



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:17 PM UTC

PDB ID : 1FBC / pdb\_00001fbc  
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 : 1992-10-14  
Resolution : 2.60 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (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

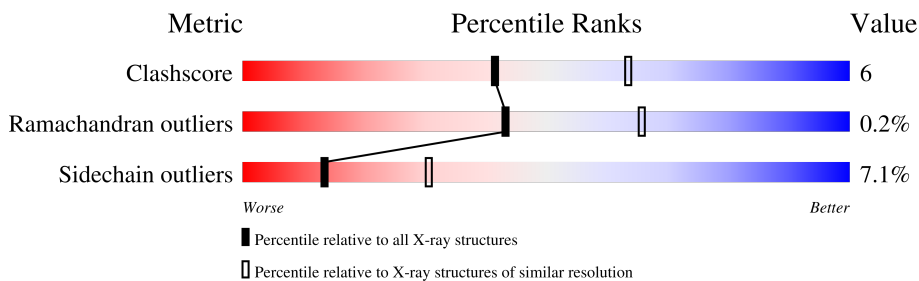
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	
1	B	335	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6198 atoms, of which 1263 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
			Total	C	H	N	O	S			
1	A	313	2921	1520	530	403	453	15	0	0	1
1	B	315	2938	1532	531	405	455	15	0	0	1

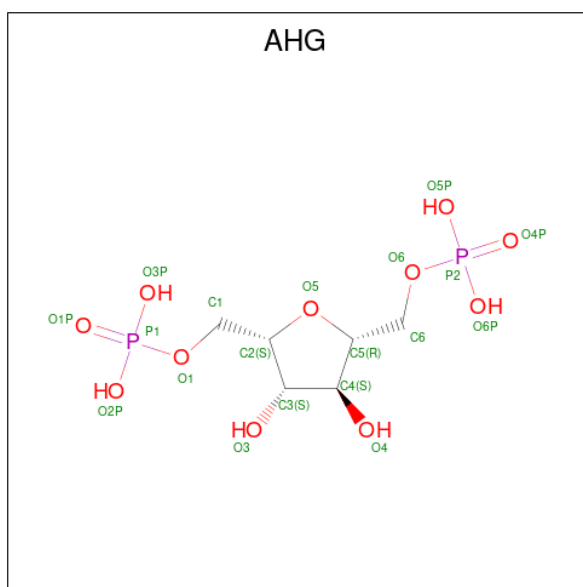
There are 6 discrepancies between the modelled and reference sequences:

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2,5-anhydro-1,6-di-O-phosphono-D-glucitol (CCD ID: AHG) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>11</sub>P<sub>2</sub>).



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		

- Molecule 4 is water.

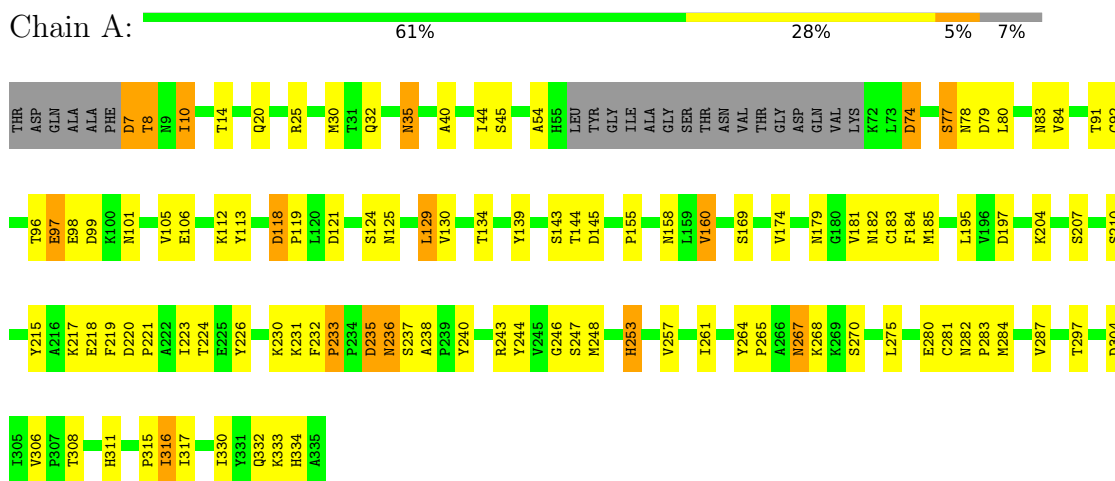
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	53	Total	H	O	0	0
			159	106	53		
4	B	44	Total	H	O	0	0
			132	88	44		

