



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:46 AM UTC

PDB ID : 1SES / pdb_00001ses
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.

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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

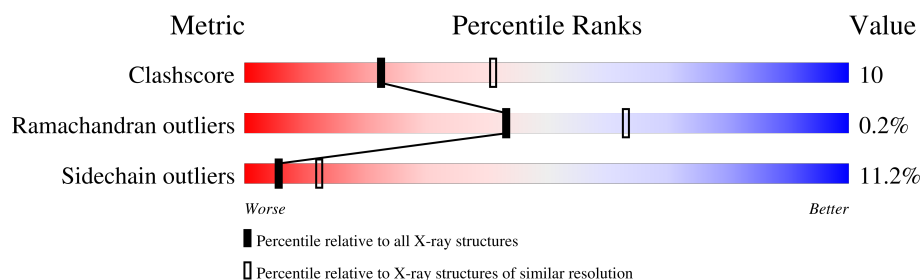
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	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.

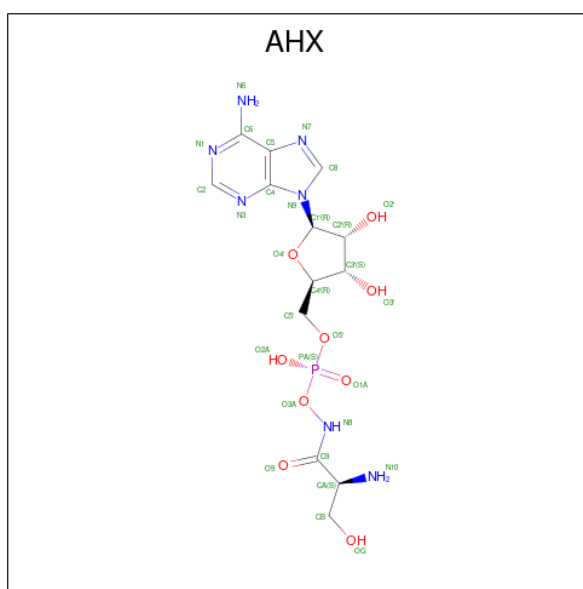
- Molecule 1 is a protein called SERYL-tRNA SYNTHETASE.

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:

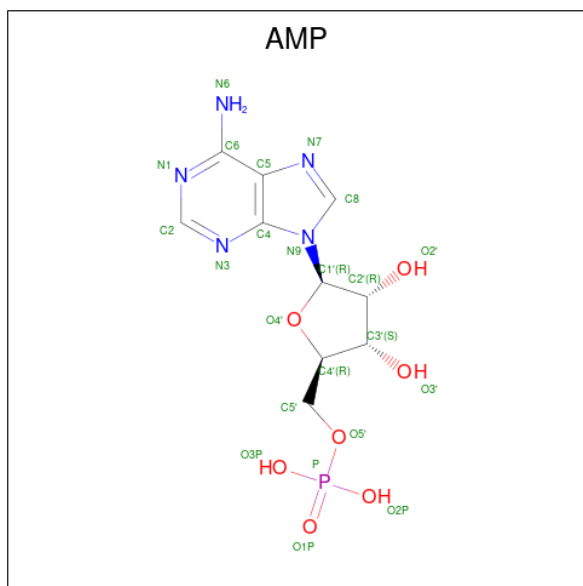
Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	conflict	UNP P34945
B	208	TYR	THR	conflict	UNP P34945

- Molecule 2 is SERYL-HYDROXAMATE-ADENOSINE MONOPHOSPHATE (CCD ID: 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 (CCD ID: 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		

