



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:27 AM UTC

PDB ID : 1FPG / pdb_00001fpg
Title : STRUCTURAL ASPECTS OF THE ALLOSTERIC INHIBITION OF FRUCTOSE-1,6-BISPHOSPHATASE BY AMP: THE BINDING OF BOTH THE SUBSTRATE ANALOGUE 2,5-ANHYDRO-D-GLUCITOL-1,6-BISPHOSPHATE AND CATALYTIC METAL IONS MONITORED BY X-RAY CRYSTALLOGRAPHY
Authors : Villeret, V.; Huang, S.; Zhang, Y.; Lipscomb, W.N.
Deposited on : 1994-12-15
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

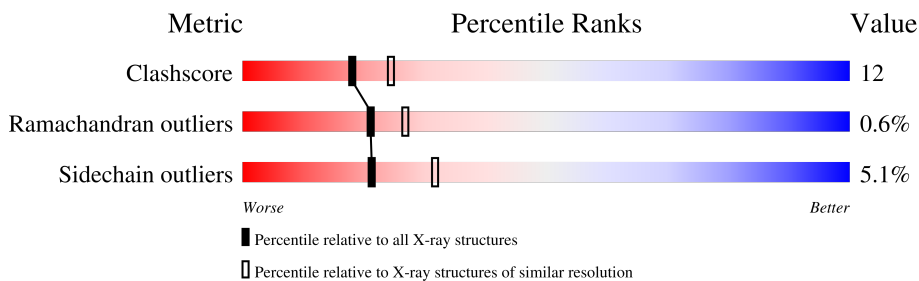
1 Overall quality at a glance

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	335	
1	B	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6509 atoms, of which 1410 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	317	Total	C	H	N	O	S	0	0	0
			2962	1546	536	409	456	15			
1	B	317	Total	C	H	N	O	S	0	0	0
			2962	1546	536	409	456	15			

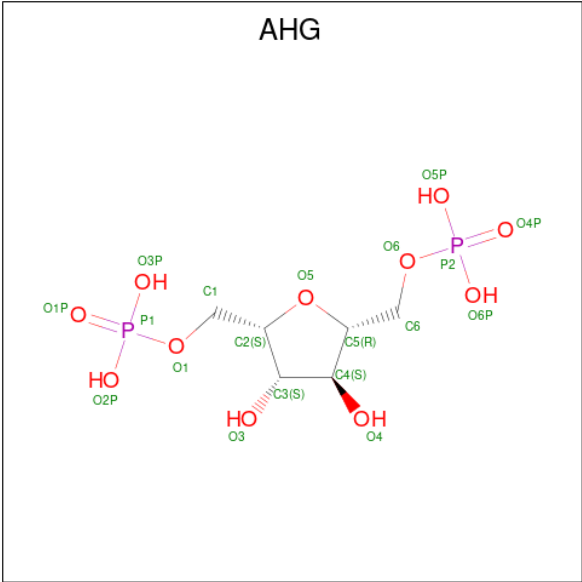
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

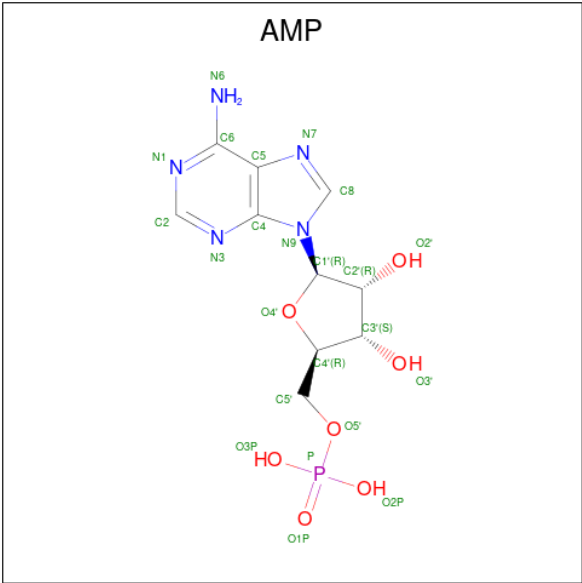
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 2,5-anhydro-1,6-di-O-phosphono-D-glucitol (CCD ID: AHG) (formula: C₆H₁₄O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			29	6	10	11	2		
3	B	1	Total	C	H	O	P	0	0
			29	6	10	11	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	85	Total	H	O	0	0
			255	170	85		
5	B	74	Total	H	O	0	0
			222	148	74		

