



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:28 PM UTC

PDB ID : 4PFK / pdb_00004pfk
Title : PHOSPHOFRUCTOKINASE. STRUCTURE AND CONTROL
Authors : Evans, P.R.; Hudson, P.J.
Deposited on : 1988-01-25
Resolution : 2.40 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

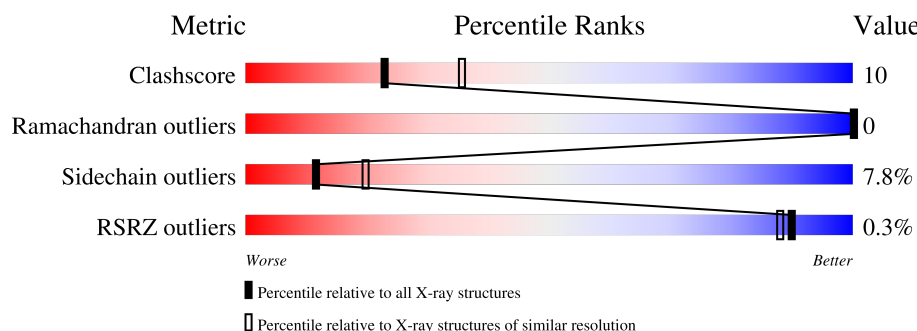
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2534 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.

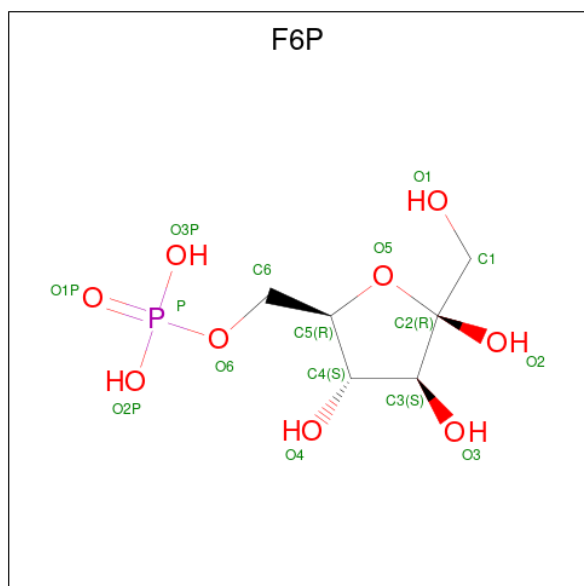
- Molecule 1 is a protein called PHOSPHOFRUCTOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2392	1494	434	456	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLN	GLU	conflict	UNP P00512

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

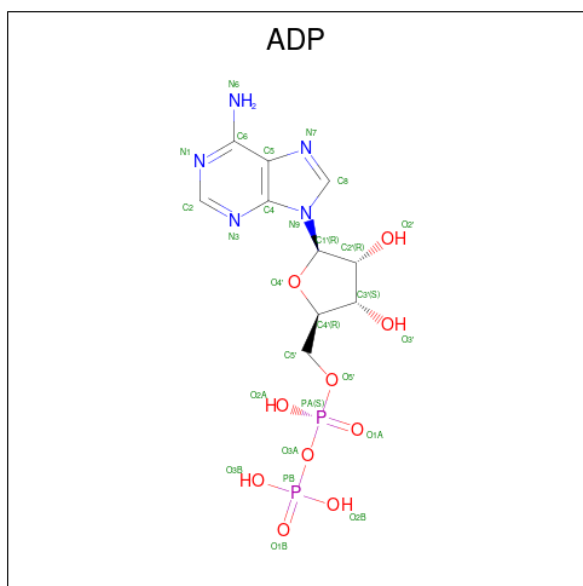


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

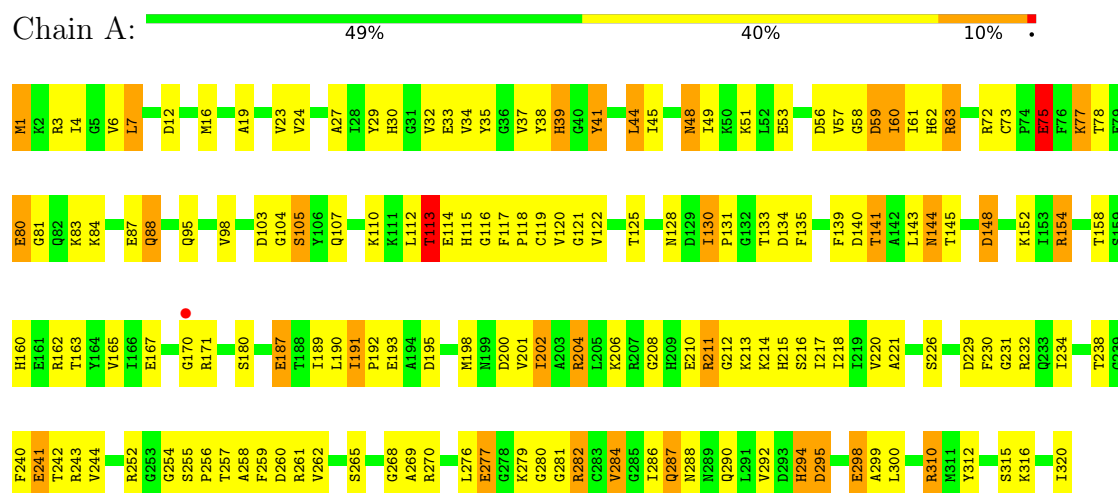
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: PHOSPHOFRUCTOKINASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.50Å 84.10Å 61.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 85.2 (30.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.38Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available) 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2534	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, F6P, ADP