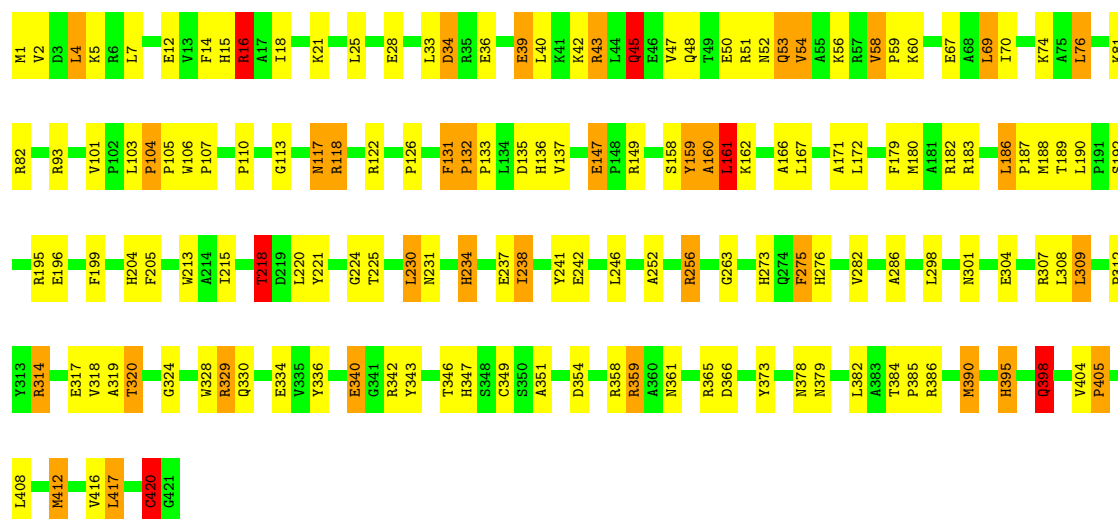
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

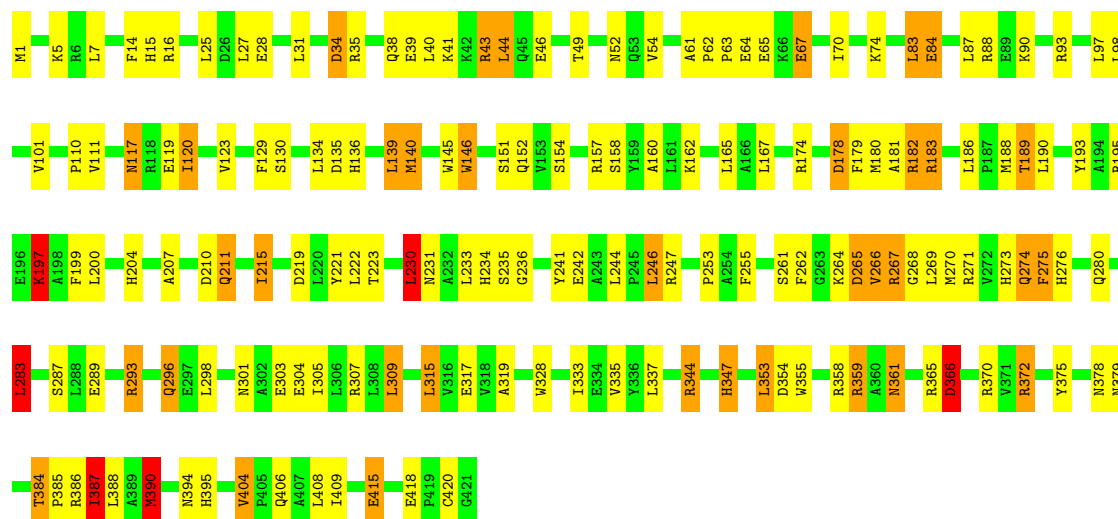
• Molecule 1: SERYL-tRNA SYNTHETASE

Chain A: 



• Molecule 1: SERYL-tRNA SYNTHETASE

Chain B: 



4 Data and refinement statistics

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, α , β , γ	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 ²)	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: AHX, AMP

