



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 PM UTC

PDB ID : 1FTA / pdb_00001fta
Title : FRUCTOSE-1,6-BISPHOSPHATASE(D-FRUCTOSE-1,6-BISPHOSPHATE, 1-PHOSPHOHYDROLASE) (E.C.3.1.3.11) COMPLEXED WITH THE ALLOSTERIC INHIBITOR AMP
Authors : Zhang, Y.; Liang, J.-Y.; Huang, S.; Lipscomb, W.N.
Deposited on : 1993-09-27
Resolution : 2.30 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

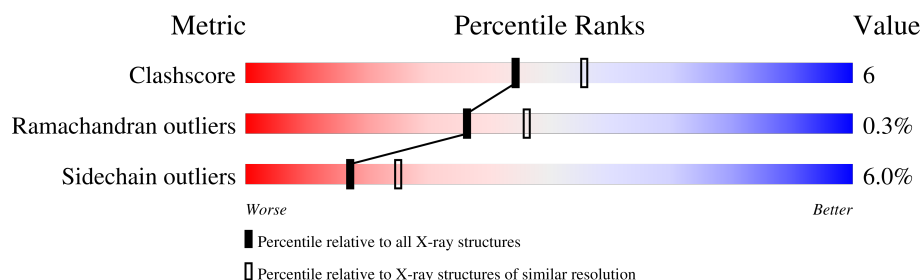
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	337	 67% 24% . . 5%
1	B	337	 73% 18% . . 6%
1	C	337	 71% 18% 5% 6%
1	D	337	 70% 19% . . 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12987 atoms, of which 2819 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 FRUCTOSE-1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	H	N	O	S	0	0	0
			2976	1559	534	408	458	17			
1	B	317	Total	C	H	N	O	S	0	0	0
			2955	1548	529	405	456	17			
1	C	317	Total	C	H	N	O	S	0	0	0
			2955	1548	529	405	456	17			
1	D	318	Total	C	H	N	O	S	0	0	0
			2968	1554	533	407	457	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ASN	conflict	UNP P09467
A	214	ALA	GLY	conflict	UNP P09467
A	316	ILE	VAL	conflict	UNP P09467
B	11	VAL	ASN	conflict	UNP P09467
B	214	ALA	GLY	conflict	UNP P09467
B	316	ILE	VAL	conflict	UNP P09467
C	11	VAL	ASN	conflict	UNP P09467
C	214	ALA	GLY	conflict	UNP P09467
C	316	ILE	VAL	conflict	UNP P09467
D	11	VAL	ASN	conflict	UNP P09467
D	214	ALA	GLY	conflict	UNP P09467
D	316	ILE	VAL	conflict	UNP P09467

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 3 is water.

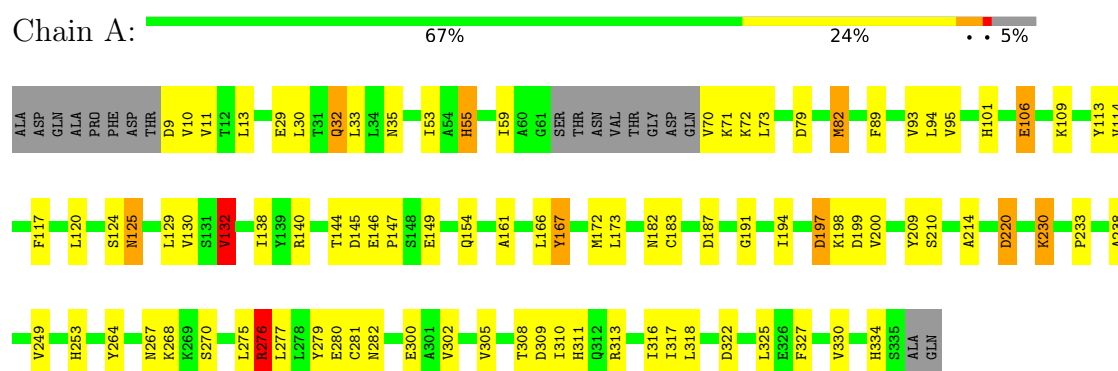
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	75	Total	H	O	0	0
			225	150	75		
3	B	89	Total	H	O	0	0
			267	178	89		
3	C	59	Total	H	O	0	0
			177	118	59		
3	D	124	Total	H	O	0	0
			372	248	124		

3 Residue-property plots

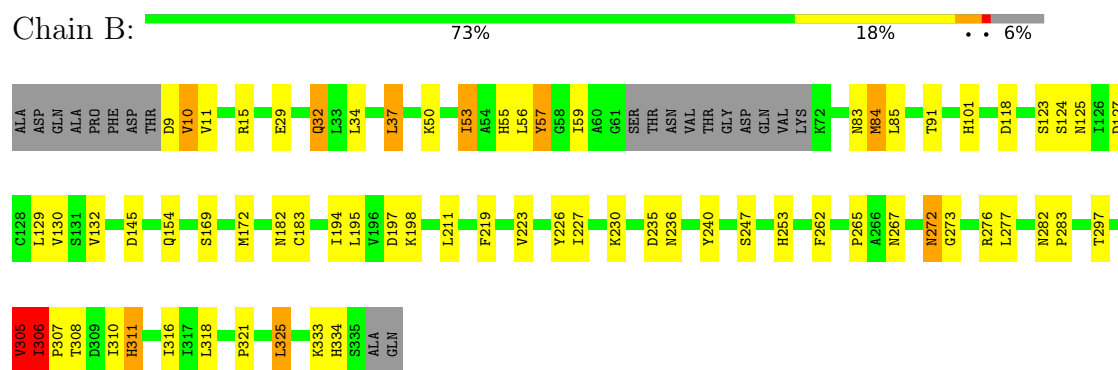
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

