



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 PM UTC

PDB ID : 1SET / pdb\_00001set  
Title : CRYSTAL STRUCTURES AT 2.5 ANGSTROMS RESOLUTION OF  
SERYL-TRNA SYNTHETASE COMPLEXED WITH TWO DIFFERENT  
ANALOGUES OF SERYL-ADENYLATE  
Authors : Cusack, S.; Belrhali, H.  
Deposited on : 1994-02-21  
Resolution : 2.55 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

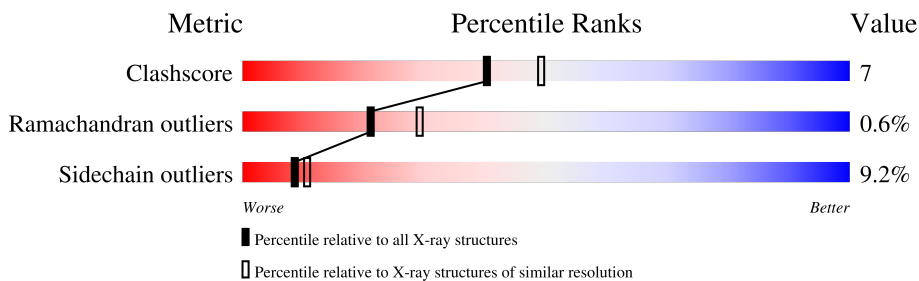
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6974 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.

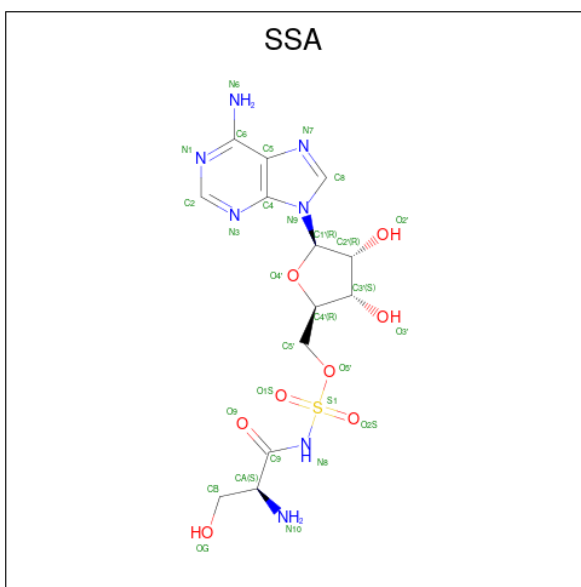
- Molecule 1 is a protein called SERYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3373	2143	606	613	11	185	0	0
1	B	421	3373	2143	606	613	11	239	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	conflict	UNP P34945
B	208	TYR	THR	conflict	UNP P34945

- Molecule 2 is 5'-O-(N-(L-SERYL)-SULFAMOYL)ADENOSINE (CCD ID: SSA) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>7</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	29	13	7	8	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	29	13	7	8	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	89	Total	O	0	0
			89	89		

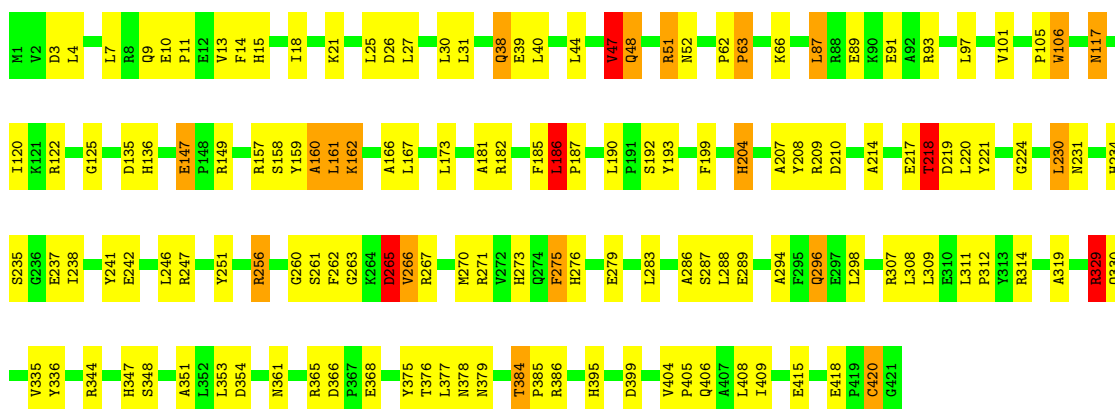
### 3 Residue-property plots

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.