### 3 Residue-property plots

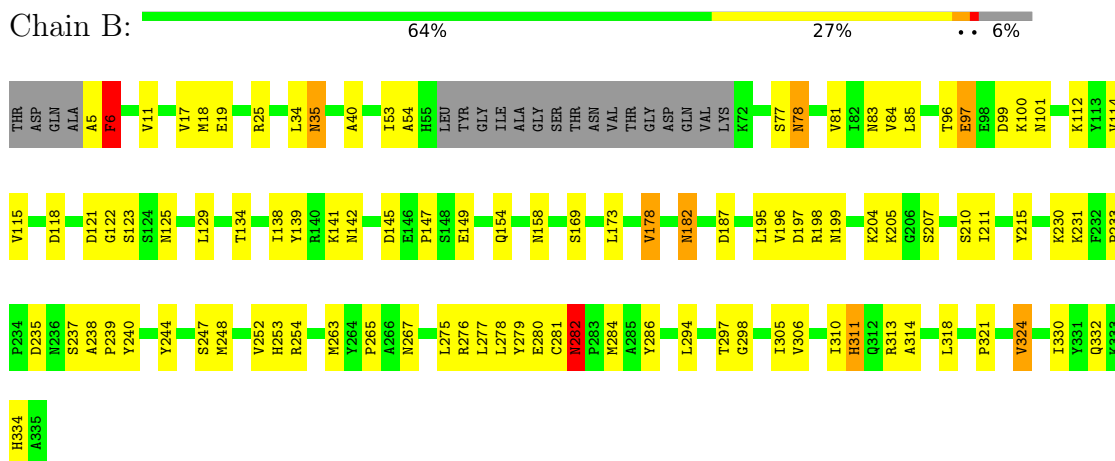
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	131.40Å 131.40Å 68.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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

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	1.02	7/2430 (0.3%)	1.80	56/3286 (1.7%)
1	B	0.99	6/2447 (0.2%)	1.76	50/3309 (1.5%)
All	All	1.01	13/4877 (0.3%)	1.78	106/6595 (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	6
1	B	0	3
All	All	0	9

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ALA	C-N	-7.07	1.23	1.33
1	A	253	HIS	CD2-NE2	-6.80	1.30	1.37
1	B	54	ALA	C-N	-6.62	1.24	1.33
1	B	311	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	160	VAL	CA-CB	6.57	1.63	1.54
1	A	334	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	334	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	253	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	311	HIS	CD2-NE2	-5.54	1.31	1.37
1	B	121	ASP	CG-OD1	5.36	1.35	1.25
1	A	253	HIS	CG-ND1	-5.17	1.32	1.38
1	A	311	HIS	CG-ND1	-5.09	1.32	1.38
1	B	253	HIS	CG-ND1	-5.00	1.32	1.38

