	2.96	0.48
1:B:136:ASN:HB2	1:B:156:ILE:HD12	1.95	0.48
1:B:399:GLU:HB3	1:B:403:LYS:HZ2	1.76	0.48
1:A:347:VAL:CG2	1:A:352:TRP:HZ2	2.26	0.48
1:A:362:LEU:HD13	1:A:386:TYR:HA	1.95	0.48
1:A:372:VAL:HG23	1:A:373:MET:HE2	1.95	0.48
1:A:202:LEU:HD23	1:A:202:LEU:N	2.28	0.47
1:B:114:HIS:HD1	1:B:115:ASP:N	2.12	0.47
1:B:297:MET:HE3	5:B:2129:HOH:O	2.13	0.47
1:B:24:LEU:HD12	1:B:29:GLN:O	2.15	0.47
1:A:369:ALA:HB1	1:A:372:VAL:HG22	1.96	0.47
2:D:1944:U:H6	2:D:1944:U:H5'	1.79	0.47
1:A:352:TRP:O	1:A:355:ASN:ND2	2.48	0.47
1:B:21:VAL:CG2	1:B:44:LEU:HD13	2.45	0.46
1:A:195:VAL:HB	1:A:202:LEU:HG	1.97	0.46
1:B:183:LEU:O	1:B:186:MET:CG	2.64	0.46
1:A:209:ALA:HB1	1:A:210:PRO:CD	2.45	0.46
1:A:115:ASP:HB2	5:A:2032:HOH:O	2.15	0.46
1:A:347:VAL:HG21	1:A:352:TRP:HZ2	1.80	0.46
1:A:207:HIS:HD2	1:A:209:ALA:O	1.97	0.46
1:B:369:ALA:HB1	1:B:372:VAL:CG2	2.46	0.46
1:B:138:LEU:O	1:B:141:THR:O	2.34	0.46
1:A:414:LEU:HB2	1:A:424:GLU:HB3	1.98	0.45
1:B:204:ILE:HD11	1:B:260:PRO:HB3	1.99	0.45
1:A:216:ARG:HH22	1:A:240:GLU:CD	2.25	0.45
2:D:1953:A:H3'	2:D:1953:A:OP1	2.17	0.45
1:B:173:LEU:HB2	1:B:174:PRO:HD3	1.99	0.45
1:A:37:LYS:NZ	1:A:58:LYS:O	2.45	0.44
1:B:411:LEU:CD1	1:B:427:VAL:HG22	2.48	0.44
1:A:409:ALA:C	1:A:410:ARG:HG2	2.42	0.44
1:B:191:HIS:CE1	1:B:206:ARG:HB2	2.51	0.44
1:B:60:GLN:NE2	2:D:1954:G:OP1	2.49	0.44
1:B:139:PRO:C	1:B:141:THR:O	2.60	0.44
1:B:201:THR:HG22	1:B:228:LEU:HD13	1.99	0.44
1:B:288:ASP:OD2	1:B:359:LYS:CD	2.65	0.44
1:A:347:VAL:HG22	1:A:352:TRP:CZ2	2.53	0.43
1:B:23:ASP:HA	1:B:46:PRO:HG3	1.99	0.43
1:A:124:PRO:HD2	5:A:2038:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:HIS:CE1	1:B:206:ARG:HB3	2.51	0.43
1:B:297:MET:CE	5:B:2129:HOH:O	2.65	0.43
1:B:245:GLU:O	1:B:246:MET:C	2.62	0.42
2:D:1944:U:H6	2:D:1944:U:C5'	2.32	0.42
1:A:134:SER:HB2	1:A:156:ILE:CD1	2.50	0.42
1:B:118:GLU:OE1	1:B:277:ARG:NH2	2.49	0.42
2:C:1954:G:O5'	2:C:1954:G:H2'	2.18	0.42
1:A:387:VAL:CG2	1:A:426:MET:HE2	2.50	0.42
1:B:129:ARG:NH1	5:B:2035:HOH:O	2.43	0.42
1:B:44:LEU:HD11	1:B:50:ALA:HB3	2.01	0.42
1:A:25:ASP:HB2	2:C:1955:U:O4	2.20	0.41
1:B:127:TYR:CZ	1:B:418:PRO:HD2	2.55	0.41
1:B:132:ARG:HD2	1:B:191:HIS:HD2	1.85	0.41
1:B:146:MET:HE1	1:B:173:LEU:O	2.20	0.41
1:A:141:THR:HB	1:A:143:GLN:HG2	2.02	0.41
1:B:50:ALA:HA	1:B:70:LEU:HD22	2.02	0.41
1:B:189:LEU:HD22	1:B:205:LEU:HD11	2.02	0.41
1:B:380:GLU:N	1:B:381:PRO:CD	2.83	0.41
1:A:150:LYS:NZ	5:A:2046:HOH:O	2.54	0.41
1:B:172:LEU:HD11	1:B:201:THR:HG21	2.02	0.41
1:A:274:MET:HG3	1:A:426:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/433 (96%)	404 (97%)	12 (3%)	0	100	100
1	B	414/433 (96%)	400 (97%)	13 (3%)	1 (0%)	43	44
All	All	830/866 (96%)	804 (97%)	25 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	LYS