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	1.06	0/2428	2.33	127/3274 (3.9%)

There are no bond length outliers.

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ASP	CA-CB-CG	18.29	130.89	112.60
1	A	75	GLU	CA-CB-CG	14.82	143.74	114.10
1	A	117	PHE	CA-CB-CG	-11.80	102.00	113.80
1	A	75	GLU	CB-CG-CD	10.29	130.10	112.60
1	A	277	GLU	CA-CB-CG	9.57	133.23	114.10
1	A	58	GLY	N-CA-C	-9.19	99.50	112.37
1	A	30	HIS	CA-CB-CG	-8.76	105.04	113.80
1	A	122	VAL	CB-CA-C	8.75	120.23	110.52
1	A	212	GLY	N-CA-C	8.48	128.14	115.08
1	A	191	ILE	O-C-N	8.42	128.39	121.40
1	A	77	LYS	CA-C-N	8.39	132.78	120.87
1	A	77	LYS	C-N-CA	8.39	132.78	120.87
1	A	148	ASP	N-CA-C	-8.38	102.23	111.36
1	A	187	GLU	CB-CG-CD	8.26	126.65	112.60
1	A	288	ASN	OD1-CG-ND2	8.21	130.81	122.60
1	A	134	ASP	CA-C-O	8.06	128.96	120.42
1	A	59	ASP	N-CA-C	8.04	122.54	112.24
1	A	241	GLU	CA-CB-CG	7.94	129.99	114.10
1	A	310	ARG	CD-NE-CZ	7.87	135.42	124.40
1	A	229	ASP	CA-CB-CG	7.84	120.44	112.60
1	A	282	ARG	CD-NE-CZ	-7.58	113.78	124.40
1	A	295	ASP	N-CA-C	-7.52	96.97	109.24
1	A	98	VAL	N-CA-CB	7.39	119.86	110.99
1	A	116	GLY	N-CA-C	7.35	125.46	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PHE	O-C-N	7.30	128.06	121.19
1	A	211	ARG	CG-CD-NE	7.30	128.06	112.00
1	A	115	HIS	N-CA-CB	7.19	120.48	110.56
1	A	48	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	284	VAL	CA-C-O	7.07	127.26	121.68
1	A	265	SER	CA-C-N	7.05	129.73	120.28
1	A	265	SER	C-N-CA	7.05	129.73	120.28
1	A	152	LYS	O-C-N	6.85	129.96	122.15
1	A	57	VAL	O-C-N	6.80	129.19	122.05
1	A	252	ARG	N-CA-C	6.74	121.25	112.89
1	A	154	ARG	CB-CA-C	6.74	122.30	110.85
1	A	104	GLY	CA-C-O	6.70	127.37	120.80
1	A	44	LEU	N-CA-C	-6.66	103.94	111.14
1	A	163	THR	CA-CB-OG1	-6.66	99.61	109.60
1	A	130	ILE	O-C-N	6.64	128.67	121.10
1	A	180	SER	O-C-N	6.61	128.88	122.07
1	A	254	GLY	CA-C-O	6.55	127.17	122.45
1	A	171	ARG	CG-CD-NE	6.54	126.40	112.00
1	A	211	ARG	CD-NE-CZ	-6.50	115.30	124.40
1	A	280	GLY	N-CA-C	-6.44	100.85	110.38
1	A	287	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	A	103	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	260	ASP	O-C-N	6.41	128.91	122.12
1	A	290	GLN	O-C-N	6.40	130.70	123.27
1	A	158	THR	O-C-N	6.33	128.92	122.09
1	A	270	ARG	CG-CD-NE	6.32	125.90	112.00
1	A	295	ASP	CA-C-O	-6.32	113.55	120.43
1	A	125	THR	CA-C-O	-6.29	113.97	120.89
1	A	87	GLU	CA-CB-CG	6.17	126.43	114.10
1	A	62	HIS	CA-CB-CG	-6.14	107.66	113.80
1	A	218	ILE	CA-C-N	6.13	130.66	122.93
1	A	218	ILE	C-N-CA	6.13	130.66	122.93
1	A	33	GLU	CA-CB-CG	6.13	126.35	114.10
1	A	288	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	294	HIS	CA-CB-CG	-6.11	107.69	113.80
1	A	105	SER	CB-CA-C	6.11	121.23	110.85
1	A	114	GLU	N-CA-C	-6.05	104.01	111.33
1	A	141	THR	CA-C-O	-5.97	114.55	120.82
1	A	201	VAL	O-C-N	5.96	127.65	121.87
1	A	39	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	286	ILE	CB-CA-C	5.93	118.99	110.33
