



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:58 PM UTC

PDB ID : 1FBG / pdb_00001fbg
Title : CRYSTALLOGRAPHIC STUDIES OF THE CATALYTIC MECHANISM OF
THE NEUTRAL FORM OF FRUCTOSE-1,6-BISPHOSPHATASE
Authors : Zhang, Y.; Liang, J.-Y.; Huang, S.; Ke, H.; Lipscomb, W.N.
Deposited on : 1992-10-16
Resolution : 3.00 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

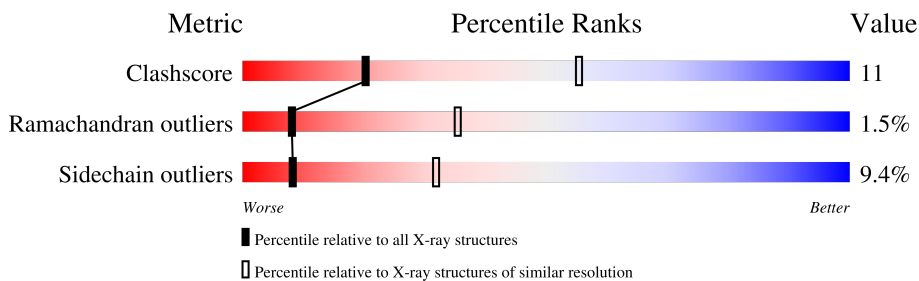
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 3 unique types of molecules in this entry. The entry contains 5907 atoms, of which 1069 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	313	Total	C	H	N	O	S	0	0	1
			2921	1520	530	403	453	15			
1	B	315	Total	C	H	N	O	S	0	0	1
			2938	1532	531	405	455	15			

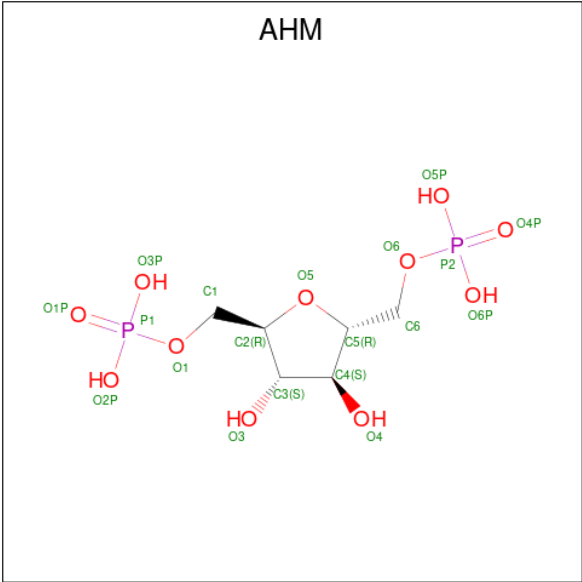
There are 6 discrepancies between the modelled and reference sequences:

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	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			23	6	4	11	2		
3	B	1	Total	C	H	O	P	0	0
			23	6	4	11	2		

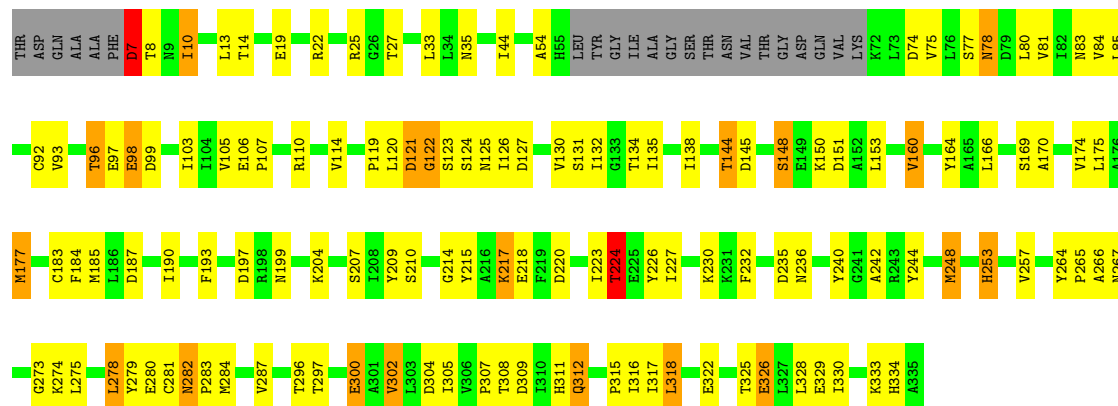
3 Residue-property plots

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.

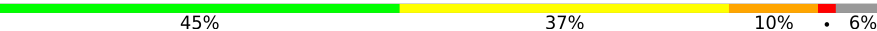
Note EDS was not executed.

