



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:16 PM UTC

PDB ID : 4KS0 / pdb_00004ks0
Title : Pyruvate kinase (PYK) from Trypanosoma cruzi in the presence of Magnesium, oxalate and F26BP
Authors : Morgan, H.P.; Zhong, W.; McNae, I.W.; Michels, P.A.M.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on : 2013-05-17
Resolution : 2.80 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

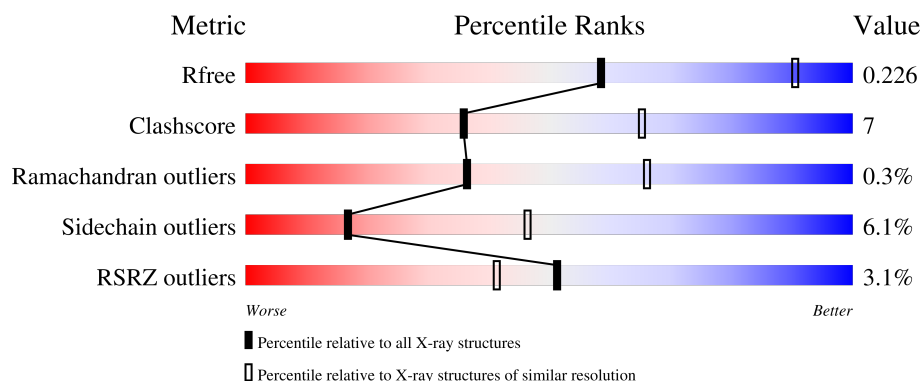
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	519	 3% 71% 17% • 10%
1	B	519	 2% 79% 16% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OXL	A	1003	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7727 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	2	0
			3591	2239	638	686	28			
1	B	499	Total	C	N	O	S	0	1	0
			3826	2392	674	732	28			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q4D9Z4
A	-18	GLY	-	expression tag	UNP Q4D9Z4
A	-17	SER	-	expression tag	UNP Q4D9Z4
A	-16	SER	-	expression tag	UNP Q4D9Z4
A	-15	HIS	-	expression tag	UNP Q4D9Z4
A	-14	HIS	-	expression tag	UNP Q4D9Z4
A	-13	HIS	-	expression tag	UNP Q4D9Z4
A	-12	HIS	-	expression tag	UNP Q4D9Z4
A	-11	HIS	-	expression tag	UNP Q4D9Z4
A	-10	HIS	-	expression tag	UNP Q4D9Z4
A	-9	SER	-	expression tag	UNP Q4D9Z4
A	-8	SER	-	expression tag	UNP Q4D9Z4
A	-7	GLY	-	expression tag	UNP Q4D9Z4
A	-6	LEU	-	expression tag	UNP Q4D9Z4
A	-5	VAL	-	expression tag	UNP Q4D9Z4
A	-4	PRO	-	expression tag	UNP Q4D9Z4
A	-3	ARG	-	expression tag	UNP Q4D9Z4
A	-2	GLY	-	expression tag	UNP Q4D9Z4
A	-1	SER	-	expression tag	UNP Q4D9Z4
A	0	HIS	-	expression tag	UNP Q4D9Z4
B	-19	MET	-	expression tag	UNP Q4D9Z4
B	-18	GLY	-	expression tag	UNP Q4D9Z4
B	-17	SER	-	expression tag	UNP Q4D9Z4
B	-16	SER	-	expression tag	UNP Q4D9Z4
B	-15	HIS	-	expression tag	UNP Q4D9Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q4D9Z4
B	-13	HIS	-	expression tag	UNP Q4D9Z4
B	-12	HIS	-	expression tag	UNP Q4D9Z4
B	-11	HIS	-	expression tag	UNP Q4D9Z4
B	-10	HIS	-	expression tag	UNP Q4D9Z4
B	-9	SER	-	expression tag	UNP Q4D9Z4
B	-8	SER	-	expression tag	UNP Q4D9Z4
B	-7	GLY	-	expression tag	UNP Q4D9Z4
B	-6	LEU	-	expression tag	UNP Q4D9Z4
B	-5	VAL	-	expression tag	UNP Q4D9Z4
B	-4	PRO	-	expression tag	UNP Q4D9Z4
B	-3	ARG	-	expression tag	UNP Q4D9Z4
B	-2	GLY	-	expression tag	UNP Q4D9Z4
B	-1	SER	-	expression tag	UNP Q4D9Z4
B	0	HIS	-	expression tag	UNP Q4D9Z4