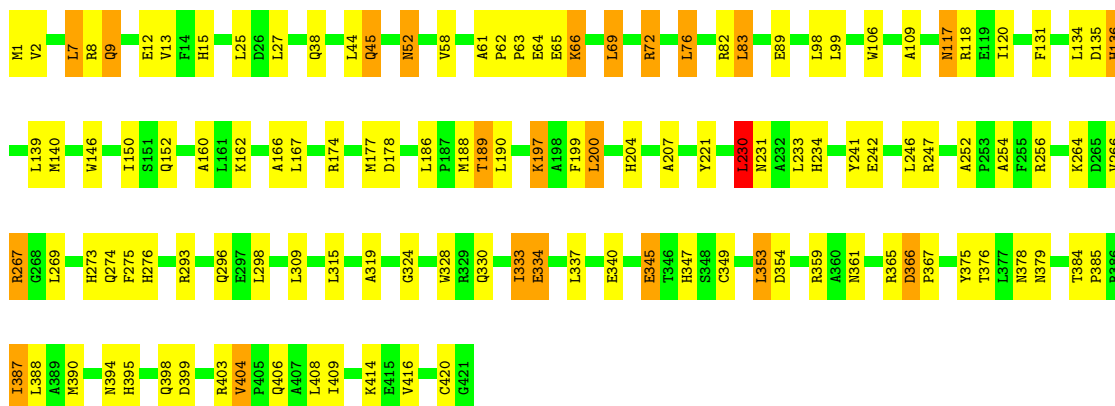
- Molecule 1: SERYL-tRNA SYNTHETASE

Chain A: 



- Molecule 1: SERYL-tRNA SYNTHETASE

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.40Å 126.30Å 62.90Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.55)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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: SSA

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	1.10	9/3448 (0.3%)	1.85	78/4667 (1.7%)
1	B	1.11	10/3448 (0.3%)	1.85	76/4667 (1.6%)
All	All	1.10	19/6896 (0.3%)	1.85	154/9334 (1.6%)

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	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	VAL	CA-CB	7.28	1.63	1.54
1	A	273	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	395	HIS	CD2-NE2	-6.83	1.30	1.37
1	B	395	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	276	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	273	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	276	HIS	CD2-NE2	-6.56	1.30	1.37
1	B	204	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	58	VAL	CA-CB	6.22	1.57	1.54
1	B	15	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	347	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	333	ILE	CA-CB	-5.70	1.47	1.54
1	B	273	HIS	CG-ND1	-5.58	1.32	1.38
1	B	347	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	15	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	347	HIS	CG-ND1	-5.13	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	HIS	CG-ND1	-5.03	1.32	1.38
1	A	237	GLU	CA-CB	-5.02	1.45	1.53
1	A	147	GLU	N-CA	-5.02	1.41	1.46

