



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 03:05 pm BST

PDB ID : 1SES  
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 : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

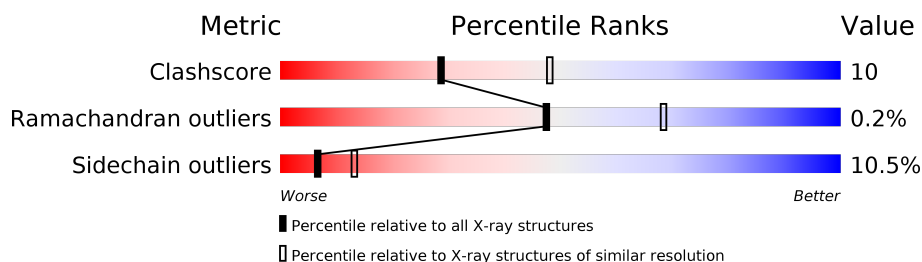
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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  $\geq 3$ , 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 4 unique types of molecules in this entry. The entry contains 6929 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.

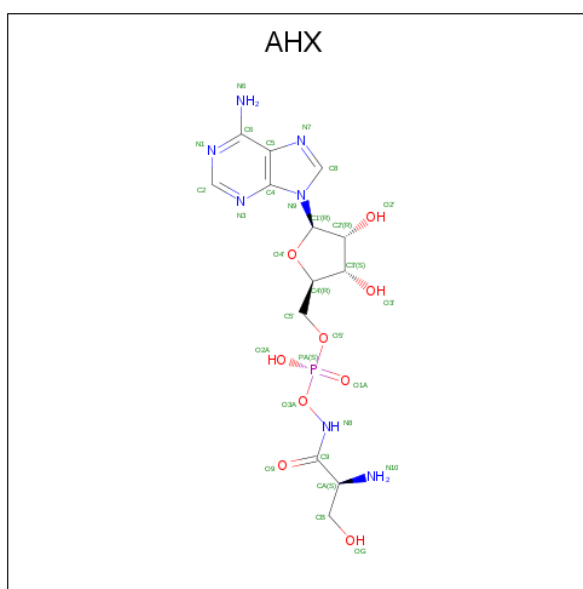
- Molecule 1 is a protein called SERYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	71	0	0
			3373	2143	606	613	11			
1	B	421	Total	C	N	O	S	64	0	0
			3373	2143	606	613	11			

There are 2 discrepancies between the modelled and reference sequences:

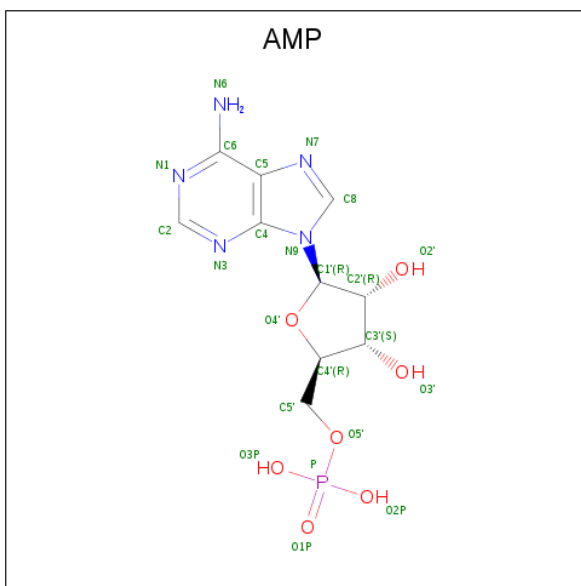
Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	CONFLICT	UNP P34945
B	208	TYR	THR	CONFLICT	UNP P34945

- Molecule 2 is SERYL-HYDROXAMATE-ADENOSINE MONOPHOSPHATE (three-letter code: AHX) (formula:  $C_{13}H_{20}N_7O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	13	7	9	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