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	LYS	N-CA-C	-10.55	100.70	112.72
1	B	278	LEU	N-CA-C	10.51	123.79	111.71
1	A	97	GLU	CB-CG-CD	9.76	129.18	112.60
1	A	121	ASP	CA-C-N	9.42	139.88	121.41
1	A	121	ASP	C-N-CA	9.42	139.88	121.41
1	A	121	ASP	CB-CG-OD1	8.96	139.00	118.40
1	B	6	PHE	CA-CB-CG	8.78	122.58	113.80
1	B	112	LYS	N-CA-C	8.52	123.51	113.20
1	B	154	GLN	OE1-CD-NE2	-8.22	114.38	122.60
1	B	235	ASP	CA-CB-CG	8.03	120.63	112.60
1	B	35	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	A	7	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	282	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	A	30	MET	CG-SD-CE	-7.58	84.22	100.90
1	B	267	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	A	217	LYS	CA-CB-CG	7.32	128.74	114.10
1	A	145	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	304	ASP	CA-CB-CG	7.22	119.82	112.60
1	B	178	VAL	N-CA-C	7.10	124.10	109.34
1	A	282	ASN	CA-C-N	7.06	126.31	118.97
1	A	282	ASN	C-N-CA	7.06	126.31	118.97
1	B	145	ASP	CA-CB-CG	7.05	119.65	112.60
1	A	121	ASP	CA-CB-CG	-7.02	105.58	112.60
1	B	35	ASN	CA-CB-CG	6.99	119.59	112.60
1	B	182	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	B	247	SER	N-CA-C	-6.86	96.87	108.26
1	B	19	GLU	CB-CG-CD	6.81	124.18	112.60
1	A	97	GLU	N-CA-C	-6.74	103.62	110.97
1	A	112	LYS	N-CA-C	6.68	121.26	113.18
1	B	142	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	35	ASN	CA-CB-CG	-6.56	106.04	112.60
1	B	129	LEU	N-CA-C	6.54	120.43	111.54
1	A	143	SER	N-CA-C	6.34	118.06	110.19
1	A	83	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	106	GLU	CA-C-N	6.31	126.06	119.05
1	A	106	GLU	C-N-CA	6.31	126.06	119.05
1	A	308	THR	N-CA-C	-6.28	106.15	113.88
1	B	280	GLU	CA-CB-CG	6.23	126.56	114.10
1	B	125	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	B	197	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	236	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	B	142	ASN	CA-CB-CG	5.97	118.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	TYR	N-CA-C	5.93	119.62	110.42
1	A	32	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	B	134	THR	CA-CB-OG1	-5.89	100.76	109.60
1	A	74	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	317	ILE	N-CA-C	-5.82	99.11	107.78
1	A	280	GLU	CB-CG-CD	5.80	122.47	112.60
1	A	121	ASP	N-CA-CB	-5.78	100.84	109.69
1	A	121	ASP	OD1-CG-OD2	-5.75	109.09	122.90
1	B	282	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	267	ASN	CA-CB-CG	5.72	118.32	112.60