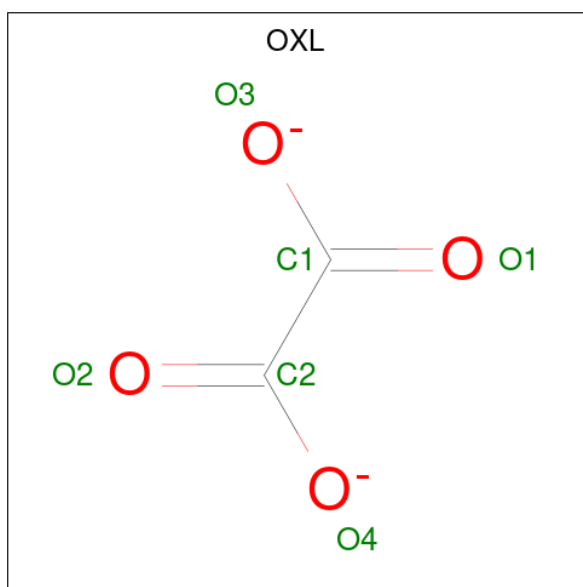
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

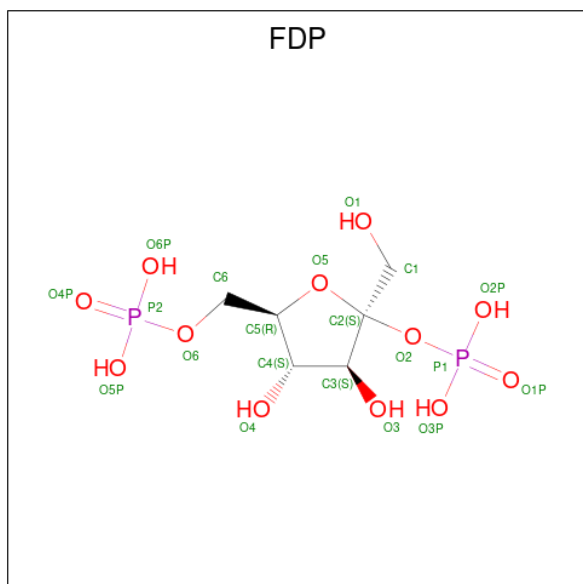
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0

- Molecule 4 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	2	4		
4	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 5 is 2,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FDP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			20	6	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	127	Total	O	0	0
			127	127		

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.77Å 173.77Å 211.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.87 – 2.80 55.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.87-2.80) 100.0 (55.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.216 0.188 , 0.226	Depositor DCC
R_{free} test set	2010 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7727	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.84	1/3649 (0.0%)	0.76	1/4927 (0.0%)
1	B	0.83	1/3887 (0.0%)	0.77	1/5250 (0.0%)
All	All	0.84	2/7536 (0.0%)	0.77	2/10177 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	HIS	CG-CD2	5.12	1.41	1.35
1	B	170	HIS	CG-CD2	5.03	1.41	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASN	N-CA-C	5.73	116.11	108.38
1	A	268	VAL	N-CA-C	-5.09	107.87	112.96

There are no chirality outliers.

There are no planarity outliers.