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	MET	CG-SD-CE	-12.79	72.77	100.90
1	A	379	ASN	OD1-CG-ND2	-10.12	112.48	122.60
1	B	378	ASN	OD1-CG-ND2	-9.43	113.17	122.60
1	A	135	ASP	CA-CB-CG	9.32	121.92	112.60
1	B	61	ALA	CA-C-N	9.31	126.46	119.66
1	B	61	ALA	C-N-CA	9.31	126.46	119.66
1	A	378	ASN	OD1-CG-ND2	-8.58	114.02	122.60
1	B	366	ASP	CA-CB-CG	8.42	121.02	112.60
1	A	266	VAL	O-C-N	8.29	130.43	122.97
1	A	366	ASP	CA-CB-CG	8.23	120.83	112.60
1	B	177	MET	CG-SD-CE	-8.02	83.25	100.90
1	B	152	GLN	CA-CB-CG	7.99	130.07	114.10
1	A	418	GLU	CA-CB-CG	-7.75	98.61	114.10
1	B	378	ASN	CB-CG-ND2	7.71	127.97	116.40
1	A	409	ILE	CA-C-O	-7.61	113.59	118.69
1	B	135	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	399	ASP	CA-CB-CG	7.47	120.07	112.60
1	B	117	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	B	399	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	117	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	162	LYS	CA-CB-CG	7.28	128.67	114.10
1	A	267	ARG	N-CA-C	-7.17	95.53	110.80
1	A	361	ASN	OD1-CG-ND2	-7.11	115.50	122.60
1	B	136	HIS	CA-CB-CG	7.05	120.85	113.80
1	A	296	GLN	CG-CD-NE2	6.93	126.80	116.40
1	A	266	VAL	CA-C-O	6.91	126.37	120.22
1	B	256	ARG	NE-CZ-NH1	6.85	128.35	121.50
1	A	207	ALA	N-CA-C	6.84	119.61	111.33
1	A	275	PHE	CA-CB-CG	6.81	120.61	113.80
1	B	231	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	218	THR	N-CA-CB	-6.77	101.03	111.46
1	B	394	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	A	415	GLU	CB-CG-CD	6.76	124.09	112.60
1	A	234	HIS	CB-CG-CD2	-6.61	122.60	131.20
1	A	3	ASP	CA-CB-CG	6.61	119.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	329	ARG	CG-CD-NE	-6.52	97.65	112.00
1	B	328	TRP	N-CA-C	-6.47	103.46	112.45
1	B	52	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	47	VAL	N-CA-C	-6.44	103.98	111.00
1	B	9	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	A	231	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	347	HIS	CA-CB-CG	6.37	120.17	113.80
1	A	273	HIS	CB-CG-CD2	-6.35	122.95	131.20
1	A	14	PHE	CA-CB-CG	-6.34	107.46	113.80
1	A	260	GLY	N-CA-C	-6.34	98.15	113.18
1	B	207	ALA	N-CA-C	6.33	118.99	111.33
1	B	61	ALA	N-CA-C	6.32	118.64	109.04
1	A	219	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	378	ASN	CB-CG-ND2	6.28	125.82	116.40
1	B	118	ARG	N-CA-CB	-6.27	100.92	110.77
1	A	330	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	B	390	MET	CG-SD-CE	6.20	114.54	100.90
1	B	120	ILE	N-CA-C	-6.17	106.51	111.81
1	A	120	ILE	N-CA-C	-6.15	105.73	111.45
1	A	351	ALA	N-CA-C	-6.14	98.38	108.76
1	A	15	HIS	CA-CB-CG	-6.07	107.73	113.80
1	B	188	MET	CG-SD-CE	-6.06	87.56	100.90
1	B	234	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	B	334	GLU	CA-C-O	-6.03	114.18	120.70
1	B	109	ALA	CA-C-N	6.01	126.03	119.90
1	B	109	ALA	C-N-CA	6.01	126.03	119.90
1	B	409	ILE	CA-C-O	-5.99	114.68	118.69
1	A	361	ASN	CB-CG-ND2	5.97	125.35	116.40
1	B	337	LEU	CA-C-N	5.96	127.29	119.84
1	B	337	LEU	C-N-CA	5.96	127.29	119.84
1	B	247	ARG	CD-NE-CZ	-5.96	116.05	124.40
1	B	296	GLN	CA-C-O	-5.92	114.28	120.55
1	B	361	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	409	ILE	CA-C-N	5.89	126.30	119.47
1	A	409	ILE	C-N-CA	5.89	126.30	119.47
1	B	204	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	A	405	PRO	CA-C-O	-5.84	114.88	121.43
1	B	273	HIS	CA-CB-CG	-5.83	107.97	113.80
1	B	45	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	287	SER	O-C-N	-5.81	116.39	123.30