1	B	182	ASN	CB-CG-ND2	5.71	124.97	116.40
1	A	79	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	220	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	196	VAL	O-C-N	-5.67	116.52	122.25
1	B	238	ALA	N-CA-C	-5.63	102.95	109.93
1	A	182	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	179	ASN	N-CA-C	5.54	119.89	113.18
1	B	178	VAL	N-CA-CB	-5.53	102.11	111.23
1	A	238	ALA	CA-C-N	5.51	125.44	119.76
1	A	238	ALA	C-N-CA	5.51	125.44	119.76
1	B	187	ASP	CA-C-N	5.50	125.21	119.82
1	B	187	ASP	C-N-CA	5.50	125.21	119.82
1	A	235	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	83	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	8	THR	N-CA-C	5.45	119.03	112.38
1	B	118	ASP	CA-C-N	5.44	125.09	119.05
1	B	118	ASP	C-N-CA	5.44	125.09	119.05
1	B	158	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	332	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	223	ILE	N-CA-C	-5.38	105.08	110.30
1	A	219	PHE	N-CA-C	5.38	118.24	110.28
1	A	264	TYR	N-CA-C	-5.38	95.65	108.40
1	B	78	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	B	97	GLU	CA-CB-CG	5.36	124.81	114.10
1	A	118	ASP	N-CA-C	-5.32	98.84	108.85
1	A	20	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	181	VAL	N-CA-C	-5.28	100.71	108.11
1	B	330	ILE	N-CA-C	-5.26	105.40	110.72
1	B	205	LYS	N-CA-C	-5.25	100.85	109.40
1	B	149	GLU	CA-CB-CG	5.24	124.59	114.10
1	A	129	LEU	N-CA-C	5.24	118.94	112.24
1	B	314	ALA	CA-C-N	5.22	125.13	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ALA	C-N-CA	5.22	125.13	119.85
1	B	324	VAL	N-CA-C	-5.22	105.41	110.42
1	A	112	LYS	CA-CB-CG	5.21	124.52	114.10
1	B	25	ARG	CA-C-O	5.18	129.28	122.44
1	B	121	ASP	CB-CG-OD1	5.16	130.26	118.40
1	A	233	PRO	CA-C-N	5.15	124.95	119.28
1	A	233	PRO	C-N-CA	5.15	124.95	119.28
1	A	98	GLU	N-CA-C	5.15	119.31	113.19
1	B	35	ASN	CB-CG-ND2	5.14	124.11	116.40
1	A	101	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	B	123	SER	CA-C-N	5.10	127.62	120.28
1	B	123	SER	C-N-CA	5.10	127.62	120.28
1	B	233	PRO	CB-CA-C	5.09	117.13	110.92
1	A	25	ARG	CB-CG-CD	5.09	123.01	111.30
1	B	173	LEU	N-CA-C	-5.08	100.89	109.07
1	B	306	VAL	CA-C-N	5.07	124.83	119.76
1	B	306	VAL	C-N-CA	5.07	124.83	119.76
1	B	101	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	298	GLY	N-CA-C	-5.05	108.17	113.58
1	A	121	ASP	CB-CA-C	5.05	117.78	109.90
1	A	267	ASN	O-C-N	-5.02	118.05	123.42
1	A	45	SER	N-CA-C	-5.02	105.70	111.07