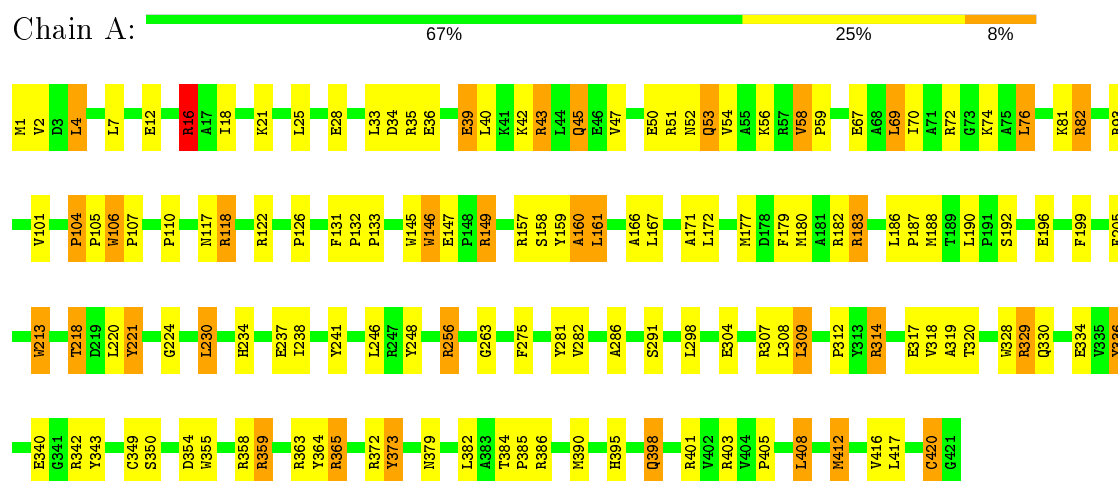
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	69	Total	O	0	0
			69	69		

### 3 Residue-property plots [i](#)

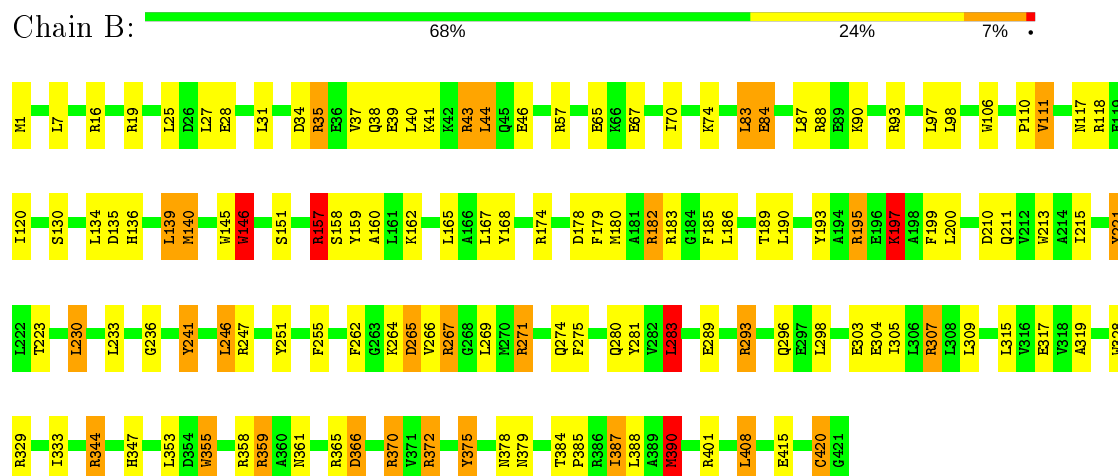
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



#### • Molecule 1: SERYL-tRNA SYNTHETASE



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	85.10Å 125.20Å 62.40Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, AHX

