Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 09:32 PM EST

PDB ID	:	1FBD
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	:	2.90 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:

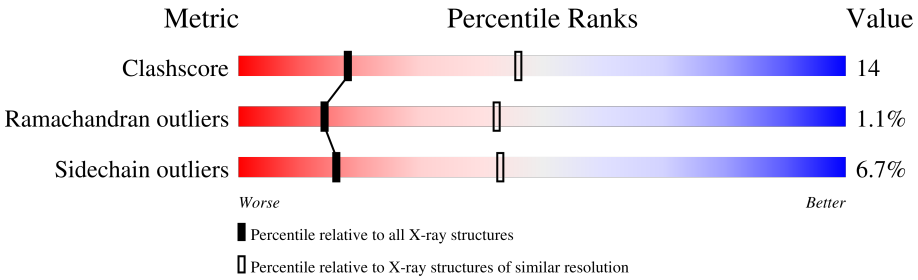
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	57% 30% 6% 7%
1	B	335	56% 32% 5% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5909 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			

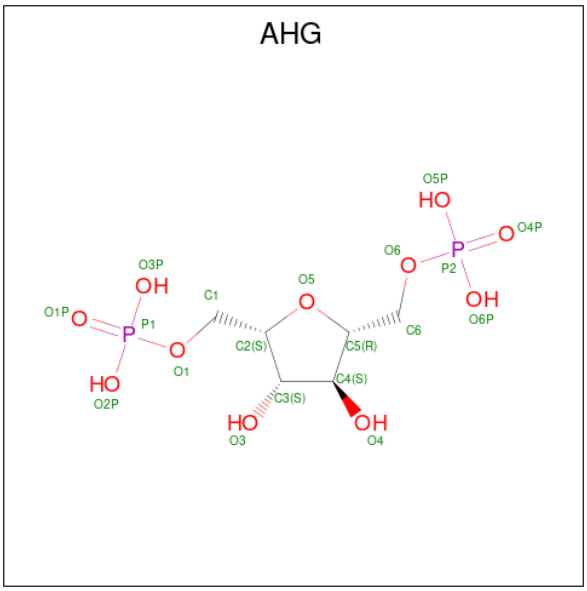
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: AHG) (formula: $C_6H_{14}O_{11}P_2$).



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		

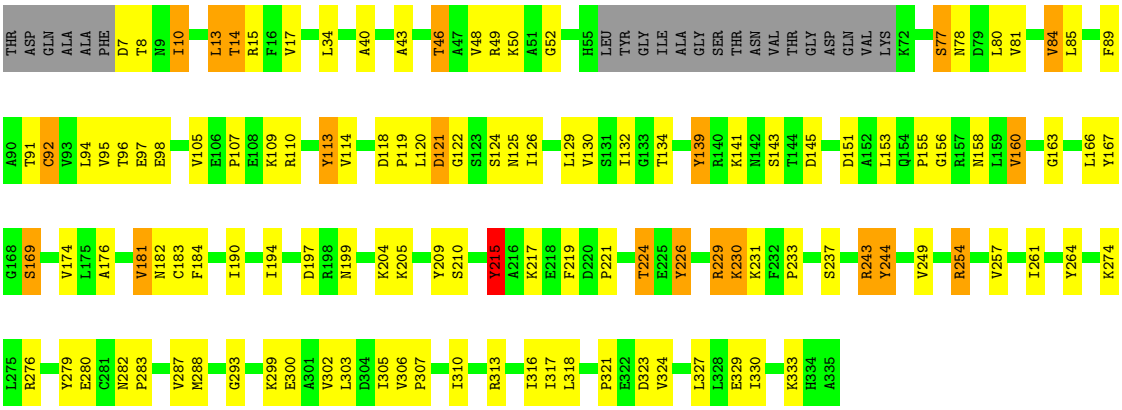
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