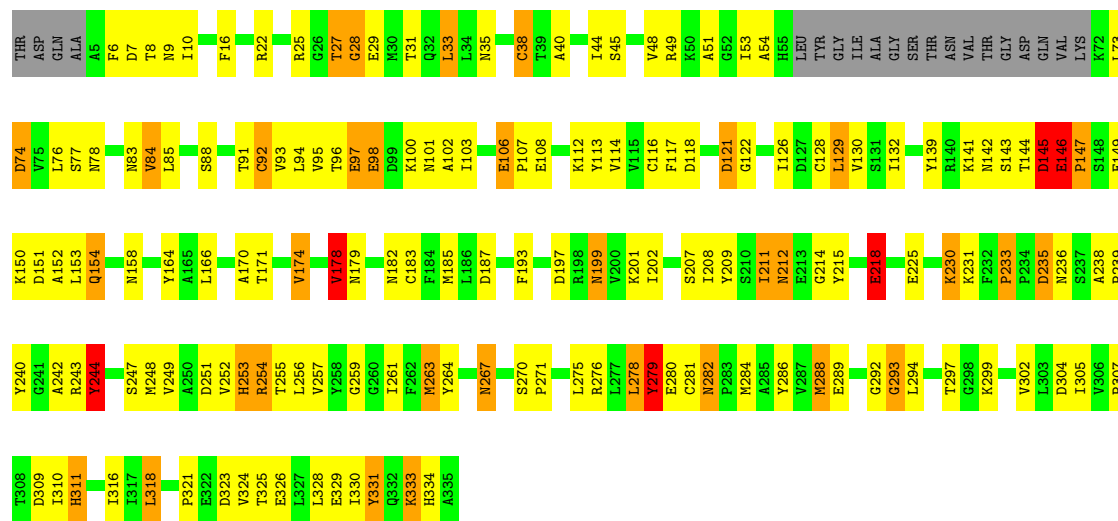
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.00Å 132.00Å 67.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5907	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: AHM, 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	1.11	11/2430 (0.5%)	1.99	65/3286 (2.0%)
1	B	0.99	7/2447 (0.3%)	1.97	90/3309 (2.7%)
All	All	1.05	18/4877 (0.4%)	1.98	155/6595 (2.4%)

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	7
All	All	0	11

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	GLY	N-CA	-7.25	1.35	1.45
1	A	54	ALA	C-N	-6.85	1.23	1.33
1	B	121	ASP	C-N	-6.73	1.25	1.33
1	A	122	GLY	N-CA	-6.60	1.36	1.45
1	A	253	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	54	ALA	C-N	-6.51	1.24	1.33
1	A	121	ASP	C-N	-6.14	1.27	1.33
1	B	311	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	334	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	334	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	311	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	160	VAL	CA-CB	5.52	1.62	1.54
1	A	264	TYR	N-CA	-5.46	1.41	1.46
1	B	311	HIS	CG-ND1	-5.29	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ILE	CA-CB	5.10	1.60	1.54
1	A	253	HIS	CG-ND1	-5.08	1.32	1.38
1	A	122	GLY	CA-C	-5.06	1.46	1.51
1	B	174	VAL	CA-CB	-5.04	1.47	1.54