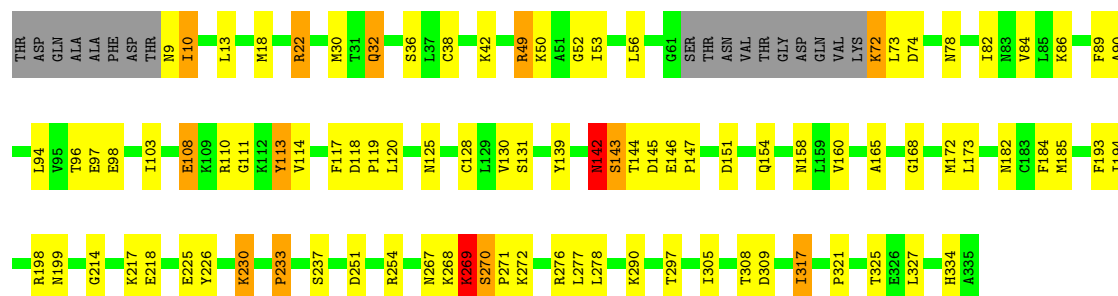
3 Residue-property plots

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.

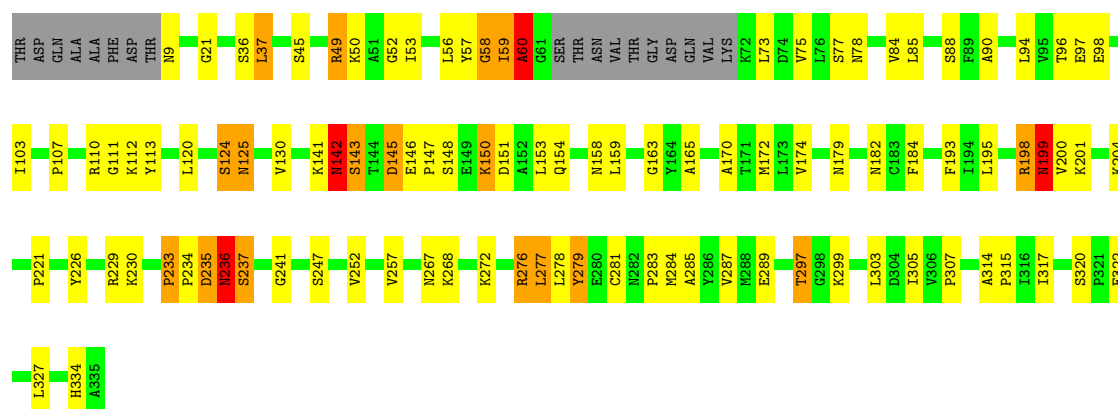
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A: 



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 166.50Å 80.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6509	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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, AHG, MN

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	1.07	11/2467 (0.4%)	1.10	11/3335 (0.3%)
1	B	1.04	8/2467 (0.3%)	1.15	20/3335 (0.6%)
All	All	1.05	19/4934 (0.4%)	1.13	31/6670 (0.5%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	SER	CA-CB	-8.30	1.39	1.53
1	B	113	TYR	CA-CB	-7.87	1.41	1.53
1	B	73	LEU	CA-CB	-7.48	1.40	1.53
1	A	97	GLU	CA-CB	-7.02	1.42	1.53
1	A	142	ASN	CA-CB	6.77	1.61	1.53
1	A	113	TYR	CA-CB	-6.72	1.43	1.53
1	B	120	LEU	CA-CB	6.62	1.61	1.52
1	A	269	LYS	CA-CB	6.55	1.64	1.53
1	B	199	ASN	CA-CB	-5.80	1.44	1.53
1	B	142	ASN	CA-CB	5.60	1.62	1.53
1	A	185	MET	CA-CB	-5.49	1.45	1.53
1	A	309	ASP	CA-CB	-5.44	1.44	1.53
1	B	143	SER	CA-CB	5.21	1.59	1.52
1	A	89	PHE	CA-CB	5.19	1.61	1.53
1	A	42	LYS	CA-CB	-5.18	1.45	1.53
1	A	110	ARG	CA-CB	-5.18	1.45	1.53
1	B	77	SER	CA-CB	-5.11	1.45	1.53
1	A	86	LYS	CA-CB	-5.03	1.45	1.53
1	B	159	LEU	CA-CB	5.01	1.61	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ASP	N-CA-C	-8.02	97.00	109.76
1	B	124	SER	N-CA-C	-8.00	102.50	111.07
1	B	59	ILE	N-CA-C	-7.43	93.88	109.34
1	A	277	LEU	N-CA-C	6.99	118.79	111.03
1	A	271	PRO	N-CA-C	-6.91	105.90	114.20
1	B	241	GLY	N-CA-C	-6.80	103.43	112.82
1	A	214	GLY	N-CA-C	-6.64	107.36	114.67
1	B	233	PRO	CA-C-N	6.52	127.99	119.84
1	B	233	PRO	C-N-CA	6.52	127.99	119.84
1	B	145	ASP	N-CA-C	-6.27	100.67	109.69
1	B	113	TYR	N-CA-C	6.21	120.16	110.17
1	A	278	LEU	N-CA-C	6.15	117.98	111.28
1	B	278	LEU	N-CA-C	6.11	117.61	111.07
1	A	111	GLY	N-CA-C	-5.96	105.63	112.79
1	B	58	GLY	N-CA-C	5.87	124.33	113.76
1	B	60	ALA	N-CA-C	5.77	123.08	110.80
1	B	56	LEU	N-CA-C	-5.76	105.14	111.82
1	A	317	ILE	N-CA-C	-5.75	99.78	108.17
1	A	82	ILE	N-CA-C	5.72	116.46	110.62
1	B	279	TYR	N-CA-C	5.67	120.20	112.88
1	B	125	ASN	N-CA-C	5.64	119.64	112.87
1	B	50	LYS	N-CA-C	5.55	119.35	111.92
1	A	233	PRO	CA-C-N	5.45	125.27	119.28
1	A	233	PRO	C-N-CA	5.45	125.27	119.28
1	A	118	ASP	N-CA-C	-5.43	96.87	108.93
1	B	277	LEU	N-CA-C	5.43	117.00	111.14
1	A	50	LYS	N-CA-C	5.40	119.17	112.58
1	B	200	VAL	N-CA-C	5.38	116.02	109.30
1	B	75	VAL	N-CA-C	-5.29	105.24	111.00
1	B	170	ALA	N-CA-C	-5.14	101.31	108.96
1	B	257	VAL	N-CA-C	5.13	116.60	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2426	536	2486	63	0
1	B	2426	536	2486	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	10	10	0	0
3	B	19	10	10	0	0
4	A	23	0	10	1	0
4	B	23	0	10	2	0
5	A	85	170	0	4	0
5	B	74	148	0	3	0
All	All	5099	1410	5012	121	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 12.