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	352/365 (96%)	321 (91%)	31 (9%)	9	5
1	B	350/365 (96%)	323 (92%)	27 (8%)	12	7
All	All	702/730 (96%)	644 (92%)	58 (8%)	10	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	17	ILE
1	A	19	VAL
1	A	22	ASN
1	A	41	ILE
1	A	71	SER
1	A	80	ARG
1	A	98	ASP
1	A	141	THR
1	A	142	GLN
1	A	160	LYS
1	A	161	GLN
1	A	175	LYS
1	A	184	GLN
1	A	186	MET
1	A	187	ARG
1	A	202	LEU
1	A	208	THR
1	A	213	SER
1	A	310	SER
1	A	330	LEU
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	347	VAL
1	A	355	ASN
1	A	362	LEU
1	A	380	GLU
1	A	382	ILE
1	A	386	TYR
1	A	393	THR
1	A	407	THR
1	A	431	ARG
1	B	17	ILE
1	B	18	THR
1	B	23	ASP
1	B	39	LEU
1	B	55	THR
1	B	56	GLU
1	B	59	LYS
1	B	66	VAL
1	B	70	LEU
1	B	102	ARG
1	B	186	MET
1	B	187	ARG
1	B	213	SER
1	B	220	GLU
1	B	223	SER
1	B	241	THR
1	B	250	ASP
1	B	272	GLN
1	B	287	GLU
1	B	297	MET
1	B	329	ARG
1	B	336	VAL
1	B	354	LYS
1	B	378	LYS
1	B	382	ILE
1	B	407	THR
1	B	430	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	29	GLN

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Mol	Chain	Res	Type
1	A	49	ASN
1	A	92	GLN
1	A	184	GLN
1	A	207	HIS
1	A	224	HIS
1	A	331	ASN
1	A	340	HIS
1	A	355	ASN
1	A	375	GLN
1	B	34	HIS
1	B	92	GLN
1	B	142	GLN
1	B	184	GLN
1	B	191	HIS
1	B	207	HIS
1	B	325	GLN
1	B	355	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	30/37 (81%)	4 (13%)	1 (3%)
2	D	29/37 (78%)	8 (27%)	5 (17%)
All	All	59/74 (79%)	12 (20%)	6 (10%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	1937	A
2	C	1938	A
2	C	1944	U
2	C	1955	U
2	D	1937	A
2	D	1938	A
2	D	1943	U
2	D	1944	U
2	D	1945	G
2	D	1953	A
2	D	1954	G
2	D	1960	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1932	A
2	D	1937	A
2	D	1943	U
2	D	1944	U
2	D	1952	A
2	D	1953	A

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

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	FMU	D	1939	2,1	19,23,24	1.34	3 (15%)	20,35,38	1.64	4 (20%)
2	FMU	C	1939	2,1	19,23,24	1.53	3 (15%)	20,35,38	2.11	7 (35%)