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASP	CA-C-N	16.94	152.67	120.66
1	A	121	ASP	C-N-CA	16.94	152.67	120.66
1	B	121	ASP	CA-C-N	11.74	140.95	121.00
1	B	121	ASP	C-N-CA	11.74	140.95	121.00
1	A	121	ASP	O-C-N	-11.65	109.56	123.19
1	A	282	ASN	OD1-CG-ND2	-10.15	112.45	122.60
1	A	308	THR	N-CA-C	-9.61	100.43	112.72
1	B	97	GLU	N-CA-C	-9.56	100.94	111.36
1	B	212	ASN	CA-CB-CG	9.54	122.14	112.60
1	B	145	ASP	N-CA-C	8.84	129.63	110.80
1	B	7	ASP	CA-CB-CG	8.71	121.31	112.60
1	A	97	GLU	CA-CB-CG	8.51	131.12	114.10
1	A	144	THR	N-CA-C	8.41	123.10	113.01
1	A	235	ASP	CA-CB-CG	8.32	120.92	112.60
1	B	182	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	A	193	PHE	CA-CB-CG	-8.04	105.76	113.80
1	B	129	LEU	N-CA-C	8.00	122.54	111.74
1	B	38	CYS	CA-CB-SG	-7.84	96.37	114.40
1	B	267	ASN	OD1-CG-ND2	-7.78	114.83	122.60
1	B	187	ASP	CA-C-N	7.76	127.41	119.19
1	B	187	ASP	C-N-CA	7.76	127.41	119.19
1	B	129	LEU	CA-C-O	7.65	130.38	121.28
1	A	78	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	A	232	PHE	CA-CB-CG	7.57	121.37	113.80
1	A	25	ARG	N-CA-C	-7.56	102.07	110.91
1	B	267	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	329	GLU	N-CA-C	-7.44	102.78	111.03
1	A	267	ASN	CA-CB-CG	7.27	119.87	112.60
1	A	333	LYS	N-CA-C	-7.22	104.47	113.28
1	A	35	ASN	CA-CB-CG	-7.19	105.41	112.60
1	B	146	GLU	N-CA-C	-7.09	98.05	109.40
1	B	235	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	14	THR	CA-CB-OG1	-7.03	99.06	109.60
1	A	7	ASP	CA-CB-CG	6.99	119.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	318	LEU	N-CA-C	6.94	118.32	108.74
1	A	97	GLU	N-CA-C	-6.87	102.86	111.11
1	B	147	PRO	N-CA-C	6.86	122.11	111.21
1	B	116	CYS	CA-CB-SG	-6.83	98.69	114.40
1	A	334	HIS	CA-CB-CG	6.80	120.60	113.80
1	A	312	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	98	GLU	N-CA-C	6.68	120.89	113.21
1	A	106	GLU	CA-C-N	6.65	126.43	119.05
1	A	106	GLU	C-N-CA	6.65	126.43	119.05
1	B	33	LEU	N-CA-C	-6.62	103.69	111.03
1	B	130	VAL	N-CA-CB	-6.60	100.30	110.86
1	A	134	THR	N-CA-C	-6.58	98.67	109.40
1	A	145	ASP	N-CA-C	6.51	120.25	109.96
1	B	117	PHE	N-CA-C	6.47	119.25	109.23
1	A	267	ASN	OD1-CG-ND2	-6.45	116.16	122.60
1	A	22	ARG	CA-CB-CG	-6.42	101.25	114.10
1	A	282	ASN	CB-CG-ND2	6.42	126.03	116.40
1	A	197	ASP	CA-CB-CG	-6.39	106.21	112.60
1	B	263	MET	CA-C-N	-6.38	114.84	123.46
1	B	263	MET	C-N-CA	-6.38	114.84	123.46
1	A	83	ASN	CA-CB-CG	-6.38	106.22	112.60
1	B	146	GLU	CA-C-N	6.38	126.35	119.78
1	B	146	GLU	C-N-CA	6.38	126.35	119.78
1	B	187	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	333	LYS	CA-CB-CG	6.24	126.59	114.10
1	B	107	PRO	N-CA-C	6.24	123.04	113.75
1	B	214	GLY	N-CA-C	-6.23	105.02	113.37
1	B	142	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	6	PHE	CA-CB-CG	6.14	119.94	113.80
1	B	83	ASN	CA-CB-CG	-6.12	106.47	112.60
1	B	236	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	B	112	LYS	N-CA-C	6.11	120.44	112.92
1	B	282	ASN	CA-C-O	-6.11	112.93	118.79
1	A	120	LEU	O-C-N	6.08	131.26	123.24
1	B	130	VAL	N-CA-C	-6.07	99.66	108.71
1	B	299	LYS	CA-CB-CG	6.04	126.19	114.10
1	B	9	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	74	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	304	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	281	CYS	N-CA-C	5.98	117.47	111.07
1	B	253	HIS	N-CA-C	5.95	118.25	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	PHE	N-CA-C	-5.93	101.06	109.96