All (121) 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:B:125:ASN:HB3	1:B:130:VAL:HB	1.49	0.93
1:A:276:ARG:HD3	5:A:370:HOH:O	1.71	0.91
1:A:78:ASN:OD1	1:A:96:THR:HG21	1.79	0.83
1:A:10:ILE:HD11	1:A:194:ILE:HD12	1.61	0.82
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.62	0.80
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.48	0.77
1:B:78:ASN:OD1	1:B:96:THR:HG21	1.84	0.77
1:B:276:ARG:NH1	5:B:403:HOH:O	2.18	0.76
1:A:182:ASN:HD22	1:A:198:ARG:HA	1.54	0.73
1:A:96:THR:HG22	1:A:98:GLU:H	1.53	0.72
1:B:37:LEU:HD13	1:B:85:LEU:HD21	1.71	0.72
1:B:96:THR:HG22	1:B:98:GLU:H	1.56	0.70
1:A:142:ASN:O	1:A:143:SER:HB3	1.93	0.69
1:A:18:MET:HE3	1:A:22:ARG:HD2	1.80	0.61
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.81	0.61
1:B:204:LYS:HE2	1:B:322:GLU:OE2	2.00	0.61
1:A:10:ILE:HB	1:B:57:TYR:O	2.01	0.61
1:B:317:ILE:HG21	1:B:327:LEU:HD23	1.83	0.60
1:B:142:ASN:H	1:B:142:ASN:ND2	2.01	0.59
1:B:283:PRO:O	1:B:287:VAL:HG23	2.02	0.59
1:A:182:ASN:ND2	1:A:198:ARG:HA	2.17	0.59
1:A:254:ARG:HD2	5:A:349:HOH:O	2.03	0.59
1:A:218:GLU:HB3	1:A:267:ASN:HB2	1.85	0.58
1:B:317:ILE:HD13	1:B:327:LEU:HD21	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:339:AMP:H8	4:A:339:AMP:O5'	1.88	0.56
1:A:90:ALA:O	1:A:113:TYR:HB2	2.06	0.56
1:B:297:THR:HG22	1:B:299:LYS:H	1.69	0.56
1:A:30:MET:HE1	1:A:160:VAL:HG12	1.87	0.56
1:B:112:LYS:NZ	4:B:339:AMP:O2P	2.35	0.56
1:A:225:GLU:OE1	1:A:334:HIS:HE1	1.89	0.56
1:B:154:GLN:HE21	1:B:158:ASN:HD22	1.54	0.55
1:B:317:ILE:HD13	1:B:327:LEU:CD2	2.36	0.55
1:B:252:VAL:HB	1:B:284:MET:HE3	1.90	0.54
1:A:94:LEU:HB2	1:A:103:ILE:HB	1.90	0.54
1:A:96:THR:OG1	1:A:117:PHE:CZ	2.55	0.54
1:B:226:TYR:CE1	1:B:230:LYS:HE3	2.43	0.54
1:A:269:LYS:HD3	1:A:269:LYS:C	2.33	0.53
1:B:142:ASN:H	1:B:142:ASN:HD22	1.54	0.53
1:A:32:GLN:NE2	1:A:32:GLN:HA	2.23	0.53
1:A:321:PRO:O	1:A:325:THR:HG23	2.09	0.53
1:A:53:ILE:HD12	1:A:56:LEU:HB2	1.91	0.53
1:A:103:ILE:HD12	1:A:103:ILE:N	2.24	0.53
1:A:226:TYR:CZ	1:A:230:LYS:HD3	2.45	0.52
1:A:182:ASN:ND2	1:A:199:ASN:H	2.08	0.52
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.92	0.51
1:A:269:LYS:HD3	1:A:269:LYS:O	2.11	0.51
1:B:182:ASN:ND2	1:B:199:ASN:H	2.08	0.51
1:A:251:ASP:OD1	1:A:254:ARG:NH2	2.43	0.51
1:B:150:LYS:HA	1:B:153:LEU:HD12	1.93	0.50
1:B:182:ASN:HD22	1:B:198:ARG:HA	1.76	0.50
1:A:218:GLU:OE2	1:A:268:LYS:HB2	2.12	0.50
1:B:148:SER:O	1:B:151:ASP:HB2	2.11	0.50
1:A:32:GLN:HA	1:A:32:GLN:HE21	1.76	0.50
1:A:218:GLU:CB	1:A:267:ASN:HB2	2.42	0.49
1:B:59:ILE:HG23	1:B:59:ILE:O	2.11	0.49
1:B:58:GLY:C	1:B:60:ALA:H	2.21	0.48
1:A:233:PRO:HG2	1:A:237:SER:O	2.13	0.48
1:A:226:TYR:CE1	1:A:230:LYS:HE3	2.48	0.48
1:A:142:ASN:O	1:A:142:ASN:ND2	2.46	0.48
1:B:107:PRO:HA	1:B:110:ARG:HD2	1.95	0.48
1:A:22:ARG:HG2	1:A:22:ARG:NH1	2.24	0.47
1:B:267:ASN:OD1	1:B:268:LYS:N	2.46	0.47
1:A:142:ASN:O	1:A:143:SER:CB	2.62	0.47