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	0.94	1/3448 (0.0%)	1.59	53/4667 (1.1%)
1	B	0.95	0/3448	1.66	66/4667 (1.4%)
All	All	0.94	1/6896 (0.0%)	1.63	119/9334 (1.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	SER	CA-CB	-5.20	1.45	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	MET	CG-SD-CE	-15.35	75.63	100.20
1	A	188	MET	CG-SD-CE	-14.17	77.53	100.20
1	B	344	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	B	344	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	B	358	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	A	359	ARG	NE-CZ-NH2	-11.67	114.47	120.30
1	B	359	ARG	NE-CZ-NH1	11.57	126.08	120.30
1	B	358	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	B	118	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	355	TRP	CD1-CG-CD2	9.56	113.95	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	B	247	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	307	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	A	106	TRP	CD1-CG-CD2	8.76	113.30	106.30
1	B	271	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	145	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	B	146	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	A	72	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	106	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	A	183	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	372	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	145	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	B	213	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	A	355	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	213	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	307	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	281	TYR	CB-CG-CD1	-7.86	116.28	121.00
1	B	157	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	363	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	72	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	359	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	157	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	149	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	267	ARG	N-CA-C	7.50	131.24	111.00
1	A	16	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	256	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	B	355	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	A	213	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	A	401	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	146	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	A	416	VAL	CG1-CB-CG2	-7.19	99.40	110.90
1	A	106	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	B	213	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	B	221	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	146	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	A	355	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	28	GLU	CA-CB-CG	6.76	128.27	113.40
1	B	375	TYR	CB-CG-CD2	-6.69	116.98	121.00
1	B	106	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	A	412	MET	CA-CB-CG	-6.67	101.97	113.30
1	B	328	TRP	CD1-CG-CD2	6.67	111.63	106.30
1	B	251	TYR	CB-CG-CD2	-6.62	117.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	146	TRP	CG-CD1-NE1	-6.55	103.55	110.10
1	A	372	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	408	LEU	CA-CB-CG	-6.47	100.41	115.30
1	B	328	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	A	146	TRP	CE2-CD2-CG	-6.38	102.19	107.30
1	B	283	LEU	CA-CB-CG	6.35	129.91	115.30
1	B	415	GLU	CA-CB-CG	6.34	127.35	113.40
1	A	307	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	328	TRP	CE2-CD2-CG	-6.31	102.25	107.30
1	B	247	ARG	CB-CG-CD	-6.30	95.22	111.60
1	A	145	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	A	401	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	281	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	19	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	328	TRP	CD1-CG-CD2	6.12	111.19	106.30
1	A	364	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	A	248	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	B	213	TRP	CG-CD1-NE1	-5.94	104.16	110.10
1	B	145	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	365	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	19	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	329	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	197	LYS	N-CA-CB	-5.81	100.14	110.60
1	B	265	ASP	CA-C-N	-5.79	104.45	117.20
1	B	355	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	A	314	ARG	CD-NE-CZ	-5.67	115.67	123.60
1	B	359	ARG	CG-CD-NE	-5.66	99.91	111.80
1	A	145	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	B	264	LYS	N-CA-C	-5.64	95.76	111.00
1	A	118	ARG	CA-CB-CG	5.63	125.78	113.40
1	A	160	ALA	N-CA-C	-5.61	95.85	111.00
1	B	265	ASP	N-CA-C	5.61	126.13	111.00
1	B	329	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	159	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	B	35	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	146	TRP	CA-CB-CG	5.51	124.17	113.70
1	B	145	TRP	CE2-CD2-CG	-5.50	102.90	107.30
1	B	106	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	B	390	MET	CB-CG-SD	-5.42	96.14	112.40
1	B	118	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	408	LEU	CA-CB-CG	-5.38	102.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	177	MET	CG-SD-CE	-5.37	91.61	100.20
1	A	213	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	B	241	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	A	82	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	336	TYR	CG-CD2-CE2	-5.28	117.07	121.30
1	A	359	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	111	VAL	CA-CB-CG1	-5.26	103.01	110.90
1	B	307	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	168	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	370	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	221	TYR	CG-CD2-CE2	-5.21	117.13	121.30
1	A	373	TYR	CG-CD2-CE2	-5.21	117.14	121.30
1	B	37	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	A	355	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	35	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	221	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	378	ASN	CB-CG-ND2	5.10	128.95	116.70
1	B	160	ALA	N-CA-C	-5.08	97.28	111.00
1	A	256	ARG	CG-CD-NE	-5.07	101.16	111.80
1	A	157	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	195	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	373	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	106	TRP	CG-CD1-NE1	-5.01	105.08	110.10
1	B	185	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	VAL	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	3373	0	3394	75	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3373	0	3394	66	2
2	A	30	0	19	2	0
3	B	23	0	12	0	0
4	A	61	0	0	1	0
4	B	69	0	0	1	0
All	All	6929	0	6819	130	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 10.