1	A	41	TYR	O-C-N	5.91	128.39	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLN	O-C-N	5.90	128.38	122.12
1	A	140	ASP	O-C-N	5.86	128.33	122.12
1	A	279	LYS	N-CA-CB	5.82	118.21	110.29
1	A	98	VAL	N-CA-C	-5.80	100.07	108.36
1	A	238	THR	O-C-N	5.78	128.70	122.34
1	A	299	ALA	N-CA-C	-5.72	105.12	111.36
1	A	258	ALA	CA-C-O	-5.72	114.78	121.07
1	A	160	HIS	CA-CB-CG	-5.71	108.09	113.80
1	A	243	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	180	SER	CA-CB-OG	-5.70	99.69	111.10
1	A	226	SER	N-CA-C	5.69	119.52	109.96
1	A	298	GLU	CA-CB-CG	5.68	125.46	114.10
1	A	113	THR	CA-C-N	5.66	128.13	120.38
1	A	113	THR	C-N-CA	5.66	128.13	120.38
1	A	63	ARG	N-CA-C	5.61	119.25	110.32
1	A	288	ASN	CB-CG-OD1	-5.61	109.57	120.80
1	A	240	PHE	O-C-N	5.54	129.55	123.01
1	A	133	THR	CA-C-O	-5.54	113.96	120.60
1	A	241	GLU	CA-C-O	5.54	127.21	120.62
1	A	144	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	6	VAL	CA-C-O	-5.50	115.01	120.90
1	A	213	LYS	O-C-N	5.50	129.70	122.93
1	A	49	ILE	N-CA-C	5.48	115.79	108.11
1	A	80	GLU	CB-CG-CD	5.47	121.90	112.60
1	A	202	ILE	O-C-N	5.46	127.58	121.90
1	A	48	ASN	CA-C-O	-5.42	115.87	122.64
1	A	114	GLU	N-CA-CB	5.41	118.17	110.06
1	A	29	TYR	CA-C-O	5.39	126.20	120.10
1	A	167	GLU	CA-C-N	5.37	130.19	122.45
1	A	167	GLU	C-N-CA	5.37	130.19	122.45
1	A	3	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	A	24	VAL	N-CA-CB	5.34	116.80	110.55
1	A	242	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	121	GLY	CA-C-N	5.32	130.78	123.28
1	A	121	GLY	C-N-CA	5.32	130.78	123.28
1	A	268	GLY	N-CA-C	-5.32	106.35	112.73
1	A	295	ASP	O-C-N	5.31	129.27	123.27
1	A	294	HIS	CA-C-O	5.30	127.64	121.49
1	A	280	GLY	CA-C-O	-5.29	116.41	121.49
1	A	113	THR	CB-CA-C	5.29	119.84	110.85
1	A	208	GLY	CA-C-O	5.28	126.26	120.66
1	A	12	ASP	CA-CB-CG	5.27	117.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	CYS	CB-CA-C	-5.27	97.86	109.56
1	A	204	ARG	CA-C-O	-5.27	114.97	120.55
1	A	217	ILE	CB-CA-C	-5.26	103.30	110.77
1	A	60	ILE	N-CA-C	-5.25	108.39	113.53
1	A	261	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	269	ALA	CA-C-N	5.18	127.47	120.38
1	A	269	ALA	C-N-CA	5.18	127.47	120.38
1	A	88	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	A	221	ALA	CA-C-O	-5.14	114.90	120.81
1	A	61	ILE	N-CA-C	5.12	115.74	110.36
1	A	110	LYS	CA-C-N	5.11	127.84	120.38
1	A	110	LYS	C-N-CA	5.11	127.84	120.38
1	A	262	VAL	CB-CA-C	5.11	118.46	111.87
1	A	134	ASP	CA-C-N	5.09	130.59	122.74
1	A	134	ASP	C-N-CA	5.09	130.59	122.74
1	A	195	ASP	N-CA-C	-5.09	102.23	110.32
1	A	231	GLY	CA-C-N	5.06	127.33	120.65
1	A	231	GLY	C-N-CA	5.06	127.33	120.65
1	A	170	GLY	N-CA-C	-5.04	101.23	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2392	0	2394	51	0
2	A	16	0	11	0	0
3	A	2	0	0	0	0
4	A	54	0	24	0	0
5	A	70	0	0	1	0
All	All	2534	0	2429	51	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 10.