1:B:145:ASP:CG	1:B:146:GLU:N	2.72	0.47
1:A:96:THR:HG23	1:A:119:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLY:C	1:B:60:ALA:N	2.70	0.47
1:B:221:PRO:HB2	1:B:334:HIS:CD2	2.49	0.47
1:A:154:GLN:HE21	1:A:158:ASN:HD22	1.62	0.47
1:B:141:LYS:HE2	1:B:147:PRO:HB3	1.97	0.47
1:B:204:LYS:O	1:B:320:SER:HB3	2.15	0.47
1:A:128:CYS:SG	5:A:369:HOH:O	2.13	0.47
1:A:125:ASN:OD1	1:A:130:VAL:HG21	2.15	0.46
1:B:165:ALA:HA	1:B:172:MET:O	2.16	0.46
1:B:94:LEU:HB2	1:B:103:ILE:HB	1.97	0.46
1:A:9:ASN:O	1:A:9:ASN:ND2	2.48	0.46
1:B:52:GLY:HA2	5:B:369:HOH:O	2.16	0.46
1:A:165:ALA:HA	1:A:172:MET:O	2.16	0.46
1:B:195:LEU:HD21	1:B:198:ARG:HG3	1.96	0.46
1:B:163:GLY:HA3	1:B:174:VAL:O	2.16	0.46
1:B:235:ASP:O	1:B:237:SER:N	2.48	0.45
1:B:21:GLY:HA2	4:B:339:AMP:C5	2.51	0.45
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.98	0.45
1:B:36:SER:OG	1:B:88:SER:HB3	2.17	0.44
1:A:72:LYS:HB3	1:A:72:LYS:NZ	2.33	0.44
1:B:45:SER:O	1:B:49:ARG:HD2	2.18	0.44
1:A:72:LYS:C	1:A:72:LYS:HD2	2.43	0.44
1:A:13:LEU:HD23	1:A:38:CYS:HB2	1.99	0.44
1:B:9:ASN:N	1:B:9:ASN:OD1	2.51	0.44
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.99	0.43
1:A:36:SER:HB3	1:A:84:VAL:HG12	2.00	0.43
1:A:217:LYS:HE3	1:B:236:ASN:HD21	1.83	0.43
1:A:270:SER:C	1:A:272:LYS:H	2.25	0.43
1:A:49:ARG:NH2	1:A:168:GLY:O	2.51	0.43
1:A:184:PHE:HA	1:A:194:ILE:O	2.18	0.43
1:B:233:PRO:HA	1:B:234:PRO:HD3	1.84	0.43
1:B:289:GLU:CD	1:B:303:LEU:HD12	2.44	0.43
1:B:142:ASN:HD22	1:B:143:SER:H	1.66	0.43
1:B:236:ASN:HD22	1:B:236:ASN:HA	1.61	0.43
1:A:270:SER:C	1:A:272:LYS:N	2.77	0.43
1:B:314:ALA:HA	1:B:315:PRO:HD3	1.82	0.43
1:A:108:GLU:H	1:A:108:GLU:HG3	1.55	0.42
1:A:317:ILE:HG21	1:A:327:LEU:HD23	2.00	0.42
1:A:290:LYS:HD3	1:A:290:LYS:HA	1.88	0.42
1:B:36:SER:HB3	1:B:84:VAL:HG12	2.01	0.42
1:B:305:ILE:O	1:B:307:PRO:HD3	2.19	0.42
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:OD1	1:A:154:GLN:NE2	2.52	0.42
1:B:90:ALA:C	1:B:111:GLY:HA3	2.45	0.41
1:A:52:GLY:HA2	5:B:365:HOH:O	2.20	0.41
1:A:145:ASP:O	1:A:146:GLU:C	2.62	0.41
1:B:179:ASN:OD1	1:B:179:ASN:N	2.53	0.41
1:B:198:ARG:HE	1:B:198:ARG:HB2	1.65	0.41
1:B:272:LYS:HB2	1:B:272:LYS:HE3	1.87	0.41
1:B:226:TYR:CZ	1:B:230:LYS:HE3	2.56	0.41
1:A:56:LEU:HD12	5:A:379:HOH:O	2.21	0.41
1:A:72:LYS:O	1:A:73:LEU:C	2.62	0.41
1:B:97:GLU:HA	1:B:279:TYR:CZ	2.56	0.40
1:A:147:PRO:HA	1:A:151:ASP:OD2	2.22	0.40
1:B:124:SER:OG	1:B:125:ASN:N	2.53	0.40
1:A:297:THR:HG21	1:A:305:ILE:HD11	2.03	0.40
1:B:285:ALA:O	1:B:289:GLU:HG3	2.22	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	313/335 (93%)	301 (96%)	10 (3%)	2 (1%)	21	27
1	B	313/335 (93%)	297 (95%)	14 (4%)	2 (1%)	21	27
All	All	626/670 (93%)	598 (96%)	24 (4%)	4 (1%)	21	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER
1	A	270	SER
1	B	60	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	236	ASN