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASP	Sidechain
1	A	139	TYR	Sidechain
1	A	215	TYR	Sidechain
1	A	232	PHE	Sidechain
1	A	240	TYR	Sidechain
1	A	244	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	244	TYR	Sidechain
1	B	286	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	2391	530	2448	28	0
1	B	2407	531	2462	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	19	4	10	1	0
3	B	19	4	10	2	0
4	A	53	106	0	0	0
4	B	44	88	0	1	0
All	All	4935	1263	4930	62	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 (62) 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:78:ASN:OD1	1:B:96:THR:HG21	1.80	0.81
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.64	0.80
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.69	0.74
1:B:248:MET:HE3	1:B:275:LEU:HD13	1.70	0.72
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.77	0.66
1:B:182:ASN:HD22	1:B:198:ARG:HA	1.61	0.66
1:B:122:GLY:HA2	3:B:336:AHG:O1	1.97	0.65
1:B:252:VAL:HG11	1:B:284:MET:SD	2.41	0.60
1:B:297:THR:HG21	1:B:305:ILE:HD11	1.83	0.60
1:A:7:ASP:HB3	1:A:10:ILE:HG23	1.84	0.58
1:A:275:LEU:HD12	1:A:316:ILE:HG21	1.86	0.57
1:B:276:ARG:NH1	1:B:313:ARG:HD3	2.20	0.57
3:B:336:AHG:O2P	4:B:376:HOH:O	2.17	0.57
1:A:40:ALA:O	1:A:44:ILE:HG13	2.06	0.56
1:B:141:LYS:HE3	1:B:147:PRO:HG3	1.90	0.54
1:A:268:LYS:HD2	1:A:268:LYS:H	1.75	0.52
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.46	0.51
1:A:210:SER:HA	1:A:243:ARG:O	2.11	0.50
1:B:114:VAL:O	1:B:138:ILE:HA	2.11	0.50
1:A:297:THR:HG22	1:A:315:PRO:O	2.12	0.49
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.54	0.48
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.94	0.48
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ILE:HB	1:B:263:MET:HE3	1.97	0.47
1:A:184:PHE:CE2	1:A:195:LEU:HB2	2.50	0.47
1:A:74:ASP:HA	1:A:77:SER:OG	2.15	0.47
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.97	0.46
1:B:5:ALA:O	1:B:6:PHE:HB3	2.14	0.46
1:B:294:LEU:O	1:B:318:LEU:HA	2.15	0.46
1:A:231:LYS:O	1:A:233:PRO:HD3	2.15	0.46
1:A:253:HIS:O	1:A:257:VAL:HG22	2.16	0.46
1:B:294:LEU:HB2	1:B:324:VAL:HG11	1.97	0.46
1:B:11:VAL:HG11	1:B:195:LEU:HD23	1.98	0.45
1:B:100:LYS:O	1:B:310:ILE:HD11	2.16	0.45
1:A:92:CYS:HA	1:A:105:VAL:HB	1.99	0.45
1:A:268:LYS:HD2	1:A:268:LYS:N	2.32	0.45
1:A:40:ALA:HB2	1:A:84:VAL:HG21	1.99	0.44
1:B:294:LEU:HD12	1:B:321:PRO:HA	1.98	0.44
1:B:97:GLU:HB2	1:B:279:TYR:CE1	2.53	0.44
1:A:226:TYR:HD1	1:A:330:ILE:HD12	1.83	0.44
1:A:283:PRO:O	1:A:287:VAL:HG23	2.17	0.44
1:A:275:LEU:HB2	1:A:281:CYS:SG	2.57	0.44
1:A:155:PRO:HD2	1:A:158:ASN:ND2	2.33	0.44
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.99	0.43
1:B:96:THR:O	1:B:311:HIS:HE1	2.01	0.43
1:A:91:THR:OG1	1:A:105:VAL:HG21	2.18	0.43
1:B:231:LYS:O	1:B:239:PRO:HB3	2.19	0.43
1:B:115:VAL:HG22	1:B:138:ILE:HG23	2.01	0.42
1:B:17:VAL:HG11	1:B:34:LEU:HD12	2.02	0.42
1:B:230:LYS:HA	1:B:230:LYS:HE2	2.02	0.42
1:A:248:MET:HE2	1:A:284:MET:HG3	2.00	0.42
1:A:155:PRO:HG3	1:A:306:VAL:HG22	2.02	0.42
1:A:218:GLU:HB2	1:A:267:ASN:HB2	2.02	0.42
1:B:230:LYS:HD3	1:B:240:TYR:CD2	2.55	0.42
1:B:204:LYS:HD3	1:B:321:PRO:HG2	2.02	0.41
1:A:119:PRO:HA	1:A:134:THR:HG23	2.02	0.41
1:B:77:SER:O	1:B:81:VAL:HG23	2.20	0.41
1:A:185:MET:HG2	1:B:53:ILE:HD11	2.02	0.41
1:B:282:ASN:HD22	1:B:282:ASN:HA	1.73	0.41
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.77	0.41
1:A:246:GLY:O	3:A:336:AHG:H4	2.21	0.41
1:B:210:SER:HB2	1:B:254:ARG:HH21	1.86	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%)	287 (93%)	22 (7%)	0	100	100
1	B	311/335 (93%)	294 (94%)	16 (5%)	1 (0%)	36	58
All	All	620/670 (92%)	581 (94%)	38 (6%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	VAL