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	3591	0	3641	59	0
1	B	3826	0	3881	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	20	0	10	0	0
5	B	20	0	10	0	0
6	A	127	0	0	3	0
6	B	127	0	0	2	0
All	All	7727	0	7542	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360[A]:GLN:HE22	1:A:414:ARG:HB3	1.28	0.96
1:A:25:VAL:HG11	1:A:329:MET:HE2	1.48	0.96
1:A:92:THR:HG22	1:A:127:ILE:HG22	1.50	0.94
1:A:135:THR:HG23	1:A:183:CYS:SG	2.09	0.93
1:B:260:MET:HE2	1:B:329:MET:HE1	1.50	0.91
1:B:260:MET:CE	1:B:329:MET:HE1	2.07	0.83
1:A:241:GLU:HG2	1:A:262:ALA:HB3	1.65	0.76
1:A:471:VAL:HG21	1:A:477:MET:CE	2.19	0.73
1:A:260:MET:HE2	1:A:329:MET:HE1	1.71	0.72
1:B:360[B]:GLN:HE22	1:B:414:ARG:HB3	1.55	0.71
1:B:471:VAL:HG11	1:B:477:MET:HE2	1.73	0.70
1:A:134:ILE:O	1:A:134:ILE:CG2	2.42	0.68
1:A:341:ASN:O	1:A:345:GLN:HG3	1.95	0.67
1:B:453:ASN:O	1:B:454:LYS:HB2	1.93	0.67
1:A:138:PRO:HB3	1:A:154:LEU:O	1.95	0.67
1:A:378:GLU:HG2	1:A:489:TYR:HB2	1.75	0.66
1:A:135:THR:CG2	1:A:183:CYS:SG	2.82	0.66
1:A:131:ARG:O	1:A:135:THR:HB	1.97	0.65
1:A:144:ILE:HG23	1:A:178:CYS:HB3	1.79	0.65
1:A:198:LEU:O	1:A:202:VAL:HG23	1.96	0.65
1:A:134:ILE:O	1:A:134:ILE:HG22	1.96	0.64
1:B:224:ARG:HH21	1:B:224:ARG:HG3	1.62	0.64
1:B:86:LYS:HD3	1:B:193:LYS:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:C	1:A:454:LYS:HG2	2.23	0.63
1:B:25:VAL:HB	1:B:329:MET:HG3	1.81	0.62
1:B:300:LEU:HD23	1:B:313:GLU:HB3	1.82	0.61
1:B:471:VAL:HG21	1:B:477:MET:CE	2.30	0.61
1:B:260:MET:HE2	1:B:329:MET:CE	2.26	0.61
1:A:471:VAL:HG21	1:A:477:MET:HE2	1.83	0.61
1:B:173:THR:HB	1:B:176:LYS:HE2	1.85	0.58
1:B:215:ARG:HG2	1:B:244:GLN:HB2	1.85	0.58
1:B:260:MET:SD	1:B:329:MET:HE1	2.44	0.58
1:A:249:ILE:HG12	1:A:282:LEU:HD22	1.86	0.57
1:A:303:MET:HE2	1:A:309:PRO:HB3	1.86	0.57
1:A:156:LYS:HE2	1:A:158:ASP:O	2.05	0.56
1:A:294:ILE:HG12	1:A:327:CYS:HB2	1.88	0.56
1:B:453:ASN:HB3	1:B:455:GLU:HG3	1.87	0.56
1:A:145:ASP:O	1:A:148:VAL:HG23	2.07	0.55
1:A:27:THR:CG2	1:A:50:ARG:NH1	2.71	0.53
1:B:436:ARG:O	1:B:437:SER:HB2	2.08	0.53
1:A:218:GLU:H	1:A:218:GLU:CD	2.15	0.53
1:A:27:THR:HG21	1:A:50:ARG:NH1	2.24	0.53
1:B:95:PHE:CD2	1:B:100:ILE:HG12	2.44	0.52
1:B:224:ARG:HG3	1:B:224:ARG:NH2	2.23	0.52
1:A:249:ILE:CD1	1:A:282:LEU:HD22	2.41	0.51
1:A:294:ILE:HG21	1:A:329:MET:HE3	1.92	0.51
1:A:395:LYS:HB2	1:A:471:VAL:HG12	1.92	0.51
1:B:38:LEU:HD13	1:B:68:LEU:HA	1.92	0.51
1:B:331:SER:O	1:B:332:GLY:C	2.54	0.51
1:A:92:THR:HG22	1:A:127:ILE:CG2	2.34	0.51
1:A:133:SER:HB2	1:A:156:LYS:HE3	1.92	0.50
1:A:494:ARG:HD2	1:B:483:ASP:HB3	1.94	0.50
1:A:235:LEU:HA	1:A:257:ASP:OD2	2.12	0.49
1:A:244:GLN:HB2	6:A:1202:HOH:O	2.12	0.49
1:B:271:PRO:HB2	1:B:274:LYS:HG3	1.95	0.49