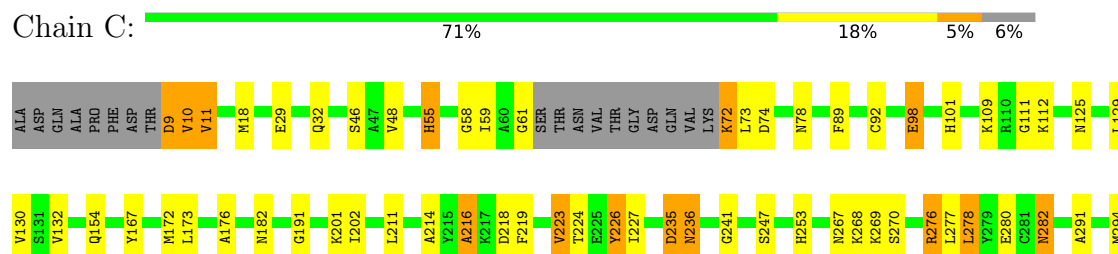
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

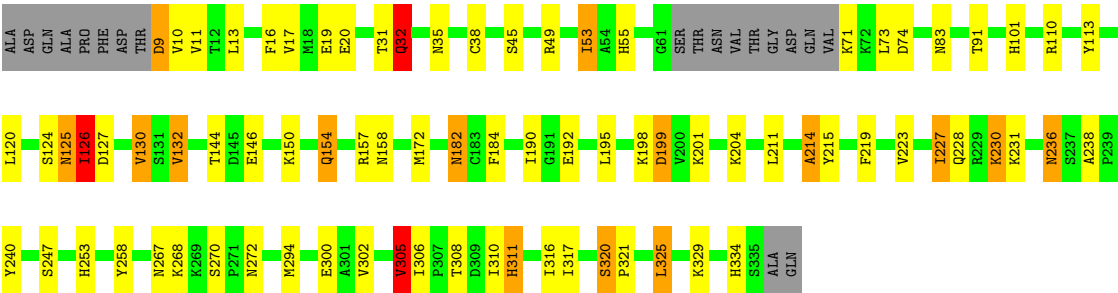


• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE





● Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.60Å 84.80Å 281.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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

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	0.84	6/2485 (0.2%)	1.61	33/3356 (1.0%)
1	B	0.88	7/2469 (0.3%)	1.62	30/3335 (0.9%)
1	C	0.89	8/2469 (0.3%)	1.65	30/3335 (0.9%)
1	D	0.88	7/2478 (0.3%)	1.64	39/3346 (1.2%)
All	All	0.87	28/9901 (0.3%)	1.63	132/13372 (1.0%)

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	4
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	9

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	311	HIS	CD2-NE2	-6.57	1.30	1.37
1	D	101	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	311	HIS	CD2-NE2	-6.53	1.30	1.37
1	C	253	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	101	HIS	CD2-NE2	-6.45	1.30	1.37
1	C	223	VAL	CA-CB	6.43	1.63	1.54
1	D	311	HIS	CD2-NE2	-6.30	1.30	1.37
1	C	311	HIS	CD2-NE2	-6.25	1.30	1.37
1	C	334	HIS	CD2-NE2	-6.22	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	55	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	55	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	334	HIS	CD2-NE2	-6.13	1.31	1.37
1	D	334	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	101	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	305	VAL	CA-CB	6.09	1.61	1.53
1	D	253	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	253	HIS	CD2-NE2	-5.83	1.31	1.37
1	C	101	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	305	VAL	CA-CB	5.74	1.60	1.53
1	A	334	HIS	CD2-NE2	-5.69	1.31	1.37
1	C	305	VAL	CA-CB	5.68	1.61	1.54
1	C	55	HIS	CD2-NE2	-5.60	1.31	1.37
1	D	311	HIS	CG-ND1	-5.58	1.32	1.38
1	A	55	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	334	HIS	CG-ND1	-5.24	1.32	1.38
1	C	334	HIS	CG-ND1	-5.11	1.32	1.38
1	A	334	HIS	CG-ND1	-5.01	1.32	1.38