All (130) 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:159:TYR:HD2	1:A:161:LEU:HD13	1.52	0.74
1:B:190:LEU:HD11	1:B:230:LEU:HD13	1.69	0.74
1:B:136:HIS:HE1	1:B:269:LEU:H	1.34	0.73
1:A:4:LEU:HD23	1:A:7:LEU:HD23	1.72	0.71
1:B:40:LEU:HB3	1:B:87:LEU:HD13	1.75	0.68
1:B:120:ILE:HD11	1:B:317:GLU:HB2	1.75	0.67
1:B:44:LEU:HG	1:B:83:LEU:HB3	1.77	0.67
1:B:43:ARG:HD3	1:B:83:LEU:HD21	1.76	0.66
1:A:412:MET:HA	1:A:412:MET:HE2	1.78	0.66
1:B:110:PRO:HG2	1:B:319:ALA:HA	1.77	0.65
1:A:67:GLU:HA	1:A:70:ILE:HD12	1.80	0.64
1:B:7:LEU:HD11	1:B:27:LEU:HD11	1.79	0.63
1:B:44:LEU:HD11	1:B:84:GLU:HA	1.81	0.63
1:A:171:ALA:HB2	1:B:174:ARG:HH12	1.64	0.62
1:A:16:ARG:HB3	1:A:16:ARG:HH11	1.64	0.61
1:A:420:CYS:SG	1:B:186:LEU:HD11	2.40	0.61
1:B:67:GLU:HA	1:B:70:ILE:HD12	1.83	0.61
1:B:41:LYS:HG2	1:B:87:LEU:HD21	1.82	0.60
1:A:21:LYS:HE3	1:A:105:PRO:HD3	1.83	0.60
1:A:218:THR:HG22	1:A:220:LEU:H	1.66	0.60
1:B:275:PHE:HB2	1:B:384:THR:O	2.01	0.60
1:A:192:SER:H	1:B:274:GLN:HE22	1.52	0.58
1:A:171:ALA:HB2	1:B:174:ARG:NH1	2.18	0.58
1:B:199:PHE:CE1	1:B:221:TYR:HB2	2.40	0.57
1:A:106:TRP:CD1	1:A:329:ARG:HG2	2.39	0.57
1:A:241:TYR:HB2	1:A:365:ARG:O	2.06	0.56
1:A:334:GLU:HB3	1:A:343:TYR:HB3	1.87	0.56
1:B:1:MET:H1	1:B:359:ARG:HE	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:TYR:HB2	1:B:365:ARG:O	2.09	0.53
1:B:384:THR:HG22	1:B:387:ILE:HD11	1.91	0.53
1:A:58:VAL:HG22	1:A:69:LEU:HB3	1.92	0.52
1:B:355:TRP:O	1:B:359:ARG:HG3	2.09	0.52
1:A:158:SER:HA	4:B:460:HOH:O	2.10	0.52
1:A:179:PHE:HD2	1:A:180:MET:HE2	1.76	0.51
1:A:312:PRO:HG2	1:A:336:TYR:HB3	1.93	0.51
1:A:42:LYS:O	1:A:45:GLN:HB2	2.10	0.51
1:A:183:ARG:NH2	1:A:304:GLU:HG2	2.26	0.50
1:B:158:SER:H	1:B:267:ARG:HH21	1.58	0.50
1:A:54:VAL:O	1:A:58:VAL:HG23	2.12	0.50
1:B:293:ARG:HH21	1:B:296:GLN:NE2	2.09	0.50
1:A:199:PHE:CE1	1:A:221:TYR:HB2	2.47	0.49
1:A:110:PRO:HD2	1:A:319:ALA:HA	1.94	0.49
1:B:134:LEU:HD12	1:B:139:LEU:HD13	1.93	0.49
1:B:136:HIS:O	1:B:140:MET:HG3	2.12	0.49
1:B:44:LEU:HA	1:B:83:LEU:HD23	1.95	0.49
1:A:53:GLN:HA	1:A:56:LYS:HE2	1.93	0.49
1:B:385:PRO:O	1:B:388:LEU:HB2	2.13	0.49
1:A:224:GLY:O	1:A:256:ARG:NH1	2.47	0.48
1:A:117:ASN:ND2	1:A:319:ALA:H	2.12	0.48
1:A:190:LEU:HD11	1:A:230:LEU:HD13	1.95	0.48
1:A:412:MET:CE	1:A:412:MET:HA	2.42	0.48
1:A:36:GLU:O	1:A:39:GLU:HG3	2.14	0.48
1:B:183:ARG:HH12	1:B:304:GLU:HG2	1.78	0.48
1:B:179:PHE:HD2	1:B:180:MET:HE2	1.78	0.48
1:A:196:GLU:HG3	1:A:205:PHE:CD2	2.49	0.47
1:A:218:THR:CG2	1:A:220:LEU:H	2.27	0.47
1:B:140:MET:HE1	1:B:146:TRP:HB3	1.94	0.47
1:B:366:ASP:HB3	1:B:372:ARG:HD2	1.95	0.47
1:A:192:SER:H	1:B:274:GLN:NE2	2.13	0.47
1:A:286:ALA:HB2	1:A:373:TYR:O	2.13	0.47
1:A:50:GLU:HG3	1:A:53:GLN:HE22	1.80	0.47
1:B:246:LEU:HB2	1:B:283:LEU:HB3	1.97	0.47
1:A:147:GLU:HB3	1:A:160:ALA:HB3	1.97	0.46
1:B:117:ASN:ND2	1:B:319:ALA:H	2.12	0.46
1:B:90:LYS:HD3	1:B:93:ARG:HH11	1.79	0.46
1:A:213:TRP:CE3	1:B:215:ILE:HD13	2.50	0.46
