



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:44 PM UTC

PDB ID : 1EYJ / pdb_00001eyj
Title : FRUCTOSE-1,6-BISPHOSPHATASE COMPLEX WITH AMP, MAGNESIUM, FRUCTOSE-6-PHOSPHATE AND PHOSPHATE (T-STATE)
Authors : Choe, J.; Honzatko, R.B.
Deposited on : 2000-05-07
Resolution : 2.28 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

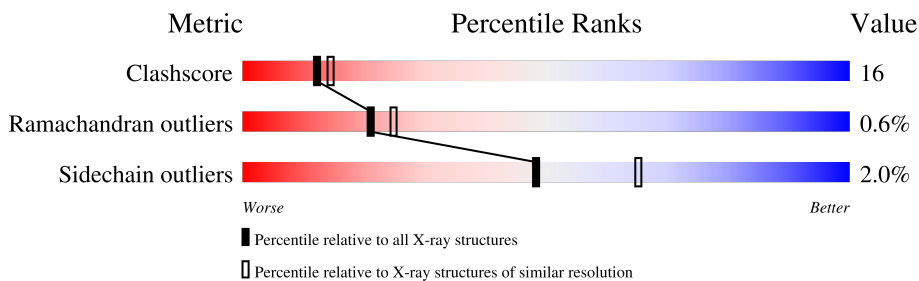
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	 69% 25% . .
1	B	337	 69% 27% . .

2 Entry composition [i](#)

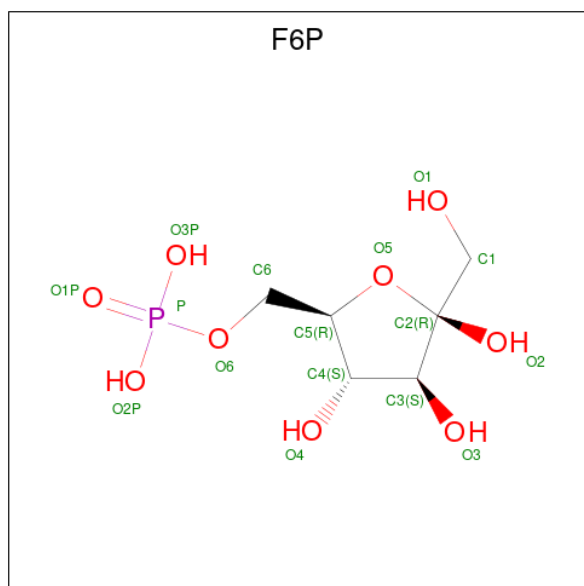
There are 6 unique types of molecules in this entry. The entry contains 5477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	327	Total	C	N	O	S	0	0	0
			2496	1587	420	474	15			
1	B	327	Total	C	N	O	S	0	0	0
			2496	1587	420	474	15			

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (CCD ID: F6P) (formula: $C_6H_{13}O_9P$).