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	1.17	15/3448 (0.4%)	1.81	66/4667 (1.4%)
1	B	1.18	17/3448 (0.5%)	1.86	86/4667 (1.8%)
All	All	1.18	32/6896 (0.5%)	1.83	152/9334 (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 (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	HIS	CD2-NE2	-7.66	1.29	1.37
1	A	276	HIS	CD2-NE2	-7.50	1.29	1.37
1	B	120	ILE	CA-CB	7.25	1.63	1.54
1	A	395	HIS	CD2-NE2	-7.22	1.29	1.37
1	B	273	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	404	VAL	CA-CB	6.61	1.62	1.54
1	B	204	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	395	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	276	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	347	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	234	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	273	HIS	CG-ND1	-6.08	1.31	1.38
1	B	15	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	273	HIS	CG-ND1	-5.95	1.31	1.38
1	A	15	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	387	ILE	CA-CB	5.86	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	HIS	CG-ND1	-5.62	1.32	1.38
1	B	409	ILE	CA-CB	5.54	1.57	1.53
1	A	54	VAL	CA-CB	5.51	1.62	1.54
1	A	204	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	136	HIS	CD2-NE2	-5.36	1.31	1.37
1	A	395	HIS	CG-ND1	-5.33	1.32	1.38
1	B	154	SER	CA-CB	-5.33	1.46	1.54
1	A	276	HIS	CG-ND1	-5.32	1.32	1.38
1	B	215	ILE	CA-CB	-5.24	1.48	1.54
1	B	234	HIS	CD2-NE2	-5.24	1.32	1.37
1	A	147	GLU	N-CA	-5.13	1.41	1.46
1	A	340	GLU	CA-CB	-5.12	1.45	1.53
1	B	178	ASP	CA-CB	-5.10	1.45	1.53
1	B	204	HIS	CG-ND1	-5.07	1.32	1.38
1	B	347	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	137	VAL	CA-CB	-5.03	1.48	1.54