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	263/278 (95%)	250 (95%)	13 (5%)	22	34
1	B	263/278 (95%)	249 (95%)	14 (5%)	20	30
All	All	526/556 (95%)	499 (95%)	27 (5%)	21	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	22	ARG
1	A	32	GLN
1	A	49	ARG
1	A	72	LYS
1	A	74	ASP
1	A	108	GLU
1	A	142	ASN
1	A	144	THR
1	A	173	LEU
1	A	230	LYS
1	A	269	LYS
1	A	308	THR
1	B	37	LEU
1	B	49	ARG
1	B	53	ILE
1	B	142	ASN
1	B	150	LYS
1	B	198	ARG
1	B	199	ASN
1	B	201	LYS
1	B	229	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	236	ASN
1	B	237	SER
1	B	247	SER
1	B	276	ARG
1	B	297	THR

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	32	GLN
1	A	35	ASN
1	A	101	ASN
1	A	154	GLN
1	A	182	ASN
1	A	282	ASN
1	A	334	HIS
1	B	9	ASN
1	B	35	ASN
1	B	142	ASN
1	B	154	GLN
1	B	182	ASN
1	B	199	ASN
1	B	236	ASN
1	B	282	ASN
1	B	332	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	AHG	A	338	2	19,19,19	1.55	5 (26%)	27,29,29	1.53	6 (22%)
4	AMP	A	339	-	25,25,25	1.89	3 (12%)	37,38,38	2.18	12 (32%)
3	AHG	B	338	2	19,19,19	1.38	3 (15%)	27,29,29	1.75	6 (22%)
4	AMP	B	339	-	25,25,25	2.12	4 (16%)	37,38,38	2.33	15 (40%)