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	ASP	CA-CB-CG	10.34	122.94	112.60
1	B	132	VAL	N-CA-CB	-9.52	99.19	112.52
1	B	9	ASP	CA-CB-CG	9.21	121.81	112.60
1	B	235	ASP	CA-CB-CG	9.04	121.64	112.60
1	C	132	VAL	N-CA-CB	-8.37	99.88	112.35
1	B	83	ASN	CA-CB-CG	-8.27	104.33	112.60
1	A	309	ASP	CA-CB-CG	8.21	120.81	112.60
1	D	124	SER	N-CA-C	-7.95	102.61	113.18
1	A	317	ILE	N-CA-C	-7.81	96.21	107.77
1	A	276	ARG	CB-CG-CD	7.35	128.19	111.30
1	D	53	ILE	CB-CA-C	-7.33	101.35	112.05
1	B	235	ASP	N-CA-C	-7.24	99.57	110.28
1	A	35	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	D	267	ASN	O-C-N	-7.07	117.81	123.11
1	D	132	VAL	N-CA-CB	-7.03	99.62	111.23
1	D	214	ALA	CB-CA-C	-6.86	99.41	110.79
1	C	98	GLU	N-CA-C	6.81	119.72	111.82
1	C	278	LEU	N-CA-C	6.79	118.76	111.36
1	C	282	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	C	182	ASN	OD1-CG-ND2	-6.65	115.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	VAL	CB-CA-C	6.62	120.91	110.52
1	D	9	ASP	CA-CB-CG	6.61	119.21	112.60
1	C	218	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	197	ASP	CA-CB-CG	6.51	119.11	112.60
1	C	176	ALA	CA-C-O	6.46	127.47	120.43
1	C	308	THR	N-CA-C	-6.40	106.10	114.04
1	A	35	ASN	CA-CB-CG	6.36	118.96	112.60
1	C	11	VAL	N-CA-C	-6.33	99.02	108.46
1	D	329	LYS	CB-CG-CD	-6.26	96.89	111.30
1	B	297	THR	N-CA-C	-6.24	105.71	113.38
1	B	32	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	C	267	ASN	CA-CB-CG	6.22	118.82	112.60
1	C	297	THR	N-CA-C	-6.17	105.75	113.28
1	B	127	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	132	VAL	O-C-N	-6.11	116.28	123.00
1	B	132	VAL	CB-CA-C	6.11	119.86	110.82
1	D	144	THR	CA-CB-OG1	-6.09	100.46	109.60
1	D	32	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	D	74	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	282	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	A	125	ASN	CA-CB-CG	5.99	118.59	112.60
1	B	247	SER	N-CA-C	-5.97	97.10	107.49
1	D	125	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	A	154	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	D	236	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	282	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	B	118	ASP	CA-C-N	5.88	125.58	119.05
1	B	118	ASP	C-N-CA	5.88	125.58	119.05
1	B	32	GLN	CG-CD-NE2	5.88	125.21	116.40
1	C	129	LEU	N-CA-C	5.86	119.74	112.24
1	C	270	SER	CA-C-N	5.86	125.72	119.28
1	C	270	SER	C-N-CA	5.86	125.72	119.28
1	D	247	SER	N-CA-C	-5.85	98.55	108.26
1	A	132	VAL	N-CA-CB	-5.84	100.02	112.00
1	C	235	ASP	N-CA-C	-5.82	98.40	110.80
1	D	113	TYR	N-CA-C	5.77	118.88	109.59
1	D	32	GLN	CG-CD-NE2	5.76	125.05	116.40
1	B	236	ASN	N-CA-C	5.73	118.22	109.62
1	A	144	THR	N-CA-C	-5.72	105.96	113.17
1	A	32	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	C	154	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	106	GLU	CA-C-N	5.66	125.77	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	GLU	C-N-CA	5.66	125.77	119.32
1	A	199	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	233	PRO	CA-C-N	5.60	124.80	118.97
1	A	233	PRO	C-N-CA	5.60	124.80	118.97
1	D	132	VAL	O-C-N	-5.60	115.57	122.57
1	A	267	ASN	CA-CB-CG	5.59	118.19	112.60
1	C	267	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	B	273	GLY	N-CA-C	-5.58	104.56	112.81
1	D	317	ILE	N-CA-C	-5.54	100.36	108.11
1	D	272	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	B	333	LYS	N-CA-C	-5.49	106.78	112.93
1	A	270	SER	CA-C-N	5.47	125.18	119.82
1	A	270	SER	C-N-CA	5.47	125.18	119.82
1	A	82	MET	CA-CB-CG	-5.43	103.25	114.10
1	D	132	VAL	CB-CA-C	5.39	120.12	111.29
1	C	236	ASN	CA-CB-CG	-5.38	107.22	112.60
1	D	154	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	B	306	ILE	CA-C-N	5.38	125.58	120.31
1	B	306	ILE	C-N-CA	5.38	125.58	120.31
1	D	35	ASN	CB-CA-C	-5.38	101.70	110.85
1	C	72	LYS	N-CA-C	-5.38	95.94	111.00
1	A	268	LYS	N-CA-C	5.37	118.62	111.75
1	C	247	SER	N-CA-C	-5.36	99.69	108.76
1	A	79	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	154	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	C	317	ILE	N-CA-C	-5.34	100.43	108.12
1	D	83	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	C	216	ALA	N-CA-C	5.32	117.77	111.33
1	D	126	ILE	CA-CB-CG1	-5.32	101.35	110.40
1	B	145	ASP	N-CA-C	5.30	117.66	110.35
1	B	145	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	306	ILE	CA-C-N	5.28	125.19	119.85
1	D	306	ILE	C-N-CA	5.28	125.19	119.85
1	D	144	THR	N-CA-CB	-5.28	101.34	110.32
1	B	197	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	11	VAL	N-CA-C	-5.26	100.54	108.12
1	B	308	THR	N-CA-C	-5.26	107.52	114.31
1	B	10	VAL	N-CA-C	5.25	120.25	109.34
1	D	320	SER	CA-C-N	5.25	124.70	119.24
1	D	320	SER	C-N-CA	5.25	124.70	119.24
1	A	238	ALA	CA-C-N	5.24	125.16	119.76
1	A	238	ALA	C-N-CA	5.24	125.16	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	127	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	10	VAL	N-CA-C	5.22	120.20	109.34
1	B	267	ASN	N-CA-C	-5.21	101.78	110.17
1	D	204	LYS	CB-CG-CD	-5.21	99.31	111.30
1	D	228	GLN	CA-CB-CG	-5.20	103.71	114.10
1	A	210	SER	CB-CA-C	-5.15	101.61	110.16
1	D	227	ILE	CB-CG1-CD1	-5.12	103.04	113.80
1	C	314	ALA	CA-C-N	5.12	125.02	119.85
1	C	314	ALA	C-N-CA	5.12	125.02	119.85
1	D	53	ILE	N-CA-CB	5.10	118.55	110.54
1	C	112	LYS	N-CA-C	5.09	119.59	113.17
1	B	235	ASP	CA-C-O	-5.08	115.47	121.16
1	A	187	ASP	CA-C-N	5.08	124.87	119.28
1	A	187	ASP	C-N-CA	5.08	124.87	119.28
1	A	145	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	9	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	182	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	279	TYR	N-CA-C	5.04	120.06	113.30
1	C	10	VAL	CB-CA-C	-5.03	103.03	111.29
1	A	140	ARG	N-CA-C	-5.03	101.51	109.96
1	D	238	ALA	CA-C-N	5.03	124.93	119.85
1	D	238	ALA	C-N-CA	5.03	124.93	119.85
1	B	91	THR	N-CA-C	5.03	117.94	109.95
1	A	322	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	272	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	D	199	ASP	N-CA-CB	-5.01	102.02	110.49
1	C	74	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	209	TYR	Sidechain
1	A	264	TYR	Sidechain
1	A	276	ARG	Sidechain
1	B	226	TYR	Sidechain
1	B	57	TYR	Sidechain
1	C	167	TYR	Sidechain
1	C	226	TYR	Sidechain
1	D	258	TYR	Sidechain