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	MET	CG-SD-CE	-11.48	75.63	100.90
1	A	188	MET	CG-SD-CE	-10.62	77.53	100.90
1	B	267	ARG	N-CA-C	9.59	131.24	110.80
1	B	366	ASP	CA-CB-CG	9.22	121.83	112.60
1	B	378	ASN	OD1-CG-ND2	-8.61	114.00	122.60
1	B	394	ASN	OD1-CG-ND2	-8.51	114.09	122.60
1	B	378	ASN	CB-CG-ND2	8.37	128.95	116.40
1	A	379	ASN	OD1-CG-ND2	-8.15	114.45	122.60
1	B	14	PHE	CA-CB-CG	-8.07	105.73	113.80
1	B	354	ASP	CA-CB-CG	8.02	120.62	112.60
1	B	242	GLU	CB-CG-CD	7.95	126.12	112.60
1	A	14	PHE	CA-CB-CG	-7.93	105.86	113.80
1	A	117	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	B	219	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	234	HIS	CB-CG-CD2	-7.67	121.23	131.20
1	A	15	HIS	CA-CB-CG	-7.32	106.48	113.80
1	B	117	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	B	273	HIS	CB-CG-CD2	-7.27	121.74	131.20
1	B	274	GLN	OE1-CD-NE2	-7.22	115.38	122.60
1	B	265	ASP	N-CA-C	7.20	126.13	110.80
1	A	160	ALA	N-CA-C	-7.14	95.85	108.13
1	A	28	GLU	CA-CB-CG	7.08	128.27	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	N-CA-C	-7.08	101.15	109.93
1	B	120	ILE	N-CA-C	-7.03	104.00	110.82
1	B	268	GLY	N-CA-C	-7.03	103.90	111.21
1	B	247	ARG	CB-CG-CD	-6.99	95.22	111.30
1	A	234	HIS	CB-CG-CD2	-6.97	122.13	131.20
1	A	231	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	B	270	MET	N-CA-C	6.78	120.03	111.69
1	B	264	LYS	N-CA-C	-6.71	95.76	108.17
1	A	34	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	415	GLU	CA-CB-CG	6.63	127.35	114.10
1	B	197	LYS	N-CA-CB	-6.61	100.14	110.06
1	B	235	SER	CA-CB-OG	-6.58	97.94	111.10
1	A	366	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	34	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	207	ALA	N-CA-C	6.45	120.00	111.75
1	A	215	ILE	N-CA-C	-6.44	98.59	107.99
1	B	328	TRP	N-CA-C	-6.43	102.77	112.04
1	A	273	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	238	ILE	N-CA-C	-6.42	97.87	107.37
1	A	135	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	136	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	405	PRO	CA-C-O	-6.37	114.16	121.36
1	B	261	SER	N-CA-C	6.25	119.72	110.48
1	A	273	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	A	28	GLU	CB-CG-CD	6.24	123.21	112.60
1	A	314	ARG	CD-NE-CZ	-6.24	115.67	124.40
1	B	160	ALA	N-CA-C	-6.22	97.28	108.48
1	A	378	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	351	ALA	N-CA-C	-6.17	99.13	109.07
1	B	183	ARG	N-CA-C	-6.13	105.39	112.92
1	A	347	HIS	CB-CG-CD2	-6.11	123.25	131.20
1	A	420	CYS	N-CA-C	-6.10	103.26	112.04
1	A	412	MET	CA-CB-CG	-6.07	101.97	114.10
1	B	129	PHE	CA-C-O	6.03	127.57	120.69
1	B	15	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	B	52	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	B	234	HIS	CB-CG-ND1	5.99	131.68	122.70
1	A	361	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	394	ASN	CB-CG-ND2	5.92	125.28	116.40
1	B	52	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	361	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	B	384	THR	O-C-N	-5.89	115.90	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	A	118	ARG	CA-CB-CG	5.84	125.78	114.10
1	B	231	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	234	HIS	CA-CB-CG	-5.80	108.00	113.80
1	B	274	GLN	CG-CD-NE2	5.80	125.10	116.40
1	B	123	VAL	N-CA-C	-5.78	99.79	108.12
1	B	358	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	A	404	VAL	CA-C-N	5.77	125.79	119.90
1	A	404	VAL	C-N-CA	5.77	125.79	119.90