1:A:494:ARG:NH2	1:B:483:ASP:OD1	2.46	0.49
1:A:400:LEU:HD22	1:A:422:ALA:HB3	1.94	0.49
1:B:198:LEU:O	1:B:202:VAL:HG23	2.13	0.49
1:A:1:MET:HE3	6:A:1211:HOH:O	2.13	0.48
1:A:489:TYR:HB2	1:A:490:PRO:HD2	1.95	0.48
1:B:278:ALA:O	1:B:282:LEU:HG	2.14	0.48
1:A:51:MET:HG2	6:A:1112:HOH:O	2.14	0.48
1:B:400:LEU:HG	1:B:481:HIS:HB3	1.96	0.47
1:B:294:ILE:HG12	1:B:327:CYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:MET:HE1	1:B:346:TYR:CB	2.45	0.47
1:A:215:ARG:HD2	1:A:219:GLN:HE22	1.79	0.46
1:B:218:GLU:O	1:B:221:GLN:HB3	2.15	0.46
1:A:400:LEU:HG	1:A:481:HIS:HB3	1.98	0.46
1:A:249:ILE:CG1	1:A:282:LEU:HD22	2.45	0.46
1:B:249:ILE:HG12	1:B:282:LEU:HD22	1.98	0.45
1:A:168:ASN:OD1	1:A:168:ASN:N	2.50	0.45
1:B:477:MET:HE3	1:B:498:VAL:CG2	2.46	0.45
1:B:51:MET:HA	6:B:1127:HOH:O	2.16	0.45
1:B:116:PHE:HA	1:B:119:ILE:HD12	1.99	0.45
1:B:65:ILE:HG12	1:B:81:LEU:HD21	1.98	0.45
1:A:27:THR:CG2	1:A:50:ARG:HH11	2.30	0.45
1:A:151:LEU:HD23	1:A:166:VAL:HA	1.99	0.44
1:B:26:CYS:SG	1:B:46:MET:HB2	2.57	0.44
1:A:454:LYS:HG3	1:A:481:HIS:CE1	2.53	0.44
1:A:483:ASP:OD1	1:A:483:ASP:C	2.60	0.44
1:A:150:SER:O	1:A:151:LEU:HD23	2.18	0.44
1:B:86:LYS:NZ	6:B:1205:HOH:O	2.50	0.44
1:B:296:ALA:HB2	1:B:329:MET:HE3	2.01	0.43
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.86	0.43
1:A:83:LEU:C	1:A:83:LEU:HD23	2.44	0.42
1:B:102:LEU:O	1:B:169:ALA:HA	2.19	0.42
1:B:179:ASN:C	1:B:181:PRO:HD3	2.44	0.42
1:B:360[B]:GLN:NE2	1:B:414:ARG:O	2.53	0.42
1:A:62:GLN:HA	1:A:65:ILE:HD12	2.00	0.42
1:B:473:PRO:HA	1:B:498:VAL:O	2.19	0.42
1:A:23:ARG:O	1:A:327:CYS:HA	2.19	0.42
1:B:38:LEU:HD12	1:B:67:ASN:HB3	2.01	0.42
1:B:453:ASN:HB3	1:B:455:GLU:H	1.84	0.42
1:B:136:VAL:HG12	1:B:153:VAL:HG21	2.02	0.42
1:B:96:LYS:O	1:B:97:ASP:HB2	2.20	0.41
1:B:150:SER:HB3	1:B:167:ASN:HB2	2.02	0.41
1:B:453:ASN:O	1:B:454:LYS:CB	2.64	0.41
1:A:145:ASP:OD1	1:A:176:LYS:HD2	2.21	0.41
1:B:91:ARG:HA	1:B:176:LYS:O	2.21	0.41
1:A:329:MET:HG2	1:A:330:LEU:N	2.36	0.41
1:B:208:MET:HE2	1:B:208:MET:HB3	1.93	0.41
1:A:378:GLU:HG3	1:A:489:TYR:CD1	2.56	0.41
1:B:412:LYS:HD3	1:B:413:TYR:CE2	2.56	0.41
1:A:241:GLU:HG2	1:A:262:ALA:CB	2.44	0.40
1:A:297:THR:HG22	1:A:298:GLN:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASN:HD22	1:A:323:ASN:HA	1.67	0.40
1:A:404:GLY:O	1:A:405:ARG:C	2.64	0.40
1:B:221:GLN:OE1	1:B:221:GLN:HA	2.20	0.40
1:B:264:GLY:HA3	1:B:297:THR:HG21	2.03	0.40
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.94	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	464/519 (89%)	437 (94%)	25 (5%)	2 (0%)	30	60
1	B	498/519 (96%)	474 (95%)	23 (5%)	1 (0%)	43	72
All	All	962/1038 (93%)	911 (95%)	48 (5%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	THR
1	A	158	ASP
1	B	297	THR