All (51) 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:45:ILE:HG23	1:A:84:LYS:HD2	1.53	0.88
1:A:107:GLN:HE21	1:A:300:LEU:HD13	1.40	0.86
1:A:78:THR:HG22	1:A:81:GLY:H	1.51	0.75
1:A:287:GLN:HB2	1:A:292:VAL:HG11	1.73	0.69
1:A:259:PHE:HB3	5:A:375:HOH:O	1.92	0.69
1:A:190:LEU:HD12	1:A:220:VAL:HG22	1.75	0.68
1:A:295:ASP:HB3	1:A:298:GLU:HG2	1.78	0.65
1:A:154:ARG:HG3	1:A:215:HIS:CE1	2.36	0.61
1:A:113:THR:HG21	1:A:281:GLY:N	2.17	0.60
1:A:1:MET:HE2	1:A:95:GLN:HB2	1.85	0.59
1:A:107:GLN:NE2	1:A:300:LEU:HD13	2.18	0.56
1:A:1:MET:HE2	1:A:95:GLN:CB	2.35	0.56
1:A:35:TYR:CZ	1:A:51:LYS:HG3	2.40	0.55
1:A:16:MET:O	1:A:19:ALA:HB3	2.07	0.55
1:A:206:LYS:O	1:A:210:GLU:HG3	2.08	0.54
1:A:84:LYS:O	1:A:88:GLN:HG2	2.09	0.53
1:A:198:MET:O	1:A:202:ILE:HG12	2.09	0.52
1:A:211:ARG:O	1:A:211:ARG:HD2	2.10	0.51
1:A:7:LEU:HB3	1:A:37:VAL:HB	1.92	0.51
1:A:80:GLU:HA	1:A:83:LYS:HD3	1.91	0.51
1:A:45:ILE:HD12	1:A:73:CYS:SG	2.50	0.51
1:A:113:THR:HG22	1:A:118:PRO:HA	1.93	0.50
1:A:32:VAL:HG21	1:A:276:LEU:HD21	1.94	0.50
1:A:230:PHE:O	1:A:234:ILE:HD12	2.12	0.50
1:A:19:ALA:O	1:A:23:VAL:HG23	2.13	0.49
1:A:200:ASP:O	1:A:204:ARG:HG3	2.13	0.49
1:A:27:ALA:HB3	1:A:34:VAL:CG2	2.43	0.48
1:A:128:ASN:OD1	1:A:135:PHE:HA	2.14	0.48
1:A:192:PRO:HD2	1:A:193:GLU:OE1	2.14	0.48
1:A:162:ARG:HG2	1:A:241:GLU:CG	2.44	0.47
1:A:75:GLU:O	1:A:81:GLY:HA3	2.15	0.47
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.78	0.46
1:A:120:VAL:HA	1:A:282:ARG:O	2.15	0.46
1:A:282:ARG:HB3	1:A:294:HIS:O	2.16	0.46
1:A:141:THR:HA	1:A:257:THR:HG23	1.98	0.45
1:A:128:ASN:HB2	1:A:139:PHE:CD2	2.52	0.45
1:A:312:TYR:CE1	1:A:316:LYS:HE3	2.52	0.44
1:A:63:ARG:HH11	1:A:63:ARG:HD2	1.64	0.43
1:A:165:VAL:O	1:A:244:VAL:HA	2.18	0.43
1:A:189:ILE:HG22	1:A:191:ILE:HG23	2.00	0.43
1:A:145:THR:O	1:A:148:ASP:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:HA	1:A:256:PRO:HD2	1.93	0.43
1:A:80:GLU:O	1:A:83:LYS:HB2	2.19	0.42
1:A:191:ILE:HB	1:A:192:PRO:CD	2.50	0.41
1:A:41:TYR:O	1:A:44:LEU:HB3	2.20	0.41
1:A:130:ILE:HA	1:A:131:PRO:HD3	1.75	0.41
1:A:53:GLU:HB2	1:A:56:ASP:OD1	2.21	0.41
1:A:214:LYS:HA	1:A:214:LYS:HD3	1.96	0.40
1:A:60:ILE:HA	1:A:63:ARG:HG3	2.03	0.40
1:A:38:TYR:O	1:A:39:HIS:HB2	2.21	0.40
1:A:144:ASN:O	1:A:148:ASP:HB2	2.22	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	317/319 (99%)	306 (96%)	11 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	244/247 (99%)	225 (92%)	19 (8%)	11	20