1	A	16	ARG	N-CA-C	-5.75	104.92	111.07
1	A	361	ASN	CB-CG-ND2	5.74	125.01	116.40
1	A	307	ARG	CA-CB-CG	-5.73	102.64	114.10
1	A	328	TRP	N-CA-C	-5.73	104.48	112.45
1	B	275	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	132	PRO	CB-CA-C	5.63	117.79	110.92
1	A	252	ALA	CA-C-N	5.61	125.62	119.90
1	A	252	ALA	C-N-CA	5.61	125.62	119.90
1	B	49	THR	N-CA-CB	-5.59	101.68	110.30
1	B	204	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	218	THR	N-CA-CB	-5.57	102.35	111.66
1	B	287	SER	CA-CB-OG	5.57	122.25	111.10
1	B	146	TRP	CA-CB-CG	5.56	124.17	113.60
1	B	230	LEU	N-CA-CB	-5.54	101.98	110.12
1	B	366	ASP	CA-C-N	5.53	125.24	119.82
1	B	366	ASP	C-N-CA	5.53	125.24	119.82
1	B	347	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	B	390	MET	CB-CG-SD	-5.52	96.14	112.70
1	B	152	GLN	N-CA-C	-5.51	105.29	112.23
1	A	186	LEU	CA-C-N	5.50	125.26	119.76
1	A	186	LEU	C-N-CA	5.50	125.26	119.76
1	A	320	THR	CA-CB-OG1	-5.50	101.35	109.60
1	B	359	ARG	CG-CD-NE	-5.50	99.91	112.00
1	B	211	GLN	N-CA-C	5.47	119.95	113.16
1	A	117	ASN	CA-C-O	-5.47	114.69	120.92
1	A	159	TYR	N-CA-C	-5.40	101.09	109.24
1	A	417	LEU	O-C-N	5.39	129.33	123.13
1	B	335	VAL	O-C-N	-5.38	117.38	122.98
1	B	406	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	276	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	B	181	ALA	O-C-N	-5.32	116.48	122.12
1	A	147	GLU	CA-C-N	5.29	124.96	119.56
1	A	147	GLU	C-N-CA	5.29	124.96	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ARG	NE-CZ-NH2	-5.26	114.47	119.20
1	B	418	GLU	CA-C-N	5.26	125.24	120.03
1	B	418	GLU	C-N-CA	5.26	125.24	120.03
1	B	344	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	398	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	61	ALA	CA-C-N	5.24	123.48	119.66
1	B	61	ALA	C-N-CA	5.24	123.48	119.66
1	B	386	ARG	CA-C-O	-5.23	115.00	120.55
1	B	283	LEU	N-CA-C	-5.23	99.89	108.41
1	A	113	GLY	CA-C-N	5.22	128.00	120.38
1	A	113	GLY	C-N-CA	5.22	128.00	120.38
1	A	234	HIS	CB-CG-ND1	5.22	130.52	122.70
1	B	309	LEU	CA-C-N	5.20	129.52	122.19
1	B	309	LEU	C-N-CA	5.20	129.52	122.19
1	A	118	ARG	N-CA-CB	5.20	119.09	110.52
1	A	275	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	48	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	416	VAL	CG1-CB-CG2	-5.18	99.40	110.80
1	B	145	TRP	CD2-CE2-CZ2	-5.18	117.22	122.40
1	B	296	GLN	CA-C-O	-5.15	115.09	120.55
1	B	372	ARG	CB-CG-CD	-5.14	99.47	111.30
1	A	60	LYS	CA-CB-CG	5.14	124.37	114.10
1	B	119	GLU	CA-C-N	5.13	128.08	120.74
1	B	119	GLU	C-N-CA	5.13	128.08	120.74
1	A	225	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	15	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	189	THR	N-CA-C	-5.12	100.83	109.07
1	A	131	PHE	N-CA-C	-5.12	103.61	108.22
1	B	146	TRP	CG-CD1-NE1	-5.12	103.55	110.20
1	B	390	MET	N-CA-C	5.11	118.66	112.23
1	B	409	ILE	O-C-N	-5.10	116.45	120.07
1	A	161	LEU	N-CA-CB	-5.10	102.69	110.85
1	B	266	VAL	N-CA-C	5.08	119.91	109.34
1	A	189	THR	N-CA-C	-5.07	101.42	109.59
1	B	62	PRO	CA-C-O	-5.06	117.26	120.90
1	B	222	LEU	N-CA-C	-5.05	101.47	109.96
1	B	5	LYS	CA-CB-CG	5.05	124.20	114.10
1	B	337	LEU	CA-C-N	5.05	126.15	119.84
1	B	337	LEU	C-N-CA	5.05	126.15	119.84
1	A	45	GLN	O-C-N	5.04	127.27	122.03
1	B	253	PRO	CA-C-O	-5.03	115.68	121.36
1	A	324	GLY	CA-C-N	5.03	124.63	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLY	C-N-CA	5.03	124.63	119.05
1	B	67	GLU	CB-CG-CD	5.02	121.14	112.60
1	B	265	ASP	CA-C-O	5.01	127.67	120.51
1	B	315	LEU	N-CA-C	-5.00	102.00	109.95