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	AHG	A	338	2	-	3/12/28/28	0/1/1/1
4	AMP	A	339	-	-	0/10/26/26	0/3/3/3
3	AHG	B	338	2	-	4/12/28/28	0/1/1/1
4	AMP	B	339	-	-	1/10/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	339	AMP	O3'-C3'	-6.91	1.25	1.43
4	B	339	AMP	O3'-C3'	-6.49	1.26	1.43
4	B	339	AMP	O2'-C2'	-6.35	1.27	1.43
4	A	339	AMP	O2'-C2'	-4.26	1.32	1.43
3	B	338	AHG	C4-C3	3.38	1.62	1.53
3	A	338	AHG	P2-O6	3.04	1.69	1.60
4	B	339	AMP	P-O2P	-2.92	1.43	1.54
3	B	338	AHG	P1-O1	2.71	1.68	1.60
3	A	338	AHG	C1-C2	2.59	1.59	1.51
4	B	339	AMP	P-O5'	-2.46	1.52	1.60
3	A	338	AHG	C4-C3	2.38	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	338	AHG	P2-O6P	-2.32	1.46	1.54
4	A	339	AMP	P-O2P	-2.32	1.46	1.54
3	A	338	AHG	O3-C3	2.27	1.48	1.43
3	B	338	AHG	P2-O6P	-2.10	1.47	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	339	AMP	C5-N7-C8	5.35	111.86	103.45
4	A	339	AMP	N3-C2-N1	-5.25	120.64	128.58
3	B	338	AHG	O4-C4-C3	5.12	128.22	111.82
4	B	339	AMP	N3-C2-N1	-5.05	120.94	128.58
4	B	339	AMP	N9-C8-N7	-4.78	107.15	113.94
4	B	339	AMP	O2'-C2'-C3'	-4.74	96.61	111.82
4	A	339	AMP	C3'-C2'-C1'	-4.42	93.11	101.46
3	A	338	AHG	O4-C4-C3	3.94	124.45	111.82
4	B	339	AMP	C4-C5-N7	-3.85	106.18	110.58
4	A	339	AMP	C4-C5-N7	-3.83	106.20	110.58
4	A	339	AMP	C5-N7-C8	3.65	109.19	103.45
4	B	339	AMP	O2P-P-O5'	3.63	116.13	106.67
3	B	338	AHG	O5-C5-C4	-3.54	98.12	105.15
4	A	339	AMP	N9-C8-N7	-3.37	109.16	113.94
3	B	338	AHG	O3-C3-C4	-3.30	101.24	111.82
4	A	339	AMP	O2P-P-O5'	3.29	115.24	106.67
4	A	339	AMP	O3'-C3'-C4'	3.05	119.83	111.08
4	A	339	AMP	C6-C5-N7	2.97	137.82	132.09
4	A	339	AMP	O2'-C2'-C1'	2.97	120.32	110.10
4	A	339	AMP	C2-N1-C6	2.95	123.57	118.73
4	A	339	AMP	C4-N9-C8	2.82	108.70	105.74
4	B	339	AMP	C6-C5-N7	2.77	137.43	132.09
3	A	338	AHG	C3-C4-C5	2.66	107.76	102.61
4	A	339	AMP	C2'-C1'-N9	2.51	119.54	113.30
4	B	339	AMP	C5-C4-N3	-2.51	123.27	126.72
3	B	338	AHG	C3-C4-C5	2.49	107.42	102.61
3	A	338	AHG	O6-P2-O4P	2.46	113.10	106.44
4	B	339	AMP	C2-N3-C4	2.37	117.63	111.83
3	B	338	AHG	C5-O5-C2	2.36	119.12	105.38
3	B	338	AHG	O3-C3-C2	2.36	117.85	111.08
4	B	339	AMP	C2'-C1'-N9	2.33	119.09	113.30
4	B	339	AMP	C1'-N9-C8	-2.30	122.00	127.09
4	B	339	AMP	O5'-P-O1P	2.28	112.61	106.44
3	A	338	AHG	O6P-P2-O5P	2.26	116.28	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	339	AMP	O2'-C2'-C1'	2.21	117.70	110.10
4	B	339	AMP	C2-N1-C6	2.03	122.06	118.73
3	A	338	AHG	C5-O5-C2	2.03	117.16	105.38
4	B	339	AMP	C4-N9-C8	2.02	107.86	105.74
3	A	338	AHG	O5-C5-C4	-2.01	101.17	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