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ILE
1	A	7	LEU
1	A	48	ASN
1	A	59	ASP
1	A	72	ARG
1	A	75	GLU
1	A	77	LYS
1	A	105	SER
1	A	112	LEU
1	A	113	THR
1	A	187	GLU
1	A	216	SER
1	A	232	ARG
1	A	277	GLU
1	A	284	VAL
1	A	310	ARG
1	A	315	SER
1	A	320	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	107	GLN
1	A	233	GLN
1	A	294	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

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
4	ADP	A	326	3	28,29,29	0.96	1 (3%)	43,45,45	0.96	1 (2%)
4	ADP	A	324	3	28,29,29	1.29	2 (7%)	43,45,45	1.92	14 (32%)
2	F6P	A	323	-	15,16,16	1.24	2 (13%)	16,25,25	0.83	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
4	ADP	A	326	3	-	0/16/32/32	0/3/3/3
4	ADP	A	324	3	-	1/16/32/32	0/3/3/3
2	F6P	A	323	-	-	1/9/28/28	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	324	ADP	PA-O3A	4.59	1.64	1.59
2	A	323	F6P	O2-C2	2.57	1.45	1.40
4	A	326	ADP	C2-N1	2.46	1.38	1.33
2	A	323	F6P	O5-C2	2.17	1.47	1.43
4	A	324	ADP	C2-N1	2.04	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	324	ADP	O4'-C1'-N9	4.32	116.39	108.09
4	A	324	ADP	O2'-C2'-C3'	4.16	125.14	111.82
4	A	324	ADP	C4-N9-C1'	-3.67	118.04	126.63
4	A	324	ADP	O3B-PB-O2B	3.34	120.32	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	324	ADP	O5'-C5'-C4'	-3.26	97.88	108.99
4	A	324	ADP	C2'-C1'-N9	-3.08	105.64	113.30
4	A	324	ADP	O4'-C4'-C3'	-3.07	99.06	105.15
4	A	324	ADP	C1'-N9-C8	2.88	133.49	127.09
4	A	324	ADP	O4'-C4'-C5'	-2.82	100.30	109.33
4	A	324	ADP	O3'-C3'-C4'	2.62	118.60	111.08
4	A	324	ADP	O2A-PA-O5'	2.52	119.01	107.57
4	A	324	ADP	N9-C8-N7	-2.46	110.45	113.94
4	A	324	ADP	C5-C4-N3	2.37	129.98	126.72
4	A	324	ADP	C4-N9-C8	2.28	108.13	105.74
4	A	326	ADP	O5'-PA-O1A	2.11	117.31	108.94

There are no chirality outliers.