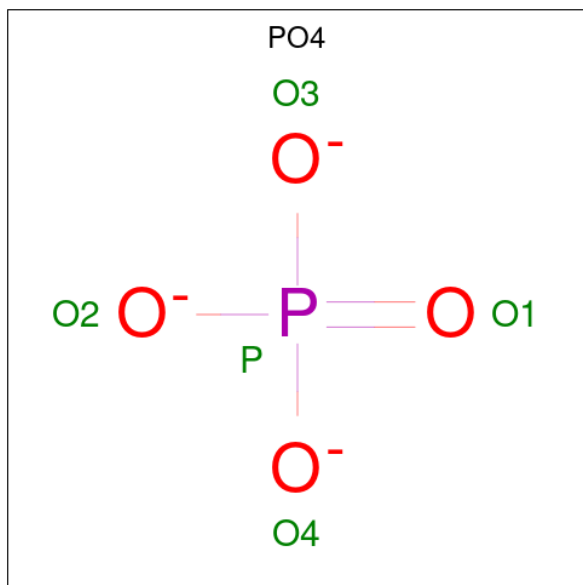


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

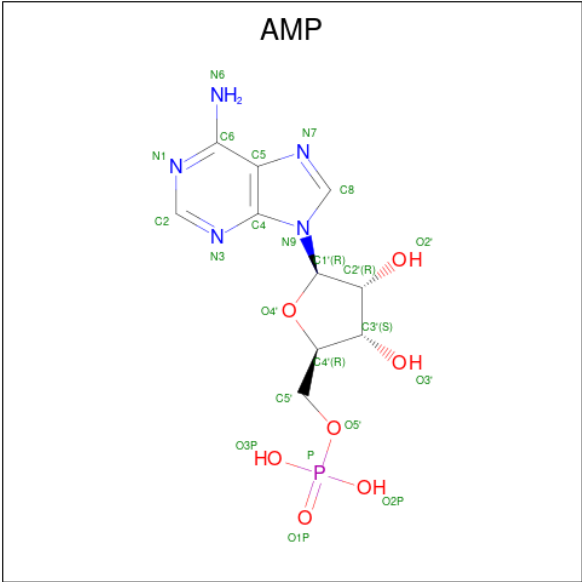
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 6 is water.

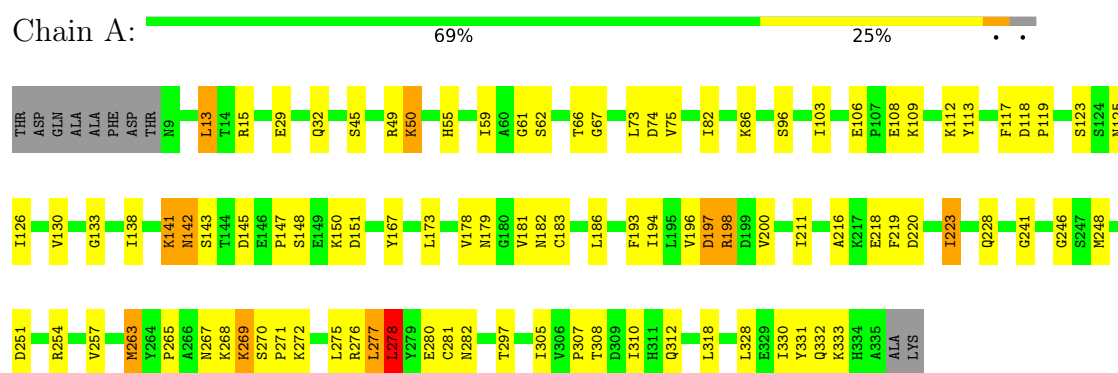
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	203	Total	O	0	0
			203	203		
6	B	192	Total	O	0	0
			192	192		

3 Residue-property plots [i](#)

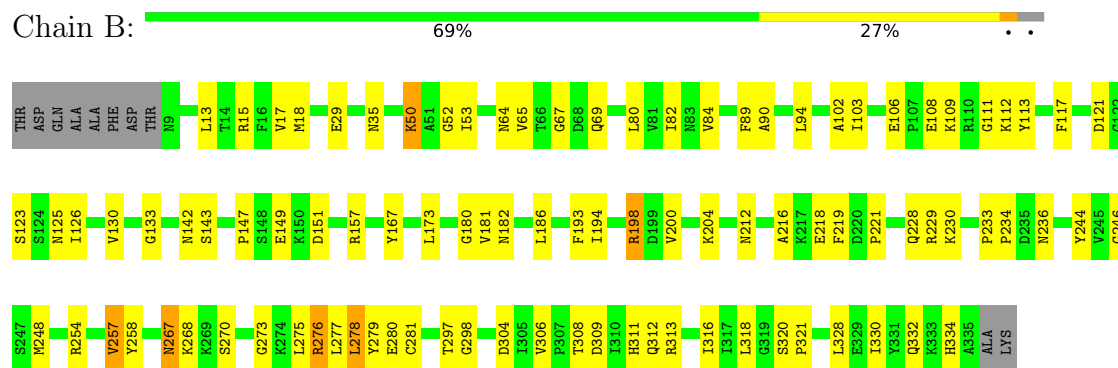
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	59.86Å 165.82Å 79.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.28	Depositor
% Data completeness (in resolution range)	89.8 (5.00-2.28)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5477	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: F6P, PO4, MG, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/2538	0.95	12/3434 (0.3%)
1	B	0.41	0/2538	0.96	11/3434 (0.3%)
All	All	0.41	0/5076	0.95	23/6868 (0.3%)