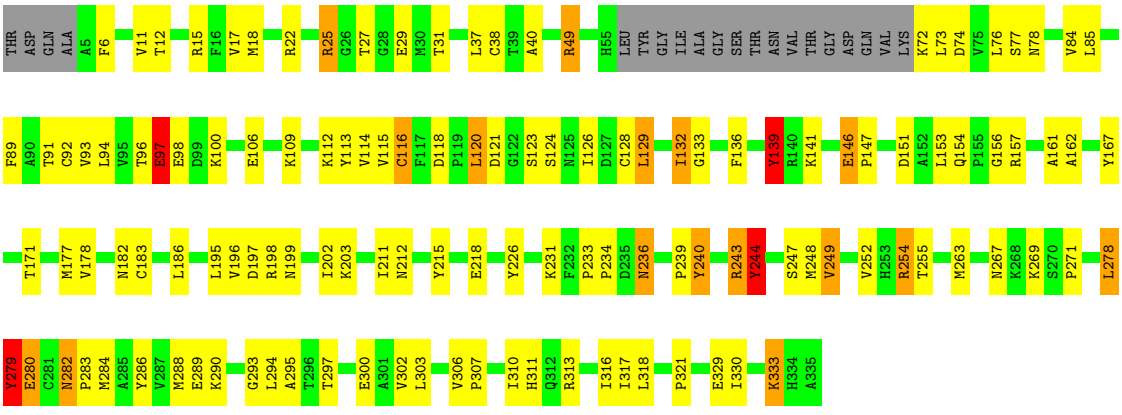
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A:



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B:



4 Data and refinement statistics (i)

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	131.60Å 131.60Å 68.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5909	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: 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	0.86	1/2430 (0.0%)	1.62	26/3286 (0.8%)
1	B	0.84	1/2447 (0.0%)	1.64	28/3309 (0.8%)
All	All	0.85	2/4877 (0.0%)	1.63	54/6595 (0.8%)

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	5
1	B	0	8
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	GLU	CD-OE1	-6.22	1.18	1.25
1	A	280	GLU	CD-OE1	-6.02	1.19	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	TYR	CB-CG-CD1	-11.02	114.39	121.00
1	B	97	GLU	OE1-CD-OE2	10.70	136.13	123.30
1	B	120	LEU	CA-C-N	-10.46	94.18	117.20
1	A	118	ASP	CB-CG-OD2	10.40	127.66	118.30
1	A	120	LEU	O-C-N	9.64	138.13	122.70
1	A	97	GLU	OE1-CD-OE2	8.91	134.00	123.30
1	B	120	LEU	O-C-N	8.66	136.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	A	118	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	B	240	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	15	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	217	LYS	CA-CB-CG	7.41	129.71	113.40
1	B	15	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	118	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	B	243	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	329	GLU	CA-CB-CG	7.05	128.92	113.40
1	B	254	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	120	LEU	CA-C-N	-6.94	101.94	117.20
1	B	313	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	121	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	B	183	CYS	CA-CB-SG	-6.73	101.89	114.00
1	A	167	TYR	CG-CD1-CE1	-6.49	116.11	121.30
1	A	254	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	244	TYR	CB-CG-CD2	6.35	124.81	121.00
1	B	17	VAL	CA-CB-CG2	-6.24	101.54	110.90
1	B	333	LYS	CA-CB-CG	6.19	127.02	113.40
1	B	139	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	B	248	MET	CA-CB-CG	-6.11	102.92	113.30
1	A	49	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	313	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	B	113	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	B	12	THR	CA-CB-CG2	-5.82	104.26	112.40
1	B	116	CYS	CA-CB-SG	-5.77	103.62	114.00
1	A	14	THR	CA-CB-OG1	-5.73	96.96	109.00
1	A	160	VAL	CG1-CB-CG2	-5.66	101.85	110.90
1	B	38	CYS	CA-CB-SG	-5.66	103.82	114.00
1	A	14	THR	CA-CB-CG2	5.62	120.27	112.40
1	B	247	SER	N-CA-C	-5.59	95.90	111.00
1	A	97	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	B	25	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	215	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	50	LYS	CA-CB-CG	5.43	125.35	113.40
1	A	118	ASP	N-CA-C	-5.42	96.37	111.00
1	A	299	LYS	CA-CB-CG	5.37	125.21	113.40
1	B	132	ILE	CA-C-N	5.33	126.86	116.20
1	A	46	THR	CA-CB-CG2	5.31	119.84	112.40
1	B	129	LEU	CA-C-N	-5.28	105.58	117.20
1	B	236	ASN	N-CA-C	5.25	125.18	111.00
1	A	181	VAL	N-CA-C	-5.24	96.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	TYR	CD1-CG-CD2	5.21	123.63	117.90
1	B	249	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	B	279	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	84	VAL	CA-CB-CG1	-5.05	103.33	110.90
1	B	49	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	139	TYR	Sidechain
1	A	215	TYR	Sidechain
1	A	226	TYR	Sidechain
1	A	244	TYR	Sidechain
1	B	139	TYR	Sidechain
1	B	167	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	240	TYR	Sidechain
1	B	244	TYR	Sidechain
1	B	279	TYR	Sidechain
1	B	286	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	2448	67	0
1	B	2407	531	2462	67	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	4	10	3	0
3	B	19	4	10	1	0
All	All	4840	1069	4930	132	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 14.