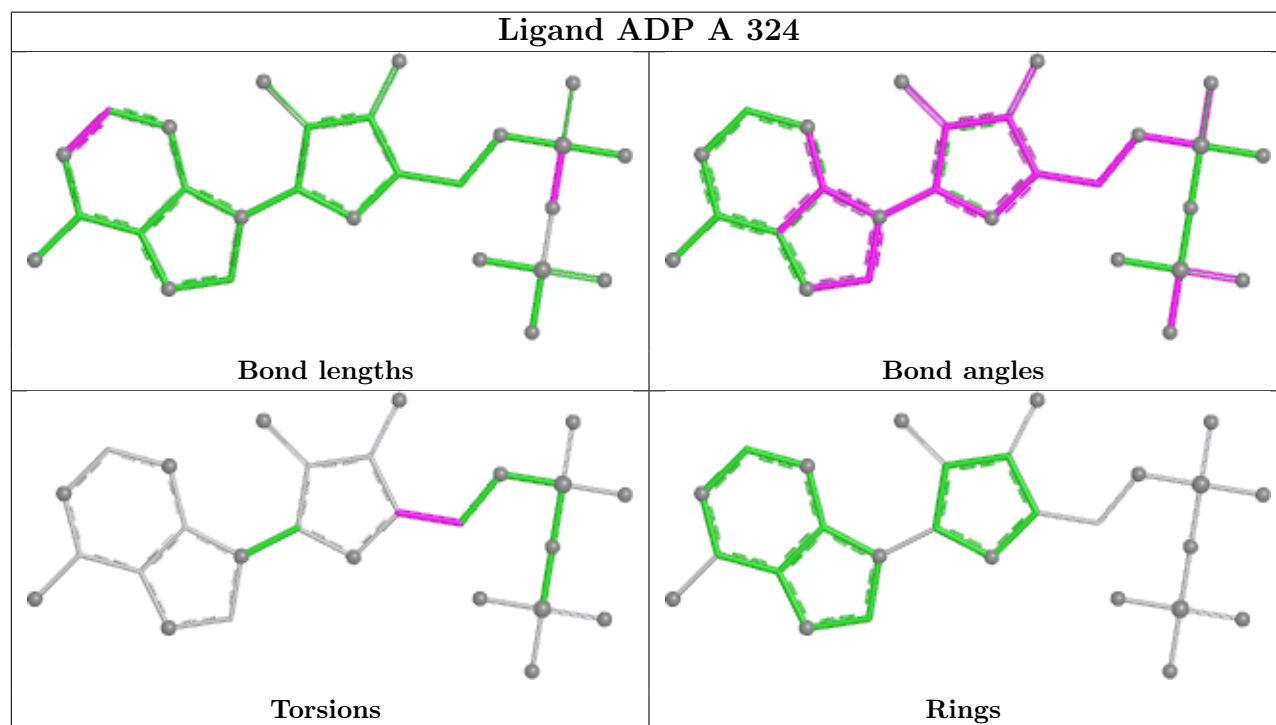
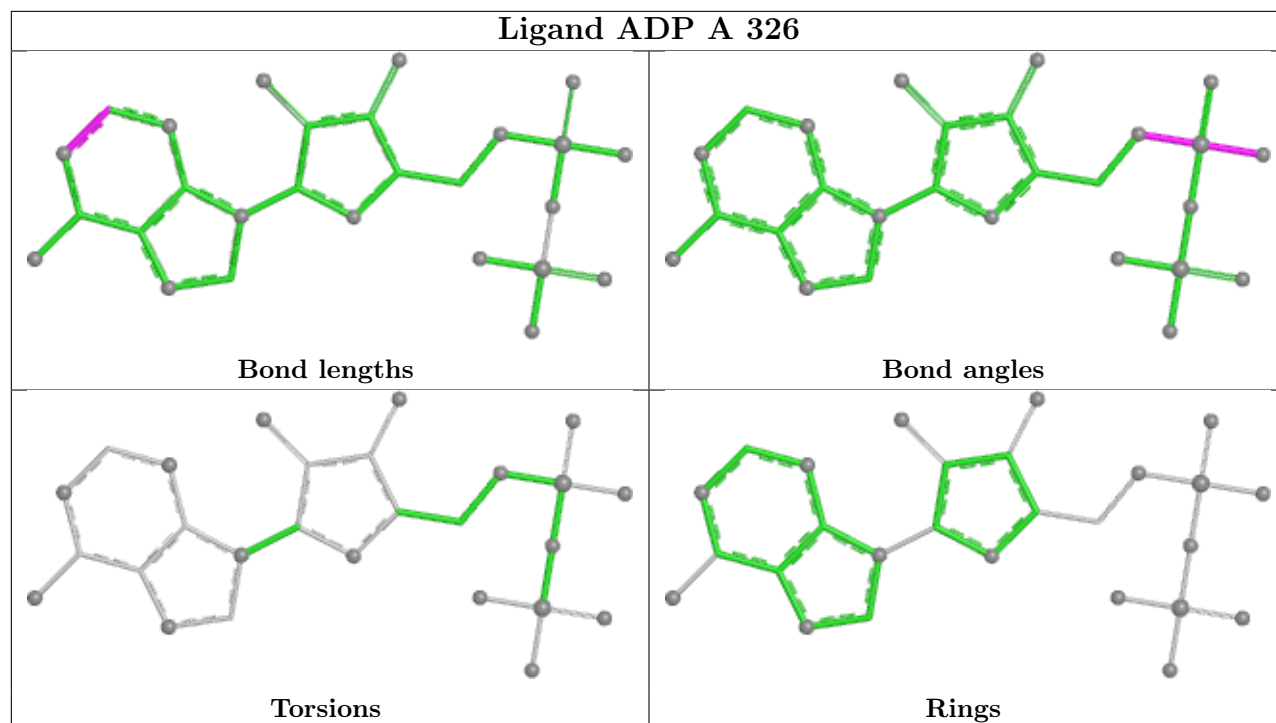
All (2) torsion outliers are listed below:

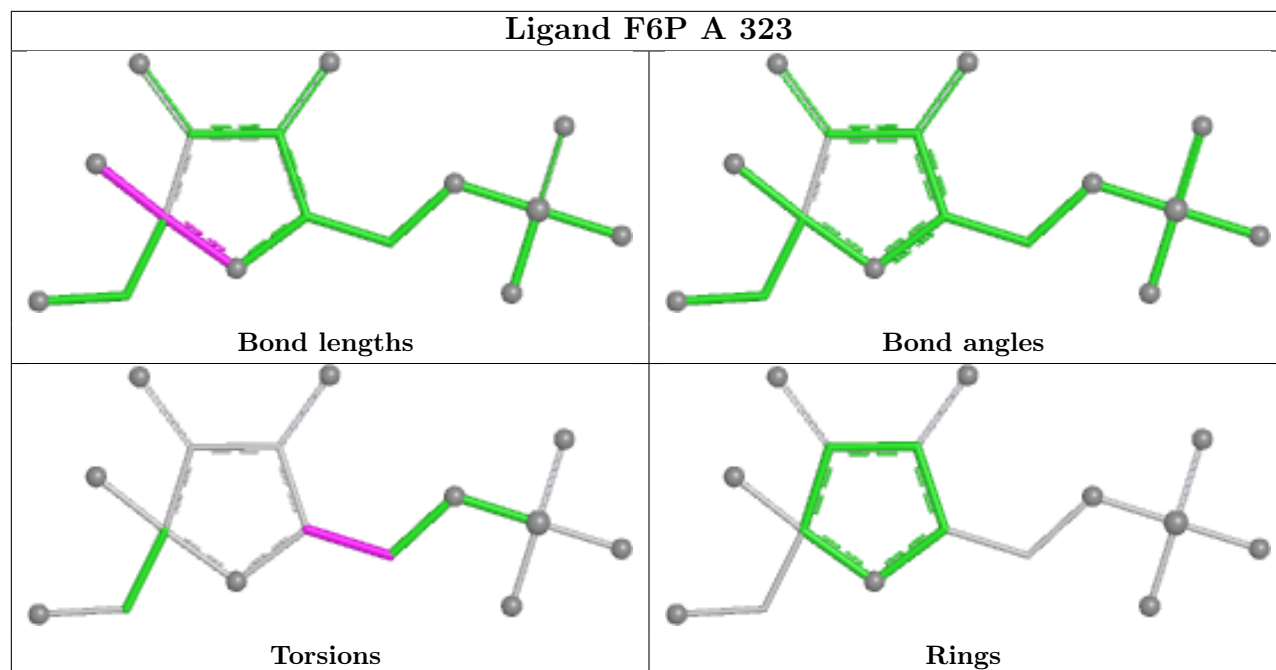
Mol	Chain	Res	Type	Atoms
2	A	323	F6P	C4-C5-C6-O6
4	A	324	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/319 (100%)	-0.43	1 (0%) 90 88	14, 41, 71, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

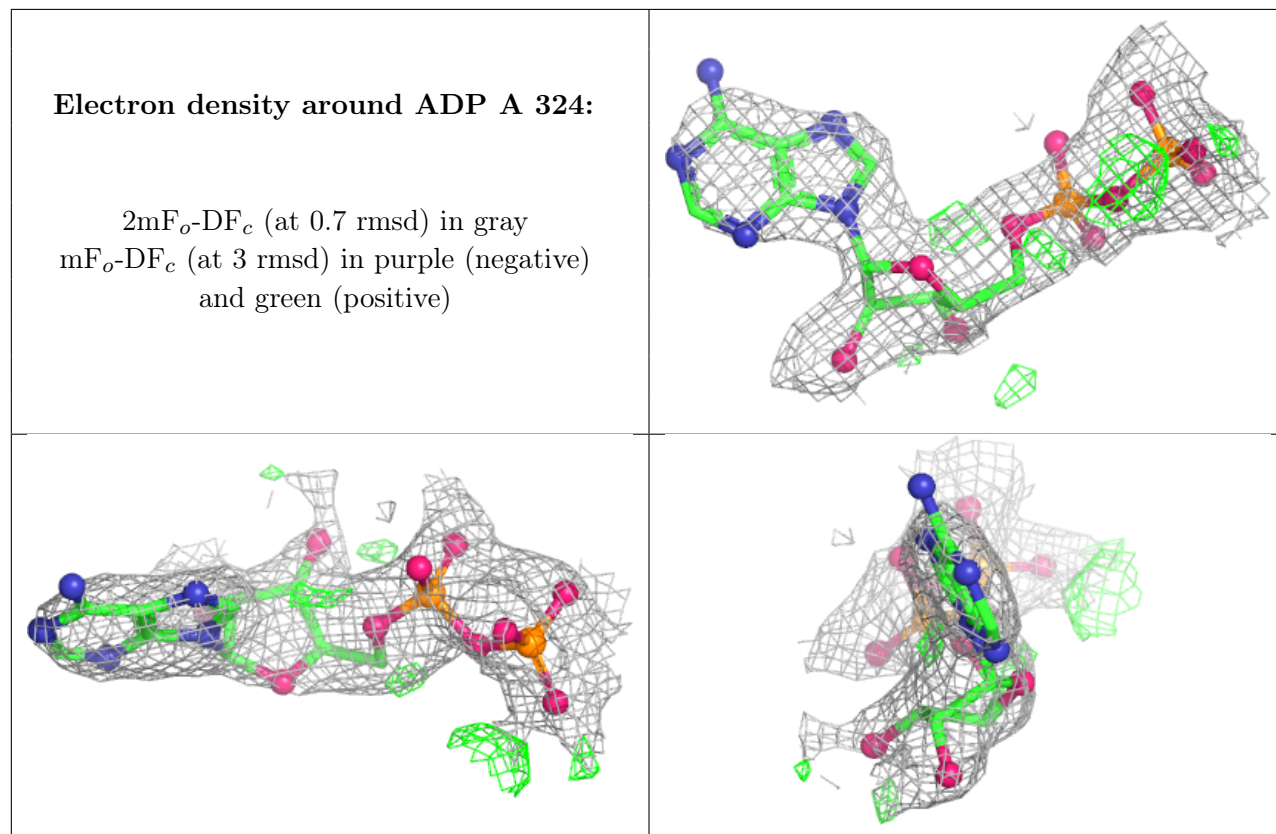
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	325	1/1	0.80	0.15	76,76,76,76	1
4	ADP	A	324	27/27	0.83	0.11	18,29,61,62	27
2	F6P	A	323	16/16	0.92	0.08	45,50,52,54	0
4	ADP	A	326	27/27	0.93	0.09	43,57,75,77	0
3	MG	A	327	1/1	0.96	0.07	35,35,35,35	0