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	B	0	1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	GLY	N-CA-C	7.43	119.59	112.08
1	B	278	LEU	N-CA-C	6.88	118.78	111.28
1	A	278	LEU	N-CA-C	6.55	118.08	111.07
1	A	297	THR	N-CA-C	-6.40	105.51	113.38
1	B	297	THR	N-CA-C	-6.38	105.50	113.28
1	B	316	ILE	N-CA-C	6.23	116.80	108.27
1	A	50	LYS	N-CA-C	6.20	120.14	112.58
1	A	257	VAL	N-CA-C	6.09	116.73	110.82
1	B	200	VAL	N-CA-C	5.71	117.08	109.37
1	A	178	VAL	N-CA-C	5.70	117.12	110.62
1	A	263	MET	N-CA-C	5.57	118.55	108.69
1	B	298	GLY	N-CA-C	-5.49	107.94	114.48
1	B	117	PHE	N-CA-C	5.28	117.11	108.76
1	B	257	VAL	N-CA-C	5.25	116.03	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	LYS	N-CA-C	5.24	118.98	112.58
1	A	118	ASP	CA-C-N	5.23	124.68	119.24
1	A	118	ASP	C-N-CA	5.23	124.68	119.24
1	B	113	TYR	N-CA-C	5.19	118.52	110.17
1	A	138	ILE	N-CA-C	5.12	115.28	108.11
1	A	200	VAL	N-CA-C	5.10	116.97	109.63
1	A	113	TYR	N-CA-C	5.09	118.36	110.17
1	B	306	VAL	N-CA-C	-5.05	102.96	107.56
1	A	241	GLY	N-CA-C	-5.01	105.05	113.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	276	ARG	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	2496	0	2552	76	0
1	B	2496	0	2552	83	0
2	A	16	0	11	1	0
2	B	16	0	10	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	23	0	12	0	0
5	B	23	0	12	0	0
6	A	203	0	0	8	0
6	B	192	0	0	7	0
All	All	5477	0	5149	159	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 16.