1	B	333	LYS	N-CA-CB	-5.93	101.87	110.70
1	A	236	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	B	247	SER	N-CA-C	-5.92	98.44	108.26
1	A	19	GLU	CA-C-O	-5.91	114.61	120.82
1	B	178	VAL	N-CA-C	5.78	121.37	109.34
1	A	322	GLU	CB-CG-CD	5.78	122.42	112.60
1	A	278	LEU	N-CA-C	5.75	118.29	111.33
1	B	278	LEU	N-CA-C	5.75	118.28	111.33
1	B	118	ASP	N-CA-CB	5.71	120.28	110.05
1	B	270	SER	N-CA-C	-5.70	99.06	108.75
1	A	127	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	85	LEU	O-C-N	5.67	127.92	122.07
1	A	326	GLU	N-CA-C	-5.67	105.00	111.07
1	A	14	THR	CA-CB-CG2	5.67	120.13	110.50
1	A	317	ILE	N-CA-C	-5.66	99.48	107.75
1	B	92	CYS	N-CA-C	-5.61	108.23	114.62
1	B	118	ASP	CB-CA-C	-5.60	103.71	110.15
1	B	154	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	108	GLU	N-CA-C	5.59	118.91	111.75
1	A	131	SER	CA-C-O	-5.58	114.56	120.92
1	A	75	VAL	CA-C-O	-5.57	114.33	120.96
1	A	273	GLY	N-CA-C	-5.57	105.41	112.65
1	B	16	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	224	THR	N-CA-CB	-5.50	102.03	110.12
1	B	288	MET	N-CA-C	5.50	117.73	111.02
1	B	22	ARG	N-CA-C	5.50	116.95	111.07
1	B	78	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	119	PRO	N-CA-C	-5.46	106.08	113.40
1	B	309	ASP	N-CA-C	-5.46	100.80	109.76
1	A	177	MET	CG-SD-CE	-5.46	88.89	100.90
1	B	193	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	312	GLN	CG-CD-NE2	5.43	124.55	116.40
1	B	150	LYS	N-CA-C	-5.43	105.53	111.82
1	A	220	ASP	CA-C-N	5.42	125.50	119.32
1	A	220	ASP	C-N-CA	5.42	125.50	119.32
1	B	211	ILE	O-C-N	-5.41	118.00	123.19
1	B	230	LYS	N-CA-C	-5.38	106.39	113.12
1	B	233	PRO	CA-C-N	5.37	124.88	119.19
1	B	233	PRO	C-N-CA	5.37	124.88	119.19
1	B	225	GLU	N-CA-C	-5.36	104.86	111.40
1	A	123	SER	N-CA-C	5.35	117.81	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	ASP	CA-CB-CG	-5.35	107.25	112.60
1	B	151	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	8	THR	N-CA-C	5.34	119.54	113.19
1	B	101	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	118	ASP	OD1-CG-OD2	-5.33	110.11	122.90
1	B	130	VAL	CB-CA-C	5.32	118.48	110.98
1	A	96	THR	CA-C-O	-5.31	115.25	121.46
1	A	96	THR	CA-C-N	5.31	127.71	120.54
1	A	96	THR	C-N-CA	5.31	127.71	120.54
1	B	98	GLU	N-CA-C	5.31	119.38	113.01
1	B	128	CYS	CA-C-N	5.30	129.66	122.19
1	B	128	CYS	C-N-CA	5.30	129.66	122.19
1	A	148	SER	N-CA-CB	-5.29	103.36	111.56
1	A	253	HIS	CA-CB-CG	-5.28	108.52	113.80
1	A	287	VAL	N-CA-C	-5.25	105.38	110.42
1	A	14	THR	N-CA-CB	-5.24	102.41	110.01
1	B	145	ASP	N-CA-CB	-5.24	101.63	110.49
1	A	138	ILE	N-CA-CB	-5.23	104.84	111.64
1	B	293	GLY	CA-C-N	-5.22	115.37	122.93
1	B	293	GLY	C-N-CA	-5.22	115.37	122.93
1	A	224	THR	CB-CA-C	5.19	119.40	110.79
1	B	299	LYS	CB-CG-CD	-5.19	99.37	111.30
1	B	158	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	131	SER	N-CA-C	-5.17	102.39	110.10
1	B	144	THR	CA-C-N	5.17	131.42	121.54
1	B	144	THR	C-N-CA	5.17	131.42	121.54
1	B	106	GLU	CA-C-N	5.15	125.19	119.32
1	B	106	GLU	C-N-CA	5.15	125.19	119.32
1	B	201	LYS	O-C-N	5.14	129.63	123.36
1	B	209	TYR	N-CA-C	-5.13	100.09	108.76
1	B	27	THR	N-CA-C	5.13	121.72	110.80
1	B	76	LEU	CA-C-O	-5.12	115.12	120.55
1	A	33	LEU	O-C-N	5.11	127.34	122.03
1	A	160	VAL	N-CA-C	-5.11	106.17	111.58
1	B	28	GLY	N-CA-C	-5.09	106.03	114.48
1	B	264	TYR	CA-CB-CG	-5.06	104.79	113.90
1	A	187	ASP	CA-C-O	5.03	122.56	119.29