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	82	2
1	B	3373	0	3394	70	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	140	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 (140) 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:179:PHE:HD2	1:A:180:MET:HE2	1.50	0.77
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:B:179:PHE:HD2	1:B:180:MET:HE2	1.53	0.73
1:A:412:MET:HA	1:A:412:MET:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD23	1:A:7:LEU:HD23	1.72	0.71
1:B:179:PHE:CD2	1:B:180:MET:HE2	2.25	0.70
1:A:179:PHE:CD2	1:A:180:MET:HE2	2.26	0.69
1:B:40:LEU:HB3	1:B:87:LEU:HD13	1.75	0.68
1:B:44:LEU:HG	1:B:83:LEU:HB3	1.77	0.67
1:B:120:ILE:HD11	1:B:317:GLU:HB2	1.75	0.67
1:B:43:ARG:HD3	1:B:83:LEU:HD21	1.76	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:HH11	1:A:16:ARG:HB3	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:A:180:MET:HE1	1:A:301:ASN:HB3	1.90	0.53
1:B:241:TYR:HB2	1:B:365:ARG:O	2.09	0.53
1:A:171:ALA:HB2	1:A:412:MET:HE3	1.90	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:1:MET:H1	1:B:359:ARG:HE	1.58	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: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:110:PRO:HD2	1:A:319:ALA:HA	1.94	0.49
1:A:199:PHE:CE1	1:A:221:TYR:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD12	1:B:139:LEU:HD13	1.93	0.49
1:B:140:MET:HE2	1:B:146:TRP:HB3	1.94	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:386:ARG:HG2	1:A:390:MET:HE2	1.94	0.49
1:A:171:ALA:CB	1:A:412:MET:HE3	2.43	0.48
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:HA	1:A:412:MET:CE	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: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:366:ASP:HB3	1:B:372:ARG:HD2	1.95	0.47
1:A:162:LYS:HG2	1:B:188:MET:HE3	1.96	0.47
1:A:192:SER:H	1:B:274:GLN:NE2	2.13	0.47
1:A:50:GLU:HG3	1:A:53:GLN:HE22	1.80	0.47
1:A:286:ALA:HB2	1:A:373:TYR:O	2.13	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:90:LYS:HD3	1:B:93:ARG:HH11	1.79	0.46
1:B:117:ASN:ND2	1:B:319:ALA:H	2.12	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:43:ARG:O	1:A:47:VAL:HG23	2.16	0.46
1:A:234:HIS:O	1:A:237:GLU:HB3	2.15	0.46
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:B:180:MET:HE3	1:B:305:ILE:HD11	1.99	0.45
1:A:51:ARG:HG2	1:A:76:LEU:HB3	1.98	0.45
1:A:186:LEU:HD12	1:A:187:PRO:HD2	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:56:LYS:O	1:A:59:PRO:HD2	2.16	0.45
1:A:132:PRO:HA	1:A:133:PRO:HD2	1.87	0.45
1:A:346:THR:CG2	1:A:390:MET:HE3	2.46	0.44
1:B:157:ARG:H	1:B:267:ARG:NE	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:CD1	1:B:420:CYS:SG	3.05	0.44
1:B:195:ARG:HB2	1:B:197:LYS:NZ	2.33	0.44
1:A:18:ILE:HD11	1:A:25:LEU:HD23	2.00	0.44
1:A:186:LEU:HD21	1:B:162:LYS:HE3	1.99	0.44
1:A:256:ARG:HH22	2:A:422:AHX:PA	2.39	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:B:140:MET:HE3	1:B:165:LEU:CD2	2.48	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:136:HIS:CE1	1:B:269:LEU:H	2.23	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:303:GLU:O	1:B:307:ARG:HG3	2.19	0.43
1:B:344:ARG:HB2	1:B:390:MET:CE	2.49	0.43
1:B:353:LEU:O	1:B:375:TYR:HA	2.19	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:B:41:LYS:HZ2	1:B:41:LYS:HB2	1.84	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:B:180:MET:HE1	1:B:301:ASN:HB3	2.01	0.42
1:A:104:PRO:HA	1:A:105:PRO:HD2	1.81	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HG2	1:A:320:THR:O	2.21	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:36:GLU:O	1:A:40:LEU:HD13	2.21	0.41
1:A:126:PRO:HB3	1:A:336:TYR:CE2	2.56	0.41
1:A:354:ASP:O	1:A:358:ARG:HG3	2.21	0.41
1:B:34:ASP:O	1:B:38:GLN:HG2	2.21	0.41
1:B:193:TYR:HA	1:B:221:TYR:O	2.20	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:HE2	1:A:81:LYS:HB3	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%)	43	63
1	B	419/421 (100%)	410 (98%)	8 (2%)	1 (0%)	43	63
All	All	838/842 (100%)	810 (97%)	26 (3%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	VAL