All (159) 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:142:ASN:HD22	1:A:142:ASN:H	1.22	0.88
1:B:125:ASN:HB3	1:B:130:VAL:HB	1.55	0.87
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.60	0.83
1:A:142:ASN:H	1:A:142:ASN:ND2	1.78	0.78
1:A:183:CYS:HB2	1:A:197:ASP:OD2	1.84	0.77
1:B:15:ARG:HG2	1:B:15:ARG:HH11	1.48	0.76
1:B:65:VAL:HG11	1:B:69:GLN:H	1.49	0.76
1:B:267:ASN:C	1:B:267:ASN:HD22	1.96	0.74
1:B:267:ASN:ND2	1:B:270:SER:H	1.86	0.71
1:A:148:SER:OG	1:A:150:LYS:HG2	1.92	0.70
1:B:182:ASN:HD22	1:B:198:ARG:HA	1.57	0.70
1:B:29:GLU:OE1	1:B:112:LYS:HG2	1.92	0.69
1:B:267:ASN:HD22	1:B:270:SER:H	1.40	0.68
1:B:276:ARG:NE	6:B:765:HOH:O	2.26	0.67
1:B:276:ARG:HH22	1:B:313:ARG:NH2	1.94	0.66
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.78	0.64
1:B:218:GLU:HG2	1:B:268:LYS:HE3	1.80	0.64
1:A:308:THR:H	1:A:312:GLN:NE2	1.95	0.64
1:A:182:ASN:HD22	1:A:198:ARG:HA	1.64	0.64
1:B:218:GLU:HG2	1:B:268:LYS:HG3	1.81	0.63
1:A:328:LEU:O	1:A:332:GLN:HG2	1.99	0.63
1:A:141:LYS:HE3	1:A:151:ASP:CG	2.24	0.63
1:A:308:THR:H	1:A:312:GLN:HE22	1.46	0.62
1:B:276:ARG:HG2	1:B:279:TYR:OH	1.98	0.62
1:B:308:THR:H	1:B:312:GLN:HE22	1.47	0.61
1:A:45:SER:O	1:A:49:ARG:HD3	2.01	0.61
1:B:248:MET:HE3	1:B:275:LEU:HD13	1.83	0.60
1:A:248:MET:HE3	1:A:275:LEU:HD13	1.84	0.60
1:A:142:ASN:ND2	1:A:143:SER:H	2.00	0.60
1:B:50:LYS:HD2	1:B:53:ILE:HD12	1.84	0.60
1:A:133:GLY:HA2	1:A:167:TYR:CD2	2.37	0.59
1:A:142:ASN:HD22	1:A:142:ASN:N	1.88	0.58
1:A:197:ASP:OD2	1:A:197:ASP:N	2.34	0.58
1:B:278:LEU:HD22	6:B:621:HOH:O	2.04	0.57
1:B:276:ARG:NH2	1:B:313:ARG:NH2	2.52	0.57
1:B:15:ARG:HG2	1:B:15:ARG:NH1	2.20	0.56
1:B:102:ALA:HB2	1:B:149:GLU:HG2	1.87	0.56
1:B:267:ASN:ND2	1:B:270:SER:N	2.54	0.56
1:A:179:ASN:HB2	6:A:894:HOH:O	2.05	0.56
1:B:216:ALA:HA	1:B:219:PHE:CD2	2.41	0.56
1:A:254:ARG:HD2	6:A:664:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:NH1	1:B:330:ILE:HD11	2.20	0.56
1:A:13:LEU:HD11	1:A:173:LEU:HD13	1.89	0.55
1:B:308:THR:H	1:B:312:GLN:NE2	2.04	0.55
1:A:251:ASP:OD1	1:A:254:ARG:NH2	2.36	0.55
1:A:318:LEU:C	1:A:318:LEU:HD12	2.31	0.55
1:B:106:GLU:H	1:B:106:GLU:CD	2.15	0.55
1:B:182:ASN:ND2	1:B:198:ARG:O	2.40	0.55
1:A:141:LYS:HE2	1:A:143:SER:OG	2.07	0.54
1:A:106:GLU:H	1:A:106:GLU:CD	2.16	0.54
1:A:186:LEU:HB2	1:A:193:PHE:CE1	2.43	0.54
1:A:32:GLN:HG3	6:A:792:HOH:O	2.08	0.53
1:B:133:GLY:HA2	1:B:167:TYR:CD2	2.44	0.53
1:B:309:ASP:HB3	1:B:312:GLN:HB2	1.89	0.53
1:A:182:ASN:ND2	1:A:198:ARG:HG3	2.24	0.52
1:A:223:ILE:HG12	1:A:265:PRO:HG3	1.92	0.52
1:B:121:ASP:HA	4:B:343:PO4:O4	2.10	0.52
1:A:194:ILE:N	1:A:194:ILE:HD12	2.24	0.52
1:B:318:LEU:C	1:B:318:LEU:HD12	2.34	0.52
1:A:130:VAL:HG13	6:B:691:HOH:O	2.10	0.52
1:A:271:PRO:C	1:A:272:LYS:HD2	2.35	0.52
1:A:106:GLU:OE1	1:A:109:LYS:HD2	2.10	0.52
1:B:194:ILE:HD12	1:B:194:ILE:N	2.25	0.52
1:B:276:ARG:HG2	1:B:279:TYR:CZ	2.45	0.52
1:B:65:VAL:HG13	1:B:69:GLN:HG2	1.92	0.51
1:B:123:SER:HA	1:B:126:ILE:HG13	1.91	0.51
1:B:254:ARG:HD2	6:B:573:HOH:O	2.10	0.51
1:B:276:ARG:HH22	1:B:313:ARG:HH22	1.59	0.51
1:A:13:LEU:HB2	1:A:193:PHE:HB2	1.92	0.51
6:A:526:HOH:O	1:B:52:GLY:HA2	2.10	0.51
1:A:96:SER:HB2	1:A:117:PHE:CZ	2.45	0.51
1:B:181:VAL:O	1:B:198:ARG:O	2.29	0.50
1:B:13:LEU:C	1:B:13:LEU:HD13	2.36	0.50
1:B:204:LYS:HA	1:B:321:PRO:HD2	1.92	0.50
1:A:74:ASP:OD1	1:A:75:VAL:HG23	2.12	0.50
1:B:123:SER:HA	1:B:126:ILE:CD1	2.42	0.49
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.47	0.49
1:B:80:LEU:O	1:B:84:VAL:HG23	2.13	0.49
1:B:13:LEU:HD13	1:B:13:LEU:O	2.12	0.49
1:A:196:VAL:HG23	1:A:197:ASP:OD2	2.12	0.49
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.93	0.49