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	FMU	D	1939	2,1	-	2/7/44/45	0/2/2/2
2	FMU	C	1939	2,1	-	4/7/44/45	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1939	FMU	F-C5	-4.09	1.34	1.42
2	C	1939	FMU	C2-N3	-3.31	1.32	1.38
2	D	1939	FMU	C2-N3	-2.94	1.32	1.38
2	C	1939	FMU	C6-N1	2.23	1.48	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1939	FMU	C4-N3	-2.10	1.34	1.37
2	D	1939	FMU	C6-C5	2.08	1.54	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1939	FMU	N3-C2-N1	6.23	122.91	116.65
2	D	1939	FMU	N3-C2-N1	4.65	121.32	116.65
2	C	1939	FMU	C5M-C5-C4	3.41	111.93	108.82
2	D	1939	FMU	C4-N3-C2	-3.01	122.13	126.67
2	D	1939	FMU	O2-C2-N3	-2.85	116.23	121.49
2	C	1939	FMU	O2-C2-N1	-2.76	119.78	123.10
2	D	1939	FMU	O4-C4-N3	-2.61	116.37	120.59
2	C	1939	FMU	O4'-C1'-N1	-2.36	106.09	109.30
2	C	1939	FMU	O2-C2-N3	-2.28	117.29	121.49
2	C	1939	FMU	C4-N3-C2	-2.26	123.26	126.67
2	C	1939	FMU	C4'-O4'-C1'	-2.15	104.72	109.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1939	FMU	O4'-C1'-N1-C6
2	D	1939	FMU	O4'-C1'-N1-C6
2	C	1939	FMU	O4'-C1'-N1-C2
2	C	1939	FMU	C2'-C1'-N1-C2
2	D	1939	FMU	O4'-C1'-N1-C2
2	C	1939	FMU	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	500	-	27,28,28	1.20	3 (11%)	36,40,40	1.95	8 (22%)
4	SF4	B	501	1	0,12,12	-	-	-		
4	SF4	A	501	1	0,12,12	-	-	-		
3	SAH	B	500	-	27,28,28	1.30	2 (7%)	36,40,40	1.99	11 (30%)

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	SAH	A	500	-	-	0/15/31/31	0/3/3/3
4	SF4	B	501	1	-	-	0/6/5/5
4	SF4	A	501	1	-	-	0/6/5/5
3	SAH	B	500	-	-	1/15/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	SAH	C5-N7	-5.26	1.29	1.39
3	A	500	SAH	C2-N3	3.61	1.40	1.33
3	A	500	SAH	C2-N1	2.71	1.38	1.33
3	B	500	SAH	C8-N7	2.51	1.36	1.31
3	A	500	SAH	OXT-C	-2.03	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	SAH	N3-C2-N1	-6.57	118.63	128.58
3	B	500	SAH	N3-C2-N1	-5.62	120.07	128.58
3	B	500	SAH	C5-C4-N3	-4.36	120.71	126.72
3	B	500	SAH	N9-C8-N7	-4.11	108.10	113.94
3	B	500	SAH	C5-N7-C8	4.08	109.86	103.45
3	A	500	SAH	C4-C5-N7	-3.49	106.59	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	SAH	C5-N7-C8	3.24	108.54	103.45
3	A	500	SAH	N9-C8-N7	-3.22	109.37	113.94
3	A	500	SAH	C5-C4-N3	-3.12	122.42	126.72
3	A	500	SAH	C2-N3-C4	3.01	119.18	111.83
3	B	500	SAH	C6-C5-C4	2.99	121.27	117.18
3	B	500	SAH	C2-N3-C4	2.82	118.71	111.83
3	B	500	SAH	C4-C5-N7	-2.61	107.60	110.58
3	B	500	SAH	C5-C4-N9	2.57	108.61	105.81
3	B	500	SAH	C2-N1-C6	2.43	122.72	118.73
3	A	500	SAH	C2-N1-C6	2.41	122.70	118.73
3	A	500	SAH	C4-N9-C8	2.34	108.19	105.74
3	B	500	SAH	N3-C4-N9	2.04	130.63	127.17
3	B	500	SAH	O4'-C1'-C2'	-2.01	102.31	106.62

There are no chirality outliers.