1	A	160	ALA	N-CA-C	-5.78	98.67	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	ASN	CB-CG-ND2	5.78	125.06	116.40
1	B	197	LYS	CB-CG-CD	5.77	124.56	111.30
1	A	368	GLU	N-CA-C	-5.75	105.84	112.92
1	A	265	ASP	O-C-N	5.75	130.24	122.59
1	A	173	LEU	O-C-N	-5.74	116.04	122.12
1	A	162	LYS	CB-CG-CD	-5.73	98.11	111.30
1	A	186	LEU	CA-C-N	5.73	125.91	119.90
1	A	186	LEU	C-N-CA	5.73	125.91	119.90
1	A	347	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	A	296	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	B	379	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	263	GLY	N-CA-C	-5.65	107.25	114.37
1	B	273	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	B	12	GLU	CA-CB-CG	5.63	125.36	114.10
1	A	66	LYS	CA-CB-CG	5.63	125.36	114.10
1	B	62	PRO	O-C-N	-5.60	118.73	121.31
1	A	238	ILE	N-CA-C	-5.59	98.40	107.28
1	B	256	ARG	CG-CD-NE	-5.57	99.75	112.00
1	A	348	SER	CA-C-N	5.54	129.78	122.30
1	A	348	SER	C-N-CA	5.54	129.78	122.30
1	B	252	ALA	CA-C-N	5.54	125.55	119.90
1	B	252	ALA	C-N-CA	5.54	125.55	119.90
1	A	279	GLU	N-CA-C	5.54	117.99	109.07
1	B	69	LEU	N-CA-C	5.54	118.08	111.71
1	A	62	PRO	CA-C-N	5.51	126.73	119.84
1	A	62	PRO	C-N-CA	5.51	126.73	119.84
1	A	52	ASN	CA-CB-CG	5.51	118.11	112.60
1	B	118	ARG	CA-CB-CG	5.47	125.04	114.10
1	A	214	ALA	O-C-N	-5.46	116.82	123.10
1	A	354	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	106	TRP	CG-CD2-CE3	5.43	139.33	133.90
1	B	117	ASN	CB-CG-ND2	5.43	124.54	116.40
1	B	15	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	B	267	ARG	N-CA-C	5.41	122.33	110.80
1	B	166	ALA	CA-C-N	5.41	127.47	120.44
1	B	166	ALA	C-N-CA	5.41	127.47	120.44
1	A	384	THR	N-CA-C	-5.39	101.85	110.10
1	B	347	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	A	117	ASN	CB-CG-ND2	5.38	124.48	116.40
1	A	404	VAL	CA-C-N	5.38	125.38	119.89
1	A	404	VAL	C-N-CA	5.38	125.38	119.89
1	B	234	HIS	CB-CG-ND1	5.37	130.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	PRO	CA-C-N	5.37	124.82	119.24
1	B	62	PRO	C-N-CA	5.37	124.82	119.24
1	A	420	CYS	N-CA-C	-5.36	98.54	108.24
1	B	340	GLU	N-CA-CB	-5.35	102.83	110.80
1	A	125	GLY	CA-C-N	5.34	125.88	120.38
1	A	125	GLY	C-N-CA	5.34	125.88	120.38
1	B	395	HIS	CA-CB-CG	5.34	119.14	113.80
1	B	178	ASP	CB-CA-C	-5.33	101.94	110.79
1	A	235	SER	CA-CB-OG	-5.32	100.45	111.10
1	B	354	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	234	HIS	CB-CG-ND1	5.28	130.63	122.70
1	A	26	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	38	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	120	ILE	CB-CG1-CD1	-5.23	102.81	113.80
1	A	210	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	347	HIS	CB-CG-ND1	5.20	130.50	122.70
1	A	262	PHE	N-CA-C	-5.18	102.71	110.23
1	B	189	THR	N-CA-C	-5.17	100.75	109.07
1	A	204	HIS	N-CA-C	-5.16	105.78	111.71
1	B	9	GLN	CG-CD-NE2	5.15	124.12	116.40
1	A	266	VAL	CA-C-N	5.11	131.31	121.54
1	A	266	VAL	C-N-CA	5.11	131.31	121.54
1	B	324	GLY	CA-C-N	5.11	124.29	118.97
1	B	324	GLY	C-N-CA	5.11	124.29	118.97
1	B	403	ARG	CA-C-N	-5.11	118.34	123.04
1	B	403	ARG	C-N-CA	-5.11	118.34	123.04
1	B	230	LEU	O-C-N	-5.10	116.72	122.12
1	B	146	TRP	CA-CB-CG	5.09	123.28	113.60
1	A	347	HIS	CB-CG-ND1	5.07	130.31	122.70
1	B	160	ALA	N-CA-C	-5.07	99.36	108.48
1	B	106	TRP	CG-CD1-NE1	-5.04	103.64	110.20
1	B	387	ILE	CB-CA-C	-5.04	100.32	111.77
1	A	136	HIS	CB-CG-ND1	5.04	130.26	122.70
1	B	345	GLU	N-CA-C	5.04	117.74	110.28
1	B	376	THR	CA-CB-OG1	-5.03	102.05	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	TYR	Sidechain