1:B:210:ASP:OD2	1:B:211:GLN:HG2	2.15	0.46
1:A:234:HIS:O	1:A:237:GLU:HB3	2.15	0.46
1:A:43:ARG:O	1:A:47:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HB	1:B:315:LEU:HB2	1.98	0.46
1:A:122:ARG:HA	1:A:314:ARG:HA	1.98	0.46
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.98	0.45
1:A:51:ARG:HG2	1:A:76:LEU:HB3	1.98	0.45
1:A:395:HIS:CE1	1:A:405:PRO:HG3	2.52	0.45
1:A:275:PHE:HB2	1:A:384:THR:O	2.16	0.45
1:B:255:PHE:CE2	1:B:274:GLN:NE2	2.85	0.45
1:A:132:PRO:HA	1:A:133:PRO:HD2	1.87	0.45
1:A:56:LYS:O	1:A:59:PRO:HD2	2.16	0.45
1:B:140:MET:HE3	1:B:165:LEU:CD2	2.47	0.44
1:B:157:ARG:H	1:B:267:ARG:NE	2.15	0.44
1:B:195:ARG:HB2	1:B:197:LYS:NZ	2.33	0.44
1:A:186:LEU:CD1	1:B:420:CYS:SG	3.05	0.44
1:A:18:ILE:HD11	1:A:25:LEU:HD23	2.00	0.44
1:A:256:ARG:HH22	2:A:422:AHX:PA	2.39	0.44
1:A:186:LEU:HD21	1:B:162:LYS:HE3	1.99	0.44
1:A:33:LEU:HD21	1:A:93:ARG:HG3	1.99	0.44
1:B:1:MET:HB2	1:B:359:ARG:HG2	1.99	0.44
1:A:340:GLU:HB3	1:A:342:ARG:HG2	1.99	0.44
1:B:179:PHE:O	1:B:183:ARG:HG2	2.18	0.44
1:B:178:ASP:O	1:B:182:ARG:HD3	2.18	0.43
1:B:183:ARG:NH1	1:B:304:GLU:HG2	2.33	0.43
1:B:333:ILE:HB	1:B:347:HIS:HB2	2.00	0.43
1:A:25:LEU:HD21	1:A:101:VAL:HG22	2.00	0.43
1:B:280:GLN:HB2	1:B:379:ASN:O	2.19	0.43
1:B:140:MET:CE	1:B:146:TRP:HB3	2.49	0.43
1:B:180:MET:CE	1:B:305:ILE:HD11	2.49	0.43
1:B:136:HIS:CE1	1:B:269:LEU:H	2.23	0.43
1:B:303:GLU:O	1:B:307:ARG:HG3	2.19	0.43
1:B:353:LEU:O	1:B:375:TYR:HA	2.19	0.43
1:B:344:ARG:HB2	1:B:390:MET:CE	2.49	0.43
1:A:309:LEU:HD21	1:A:382:LEU:HD11	2.00	0.43
1:A:386:ARG:NH1	2:A:422:AHX:H2'	2.34	0.43
1:A:318:VAL:HB	1:A:330:GLN:HB3	2.01	0.42
1:A:2:VAL:HA	4:A:449:HOH:O	2.17	0.42
1:A:420:CYS:SG	1:B:186:LEU:CD1	3.07	0.42
1:A:149:ARG:HD3	1:B:233:LEU:O	2.20	0.42
1:A:1:MET:N	1:A:359:ARG:HH11	2.17	0.42
1:B:236:GLY:HA2	1:B:361:ASN:ND2	2.35	0.42
1:A:131:PHE:HB3	1:A:398:GLN:NE2	2.35	0.42
1:A:104:PRO:HA	1:A:105:PRO:HD2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:O	1:B:359:ARG:HD3	2.20	0.42
1:A:1:MET:H3	1:A:359:ARG:HD2	1.85	0.42
1:A:218:THR:CG2	1:A:220:LEU:HB2	2.49	0.42
1:B:157:ARG:NH2	1:B:271:ARG:HD2	2.34	0.42
1:B:199:PHE:CZ	1:B:223:THR:HG22	2.55	0.41
1:A:246:LEU:O	1:A:282:VAL:HA	2.20	0.41
1:A:330:GLN:HA	1:A:349:CYS:O	2.21	0.41
1:A:1:MET:HB3	1:A:358:ARG:HB2	2.02	0.41
1:A:21:LYS:HG2	1:A:320:THR:O	2.21	0.41
1:B:179:PHE:CE2	1:B:180:MET:HE1	2.55	0.41
1:A:317:GLU:OE1	1:A:329:ARG:NH1	2.54	0.41
1:A:172:LEU:HB3	1:A:382:LEU:HD21	2.02	0.41
1:A:126:PRO:HB3	1:A:336:TYR:CE2	2.56	0.41
1:A:36:GLU:O	1:A:40:LEU:HD13	2.21	0.41
1:B:193:TYR:HA	1:B:221:TYR:O	2.20	0.41
1:B:34:ASP:O	1:B:38:GLN:HG2	2.21	0.41
1:A:354:ASP:O	1:A:358:ARG:HG3	2.21	0.41
1:A:166:ALA:HB1	1:B:189:THR:HG23	2.03	0.41
1:A:106:TRP:HA	1:A:107:PRO:HD2	1.88	0.40
1:A:81:LYS:HB3	1:A:81:LYS:HE2	1.81	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:82:ARG:NH2	1:B:111:VAL:O[2_657]	1.96	0.24
1:A:50:GLU:OE2	1:B:16:ARG:NH1[2_657]	2.10	0.10