All (132) 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:114:VAL:HB	1:B:139:TYR:HB2	1.58	0.83
1:B:182:ASN:ND2	1:B:198:ARG:HA	1.96	0.80
1:A:92:CYS:HA	1:A:105:VAL:HB	1.65	0.77
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.68	0.75
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.69	0.74
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.75	0.69
1:B:252:VAL:HG11	1:B:284:MET:SD	2.32	0.69
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.28	0.69
1:A:121:ASP:HA	3:A:336:AHG:O2P	1.93	0.68
1:A:96:THR:HG22	1:A:98:GLU:H	1.59	0.67
1:A:17:VAL:HG11	1:A:34:LEU:HD12	1.78	0.65
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.78	0.64
1:B:93:VAL:HB	1:B:114:VAL:HG13	1.80	0.63
1:B:96:THR:HG22	1:B:98:GLU:H	1.62	0.63
1:B:121:ASP:O	1:B:132:ILE:HB	2.00	0.60
1:B:121:ASP:HA	3:B:336:AHG:O2P	2.02	0.60
1:A:226:TYR:HD1	1:A:330:ILE:HD12	1.66	0.59
1:B:154:GLN:O	1:B:307:PRO:HG2	2.03	0.58
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.86	0.58
1:A:107:PRO:HA	1:A:110:ARG:HG3	1.87	0.57
1:A:274:LYS:NZ	3:A:336:AHG:H61	2.19	0.57
1:B:100:LYS:O	1:B:310:ILE:HD11	2.06	0.56
1:A:229:ARG:HG3	1:A:230:LYS:HD2	1.87	0.56
1:B:288:MET:HG3	1:B:318:LEU:HB2	1.86	0.55
1:B:302:VAL:HG21	1:B:316:ILE:HD12	1.88	0.55
1:A:48:VAL:HG11	1:A:132:ILE:HD11	1.88	0.54
1:B:11:VAL:HG11	1:B:195:LEU:HD23	1.90	0.54
1:B:74:ASP:HB3	1:B:120:LEU:HB3	1.89	0.53
1:A:282:ASN:HD22	1:A:302:VAL:HG12	1.73	0.53
1:B:89:PHE:HA	1:B:109:LYS:O	2.08	0.53
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.91	0.53
1:A:215:TYR:HB2	1:A:219:PHE:CE1	2.43	0.53
1:A:316:ILE:HD11	1:A:318:LEU:HD23	1.89	0.52
1:A:7:ASP:HB3	1:A:10:ILE:HG23	1.92	0.52
1:B:231:LYS:O	1:B:239:PRO:HB3	2.10	0.52
1:A:317:ILE:HG22	1:A:324:VAL:HG13	1.91	0.51
1:B:74:ASP:HA	1:B:77:SER:OG	2.10	0.51
1:A:95:VAL:HG13	1:A:310:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HG3	1:A:306:VAL:HG22	1.92	0.50
1:A:91:THR:HB	1:A:94:LEU:HD21	1.92	0.50
1:B:267:ASN:O	1:B:271:PRO:HA	2.12	0.50
1:B:282:ASN:ND2	1:B:302:VAL:HG12	2.27	0.50
1:B:153:LEU:O	1:B:307:PRO:HD2	2.12	0.50
1:A:288:MET:HG3	1:A:318:LEU:HD13	1.93	0.49