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Mol	Chain	Res	Type
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%)	7	16
1	B	347/347 (100%)	303 (87%)	44 (13%)	4	9
All	All	694/694 (100%)	616 (89%)	78 (11%)	6	12

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LYS
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
1	A	161	LEU
1	A	167	LEU
1	A	182	ARG
1	A	195	ARG
1	A	218	THR
1	A	230	LEU
1	A	238	ILE

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Mol	Chain	Res	Type
1	A	242	GLU
1	A	256	ARG
1	A	298	LEU
1	A	308	LEU
1	A	309	LEU
1	A	329	ARG
1	A	385	PRO
1	A	390	MET
1	A	398	GLN
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	54	VAL
1	B	63	PRO
1	B	64	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	101	VAL
1	B	130	SER
1	B	135	ASP
1	B	139	LEU
1	B	151	SER
1	B	167	LEU
1	B	182	ARG
1	B	197	LYS
1	B	230	LEU
1	B	244	LEU
1	B	246	LEU
1	B	262	PHE

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Mol	Chain	Res	Type
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	353	LEU
1	B	366	ASP
1	B	370	ARG
1	B	387	ILE
1	B	390	MET
1	B	404	VAL
1	B	408	LEU
1	B	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	117	ASN
1	A	280	GLN
1	A	301	ASN
1	A	379	ASN
1	B	45	GLN
1	B	117	ASN
1	B	136	HIS
1	B	274	GLN
1	B	276	HIS
1	B	280	GLN
1	B	296	GLN
1	B	301	ASN
1	B	361	ASN
1	B	394	ASN
1	B	398	GLN

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 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	AHX	A	422	-	31,32,32	0.85	1 (3%)	41,47,47	1.05	1 (2%)
3	AMP	B	423	-	25,25,25	1.43	2 (8%)	37,38,38	1.21	4 (10%)

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	AHX	A	422	-	-	0/18/38/38	0/3/3/3
3	AMP	B	423	-	-	0/10/26/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	423	AMP	P-O1P	5.41	1.67	1.50
3	B	423	AMP	P-O2P	-2.45	1.45	1.54
2	A	422	AHX	C9-N8	-2.27	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	423	AMP	O4'-C1'-N9	3.22	114.27	108.09
2	A	422	AHX	C9-CA-N10	-2.96	98.19	109.37
3	B	423	AMP	O5'-P-O1P	-2.84	98.77	106.44
3	B	423	AMP	O3P-P-O2P	2.73	118.02	107.80
3	B	423	AMP	O2P-P-O5'	2.02	111.93	106.67

There are no chirality outliers.

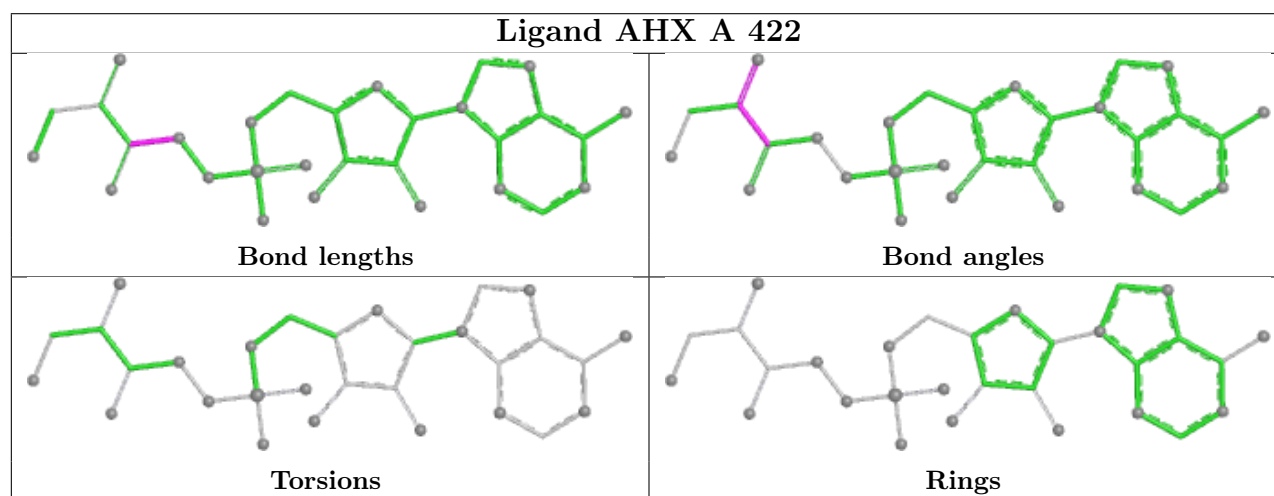
There are no torsion outliers.