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	397/437 (91%)	365 (92%)	32 (8%)	11	33
1	B	421/437 (96%)	403 (96%)	18 (4%)	26	60
All	All	818/874 (94%)	768 (94%)	50 (6%)	17	46

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	31	SER
1	A	132	LEU
1	A	133	SER
1	A	135	THR
1	A	137	ARG
1	A	161	THR
1	A	162	LEU
1	A	173	THR
1	A	183	CYS
1	A	184	GLU
1	A	218	GLU
1	A	225	GLU
1	A	229	GLU
1	A	230	LYS
1	A	232	LYS
1	A	303	MET
1	A	308	ARG
1	A	315	SER
1	A	365	ASN
1	A	369	LYS
1	A	373	LEU
1	A	378	GLU
1	A	405	ARG
1	A	426	MET
1	A	435	THR
1	A	450	GLU
1	A	452	GLU
1	A	467	LYS
1	A	468	LYS
1	A	494	ARG
1	A	499	SER
1	B	1	MET
1	B	96	LYS
1	B	119	ILE

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Mol	Chain	Res	Type
1	B	122	LYS
1	B	123	GLU
1	B	180	LEU
1	B	192	GLU
1	B	221	GLN
1	B	241	GLU
1	B	268	VAL
1	B	305	THR
1	B	365	ASN
1	B	372	LYS
1	B	373	LEU
1	B	399	VAL
1	B	405	ARG
1	B	467	LYS
1	B	485	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	33	GLN
1	A	167	ASN
1	A	219	GLN
1	B	19	HIS
1	B	243	HIS
1	B	247	GLN
1	B	306	ASN
1	B	345	GLN
1	B	492	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 4 are monoatomic - leaving 4 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	FDP	A	1004	-	19,20,20	0.96	1 (5%)	29,32,32	1.09	4 (13%)
4	OXL	A	1003	2	5,5,5	2.23	1 (20%)	6,6,6	2.06	2 (33%)
4	OXL	B	1003	2	5,5,5	2.22	1 (20%)	6,6,6	2.09	2 (33%)
5	FDP	B	1004	-	19,20,20	0.71	0	29,32,32	1.02	2 (6%)

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
5	FDP	A	1004	-	-	1/12/34/34	0/1/1/1
4	OXL	A	1003	2	-	4/4/4/4	-
4	OXL	B	1003	2	-	0/4/4/4	-
5	FDP	B	1004	-	-	5/12/34/34	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	OXL	C2-C1	-3.99	1.47	1.54
4	B	1003	OXL	C2-C1	-3.96	1.47	1.54
5	A	1004	FDP	P1-O2	3.12	1.65	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	OXL	O3-C1-C2	3.98	120.54	112.83
4	A	1003	OXL	O3-C1-C2	3.76	120.13	112.83
4	A	1003	OXL	O4-C2-C1	2.85	118.37	112.83
4	B	1003	OXL	O4-C2-C1	2.65	117.97	112.83
5	A	1004	FDP	O6P-P2-O5P	2.56	117.40	107.80
5	B	1004	FDP	O3P-P1-O2P	2.54	117.33	107.80
5	B	1004	FDP	O1-C1-C2	-2.31	103.84	111.54
5	A	1004	FDP	O3P-P1-O2P	2.27	116.31	107.80
5	A	1004	FDP	O5-C2-C1	2.15	113.18	107.94
5	A	1004	FDP	O5-C2-C3	-2.06	101.27	105.42

There are no chirality outliers.