1:A:283:PRO:O	1:A:287:VAL:HG23	2.12	0.49
1:B:73:LEU:HD23	1:B:126:ILE:HD13	1.93	0.49
1:A:221:PRO:HA	1:A:224:THR:HG22	1.95	0.49
1:B:171:THR:HB	1:B:186:LEU:HD23	1.94	0.49
1:B:254:ARG:O	1:B:254:ARG:HG2	2.08	0.49
1:A:302:VAL:O	1:A:305:ILE:HD12	2.12	0.49
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.12	0.48
1:B:202:ILE:HG23	1:B:203:LYS:O	2.12	0.48
1:B:243:ARG:O	1:B:244:TYR:HB2	2.13	0.48
1:B:96:THR:HG22	1:B:97:GLU:N	2.29	0.48
1:A:156:GLY:C	1:A:303:LEU:HD22	2.35	0.47
1:B:161:ALA:HB2	1:B:177:MET:HG2	1.96	0.47
1:A:13:LEU:HA	1:A:184:PHE:CE2	2.49	0.47
1:B:243:ARG:HB3	1:B:254:ARG:NH1	2.30	0.47
1:A:274:LYS:HZ3	3:A:336:AHG:H61	1.79	0.47
1:B:282:ASN:HD22	1:B:282:ASN:HA	1.61	0.47
1:A:210:SER:HB2	1:A:254:ARG:HH22	1.80	0.47
1:B:78:ASN:OD1	1:B:96:THR:HG21	2.15	0.47
1:A:155:PRO:O	1:A:158:ASN:HB2	2.15	0.47
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.50	0.46
1:A:163:GLY:HA3	1:A:174:VAL:O	2.15	0.46
1:B:280:GLU:O	1:B:283:PRO:HD2	2.16	0.46
1:A:13:LEU:HD12	1:A:184:PHE:CD1	2.51	0.46
1:B:269:LYS:HD3	1:B:269:LYS:HA	1.70	0.46
1:A:40:ALA:HB2	1:A:84:VAL:HG21	1.98	0.46
1:A:13:LEU:HD12	1:A:184:PHE:CE1	2.51	0.45
1:B:133:GLY:HA3	1:B:249:VAL:HG21	1.98	0.45
1:A:190:ILE:HD11	1:A:194:ILE:HD11	1.98	0.45
1:A:125:ASN:OD1	1:A:130:VAL:HG21	2.16	0.45
1:A:77:SER:O	1:A:81:VAL:HG23	2.17	0.45
1:A:7:ASP:O	1:A:10:ILE:HG12	2.17	0.44
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.77	0.44
1:A:324:VAL:O	1:A:327:LEU:HB3	2.17	0.44
1:B:267:ASN:HD21	1:B:269:LYS:HB2	1.81	0.44
1:B:116:CYS:SG	1:B:278:LEU:CD1	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ILE:HG13	1:B:263:MET:O	2.16	0.44
1:B:294:LEU:HD12	1:B:321:PRO:HA	1.99	0.44
1:A:293:GLY:HA2	1:A:321:PRO:HD3	1.98	0.44
1:B:295:ALA:HA	1:B:317:ILE:O	2.18	0.44
1:A:257:VAL:HG21	1:B:128:CYS:HA	1.99	0.44
1:A:276:ARG:HA	1:A:313:ARG:HA	1.98	0.44
1:B:156:GLY:HA3	1:B:303:LEU:HD22	2.00	0.44
1:A:288:MET:CG	1:A:318:LEU:HD13	2.47	0.44
1:B:178:VAL:HA	1:B:290:LYS:HE3	2.00	0.44
1:B:330:ILE:HA	1:B:333:LYS:HD3	1.99	0.44
1:A:119:PRO:HA	1:A:134:THR:HG23	2.00	0.43
1:A:209:TYR:HA	1:A:261:ILE:CG2	2.48	0.43