### 5.3.2 Protein sidechains [i](#)

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	16
1	B	262/278 (94%)	251 (96%)	11 (4%)	26	52
All	All	523/556 (94%)	486 (93%)	37 (7%)	13	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	10	ILE
1	A	14	THR
1	A	35	ASN
1	A	77	SER

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Mol	Chain	Res	Type
1	A	80	LEU
1	A	97	GLU
1	A	99	ASP
1	A	124	SER
1	A	129	LEU
1	A	144	THR
1	A	160	VAL
1	A	169	SER
1	A	204	LYS
1	A	207	SER
1	A	221	PRO
1	A	224	THR
1	A	230	LYS
1	A	235	ASP
1	A	236	ASN
1	A	237	SER
1	A	247	SER
1	A	261	ILE
1	A	265	PRO
1	A	270	SER
1	A	316	ILE
1	B	6	PHE
1	B	18	MET
1	B	35	ASN
1	B	99	ASP
1	B	169	SER
1	B	199	ASN
1	B	207	SER
1	B	237	SER
1	B	265	PRO
1	B	282	ASN
1	B	332	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	GLN
1	A	32	GLN
1	A	101	ASN
1	A	154	GLN
1	A	158	ASN

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Mol	Chain	Res	Type
1	A	228	GLN
1	B	35	ASN
1	B	83	ASN
1	B	101	ASN
1	B	182	ASN
1	B	228	GLN
1	B	282	ASN
1	B	334	HIS

### 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	AHG	B	336	2	19,19,19	0.63	0	27,29,29	0.90	1 (3%)
3	AHG	A	336	2	19,19,19	0.64	0	27,29,29	0.85	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	AHG	B	336	2	-	7/12/28/28	0/1/1/1
3	AHG	A	336	2	-	5/12/28/28	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	336	AHG	O2P-P1-O1P	2.19	119.38	110.83
3	A	336	AHG	O2P-P1-O1P	2.03	118.75	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

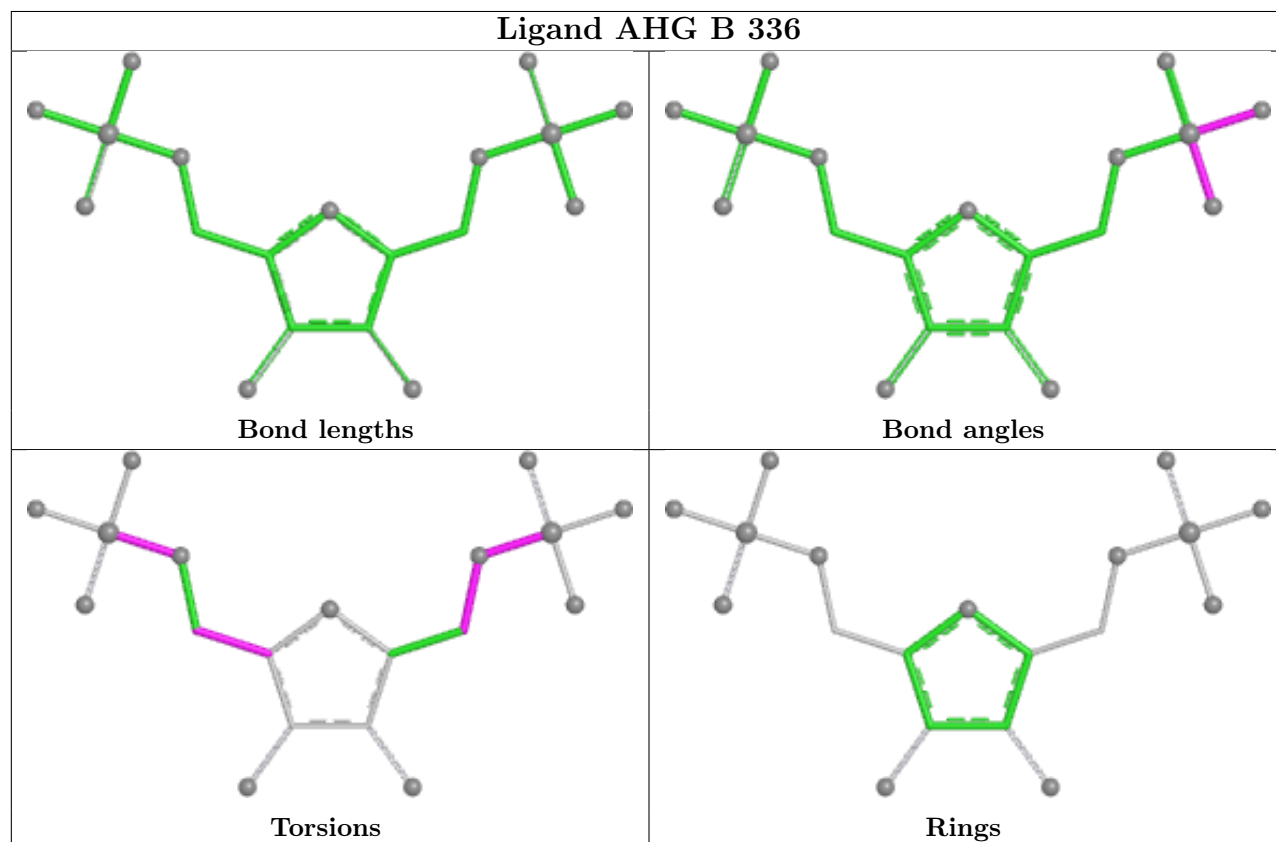
There are no ring outliers.