## 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	3373	0	3394	53	9
1	B	3373	0	3394	37	9
2	A	29	0	19	0	0
2	B	29	0	19	0	0
3	A	81	0	0	0	0
3	B	89	0	0	4	0
All	All	6974	0	6826	84	9

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.

All (84) 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:246:LEU:HD12	1:A:283:LEU:HD23	1.72	0.71
1:A:186:LEU:HD11	1:B:162:LYS:HE2	1.71	0.71
1:A:21:LYS:HE3	1:A:105:PRO:HD3	1.77	0.66
1:A:186:LEU:HD21	1:B:420:CYS:SG	2.36	0.64
1:A:190:LEU:HD11	1:A:230:LEU:HD13	1.80	0.63
1:A:157:ARG:HE	1:A:266:VAL:HG21	1.64	0.63
1:A:157:ARG:HH22	1:A:271:ARG:HH21	1.45	0.63
1:A:159:TYR:HD2	1:A:161:LEU:HD13	1.65	0.61
1:B:241:TYR:HB2	1:B:365:ARG:O	2.05	0.57
1:A:157:ARG:NH2	1:A:271:ARG:HH21	2.02	0.57
1:A:117:ASN:ND2	1:A:319:ALA:H	2.03	0.56
1:A:4:LEU:HD23	1:A:7:LEU:HD23	1.87	0.56
1:A:241:TYR:HB2	1:A:365:ARG:O	2.06	0.56
1:B:315:LEU:HD22	1:B:333:ILE:HG12	1.87	0.56
1:B:7:LEU:HD21	1:B:27:LEU:HD11	1.90	0.54
1:B:63:PRO:HA	1:B:66:LYS:HG3	1.90	0.54
1:A:106:TRP:CD1	1:A:329:ARG:HG2	2.42	0.54
1:B:190:LEU:HD11	1:B:230:LEU:HD13	1.90	0.54
1:A:157:ARG:HG2	1:A:266:VAL:HG11	1.90	0.54
1:A:7:LEU:HD11	1:A:27:LEU:HD11	1.90	0.54
1:A:266:VAL:CG2	1:A:271:ARG:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:HB3	1:A:160:ALA:HB3	1.90	0.53
1:A:312:PRO:HG2	1:A:336:TYR:HB3	1.91	0.52
1:B:131:PHE:CD2	1:B:398:GLN:HG2	2.45	0.52
1:A:275:PHE:HB2	1:A:384:THR:O	2.10	0.52
1:B:44:LEU:HA	1:B:83:LEU:HD23	1.91	0.51
1:A:193:TYR:HA	1:A:221:TYR:O	2.12	0.50
1:A:192:SER:H	1:B:274:GLN:HE22	1.58	0.50
1:B:334:GLU:HA	1:B:345:GLU:HA	1.94	0.50
1:A:87:LEU:O	1:A:91:GLU:HB2	2.13	0.49
1:B:136:HIS:HE1	1:B:269:LEU:H	1.59	0.49
1:B:275:PHE:HB2	1:B:384:THR:O	2.11	0.49
1:A:199:PHE:CE2	1:A:221:TYR:HB2	2.47	0.49
1:A:30:LEU:HD12	1:A:97:LEU:HB3	1.94	0.47
1:B:99:LEU:O	1:B:359:ARG:NH2	2.48	0.47
1:A:157:ARG:HE	1:A:266:VAL:HG11	1.80	0.46
1:A:47:VAL:O	1:A:51:ARG:HB2	2.16	0.46
1:A:18:ILE:HD11	1:A:25:LEU:HD23	1.96	0.46