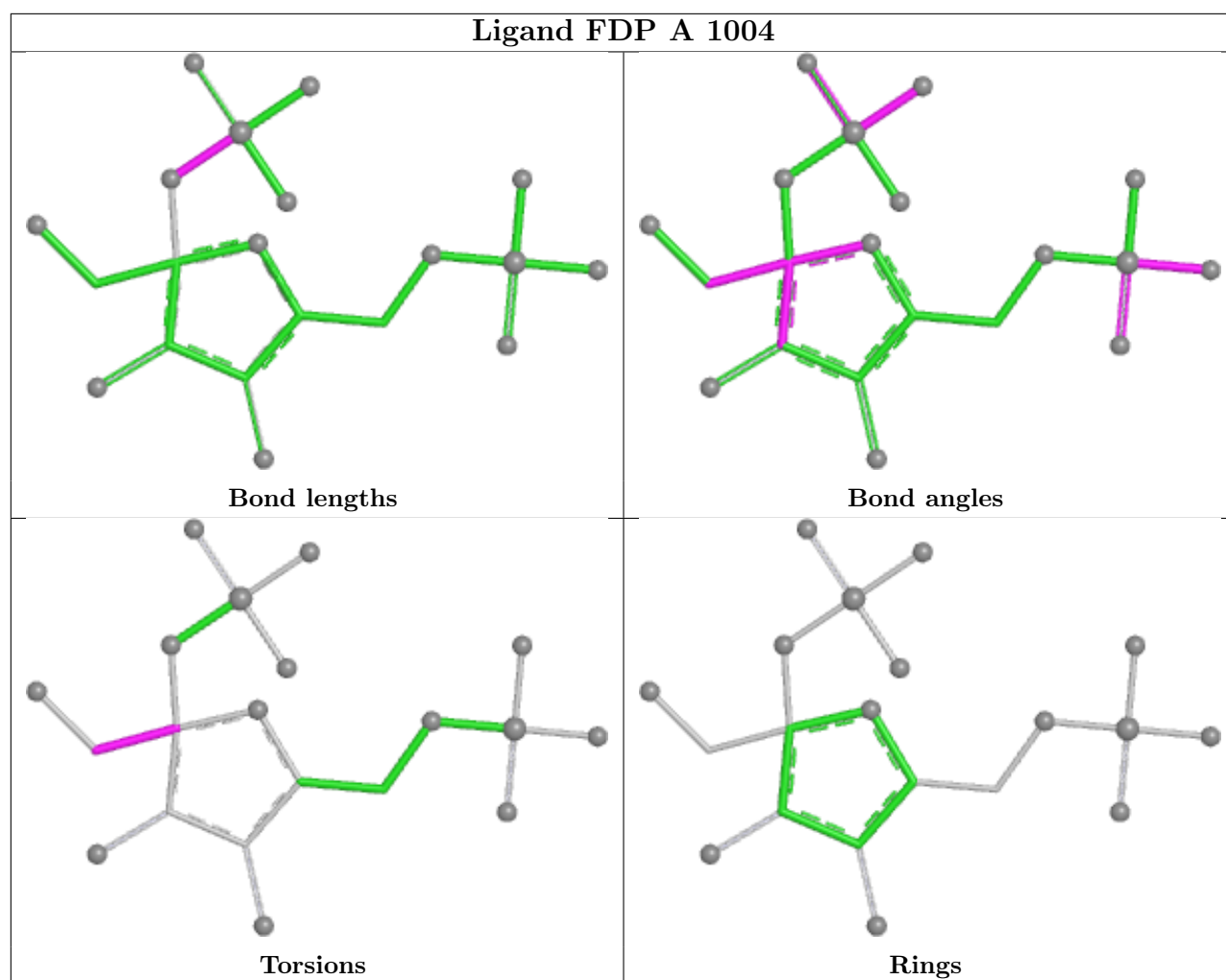
All (10) torsion outliers are listed below:

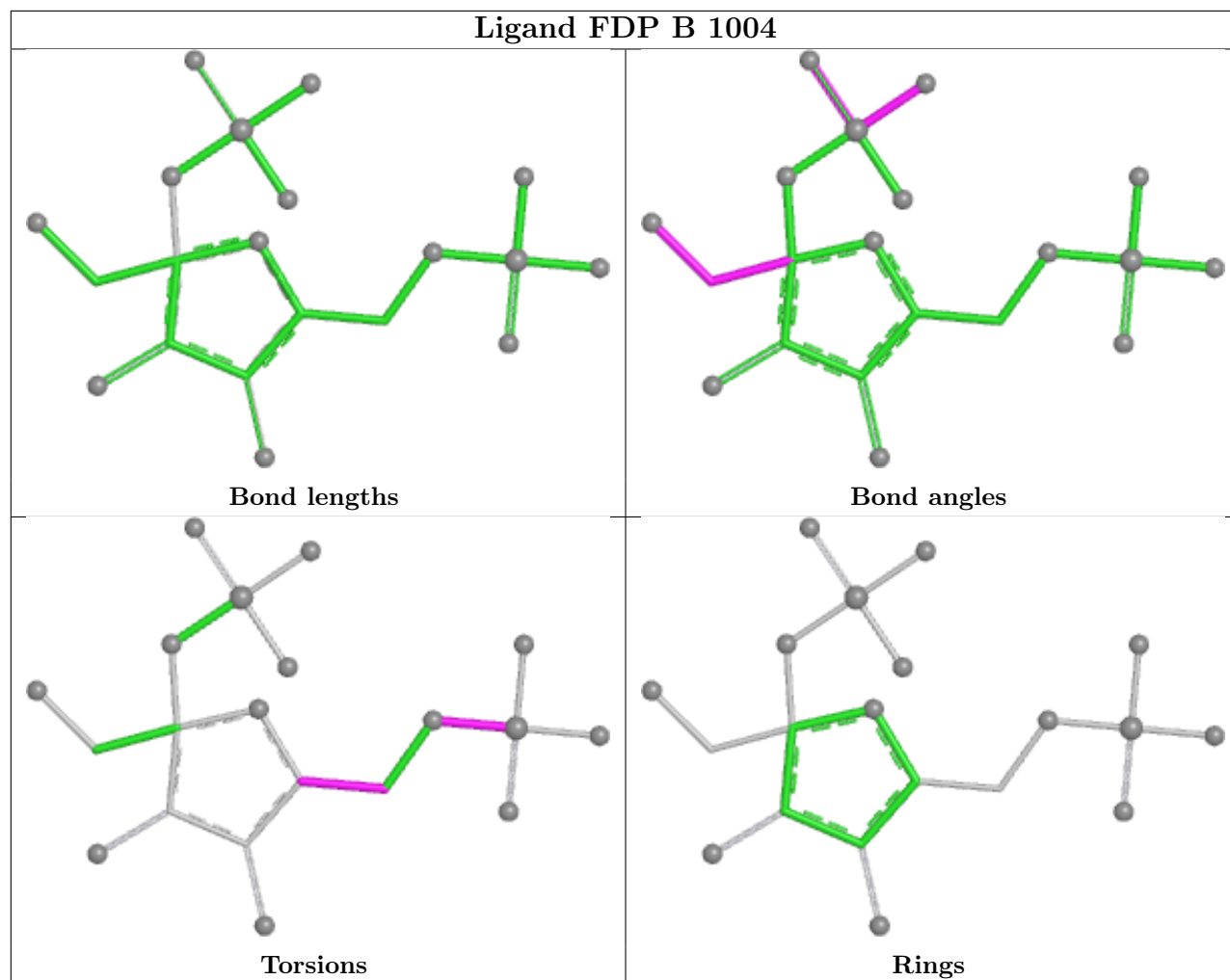
Mol	Chain	Res	Type	Atoms
5	B	1004	FDP	C6-O6-P2-O4P
5	B	1004	FDP	C6-O6-P2-O6P
5	B	1004	FDP	C4-C5-C6-O6
4	A	1003	OXL	O3-C1-C2-O4
4	A	1003	OXL	O1-C1-C2-O2
4	A	1003	OXL	O3-C1-C2-O2
4	A	1003	OXL	O1-C1-C2-O4
5	B	1004	FDP	O5-C5-C6-O6
5	B	1004	FDP	C6-O6-P2-O5P
5	A	1004	FDP	O1-C1-C2-C3