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	2442	534	2498	37	0
1	B	2426	529	2476	27	0
1	C	2426	529	2476	28	0
1	D	2435	533	2489	36	0
2	A	23	0	12	1	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	0	0
3	A	75	150	0	0	0
3	B	89	178	0	1	0
3	C	59	118	0	1	0
3	D	124	248	0	3	0
All	All	10168	2819	9987	118	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 6.

All (118) 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:125:ASN:HB3	1:A:130:VAL:HB	1.66	0.78
1:A:302:VAL:O	1:A:305:VAL:HG12	1.92	0.70
1:C:241:GLY:HA2	1:D:214:ALA:HB2	1.74	0.70
1:D:211:LEU:HD11	1:D:227:ILE:HD11	1.74	0.67
1:B:211:LEU:HD11	1:B:227:ILE:HD11	1.77	0.67
1:D:182:ASN:HD22	1:D:198:LYS:HA	1.60	0.67
1:D:302:VAL:HG21	1:D:316:ILE:HD13	1.77	0.67
1:A:183:CYS:SG	1:A:200:VAL:HG21	2.36	0.65
1:B:182:ASN:HD22	1:B:198:LYS:HA	1.61	0.64
1:A:82:MET:HE3	1:A:117:PHE:HZ	1.64	0.62
1:A:82:MET:HE3	1:A:117:PHE:CZ	2.34	0.62
1:B:32:GLN:HE21	1:B:32:GLN:HA	1.64	0.61
1:A:30:LEU:HD12	1:A:33:LEU:HD23	1.83	0.60
1:D:182:ASN:ND2	1:D:198:LYS:HA	2.16	0.60
1:B:37:LEU:HD23	1:B:85:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:HE2	1:B:84:MET:HA	1.87	0.57
1:D:302:VAL:HG21	1:D:316:ILE:CD1	2.34	0.57
1:A:129:LEU:HD11	1:B:172:MET:HB2	1.86	0.55
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.88	0.55
1:D:154:GLN:HE21	1:D:158:ASN:HD22	1.52	0.55
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.89	0.55
1:C:211:LEU:HD11	1:C:227:ILE:HD11	1.89	0.55
1:C:278:LEU:HD12	1:C:310:ILE:HA	1.89	0.54
1:D:230:LYS:HA	1:D:230:LYS:HE2	1.89	0.54
1:B:219:PHE:HB3	1:B:223:VAL:HG13	1.90	0.54
1:B:172:MET:SD	1:B:183:CYS:HB3	2.48	0.53
1:D:32:GLN:HE21	1:D:32:GLN:HA	1.73	0.53
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.90	0.53
1:D:294:MET:HE1	1:D:325:LEU:HD13	1.91	0.53
1:A:89:PHE:CD2	1:A:109:LYS:HA	2.45	0.52
1:C:9:ASP:HA	3:D:416:HOH:O	2.09	0.51
1:D:195:LEU:HD21	1:D:198:LYS:HG2	1.91	0.51
1:C:58:GLY:O	1:D:9:ASP:N	2.43	0.51
1:D:45:SER:O	1:D:49:ARG:HD3	2.10	0.51
1:A:32:GLN:HE21	1:A:32:GLN:HA	1.76	0.50
1:B:32:GLN:HA	1:B:32:GLN:NE2	2.27	0.50
1:C:214:ALA:HB1	1:D:240:TYR:O	2.12	0.50
1:C:89:PHE:HD1	1:C:109:LYS:HA	1.78	0.49
1:A:10:VAL:HG11	1:B:59:ILE:HA	1.93	0.49
1:B:125:ASN:HB3	1:B:130:VAL:HB	1.93	0.49
1:A:138:ILE:HD12	1:A:161:ALA:HB3	1.95	0.48
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.94	0.48
1:A:214:ALA:HB1	1:B:240:TYR:O	2.12	0.48
1:D:19:GLU:HG2	3:D:344:HOH:O	2.11	0.48
1:B:195:LEU:HD21	1:B:198:LYS:HG2	1.96	0.48
1:A:276:ARG:HD3	1:A:313:ARG:HG2	1.94	0.48
1:B:262:PHE:HB3	1:B:318:LEU:HD12	1.95	0.48
1:C:32:GLN:HE21	1:C:32:GLN:HA	1.78	0.48
1:D:126:ILE:HD12	1:D:132:VAL:HG21	1.96	0.47
1:C:316:ILE:HD11	1:C:318:LEU:HD23	1.95	0.47
1:C:294:MET:HE3	1:C:321:PRO:HA	1.96	0.47
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.96	0.47
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.50	0.47
1:A:95:VAL:HG13	1:A:310:ILE:HD12	1.97	0.46
1:A:32:GLN:HA	1:A:32:GLN:NE2	2.31	0.45
1:B:316:ILE:HD11	1:B:318:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASN:HB3	1:C:130:VAL:HB	1.97	0.45