1:B:200:LEU:O	1:B:359:ARG:HD3	2.16	0.46
1:B:414:LYS:HD3	1:B:416:VAL:O	2.16	0.46
1:A:204:HIS:HA	1:A:208:TYR:HD2	1.81	0.45
1:A:256:ARG:HD3	1:A:275:PHE:HE1	1.81	0.45
1:A:25:LEU:HD21	1:A:101:VAL:HG22	1.99	0.45
1:A:158:SER:HA	3:B:429:HOH:O	2.17	0.45
1:B:174:ARG:HA	1:B:174:ARG:HD2	1.88	0.44
1:A:166:ALA:HB1	1:B:189:THR:HG23	1.99	0.44
1:B:174:ARG:HG2	3:B:475:HOH:O	2.17	0.44
1:A:44:LEU:O	1:A:48:GLN:HB2	2.17	0.44
1:A:353:LEU:O	1:A:375:TYR:HA	2.18	0.44
1:A:185:PHE:CD2	1:A:247:ARG:HB3	2.53	0.44
1:A:181:ALA:HB2	1:A:187:PRO:HG3	2.00	0.43
1:B:7:LEU:CD2	1:B:27:LEU:HD11	2.48	0.43
1:A:89:GLU:HB3	1:A:93:ARG:NH2	2.34	0.43
1:B:1:MET:HB2	1:B:359:ARG:CG	2.49	0.43
1:A:122:ARG:HA	1:A:314:ARG:HA	2.01	0.43
1:A:149:ARG:HD3	1:B:233:LEU:O	2.19	0.43
1:B:64:GLU:HG2	1:B:65:GLU:HG3	2.00	0.43
1:B:353:LEU:O	1:B:375:TYR:HA	2.19	0.43
1:B:38:GLN:HG3	3:B:449:HOH:O	2.18	0.42
1:A:294:ALA:HB3	1:A:377:LEU:HD13	2.01	0.42
1:A:311:LEU:HD13	1:A:335:VAL:HG11	2.02	0.42
1:A:218:THR:CG2	1:A:220:LEU:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HB3	1:A:31:LEU:HD11	2.01	0.42
1:A:283:LEU:HD13	1:A:376:THR:HG22	2.01	0.42
1:A:294:ALA:CB	1:A:377:LEU:HD13	2.49	0.42
1:B:1:MET:H3	1:B:359:ARG:HG3	1.83	0.42
1:B:241:TYR:CZ	1:B:367:PRO:HG3	2.55	0.42
1:A:10:GLU:O	1:A:13:VAL:HG22	2.20	0.41
1:A:218:THR:HG22	1:A:220:LEU:H	1.86	0.41
1:B:117:ASN:ND2	1:B:319:ALA:H	2.18	0.41
1:A:162:LYS:HD3	1:B:186:LEU:HD21	2.02	0.41
1:A:224:GLY:O	1:A:256:ARG:NH1	2.51	0.41
1:B:264:LYS:HB2	1:B:264:LYS:HE3	1.87	0.41
1:B:365:ARG:HD2	3:B:492:HOH:O	2.20	0.41
1:A:157:ARG:NE	1:A:266:VAL:HG21	2.32	0.41
1:B:76:LEU:HD13	1:B:76:LEU:HA	1.96	0.41
1:A:270:MET:HE3	1:A:270:MET:HB3	1.83	0.41
1:B:385:PRO:O	1:B:388:LEU:HB2	2.21	0.41
1:B:254:ALA:O	1:B:274:GLN:HA	2.21	0.41
1:A:265:ASP:HB2	1:A:344:ARG:NH2	2.36	0.40
1:A:386:ARG:HH11	1:A:386:ARG:HD3	1.74	0.40
1:B:199:PHE:CE2	1:B:221:TYR:HB2	2.56	0.40
1:B:330:GLN:HA	1:B:349:CYS:O	2.20	0.40
1:B:150:ILE:HD12	1:B:150:ILE:HA	1.74	0.40