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	TYR	Sidechain
1	A	215	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	244	TYR	Sidechain
1	B	164	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	238	ALA	Peptide
1	B	244	TYR	Sidechain
1	B	279	TYR	Sidechain
1	B	286	TYR	Sidechain
1	B	331	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2391	530	2447	46	0
1	B	2407	531	2462	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	19	4	10	6	0
3	B	19	4	10	1	0
All	All	4838	1069	4929	110	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 11.

All (110) 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:150:LYS:HA	1:A:153:LEU:HD12	1.52	0.91
1:B:141:LYS:HE3	1:B:147:PRO:HG3	1.62	0.81
1:B:297:THR:HG21	1:B:305:ILE:HD11	1.67	0.75
1:A:248:MET:HE3	1:A:275:LEU:HD13	1.69	0.74
1:A:121:ASP:OD1	3:A:336:AHM:H11	1.88	0.73
1:B:281:CYS:HB3	1:B:316:ILE:HD12	1.71	0.72
1:B:96:THR:HG22	1:B:98:GLU:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HG23	1:B:263:MET:HE2	1.72	0.70
1:A:92:CYS:HA	1:A:105:VAL:HB	1.73	0.70
1:A:121:ASP:HA	3:A:336:AHM:O2P	1.92	0.69
1:A:96:THR:HG22	1:A:98:GLU:H	1.56	0.69
1:B:121:ASP:HA	3:B:336:AHM:O2P	1.93	0.69
1:A:226:TYR:HE2	1:A:326:GLU:HB3	1.59	0.67
1:A:224:THR:HA	1:A:227:ILE:HD12	1.77	0.67
1:B:93:VAL:HB	1:B:114:VAL:HG13	1.76	0.67
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.76	0.66
1:B:252:VAL:HG11	1:B:284:MET:SD	2.36	0.66
1:A:302:VAL:HA	1:A:305:ILE:HD12	1.79	0.65
1:A:122:GLY:N	3:A:336:AHM:O2P	2.30	0.64
1:A:278:LEU:HD21	1:A:307:PRO:HG3	1.80	0.64
1:A:226:TYR:HD2	1:A:330:ILE:HD12	1.63	0.63
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.80	0.62
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.83	0.61
1:A:296:THR:HG21	1:A:328:LEU:HD21	1.83	0.61
1:B:289:GLU:HA	1:B:293:GLY:O	2.01	0.60
1:A:175:LEU:HD21	1:A:177:MET:HE2	1.84	0.60
1:A:274:LYS:NZ	3:A:336:AHM:H61	2.16	0.60
1:B:33:LEU:HA	1:B:88:SER:HB2	1.82	0.59
1:A:13:LEU:HA	1:A:184:PHE:CE2	2.37	0.59
1:A:153:LEU:HA	1:A:307:PRO:HG2	1.85	0.58
1:B:288:MET:HE3	1:B:318:LEU:HD13	1.84	0.58
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.39	0.57
1:A:253:HIS:O	1:A:257:VAL:HG22	2.04	0.57
1:B:73:LEU:HD23	1:B:126:ILE:HD13	1.85	0.56
1:B:29:GLU:HB3	1:B:113:TYR:HE2	1.70	0.56
1:B:267:ASN:O	1:B:271:PRO:HA	2.05	0.56
1:B:253:HIS:O	1:B:257:VAL:HG22	2.07	0.54
1:A:209:TYR:CZ	1:A:242:ALA:HB2	2.41	0.54
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.47	0.54
1:B:292:GLY:O	1:B:321:PRO:HD3	2.08	0.54
1:B:294:LEU:HB2	1:B:324:VAL:HG11	1.90	0.54
1:B:103:ILE:H	1:B:103:ILE:HD12	1.73	0.54
1:A:217:LYS:HE2	1:B:233:PRO:HD2	1.90	0.53
1:B:325:THR:HA	1:B:328:LEU:HB2	1.90	0.53
1:B:126:ILE:HG12	1:B:132:ILE:HD13	1.89	0.53
1:B:170:ALA:CB	1:B:185:MET:HE2	2.39	0.52
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.45	0.52
1:B:252:VAL:HG21	1:B:284:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:O	1:B:48:VAL:HG23	2.12	0.50
1:A:135:ILE:HD13	1:A:284:MET:HE2	1.93	0.49