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	466/519 (89%)	-0.37	18 (3%) 43 34	22, 46, 136, 181	2 (0%)
1	B	499/519 (96%)	-0.11	12 (2%) 59 49	23, 46, 77, 105	1 (0%)
All	All	965/1038 (92%)	-0.24	30 (3%) 51 41	22, 46, 110, 181	3 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PHE	4.2
1	A	161	THR	3.9
1	A	160	TYR	3.7
1	A	126	TYR	3.7
1	B	119	ILE	3.0
1	A	92	THR	2.8
1	A	173	THR	2.7
1	A	154	LEU	2.6
1	A	172	LEU	2.6
1	A	134	ILE	2.6
1	B	173	THR	2.6
1	B	106	ASP	2.5
1	A	169	ALA	2.4
1	B	484	HIS	2.4
1	B	104	PRO	2.3
1	A	166	VAL	2.3
1	B	98	GLY	2.3
1	B	99	GLY	2.3
1	A	163	LYS	2.3
1	A	18	HIS	2.2
1	A	127	ILE	2.2
1	B	122	LYS	2.2
1	A	162	LEU	2.1
1	A	155	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	484	HIS	2.0
1	B	18	HIS	2.0
1	B	105	GLY	2.0
1	B	120	GLY	2.0
1	B	123	GLU	2.0
1	A	136	VAL	2.0

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](#)