1:A:43:ALA:HB3	1:A:80:LEU:HD21	2.00	0.43
1:A:114:VAL:HB	1:A:139:TYR:HB2	2.01	0.43
1:A:126:ILE:HG12	1:A:132:ILE:HD13	2.00	0.43
1:A:141:LYS:HE3	1:A:143:SER:O	2.18	0.43
1:B:252:VAL:O	1:B:255:THR:HB	2.19	0.43
1:A:176:ALA:HA	1:A:181:VAL:HA	2.00	0.43
1:A:210:SER:HB2	1:A:254:ARG:NH2	2.33	0.43
1:A:89:PHE:CE1	1:A:109:LYS:HG2	2.54	0.43
1:B:306:VAL:HA	1:B:307:PRO:HD3	1.73	0.43
1:A:174:VAL:HA	1:A:182:ASN:O	2.19	0.42
1:B:133:GLY:CA	1:B:249:VAL:HG21	2.49	0.42
1:A:209:TYR:HA	1:A:261:ILE:HG23	1.99	0.42
1:A:153:LEU:HA	1:A:307:PRO:HG2	2.01	0.42
1:A:122:GLY:O	1:A:125:ASN:HB2	2.18	0.42
1:B:29:GLU:OE1	1:B:112:LYS:HG2	2.19	0.42
1:B:72:LYS:NZ	1:B:76:LEU:HD21	2.34	0.42
1:B:126:ILE:O	1:B:129:LEU:HD23	2.20	0.42
1:A:141:LYS:HG3	1:A:151:ASP:OD1	2.18	0.42
1:B:37:LEU:HD21	1:B:136:PHE:CD2	2.54	0.42
1:B:116:CYS:SG	1:B:278:LEU:HD13	2.60	0.42
1:A:91:THR:HA	1:A:113:TYR:O	2.19	0.41
1:A:85:LEU:HB3	1:A:91:THR:HG21	2.01	0.41
1:B:297:THR:HG23	1:B:300:GLU:O	2.20	0.41
1:B:211:ILE:HD12	1:B:263:MET:SD	2.59	0.41
1:A:81:VAL:HA	1:A:84:VAL:HG22	2.03	0.41
1:A:329:GLU:O	1:A:333:LYS:N	2.53	0.41
1:B:146:GLU:HA	1:B:147:PRO:HD3	1.92	0.41
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.48	0.41
1:A:231:LYS:O	1:A:233:PRO:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ALA:HB1	1:B:283:PRO:HB3	2.01	0.41
1:B:254:ARG:HH11	1:B:254:ARG:HD3	1.70	0.41
1:B:141:LYS:HG3	1:B:151:ASP:OD1	2.21	0.41
1:B:218:GLU:CB	1:B:267:ASN:HB2	2.42	0.41
1:A:210:SER:HA	1:A:243:ARG:O	2.20	0.40
1:B:18:MET:O	1:B:22:ARG:HB3	2.21	0.40
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.61	0.40
1:B:289:GLU:HA	1:B:293:GLY:O	2.22	0.40
1:A:205:LYS:HA	1:A:323:ASP:OD1	2.22	0.40
1:A:169:SER:O	1:B:49:ARG:HA	2.22	0.40
1:B:94:LEU:HA	1:B:115:VAL:O	2.21	0.40
1:B:233:PRO:HA	1:B:234:PRO:HD2	1.84	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%)	289 (94%)	18 (6%)	2 (1%)	25 58
1	B	311/335 (93%)	273 (88%)	33 (11%)	5 (2%)	9 32
All	All	620/670 (92%)	562 (91%)	51 (8%)	7 (1%)	14 42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	THR
1	B	236	ASN
1	B	244	TYR
1	A	92	CYS
1	A	52	GLY
1	B	6	PHE