1:A:121:ASP:CA	3:A:336:AHM:O2P	2.59	0.49
1:A:170:ALA:HA	1:B:49:ARG:HG3	1.95	0.49
1:B:40:ALA:O	1:B:44:ILE:HG13	2.12	0.49
1:B:302:VAL:HG21	1:B:316:ILE:HG13	1.94	0.48
1:B:251:ASP:HA	1:B:254:ARG:NH2	2.28	0.48
1:B:330:ILE:HA	1:B:333:LYS:HB3	1.95	0.48
1:A:7:ASP:O	1:A:10:ILE:HG23	2.13	0.47
1:B:243:ARG:HB3	1:B:254:ARG:NH1	2.29	0.47
1:A:126:ILE:HG12	1:A:132:ILE:HD13	1.95	0.47
1:B:102:ALA:HB3	1:B:149:GLU:HB3	1.97	0.47
1:A:266:ALA:HB2	1:A:315:PRO:HG3	1.96	0.47
1:B:255:THR:HA	1:B:259:GLY:O	2.15	0.47
1:A:166:LEU:HD23	1:B:129:LEU:HD12	1.95	0.46
1:A:316:ILE:HD11	1:A:318:LEU:HD23	1.98	0.46
1:B:154:GLN:O	1:B:307:PRO:HG2	2.15	0.46
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.16	0.46
1:A:81:VAL:O	1:A:85:LEU:HG	2.16	0.46
1:B:33:LEU:HA	1:B:88:SER:CB	2.46	0.46
1:B:230:LYS:HB3	1:B:240:TYR:HB2	1.98	0.46
1:B:28:GLY:O	1:B:31:THR:HB	2.16	0.45
1:B:248:MET:HE3	1:B:275:LEU:HD13	1.98	0.45
1:A:274:LYS:HZ3	3:A:336:AHM:H61	1.80	0.45
1:A:223:ILE:O	1:A:227:ILE:HG13	2.16	0.45
1:B:35:ASN:O	1:B:38:CYS:HB2	2.17	0.45
1:A:93:VAL:HA	1:A:103:ILE:O	2.17	0.45
1:B:178:VAL:HG13	1:B:179:ASN:OD1	2.16	0.44
1:B:95:VAL:HG11	1:B:310:ILE:HB	1.98	0.44
1:A:175:LEU:CD2	1:A:177:MET:HE2	2.47	0.44
1:A:148:SER:O	1:A:151:ASP:HB2	2.18	0.44
1:A:214:GLY:HA3	1:B:240:TYR:O	2.18	0.44
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.98	0.44
1:B:40:ALA:HB2	1:B:84:VAL:CG2	2.47	0.44
1:B:330:ILE:HA	1:B:333:LYS:HD3	1.98	0.44
1:A:107:PRO:HA	1:A:110:ARG:HG3	2.00	0.44
1:B:166:LEU:O	1:B:171:THR:HA	2.17	0.44
1:B:48:VAL:HA	1:B:51:ALA:HB2	2.00	0.44
1:B:202:ILE:HG13	1:B:256:LEU:O	2.18	0.43
1:B:145:ASP:HB2	1:B:146:GLU:H	1.67	0.43
1:B:276:ARG:HB2	1:B:279:TYR:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HG22	1:B:97:GLU:N	2.35	0.42
1:A:297:THR:OG1	1:A:300:GLU:HG2	2.18	0.42
1:A:125:ASN:O	1:A:130:VAL:HB	2.20	0.42
1:B:149:GLU:O	1:B:153:LEU:HG	2.20	0.42
1:B:242:ALA:O	1:B:243:ARG:NH1	2.52	0.41
1:B:252:VAL:O	1:B:255:THR:HB	2.21	0.41
1:B:174:VAL:HG13	1:B:183:CYS:SG	2.60	0.41
1:A:44:ILE:HG13	1:A:80:LEU:HD23	2.01	0.41
1:A:81:VAL:HA	1:A:84:VAL:HG22	2.02	0.41
1:A:309:ASP:HB3	1:A:312:GLN:HB3	2.02	0.41
1:B:53:ILE:O	1:B:53:ILE:HG22	2.20	0.41
1:B:254:ARG:O	1:B:254:ARG:HG2	2.17	0.41
1:A:93:VAL:HB	1:A:114:VAL:HG13	2.02	0.41
1:B:74:ASP:HA	1:B:77:SER:OG	2.20	0.41
1:B:93:VAL:O	1:B:94:LEU:HD23	2.20	0.41
1:A:280:GLU:O	1:A:283:PRO:HD2	2.20	0.41
1:A:185:MET:SD	1:B:53:ILE:HG13	2.61	0.41
1:B:114:VAL:HG11	1:B:152:ALA:HA	2.03	0.41
1:B:231:LYS:O	1:B:239:PRO:HB3	2.20	0.41
1:B:211:ILE:HD12	1:B:263:MET:CB	2.47	0.40
1:B:154:GLN:C	1:B:307:PRO:HG2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/335 (92%)	284 (92%)	24 (8%)	1 (0%)	36	70
1	B	311/335 (93%)	271 (87%)	32 (10%)	8 (3%)	4	23
All	All	620/670 (92%)	555 (90%)	56 (9%)	9 (2%)	8	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ARG
1	B	145	ASP
1	B	199	ASN
1	B	27	THR
1	B	244	TYR
1	B	100	LYS
1	B	178	VAL
1	B	218	GLU
1	A	74	ASP