1:B:276:ARG:O	1:B:280:GLU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:LYS:HA	1:B:230:LYS:HE2	1.93	0.49
1:A:181:VAL:O	1:A:198:ARG:O	2.31	0.49
1:A:211:ILE:HB	1:A:263:MET:HE3	1.95	0.48
6:A:659:HOH:O	1:B:130:VAL:HA	2.14	0.48
1:B:277:LEU:HD12	1:B:278:LEU:HD23	1.95	0.48
1:B:267:ASN:C	1:B:267:ASN:ND2	2.68	0.48
1:B:270:SER:HB3	1:B:273:GLY:C	2.39	0.48
1:B:279:TYR:OH	1:B:311:HIS:HD2	1.97	0.47
1:B:328:LEU:O	1:B:332:GLN:HG3	2.14	0.47
1:A:269:LYS:HB2	1:A:269:LYS:NZ	2.28	0.47
1:A:173:LEU:C	1:A:173:LEU:HD23	2.39	0.47
1:A:223:ILE:HD13	1:A:331:TYR:OH	2.13	0.47
1:A:147:PRO:HA	1:A:151:ASP:OD1	2.14	0.47
1:B:157:ARG:HD3	1:B:304:ASP:OD2	2.15	0.47
1:B:142:ASN:O	1:B:143:SER:HB2	2.14	0.47
1:A:112:LYS:O	1:A:141:LYS:HB2	2.15	0.47
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.15	0.47
1:A:108:GLU:HG3	1:A:109:LYS:HG3	1.97	0.46
1:A:272:LYS:HD2	1:A:272:LYS:N	2.30	0.46
1:B:90:ALA:C	1:B:111:GLY:HA3	2.40	0.46
1:B:65:VAL:HG12	1:B:67:GLY:H	1.80	0.46
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.50	0.46
1:A:278:LEU:HD22	6:A:732:HOH:O	2.15	0.46
1:B:173:LEU:C	1:B:173:LEU:HD23	2.40	0.46
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.97	0.46
1:A:103:ILE:HD12	1:A:103:ILE:N	2.32	0.45
1:B:228:GLN:HA	1:B:228:GLN:OE1	2.17	0.45
1:A:142:ASN:HD22	1:A:143:SER:H	1.62	0.45
1:B:15:ARG:NH1	1:B:15:ARG:CG	2.80	0.45
1:B:108:GLU:HG3	1:B:109:LYS:HG3	1.99	0.45
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.82	0.45
1:B:246:GLY:O	2:B:341:F6P:H4	2.17	0.44
1:A:73:LEU:HD13	6:A:696:HOH:O	2.17	0.44
1:B:17:VAL:HG23	1:B:18:MET:N	2.32	0.44
1:A:246:GLY:O	2:A:338:F6P:H4	2.18	0.44
1:B:94:LEU:HB2	1:B:103:ILE:HB	2.00	0.44
1:A:141:LYS:HE3	1:A:151:ASP:OD2	2.16	0.44
1:B:257:VAL:HG12	1:B:258:TYR:CD2	2.52	0.44
1:B:233:PRO:HA	1:B:234:PRO:HD2	1.95	0.43
1:A:61:GLY:O	1:A:62:SER:HB3	2.17	0.43
1:A:220:ASP:OD2	1:A:220:ASP:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HB2	1:B:193:PHE:CE1	2.52	0.43
1:A:183:CYS:HB2	1:A:197:ASP:CG	2.43	0.43
1:A:276:ARG:O	1:A:280:GLU:HB2	2.19	0.43
1:A:117:PHE:CE2	1:A:119:PRO:HG3	2.53	0.43
1:A:218:GLU:OE1	1:A:268:LYS:HB2	2.18	0.43
1:A:277:LEU:HD22	1:A:282:ASN:ND2	2.34	0.43
1:A:74:ASP:OD1	1:A:75:VAL:N	2.51	0.43
1:B:182:ASN:ND2	1:B:198:ARG:C	2.77	0.42
1:B:82:ILE:HD12	1:B:103:ILE:HD12	2.01	0.42
1:B:270:SER:HB3	1:B:273:GLY:O	2.19	0.42
1:B:276:ARG:NH2	6:B:765:HOH:O	2.52	0.42
1:B:17:VAL:HG21	1:B:35:ASN:ND2	2.35	0.42
1:A:117:PHE:HE2	1:A:119:PRO:HG3	1.84	0.42
1:A:125:ASN:CB	1:A:130:VAL:HB	2.49	0.42
1:B:276:ARG:NH2	1:B:313:ARG:HH22	2.17	0.42
1:B:228:GLN:HG2	6:B:519:HOH:O	2.19	0.41
1:A:267:ASN:O	1:A:268:LYS:C	2.61	0.41
1:A:318:LEU:HD12	1:A:318:LEU:O	2.20	0.41
1:A:123:SER:HA	1:A:126:ILE:HG13	2.02	0.41
1:A:267:ASN:O	1:A:270:SER:C	2.63	0.41
1:B:89:PHE:CD2	1:B:109:LYS:HA	2.56	0.41
1:B:147:PRO:HA	1:B:151:ASP:OD1	2.20	0.41
1:B:182:ASN:ND2	1:B:198:ARG:HA	2.32	0.41
1:A:66:THR:O	1:A:66:THR:HG23	2.20	0.41
1:A:228:GLN:HG2	6:A:511:HOH:O	2.21	0.41
1:A:330:ILE:O	1:A:333:LYS:HB3	2.20	0.41
1:B:267:ASN:O	1:B:268:LYS:C	2.63	0.41
1:A:49:ARG:O	1:A:50:LYS:HB2	2.21	0.41
1:A:269:LYS:NZ	1:A:269:LYS:CB	2.84	0.41
1:B:236:ASN:O	1:B:236:ASN:CG	2.64	0.41
1:B:276:ARG:CZ	6:B:765:HOH:O	2.68	0.41
1:A:82:ILE:O	1:A:86:LYS:HG3	2.22	0.40
1:B:218:GLU:OE1	1:B:268:LYS:HB2	2.21	0.40
1:B:221:PRO:HB2	1:B:334:HIS:HD2	1.87	0.40
1:B:320:SER:HA	1:B:321:PRO:HD3	1.92	0.40
1:A:305:ILE:O	1:A:307:PRO:HD3	2.21	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	325/337 (96%)	309 (95%)	14 (4%)	2 (1%)	21	25
1	B	325/337 (96%)	311 (96%)	12 (4%)	2 (1%)	21	25
All	All	650/674 (96%)	620 (95%)	26 (4%)	4 (1%)	21	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ARG
1	B	64	ASN
1	B	198	ARG
1	A	67	GLY