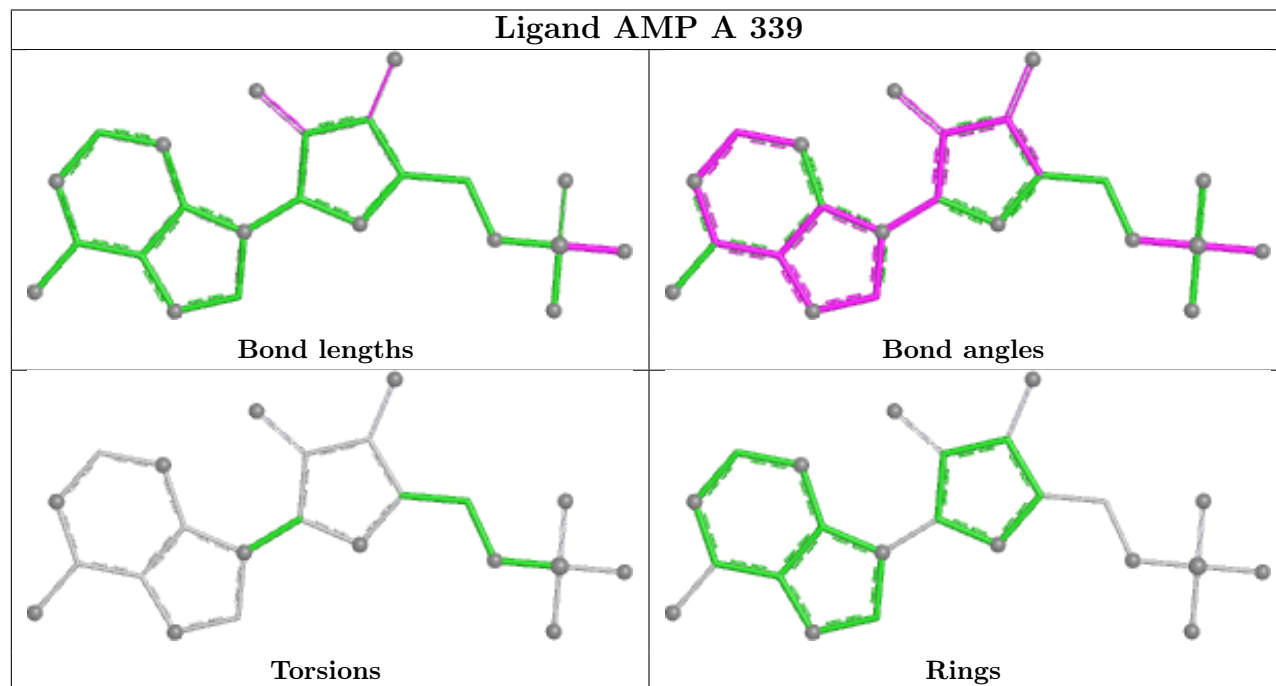
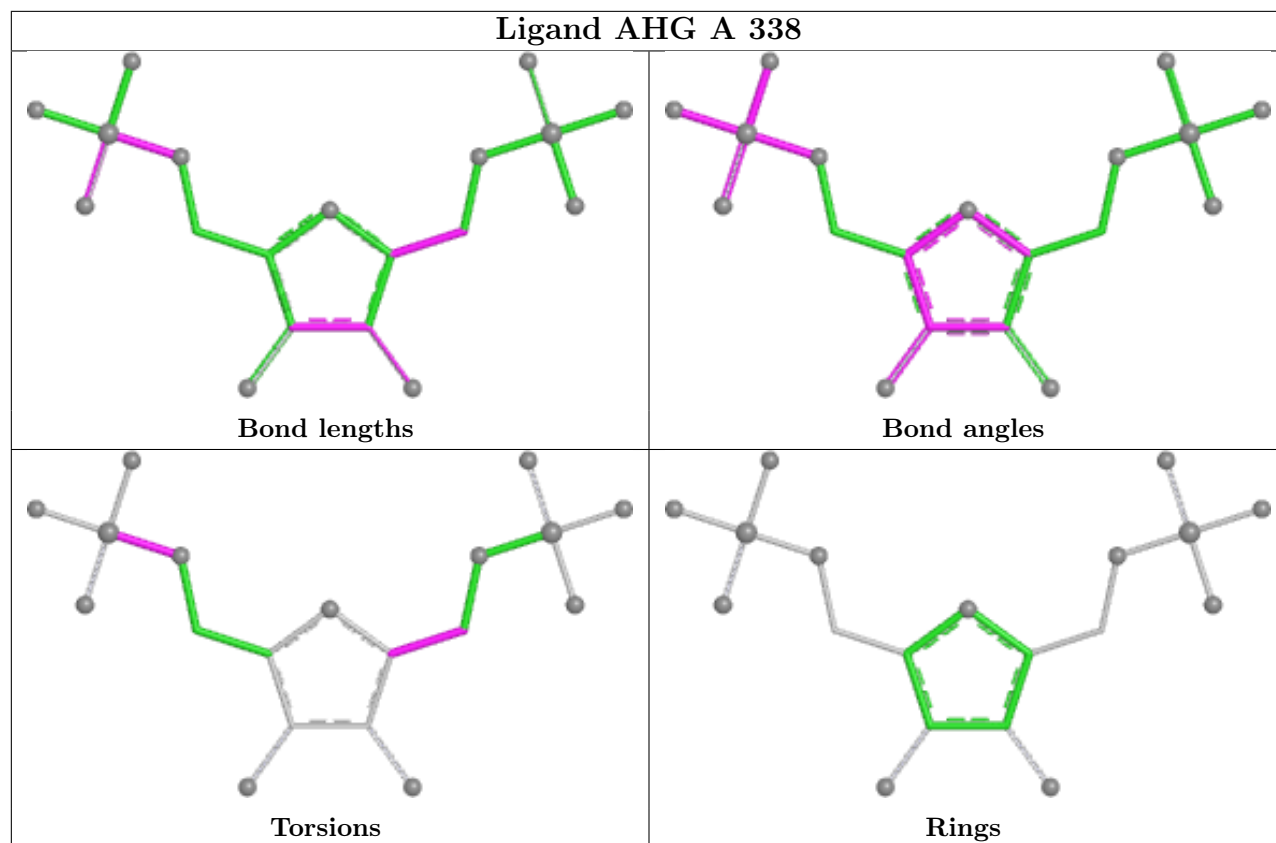
Mol	Chain	Res	Type	Atoms
3	A	338	AHG	O1-C1-C2-O5
3	A	338	AHG	C6-O6-P2-O4P
3	B	338	AHG	C6-O6-P2-O5P
3	B	338	AHG	C6-O6-P2-O6P
4	B	339	AMP	C5'-O5'-P-O1P
3	A	338	AHG	O1-C1-C2-C3
3	B	338	AHG	C4-C5-C6-O6
3	B	338	AHG	C6-O6-P2-O4P