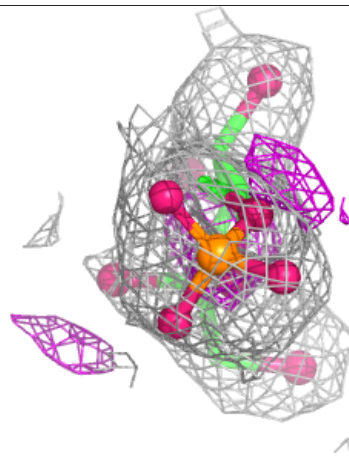
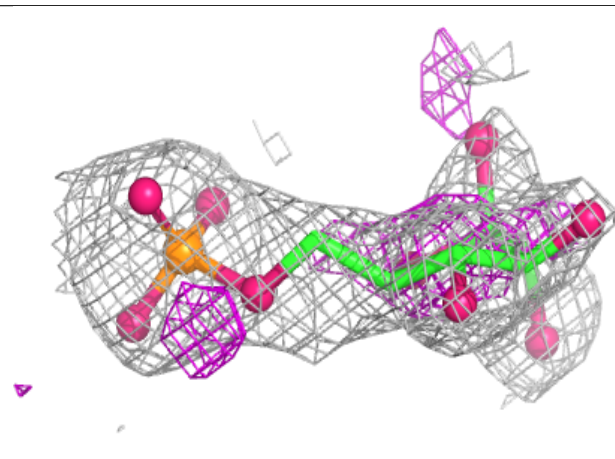
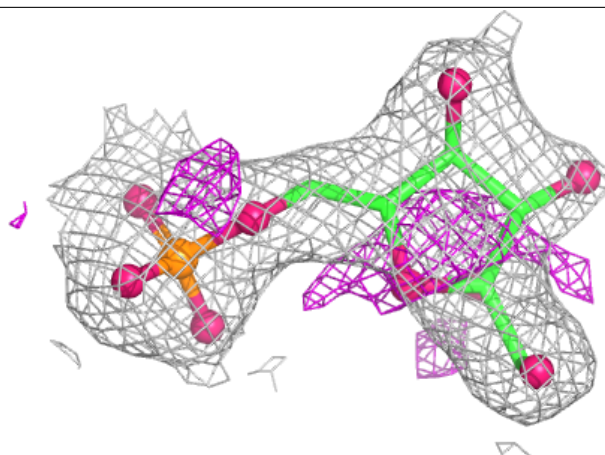
The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



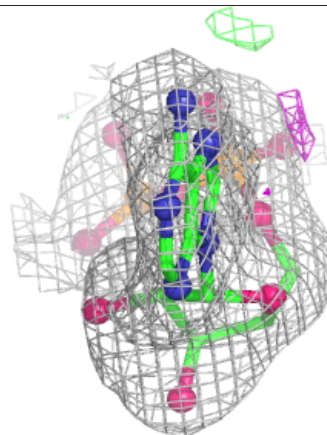
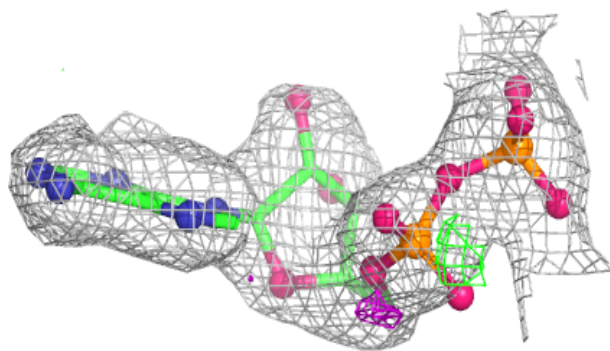
Electron density around F6P A 323:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 326:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.