1:C:55:HIS:HA	1:C:59:ILE:HG22	1.99	0.45
1:C:202:ILE:HG22	1:C:291:ALA:O	2.17	0.45
1:C:48:VAL:HA	1:C:73:LEU:HD21	1.99	0.45
1:A:120:LEU:HA	1:A:120:LEU:HD12	1.78	0.45
1:A:316:ILE:HD11	1:A:318:LEU:HD23	1.99	0.45
1:B:84:MET:HA	1:B:84:MET:CE	2.46	0.44
1:A:82:MET:HG3	1:A:94:LEU:HD13	2.00	0.44
1:D:172:MET:HG3	1:D:184:PHE:O	2.17	0.44
1:A:132:VAL:HG12	1:A:167:TYR:HD2	1.82	0.44
1:A:13:LEU:HD22	1:A:173:LEU:HD22	1.99	0.44
1:B:15:ARG:HA	1:D:32:GLN:HE22	1.83	0.44
1:C:29:GLU:HB2	2:C:338:AMP:O1P	2.17	0.44
1:C:294:MET:HE1	1:C:325:LEU:HD22	1.99	0.44
1:D:302:VAL:O	1:D:305:VAL:HG12	2.18	0.43
1:A:113:TYR:OH	2:A:338:AMP:H3'	2.18	0.43
1:C:226:TYR:HB2	1:C:330:VAL:HG21	2.00	0.43
1:A:9:ASP:HA	3:C:396:HOH:O	2.18	0.43
1:B:321:PRO:O	1:B:325:LEU:HB2	2.19	0.43
1:A:275:LEU:HD12	1:A:316:ILE:HG21	2.01	0.43
1:A:276:ARG:HA	1:A:313:ARG:HA	1.99	0.43
1:B:182:ASN:ND2	1:B:198:LYS:HA	2.30	0.43
1:C:92:CYS:HB3	1:C:111:GLY:O	2.18	0.43
1:D:182:ASN:ND2	1:D:199:ASP:H	2.17	0.43
1:D:227:ILE:HG22	1:D:231:LYS:HE3	2.00	0.43
1:A:183:CYS:HB2	1:A:197:ASP:HB3	2.01	0.43
1:D:73:LEU:HG	1:D:120:LEU:CD2	2.49	0.43
1:D:154:GLN:NE2	1:D:158:ASN:HD22	2.15	0.43
1:B:230:LYS:HA	1:B:230:LYS:HE2	2.02	0.42
1:D:157:ARG:HD3	1:D:157:ARG:HA	1.87	0.42
1:C:89:PHE:CD1	1:C:109:LYS:HA	2.54	0.42
1:D:215:TYR:HB2	1:D:219:PHE:CE1	2.54	0.42
1:D:17:VAL:HG12	1:D:31:THR:HG23	2.02	0.42
1:D:71:LYS:N	3:D:445:HOH:O	2.52	0.42
1:D:190:ILE:HG13	1:D:192:GLU:HB2	2.00	0.42
1:A:327:PHE:O	1:A:330:VAL:HG22	2.20	0.42
1:C:78:ASN:HB2	1:C:98:GLU:HG3	2.02	0.42
1:C:306:ILE:HA	1:C:307:PRO:HD3	1.88	0.42
1:A:146:GLU:HA	1:A:147:PRO:HD2	1.91	0.42
1:A:172:MET:HB2	1:B:129:LEU:HD11	2.02	0.42
1:B:306:ILE:HA	1:B:307:PRO:HD3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:N	1:A:230:LYS:HD2	2.35	0.41
1:B:29:GLU:HG3	3:B:355:HOH:O	2.20	0.41
1:B:50:LYS:O	1:B:53:ILE:HG13	2.20	0.41
1:C:268:LYS:HD2	1:C:268:LYS:HA	1.91	0.41
1:D:310:ILE:HG13	1:D:311:HIS:CD2	2.55	0.41
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.55	0.41
1:C:320:SER:HB2	1:C:323:ASP:OD2	2.20	0.41
1:A:70:VAL:HG22	1:A:71:LYS:H	1.84	0.41
1:A:276:ARG:O	1:A:280:GLU:HB2	2.19	0.41
1:D:16:PHE:O	1:D:20:GLU:HB2	2.20	0.41
1:D:91:THR:O	1:D:110:ARG:HA	2.21	0.41
1:C:61:GLY:O	1:D:9:ASP:N	2.53	0.41
1:C:277:LEU:HD22	1:C:312:GLN:NE2	2.36	0.41
1:A:182:ASN:HD22	1:A:198:LYS:HA	1.85	0.41
1:D:125:ASN:HB3	1:D:130:VAL:HG23	2.03	0.41
1:A:93:VAL:O	1:A:114:VAL:HA	2.21	0.40
1:D:13:LEU:HD23	1:D:38:CYS:SG	2.61	0.40
1:C:276:ARG:O	1:C:280:GLU:HB2	2.21	0.40
1:D:320:SER:HA	1:D:321:PRO:HD3	1.88	0.40
1:B:53:ILE:HG22	1:B:56:LEU:HD12	2.02	0.40
1:B:277:LEU:HD11	1:B:305:VAL:HG13	2.04	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	315/337 (94%)	304 (96%)	11 (4%)	0	100	100
1	B	313/337 (93%)	296 (95%)	16 (5%)	1 (0%)	36	46
1	C	313/337 (93%)	299 (96%)	12 (4%)	2 (1%)	21	27
1	D	314/337 (93%)	300 (96%)	13 (4%)	1 (0%)	36	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1255/1348 (93%)	1199 (96%)	52 (4%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ASP
1	C	269	LYS
1	D	270	SER
1	B	57	TYR