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	272/279 (98%)	262 (96%)	10 (4%)	30	43
1	B	272/279 (98%)	271 (100%)	1 (0%)	84	91
All	All	544/558 (98%)	533 (98%)	11 (2%)	48	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	141	LYS

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Mol	Chain	Res	Type
1	A	142	ASN
1	A	145	ASP
1	A	197	ASP
1	A	223	ILE
1	A	269	LYS
1	A	277	LEU
1	A	278	LEU
1	A	310	ILE
1	B	267	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	55	HIS
1	A	69	GLN
1	A	101	ASN
1	A	142	ASN
1	A	154	GLN
1	A	158	ASN
1	A	179	ASN
1	A	182	ASN
1	A	228	GLN
1	A	311	HIS
1	A	312	GLN
1	B	35	ASN
1	B	55	HIS
1	B	142	ASN
1	B	154	GLN
1	B	158	ASN
1	B	182	ASN
1	B	267	ASN
1	B	311	HIS
1	B	312	GLN
1	B	334	HIS

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
5	AMP	A	341	-	25,25,25	0.34	0	37,38,38	0.35	0
2	F6P	A	338	3	15,16,16	0.59	0	16,25,25	0.58	0
4	PO4	A	340	3	4,4,4	1.68	0	6,6,6	0.47	0
5	AMP	B	342	-	25,25,25	0.35	0	37,38,38	0.39	0
2	F6P	B	341	3	15,16,16	0.58	0	16,25,25	0.69	0
4	PO4	B	343	3	4,4,4	1.72	0	6,6,6	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F6P	B	341	3	-	2/9/28/28	0/1/1/1
5	AMP	B	342	-	-	0/10/26/26	0/3/3/3
2	F6P	A	338	3	-	3/9/28/28	0/1/1/1
5	AMP	A	341	-	-	0/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