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Mol	Chain	Res	Type
1	B	25	ARG

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%)	241 (92%)	20 (8%)	13	35
1	B	262/278 (94%)	247 (94%)	15 (6%)	20	51
All	All	523/556 (94%)	488 (93%)	35 (7%)	16	43

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	10	ILE
1	A	13	LEU
1	A	14	THR
1	A	46	THR
1	A	77	SER
1	A	124	SER
1	A	129	LEU
1	A	145	ASP
1	A	160	VAL
1	A	169	SER
1	A	199	ASN
1	A	204	LYS
1	A	224	THR
1	A	229	ARG
1	A	230	LYS
1	A	237	SER
1	A	264	TYR
1	A	279	TYR
1	A	300	GLU
1	B	31	THR
1	B	91	THR

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Mol	Chain	Res	Type
1	B	92	CYS
1	B	97	GLU
1	B	106	GLU
1	B	123	SER
1	B	124	SER
1	B	146	GLU
1	B	157	ARG
1	B	196	VAL
1	B	197	ASP
1	B	199	ASN
1	B	278	LEU
1	B	279	TYR
1	B	282	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	182	ASN
1	A	199	ASN
1	A	282	ASN
1	B	154	GLN
1	B	182	ASN
1	B	199	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	0.67	0	29,29,29	0.88	1 (3%)
3	AHG	A	336	2	19,19,19	0.68	0	29,29,29	0.90	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	-	9/12/28/28	0/1/1/1
3	AHG	A	336	2	-	8/12/28/28	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(^{o})	Ideal(^{o})
3	B	336	AHG	O2P-P1-O1P	2.22	119.36	110.68
3	A	336	AHG	O2P-P1-O1P	2.17	119.19	110.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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

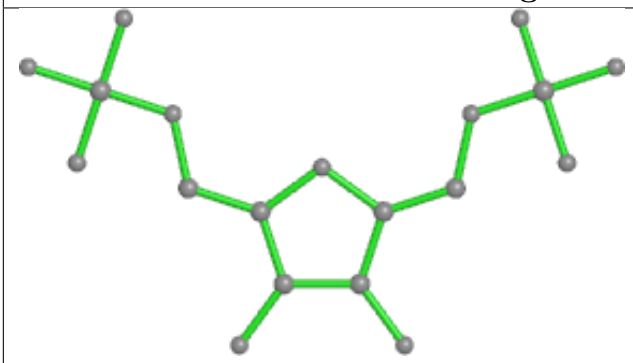
There are no ring outliers.

2 monomers are involved in 4 short contacts:

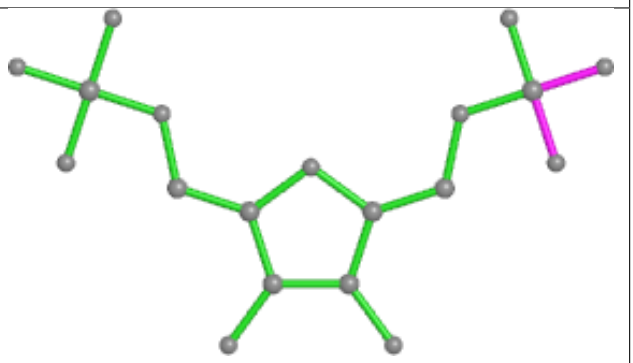
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	336	AHG	1	0
3	A	336	AHG	3	0

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 then 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.