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	266/280 (95%)	250 (94%)	16 (6%)	17	25
1	B	264/280 (94%)	247 (94%)	17 (6%)	16	23
1	C	264/280 (94%)	248 (94%)	16 (6%)	17	24
1	D	265/280 (95%)	250 (94%)	15 (6%)	18	27
All	All	1059/1120 (95%)	995 (94%)	64 (6%)	17	25

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

Mol	Chain	Res	Type
1	A	11	VAL
1	A	29	GLU
1	A	53	ILE
1	A	72	LYS
1	A	73	LEU
1	A	106	GLU
1	A	124	SER
1	A	132	VAL
1	A	149	GLU
1	A	194	ILE
1	A	220	ASP

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Mol	Chain	Res	Type
1	A	230	LYS
1	A	276	ARG
1	A	300	GLU
1	A	308	THR
1	A	325	LEU
1	B	10	VAL
1	B	11	VAL
1	B	34	LEU
1	B	37	LEU
1	B	53	ILE
1	B	84	MET
1	B	123	SER
1	B	124	SER
1	B	169	SER
1	B	194	ILE
1	B	265	PRO
1	B	272	ASN
1	B	276	ARG
1	B	283	PRO
1	B	305	VAL
1	B	306	ILE
1	B	325	LEU
1	C	10	VAL
1	C	11	VAL
1	C	18	MET
1	C	46	SER
1	C	72	LYS
1	C	172	MET
1	C	173	LEU
1	C	201	LYS
1	C	223	VAL
1	C	224	THR
1	C	236	ASN
1	C	276	ARG
1	C	282	ASN
1	C	305	VAL
1	C	306	ILE
1	C	325	LEU
1	D	32	GLN
1	D	53	ILE
1	D	126	ILE
1	D	130	VAL

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Mol	Chain	Res	Type
1	D	146	GLU
1	D	150	LYS
1	D	201	LYS
1	D	223	VAL
1	D	230	LYS
1	D	236	ASN
1	D	268	LYS
1	D	300	GLU
1	D	305	VAL
1	D	308	THR
1	D	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	35	ASN
1	A	83	ASN
1	A	154	GLN
1	A	182	ASN
1	B	32	GLN
1	B	182	ASN
1	B	282	ASN
1	C	32	GLN
1	C	83	ASN
1	C	267	ASN
1	C	282	ASN
1	D	32	GLN
1	D	35	ASN
1	D	154	GLN
1	D	182	ASN
1	D	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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	$\# Z > 2$
2	AMP	D	338	-	25,25,25	1.16	3 (12%)	37,38,38	1.69	8 (21%)
2	AMP	B	338	-	25,25,25	1.17	3 (12%)	37,38,38	1.90	9 (24%)
2	AMP	A	338	-	25,25,25	1.19	4 (16%)	37,38,38	1.65	7 (18%)
2	AMP	C	338	-	25,25,25	1.12	2 (8%)	37,38,38	1.73	9 (24%)

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	AMP	D	338	-	-	0/10/26/26	0/3/3/3
2	AMP	B	338	-	-	2/10/26/26	0/3/3/3
2	AMP	A	338	-	-	0/10/26/26	0/3/3/3
2	AMP	C	338	-	-	3/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	338	AMP	C8-N7	3.28	1.38	1.31
2	A	338	AMP	C8-N7	3.12	1.37	1.31
2	C	338	AMP	C8-N7	3.09	1.37	1.31
2	B	338	AMP	C8-N7	2.94	1.37	1.31
2	B	338	AMP	C1'-N9	2.40	1.53	1.46
2	A	338	AMP	C2-N1	2.30	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	338	AMP	C2-N1	2.29	1.38	1.33
2	A	338	AMP	C1'-N9	2.23	1.52	1.46
2	B	338	AMP	C2-N1	2.15	1.37	1.33
2	A	338	AMP	C5'-C4'	-2.15	1.45	1.51
2	D	338	AMP	C2-N1	2.14	1.37	1.33
2	D	338	AMP	C5'-C4'	-2.06	1.45	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	338	AMP	C5-C4-N3	-4.44	120.60	126.72
2	B	338	AMP	C5-C4-N3	-4.39	120.67	126.72
2	A	338	AMP	C5-C4-N3	-4.24	120.89	126.72
2	D	338	AMP	C5-C4-N3	-4.22	120.90	126.72
2	D	338	AMP	N3-C2-N1	-4.21	122.21	128.58
2	B	338	AMP	N3-C2-N1	-3.91	122.66	128.58
2	C	338	AMP	C6-C5-C4	3.80	122.37	117.18
2	A	338	AMP	C6-C5-C4	3.70	122.23	117.18
2	A	338	AMP	N3-C2-N1	-3.68	123.02	128.58
2	B	338	AMP	C6-C5-C4	3.61	122.11	117.18
2	D	338	AMP	C6-C5-C4	3.58	122.07	117.18
2	B	338	AMP	O5'-P-O1P	3.33	115.45	106.44
2	B	338	AMP	O2P-P-O5'	3.33	115.35	106.67
2	B	338	AMP	C6-C5-N7	-3.23	125.87	132.09
2	C	338	AMP	N3-C2-N1	-3.00	124.04	128.58
2	B	338	AMP	O3P-P-O1P	-2.80	99.94	110.83
2	C	338	AMP	O5'-P-O1P	2.77	113.93	106.44
2	A	338	AMP	C6-C5-N7	-2.74	126.82	132.09
2	C	338	AMP	C2'-C1'-N9	-2.70	106.60	113.30
2	C	338	AMP	O2P-P-O5'	2.66	113.60	106.67
2	D	338	AMP	C6-C5-N7	-2.57	127.14	132.09
2	D	338	AMP	N3-C4-N9	2.42	131.28	127.17
2	C	338	AMP	N9-C8-N7	-2.36	110.59	113.94
2	D	338	AMP	O4'-C1'-N9	2.32	112.55	108.09
2	B	338	AMP	O3'-C3'-C4'	2.28	117.63	111.08
2	C	338	AMP	C6-C5-N7	-2.24	127.77	132.09
2	C	338	AMP	N3-C4-N9	2.24	130.97	127.17
2	A	338	AMP	C5-C4-N9	2.20	108.21	105.81
2	D	338	AMP	N9-C8-N7	-2.18	110.85	113.94
2	A	338	AMP	C3'-C2'-C1'	2.17	105.57	101.46
2	D	338	AMP	O5'-P-O1P	2.15	112.24	106.44
2	B	338	AMP	N6-C6-N1	2.03	122.89	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	338	AMP	O2P-P-O5'	2.03	111.95	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