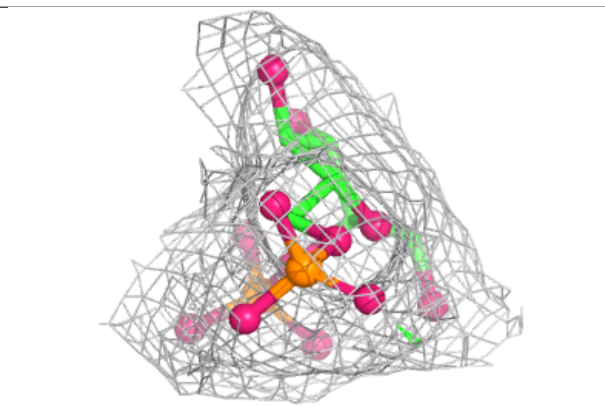
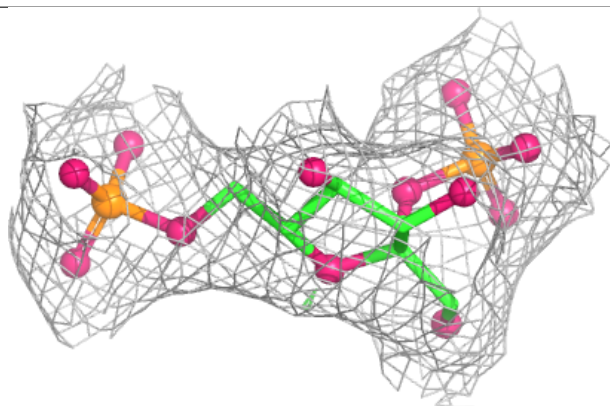
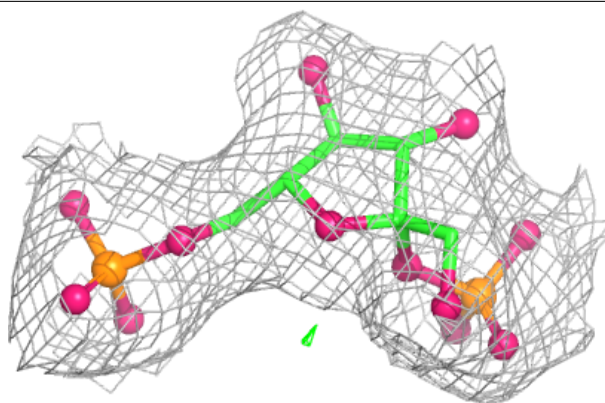
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OXL	A	1003	6/6	0.96	0.08	54,62,64,65	0
3	K	B	1002	1/1	0.97	0.07	52,52,52,52	0
4	OXL	B	1003	6/6	0.97	0.07	42,46,46,47	0
5	FDP	A	1004	20/20	0.98	0.05	26,39,45,47	0
2	MG	B	1001	1/1	0.99	0.03	44,44,44,44	0
3	K	A	1002	1/1	0.99	0.05	55,55,55,55	0
5	FDP	B	1004	20/20	0.99	0.04	32,39,45,46	0
2	MG	A	1001	1/1	1.00	0.02	35,35,35,35	0

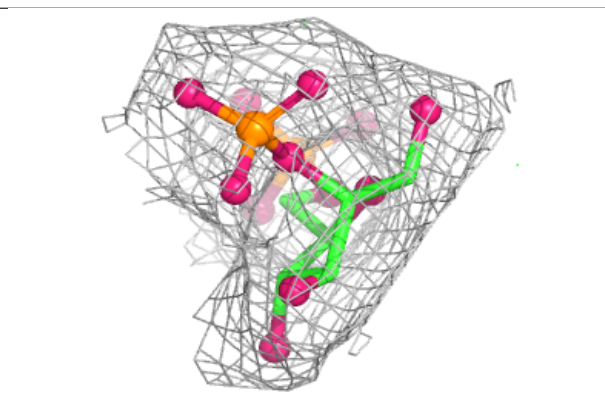
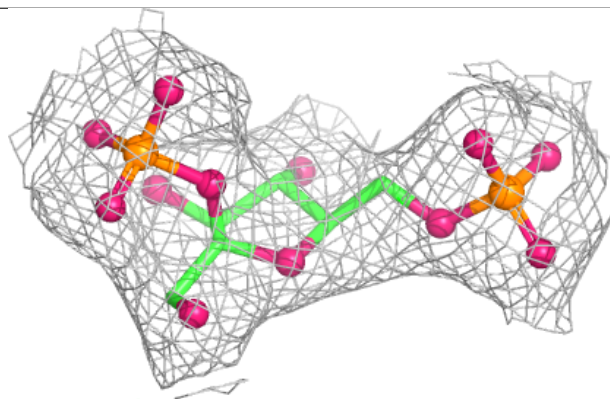
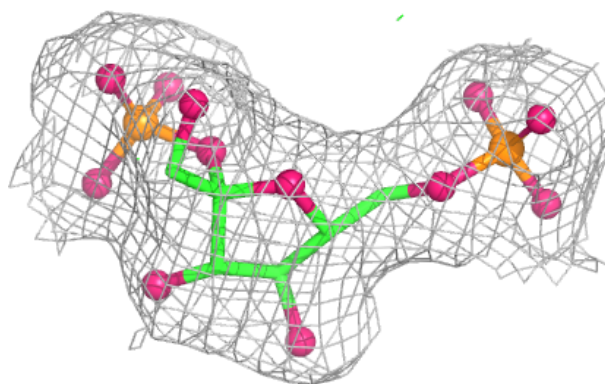
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDP A 1004:

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

**Electron density around FDP B 1004:**

$2mF_o - DF_c$ (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.