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	261/278 (94%)	235 (90%)	26 (10%)	7	29
1	B	262/278 (94%)	239 (91%)	23 (9%)	9	35
All	All	523/556 (94%)	474 (91%)	49 (9%)	8	32

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	THR
1	A	10	ILE
1	A	27	THR
1	A	77	SER
1	A	99	ASP
1	A	124	SER
1	A	144	THR
1	A	160	VAL
1	A	169	SER
1	A	199	ASN
1	A	204	LYS
1	A	207	SER
1	A	210	SER

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Mol	Chain	Res	Type
1	A	217	LYS
1	A	218	GLU
1	A	224	THR
1	A	230	LYS
1	A	248	MET
1	A	265	PRO
1	A	279	TYR
1	A	282	ASN
1	A	300	GLU
1	A	302	VAL
1	A	318	LEU
1	A	325	THR
1	B	10	ILE
1	B	45	SER
1	B	84	VAL
1	B	91	THR
1	B	92	CYS
1	B	106	GLU
1	B	143	SER
1	B	146	GLU
1	B	197	ASP
1	B	199	ASN
1	B	207	SER
1	B	208	ILE
1	B	218	GLU
1	B	235	ASP
1	B	249	VAL
1	B	254	ARG
1	B	278	LEU
1	B	279	TYR
1	B	280	GLU
1	B	282	ASN
1	B	326	GLU
1	B	329	GLU
1	B	331	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	154	GLN
1	A	199	ASN

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Mol	Chain	Res	Type
1	B	154	GLN
1	B	182	ASN
1	B	199	ASN
1	B	282	ASN
1	B	332	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	AHM	A	336	2	19,19,19	0.72	0	27,29,29	0.87	0
3	AHM	B	336	2	19,19,19	0.75	0	27,29,29	0.88	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	AHM	A	336	2	-	5/12/28/28	0/1/1/1
3	AHM	B	336	2	-	9/12/28/28	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	336	AHM	O2P-P1-O1P	2.01	118.67	110.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	336	AHM	C1-O1-P1-O1P
3	A	336	AHM	C1-O1-P1-O3P
3	B	336	AHM	C1-O1-P1-O2P
3	B	336	AHM	C6-O6-P2-O4P
3	B	336	AHM	C6-O6-P2-O5P
3	B	336	AHM	C6-O6-P2-O6P
3	A	336	AHM	O1-C1-C2-C3
3	A	336	AHM	O1-C1-C2-O5
3	B	336	AHM	C4-C5-C6-O6
3	B	336	AHM	O5-C5-C6-O6
3	B	336	AHM	C1-O1-P1-O1P
3	B	336	AHM	C2-C1-O1-P1
3	A	336	AHM	O5-C5-C6-O6
3	B	336	AHM	O1-C1-C2-O5

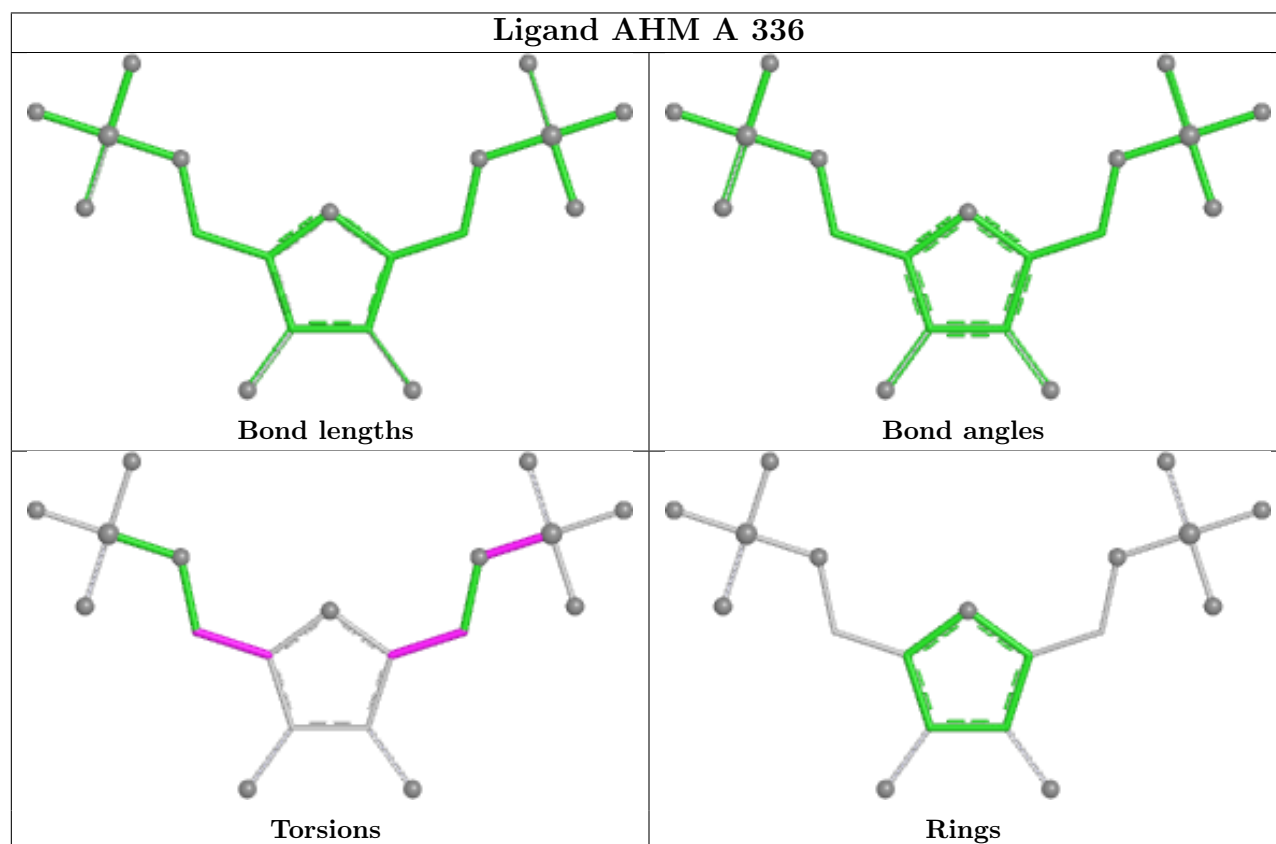
There are no ring outliers.