## 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	419/421 (100%)	400 (96%)	18 (4%)	1 (0%)	47	68
1	B	419/421 (100%)	410 (98%)	8 (2%)	1 (0%)	47	68
All	All	838/842 (100%)	810 (97%)	26 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	VAL
1	A	263	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/347 (100%)	313 (90%)	34 (10%)	8	15
1	B	347/347 (100%)	308 (89%)	39 (11%)	6	11
All	All	694/694 (100%)	621 (90%)	73 (10%)	7	13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	12	GLU
1	A	16	ARG
1	A	34	ASP
1	A	39	GLU
1	A	43	ARG
1	A	45	GLN
1	A	52	ASN
1	A	53	GLN
1	A	69	LEU
1	A	74	LYS
1	A	76	LEU
1	A	104	PRO
1	A	118	ARG

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Mol	Chain	Res	Type
1	A	146	TRP
1	A	161	LEU
1	A	167	LEU
1	A	182	ARG
1	A	218	THR
1	A	230	LEU
1	A	238	ILE
1	A	291	SER
1	A	298	LEU
1	A	308	LEU
1	A	309	LEU
1	A	329	ARG
1	A	379	ASN
1	A	385	PRO
1	A	390	MET
1	A	398	GLN
1	A	403	ARG
1	A	408	LEU
1	A	417	LEU
1	A	420	CYS
1	B	25	LEU
1	B	28	GLU
1	B	31	LEU
1	B	35	ARG
1	B	39	GLU
1	B	43	ARG
1	B	44	LEU
1	B	46	GLU
1	B	65	GLU
1	B	74	LYS
1	B	83	LEU
1	B	84	GLU
1	B	88	ARG
1	B	97	LEU
1	B	98	LEU
1	B	130	SER
1	B	135	ASP
1	B	139	LEU
1	B	146	TRP
1	B	151	SER
1	B	157	ARG
1	B	167	LEU