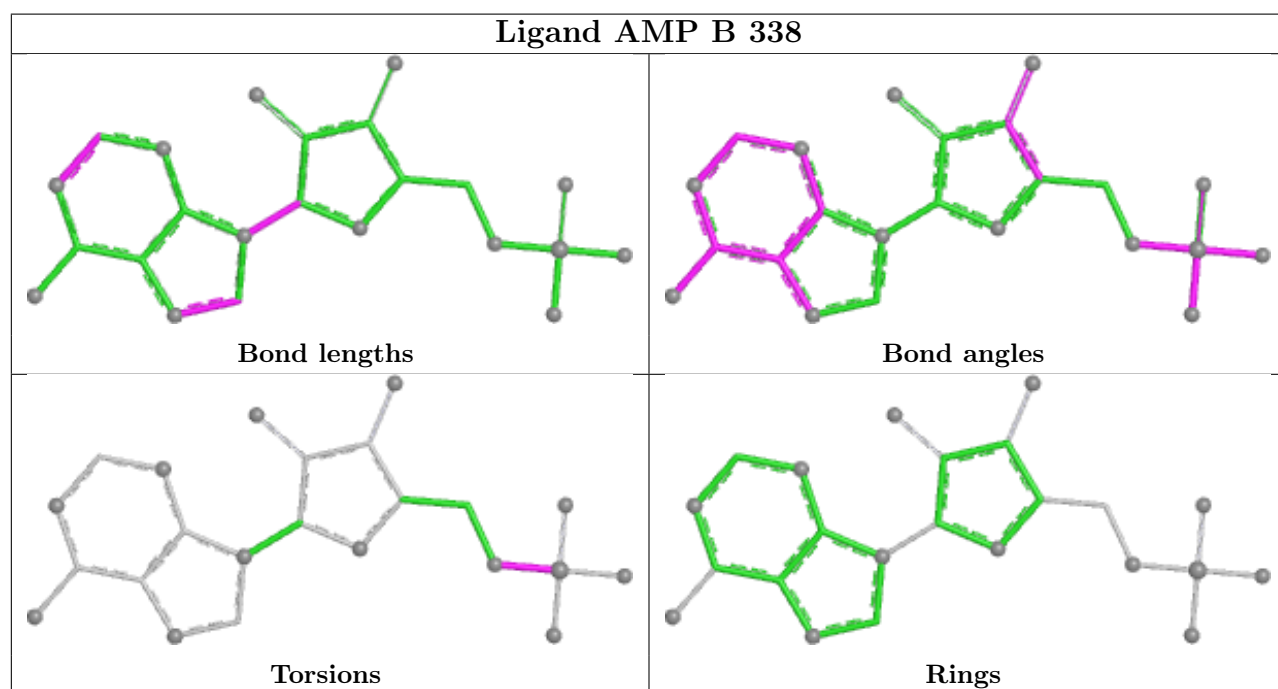
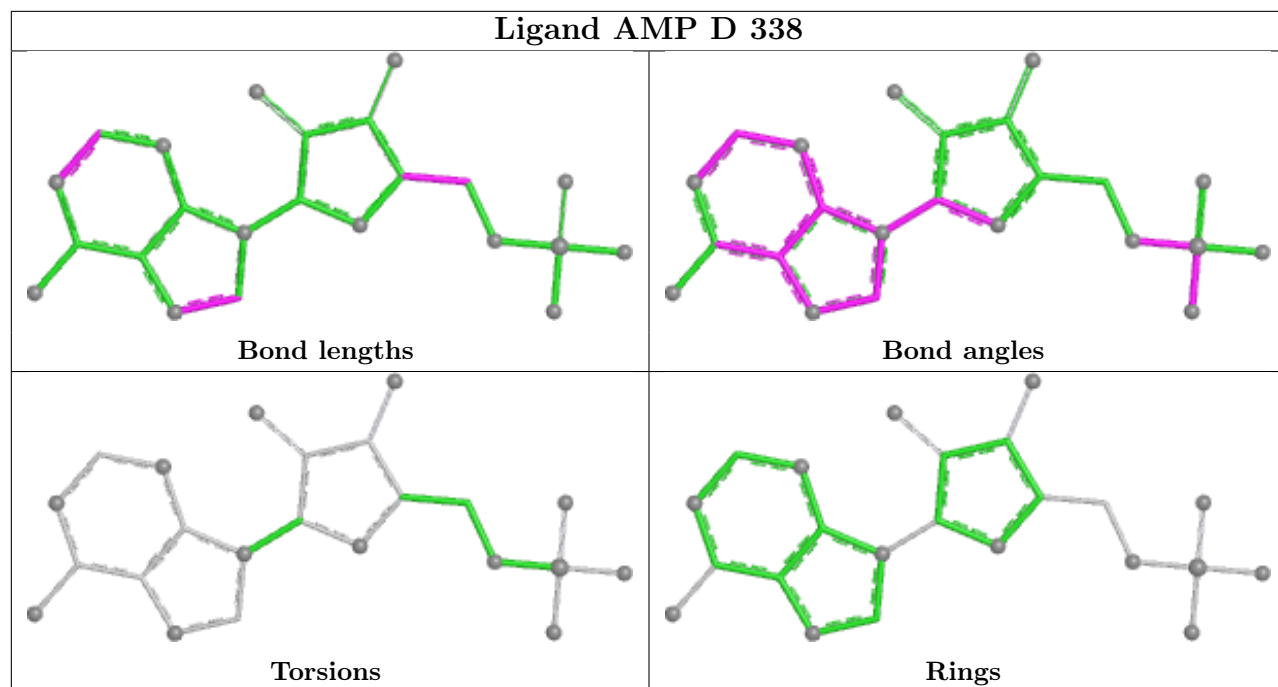
Mol	Chain	Res	Type	Atoms
2	B	338	AMP	C5'-O5'-P-O3P
2	C	338	AMP	C5'-O5'-P-O3P
2	B	338	AMP	C5'-O5'-P-O1P
2	C	338	AMP	C5'-O5'-P-O1P
2	C	338	AMP	C5'-O5'-P-O2P