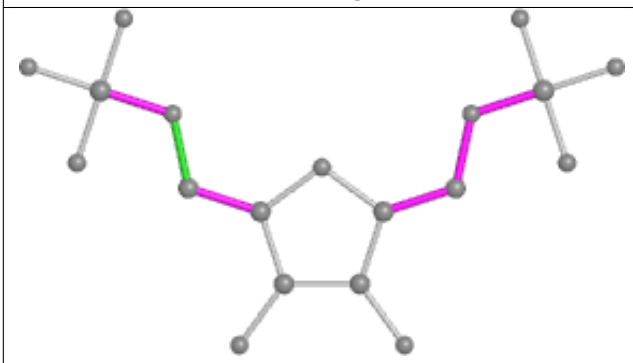
Ligand AHG B 336



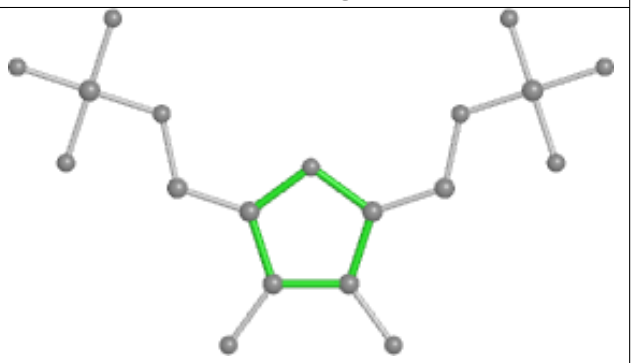
Bond lengths



Bond angles

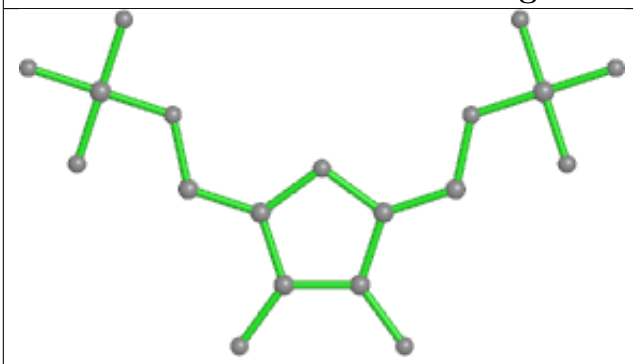


Torsions

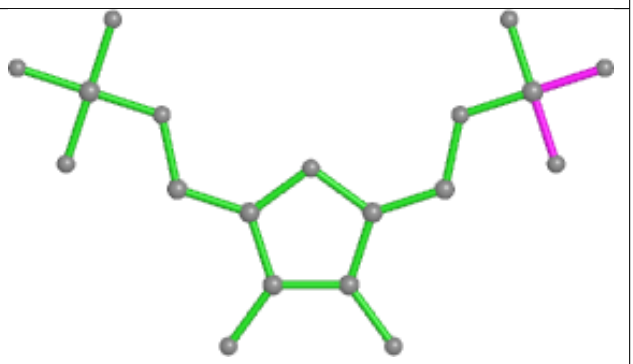


Rings

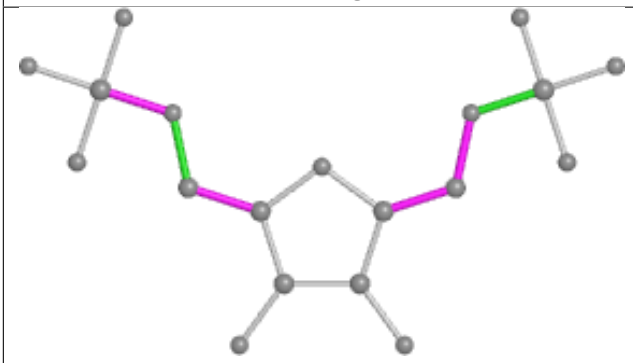
Ligand AHG A 336



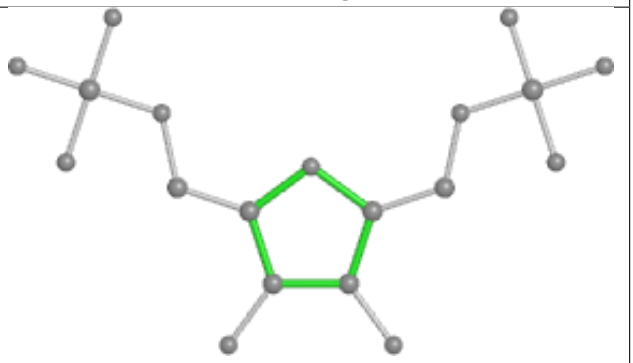
Bond lengths



Bond angles



Torsions



Rings

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.