All (9) 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:406:GLN:NE2	1:B:72:ARG:NH2[1_656]	0.70	1.50
1:A:406:GLN:NE2	1:B:72:ARG:CZ[1_656]	0.73	1.47
1:A:406:GLN:CD	1:B:72:ARG:NH2[1_656]	1.04	1.16
1:A:406:GLN:NE2	1:B:72:ARG:NH1[1_656]	1.69	0.51
1:A:406:GLN:CD	1:B:72:ARG:CZ[1_656]	1.84	0.36
1:A:406:GLN:NE2	1:B:72:ARG:NE[1_656]	1.88	0.32
1:A:406:GLN:OE1	1:B:72:ARG:NH2[1_656]	2.02	0.18
1:A:406:GLN:CG	1:B:72:ARG:NH2[1_656]	2.06	0.14
1:A:406:GLN:OE1	1:B:72:ARG:NE[1_656]	2.11	0.09

## 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	419/421 (100%)	407 (97%)	8 (2%)	4 (1%)	12	17
1	B	419/421 (100%)	414 (99%)	4 (1%)	1 (0%)	43	56
All	All	838/842 (100%)	821 (98%)	12 (1%)	5 (1%)	21	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	B	267	ARG
1	A	261	SER
1	A	286	ALA
1	A	63	PRO

### 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	347/347 (100%)	317 (91%)	30 (9%)	10	13
1	B	347/347 (100%)	313 (90%)	34 (10%)	7	9
All	All	694/694 (100%)	630 (91%)	64 (9%)	8	10

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	38	GLN
1	A	39	GLU
1	A	40	LEU
1	A	47	VAL
1	A	48	GLN
1	A	51	ARG
1	A	63	PRO
1	A	87	LEU
1	A	161	LEU
1	A	167	LEU
1	A	182	ARG
1	A	186	LEU
1	A	209	ARG
1	A	217	GLU
1	A	218	THR
1	A	230	LEU
1	A	242	GLU
1	A	256	ARG
1	A	288	LEU
1	A	289	GLU
1	A	296	GLN
1	A	298	LEU
1	A	307	ARG
1	A	308	LEU
1	A	309	LEU
1	A	329	ARG
1	A	385	PRO
1	A	408	LEU
1	A	420	CYS
1	B	2	VAL
1	B	7	LEU
1	B	8	ARG
1	B	9	GLN
1	B	13	VAL
1	B	25	LEU
1	B	45	GLN
1	B	52	ASN
1	B	66	LYS
1	B	69	LEU
1	B	72	ARG
1	B	76	LEU
1	B	82	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	83	LEU
1	B	89	GLU
1	B	98	LEU
1	B	134	LEU
1	B	139	LEU
1	B	167	LEU
1	B	197	LYS
1	B	200	LEU
1	B	230	LEU
1	B	242	GLU
1	B	246	LEU
1	B	266	VAL
1	B	293	ARG
1	B	298	LEU
1	B	309	LEU
1	B	353	LEU
1	B	366	ASP
1	B	387	ILE
1	B	404	VAL
1	B	406	GLN
1	B	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	48	GLN
1	A	117	ASN
1	A	280	GLN
1	A	301	ASN
1	A	379	ASN
1	B	117	ASN
1	B	136	HIS
1	B	211	GLN
1	B	274	GLN
1	B	276	HIS
1	B	280	GLN
1	B	301	ASN
1	B	398	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 oligosaccharides 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
2	SSA	B	423	-	30,31,31	1.18	2 (6%)	41,46,46	2.07	6 (14%)
2	SSA	A	422	-	30,31,31	1.12	2 (6%)	41,46,46	1.52	6 (14%)

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	SSA	B	423	-	-	3/20/37/37	0/3/3/3
2	SSA	A	422	-	-	1/20/37/37	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	422	SSA	C9-N8	-3.92	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	423	SSA	O5'-S1	-3.25	1.53	1.60
2	B	423	SSA	C9-N8	-2.63	1.32	1.37
2	A	422	SSA	O5'-S1	-2.12	1.55	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	423	SSA	O2S-S1-O1S	-11.23	104.04	120.85
2	A	422	SSA	O2S-S1-O1S	-6.16	111.63	120.85
2	A	422	SSA	O4'-C1'-N9	2.98	113.81	108.09
2	B	423	SSA	O9-C9-N8	2.90	128.25	122.98
2	A	422	SSA	O5'-S1-O1S	2.89	114.23	105.48
2	A	422	SSA	O4'-C4'-C5'	2.74	118.11	109.33
2	B	423	SSA	O5'-S1-O1S	2.74	113.75	105.48
2	B	423	SSA	C5'-O5'-S1	-2.50	111.73	116.97
2	B	423	SSA	O2'-C2'-C1'	-2.23	102.43	110.10
2	B	423	SSA	O5'-C5'-C4'	2.21	111.50	107.57
2	A	422	SSA	O5'-S1-N8	2.09	111.10	105.69
2	A	422	SSA	C5'-C4'-C3'	-2.01	107.96	115.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