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Mol	Chain	Res	Type
1	B	182	ARG
1	B	197	LYS
1	B	230	LEU
1	B	246	LEU
1	B	262	PHE
1	B	265	ASP
1	B	283	LEU
1	B	289	GLU
1	B	293	ARG
1	B	298	LEU
1	B	309	LEU
1	B	366	ASP
1	B	370	ARG
1	B	387	ILE
1	B	390	MET
1	B	408	LEU
1	B	420	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	117	ASN
1	A	280	GLN
1	A	301	ASN
1	A	361	ASN
1	A	379	ASN
1	B	117	ASN
1	B	136	HIS
1	B	231	ASN
1	B	274	GLN
1	B	276	HIS
1	B	280	GLN
1	B	296	GLN
1	B	301	ASN
1	B	361	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	AMP	B	423	-	22,25,25	1.72	5 (22%)	25,38,38	1.39	4 (16%)
2	AHX	A	422	-	29,32,32	1.02	3 (10%)	29,47,47	1.24	1 (3%)

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	AMP	B	423	-	-	0/6/26/26	0/3/3/3
2	AHX	A	422	-	-	2/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	423	AMP	P-O1P	5.19	1.67	1.50
3	B	423	AMP	O4'-C1'	2.55	1.44	1.41
3	B	423	AMP	C2'-C1'	-2.47	1.50	1.53
3	B	423	AMP	C8-N7	-2.43	1.30	1.34
3	B	423	AMP	P-O2P	-2.38	1.45	1.54
2	A	422	AHX	C9-N8	-2.27	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	422	AHX	O4'-C1'	2.19	1.44	1.41
2	A	422	AHX	O3A-N8	-2.02	1.38	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	422	AHX	C9-CA-N10	-2.90	98.19	109.40
3	B	423	AMP	O5'-P-O1P	-2.75	98.77	106.47
3	B	423	AMP	O3P-P-O2P	2.72	118.02	107.64
3	B	423	AMP	O4'-C1'-C2'	-2.53	103.23	106.93
3	B	423	AMP	C4-C5-N7	2.51	112.02	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