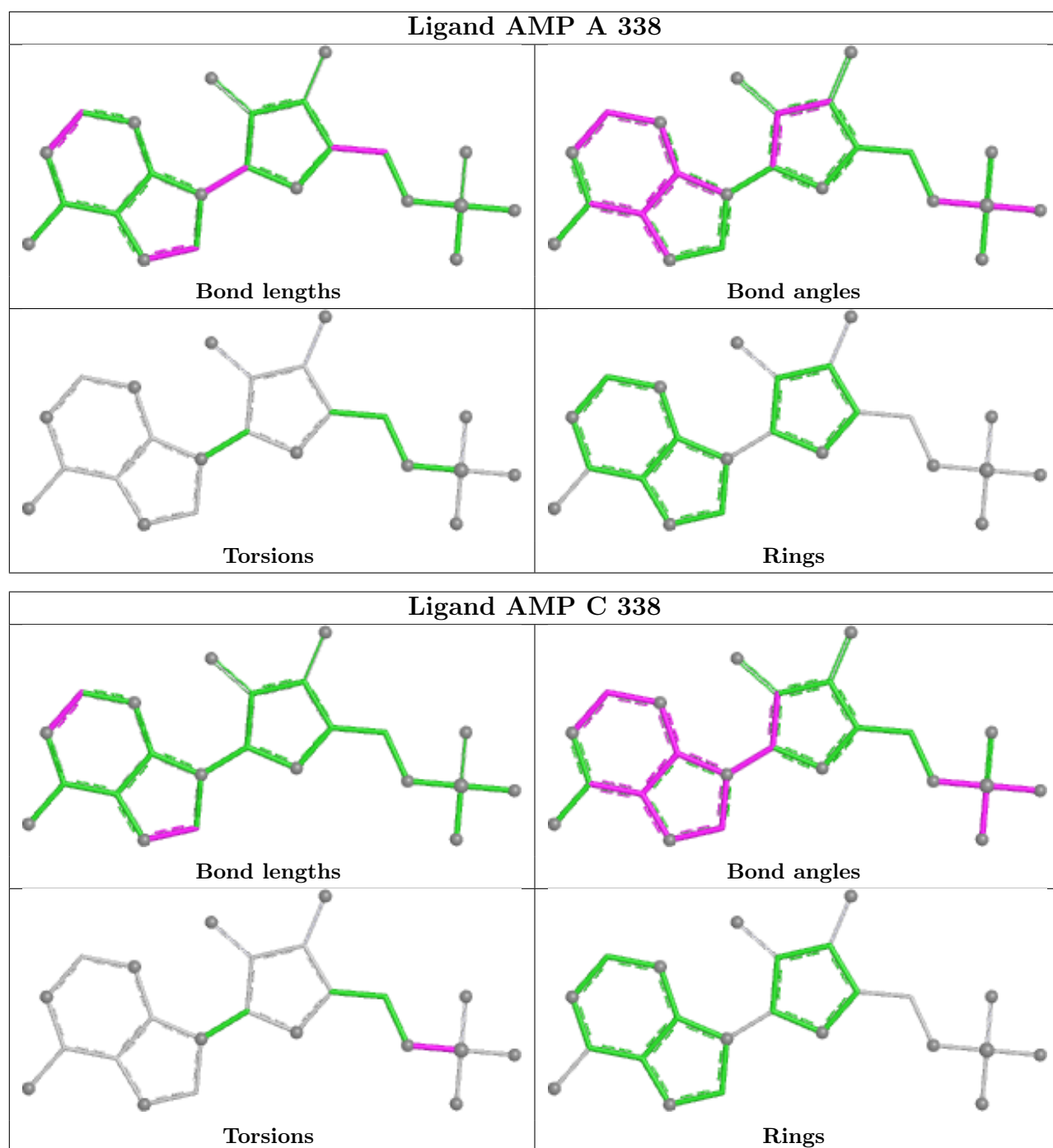
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	AMP	1	0
2	C	338	AMP	1	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.