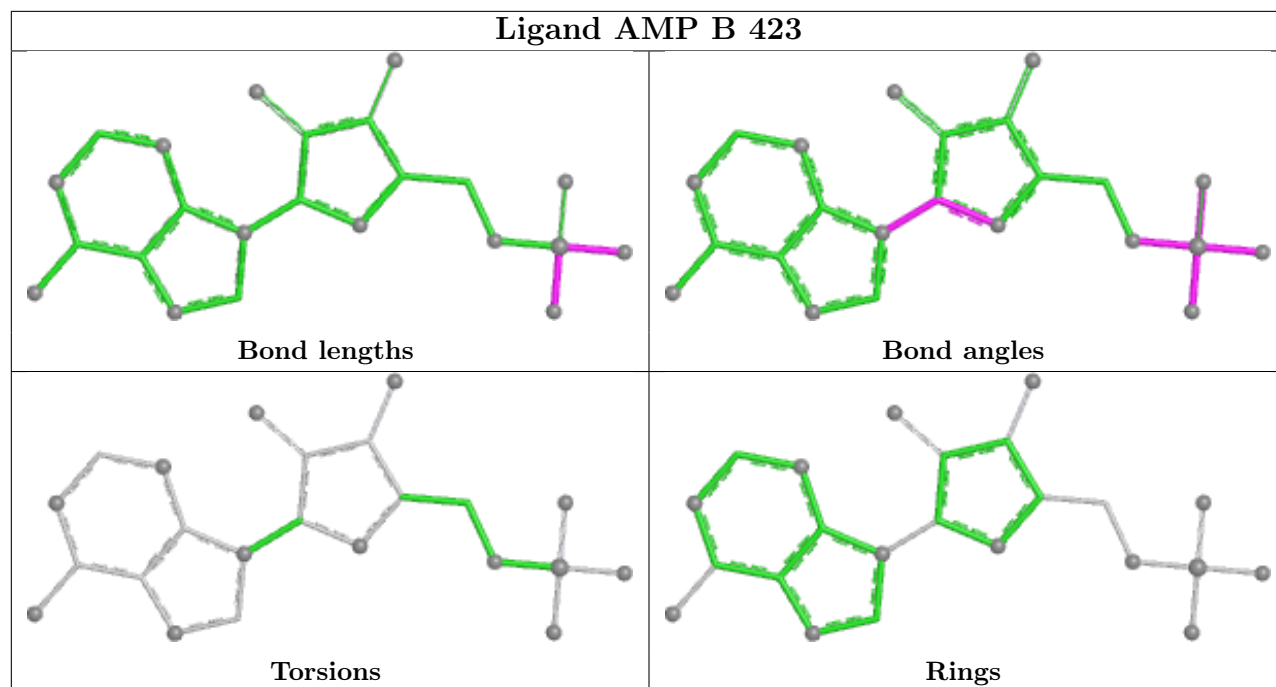
There are no ring outliers.

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.