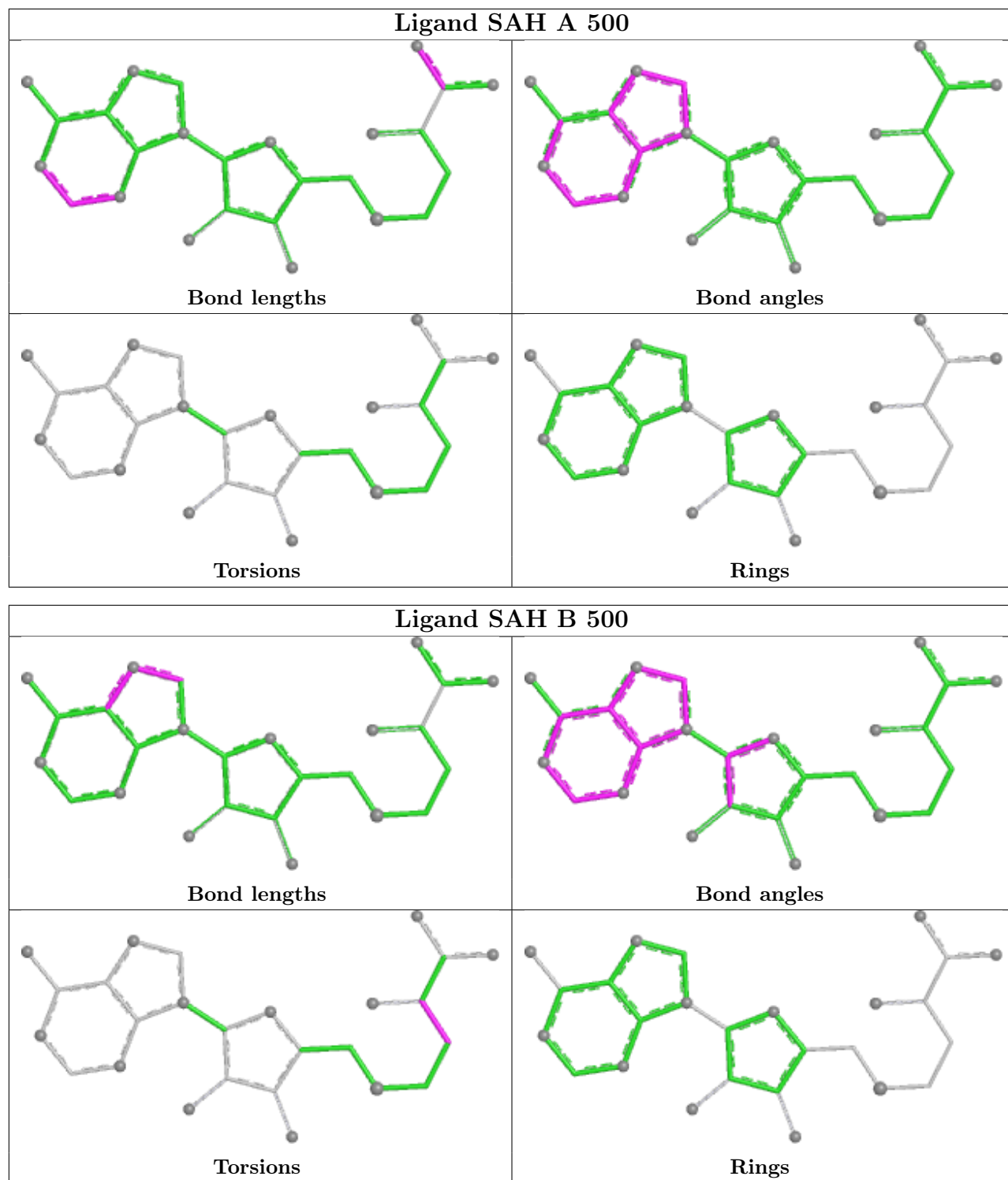
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	500	SAH	C-CA-CB-CG

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 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.