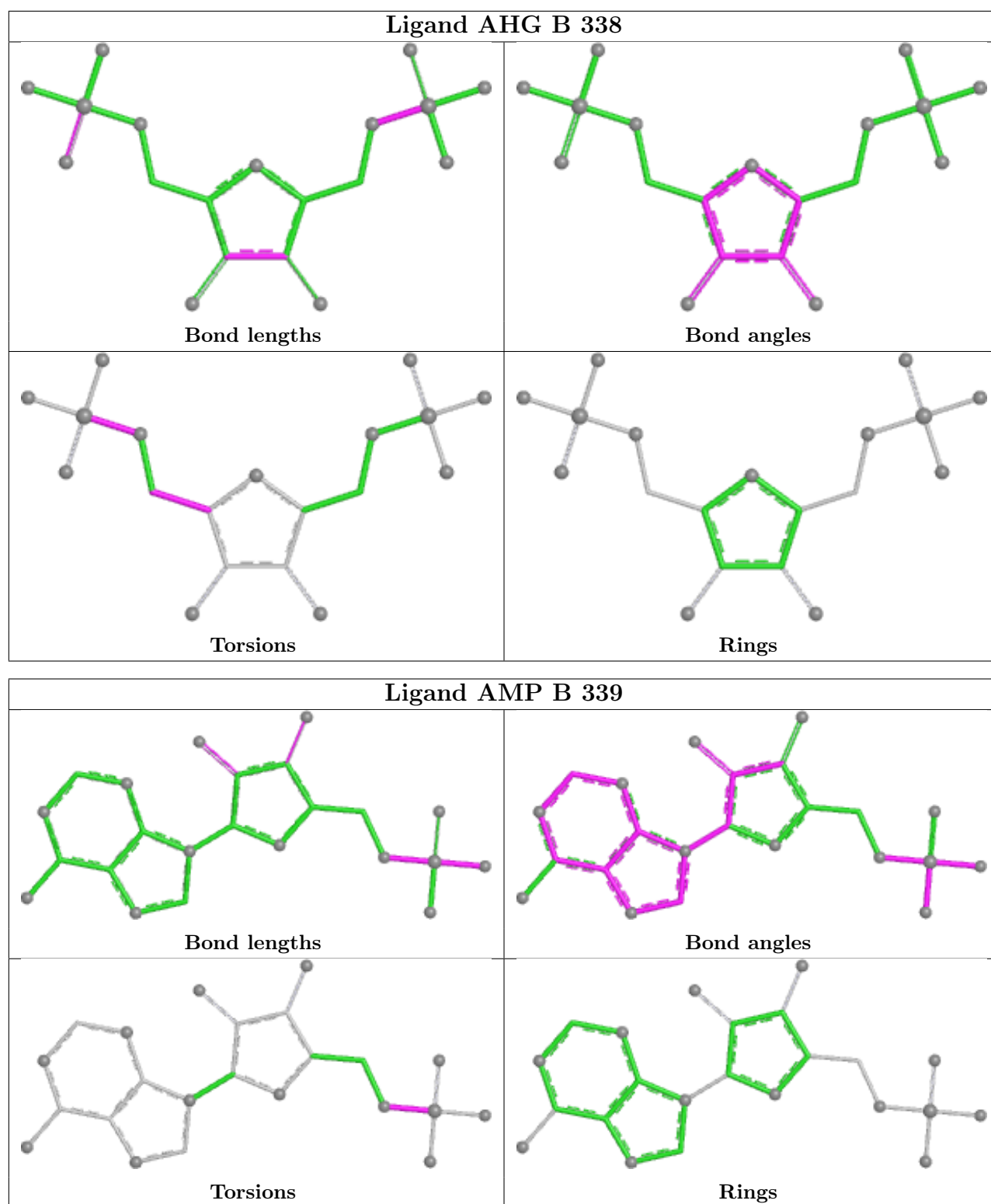
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	339	AMP	1	0
4	B	339	AMP	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 ⓘ

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.