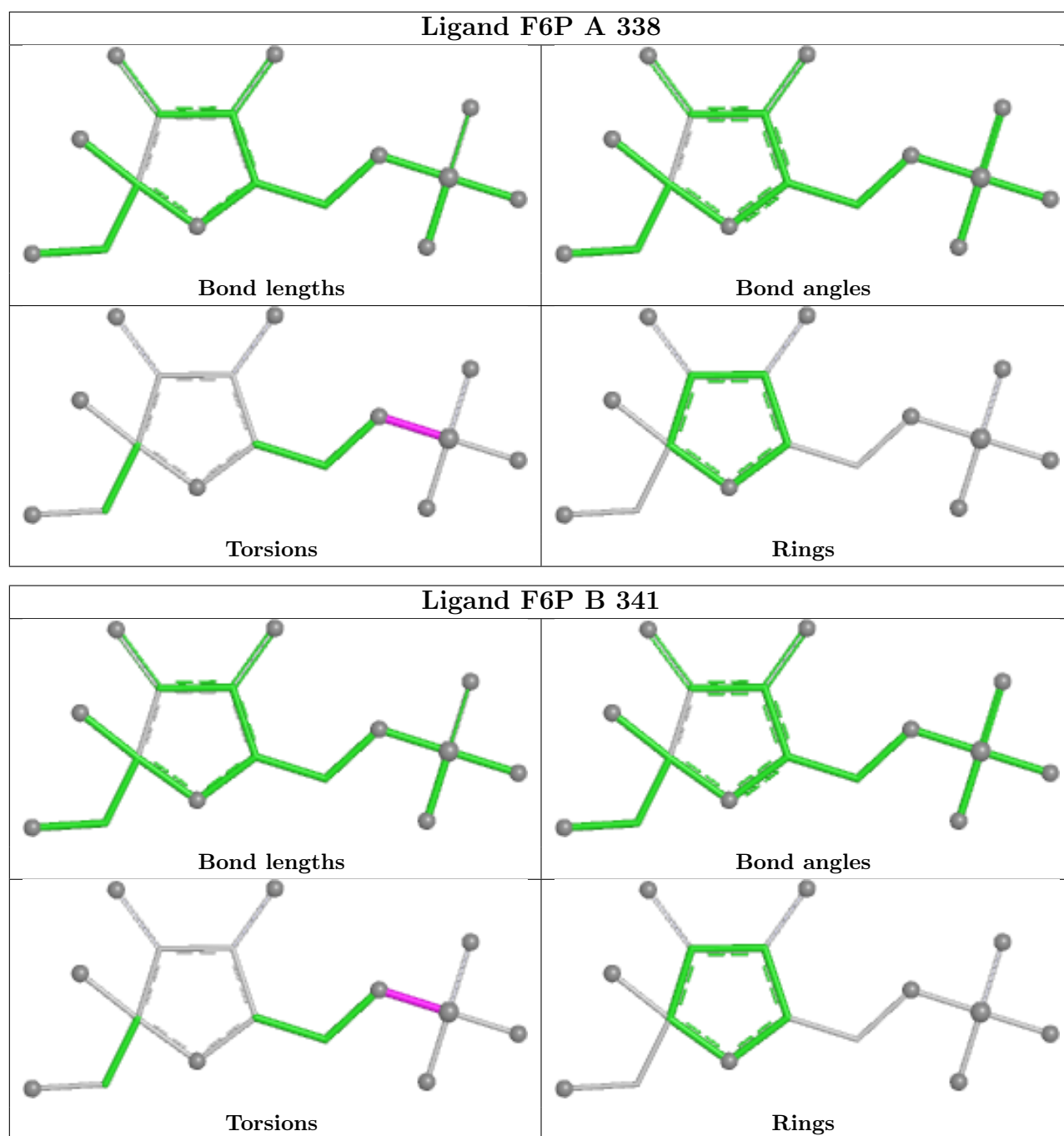
Mol	Chain	Res	Type	Atoms
2	A	338	F6P	C6-O6-P-O2P
2	A	338	F6P	C6-O6-P-O3P
2	A	338	F6P	C6-O6-P-O1P
2	B	341	F6P	C6-O6-P-O1P
2	B	341	F6P	C6-O6-P-O2P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	F6P	1	0
2	B	341	F6P	1	0
4	B	343	PO4	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.