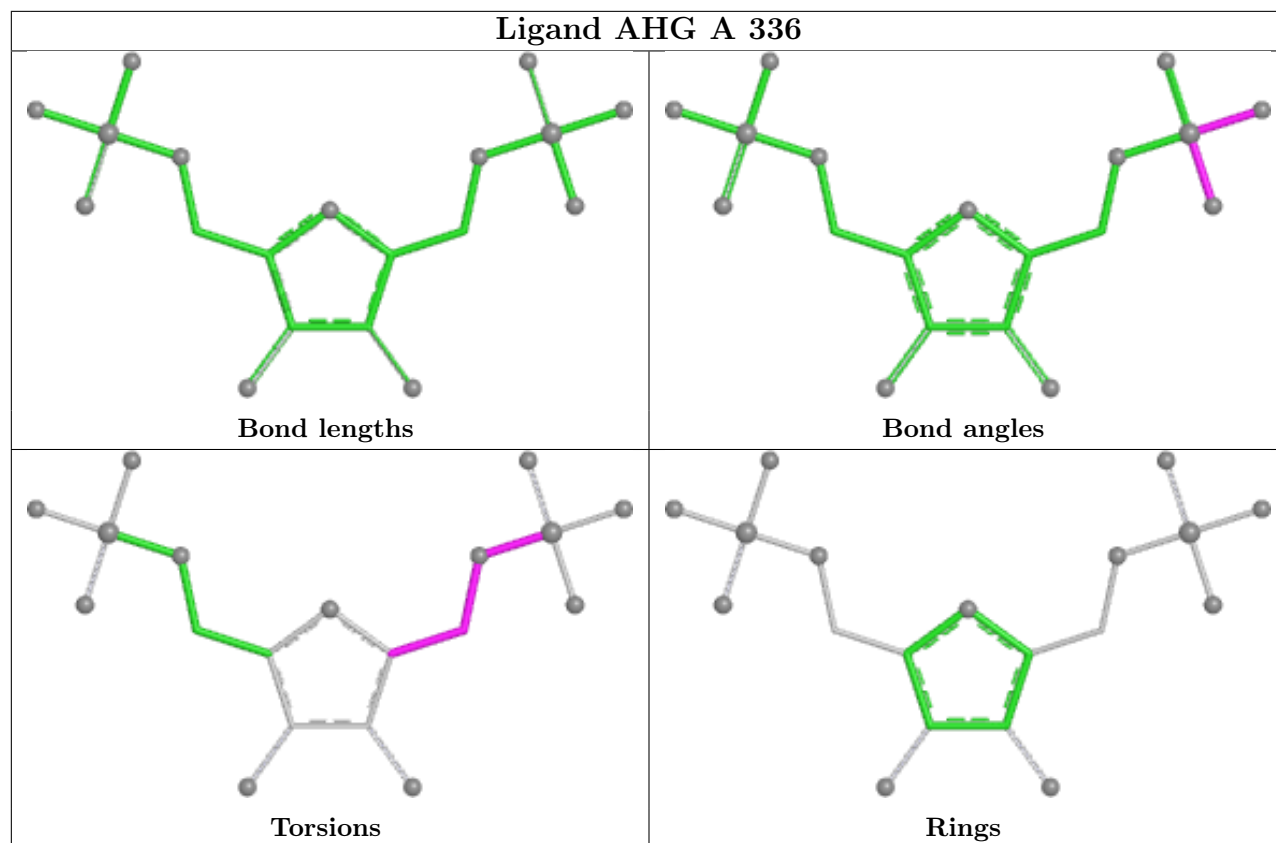
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	336	AHG	2	0
3	A	336	AHG	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.