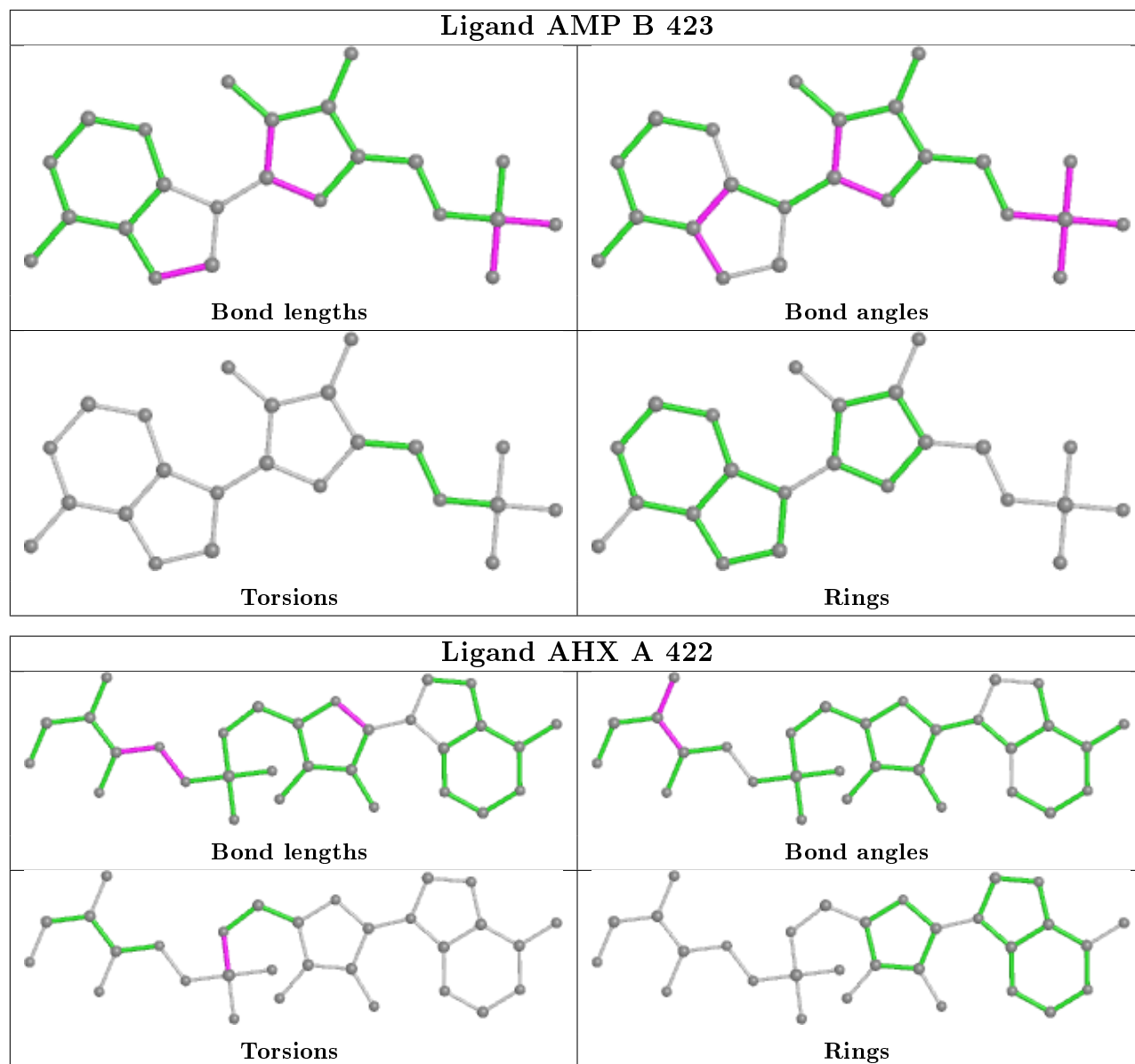
Mol	Chain	Res	Type	Atoms
2	A	422	AHX	C5'-O5'-PA-O1A
2	A	422	AHX	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	422	AHX	2	0

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 [i](#)

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.