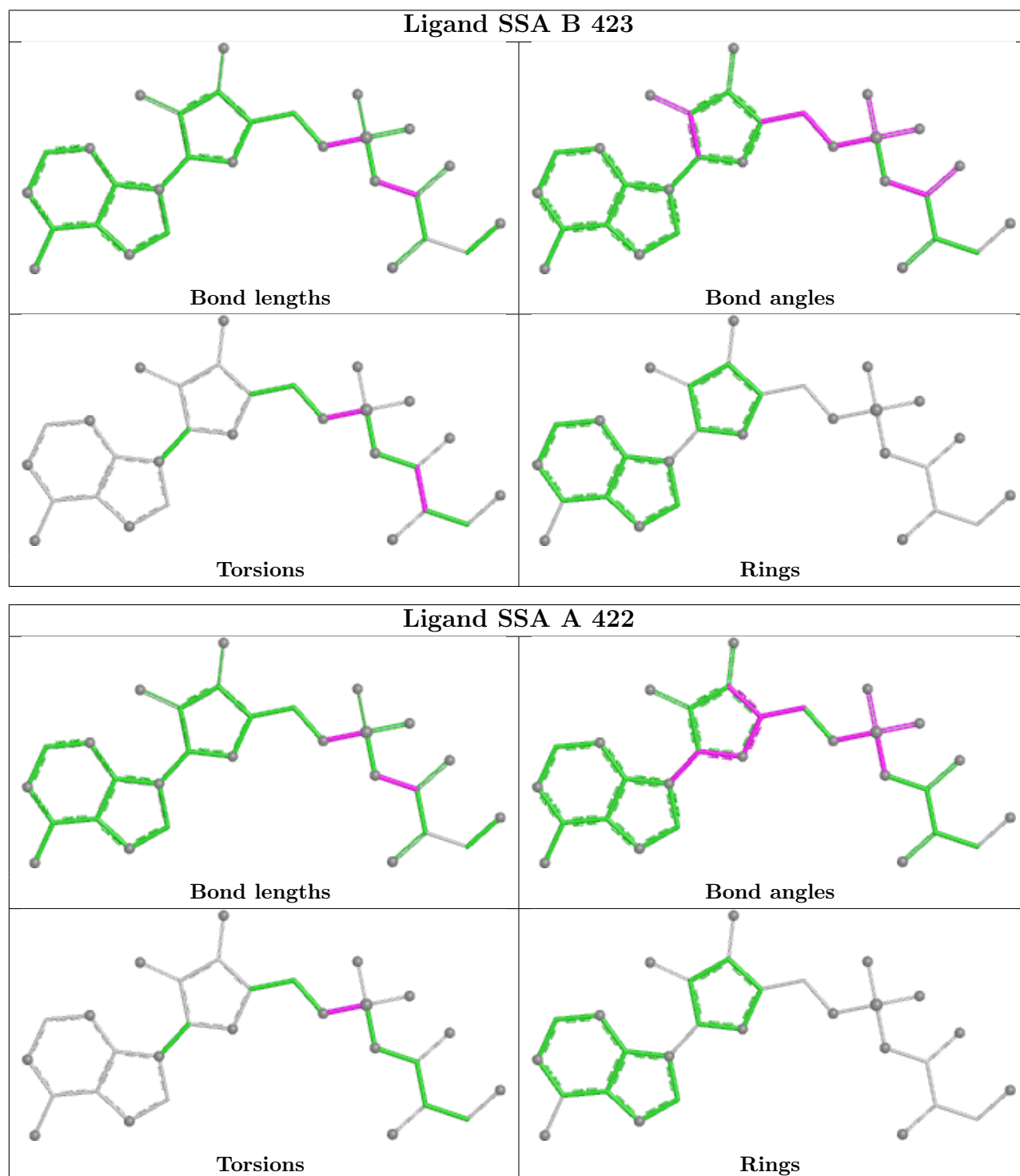
Mol	Chain	Res	Type	Atoms
2	B	423	SSA	O9-C9-CA-CB
2	B	423	SSA	N8-C9-CA-CB
2	A	422	SSA	C5'-O5'-S1-N8
2	B	423	SSA	C5'-O5'-S1-N8

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 ⓘ

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.