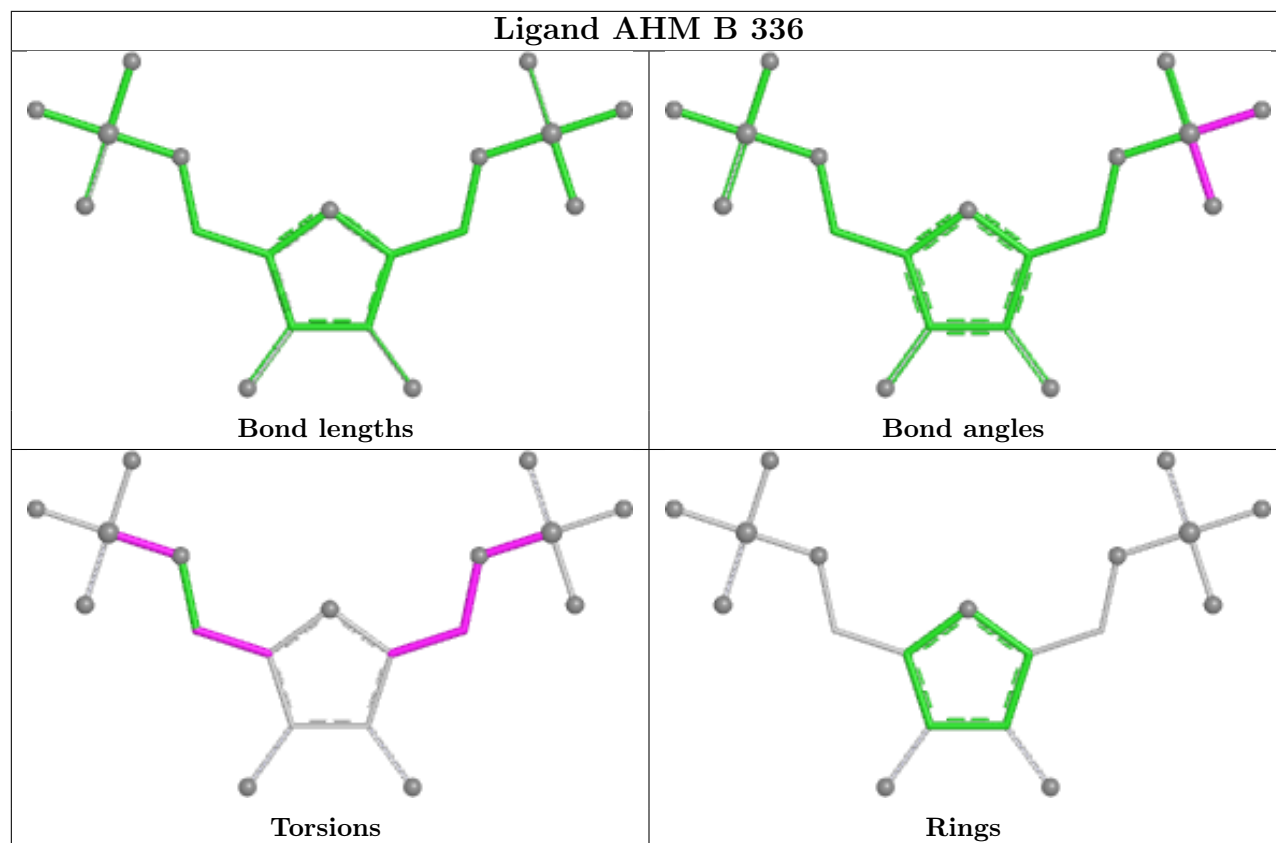
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	336	AHM	6	0
3	B	336	AHM	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.