WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 01:48 am GMT

PDB ID	:	5LNW
Title	:	Crystal structure of Arabidopsis thaliana Pdx1-I320-G3P complex
Authors	:	Rodrigues, M.J.; Windeisen, V.; Zhang, Y.; Guedez, G.; Weber, S.; Strohmeier, M.; Hanes, J.W.; Royant, A.; Evans, G.; Sinning, I.; Ealick, S.E.; Begley, T.P.; Tews, I.
Deposited on	:	2016-08-06
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

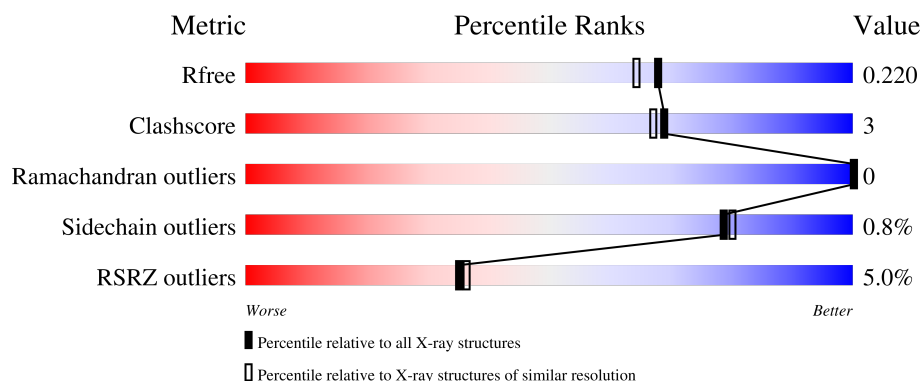|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.90 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		5.0%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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% 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	316	3% / 78% / 8% / 13%
1	B	316	5% / 79% / 7% / 14%
1	C	316	5% / 76% / 8% / 16%
1	D	316	4% / 75% / 8% / 17%

2　Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8862 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 Pyridoxal 5'-phosphate synthase subunit PDX1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2090	C 1304	N 383	O 385	S 18	0	4	0
1	B	272	Total 2069	C 1290	N 378	O 383	S 18	0	3	0
1	C	266	Total 2008	C 1256	N 370	O 365	S 17	0	2	0
1	D	262	Total 1999	C 1250	N 367	O 365	S 17	0	3	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	GLU	-	expression tag	UNP Q8L940
A	312	HIS	-	expression tag	UNP Q8L940
A	313	HIS	-	expression tag	UNP Q8L940
A	314	HIS	-	expression tag	UNP Q8L940
A	315	HIS	-	expression tag	UNP Q8L940
A	316	HIS	-	expression tag	UNP Q8L940
A	317	HIS	-	expression tag	UNP Q8L940
B	311	GLU	-	expression tag	UNP Q8L940
B	312	HIS	-	expression tag	UNP Q8L940
B	313	HIS	-	expression tag	UNP Q8L940
B	314	HIS	-	expression tag	UNP Q8L940
B	315	HIS	-	expression tag	UNP Q8L940
B	316	HIS	-	expression tag	UNP Q8L940
B	317	HIS	-	expression tag	UNP Q8L940
C	311	GLU	-	expression tag	UNP Q8L940
C	312	HIS	-	expression tag	UNP Q8L940
C	313	HIS	-	expression tag	UNP Q8L940
C	314	HIS	-	expression tag	UNP Q8L940
C	315	HIS	-	expression tag	UNP Q8L940
C	316	HIS	-	expression tag	UNP Q8L940
C	317	HIS	-	expression tag	UNP Q8L940

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	311	GLU	-	expression tag	UNP Q8L940
D	312	HIS	-	expression tag	UNP Q8L940
D	313	HIS	-	expression tag	UNP Q8L940
D	314	HIS	-	expression tag	UNP Q8L940
D	315	HIS	-	expression tag	UNP Q8L940
D	316	HIS	-	expression tag	UNP Q8L940
D	317	HIS	-	expression tag	UNP Q8L940

- Molecule 2 is [(2 {R},3 {R})-2,3-bis(oxidanyl)-3-[[(2 {S})-3-oxidanylidenepent-4-en-2-yl]amino]propyl] dihydrogen phosphate (three-letter code: K8P) (formula: $C_8H_{16}NO_7P$).
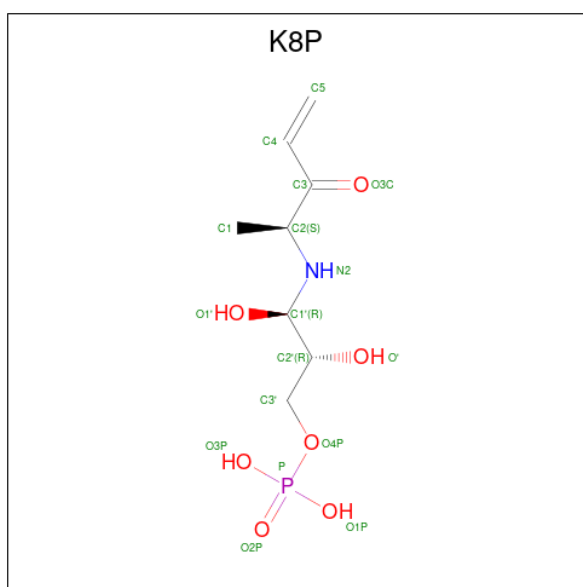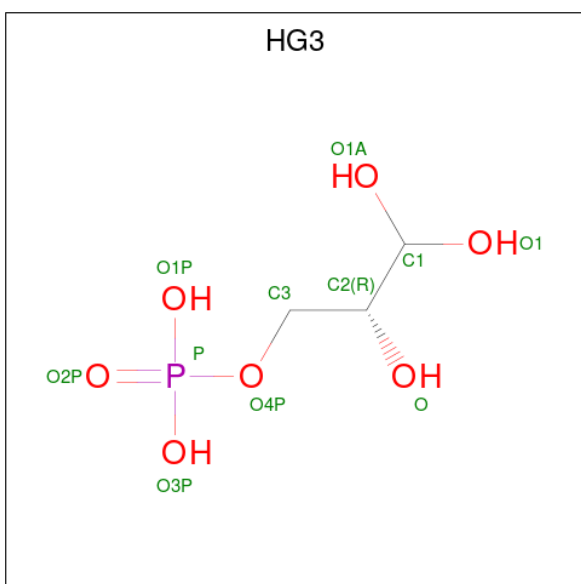

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total C N O P				0	0
			17 8 1 7 1					
2	B	1	Total C N O P				0	0
			17 8 1 7 1					
2	C	1	Total C N O P				0	0
			17 8 1 7 1					
2	D	1	Total C N O P				0	0
			17 8 1 7 1					

- Molecule 3 is 5-O-phosphono-beta-D-ribofuranose (three-letter code: RP5) (formula: $C_5H_{11}O_8P$).

RP5
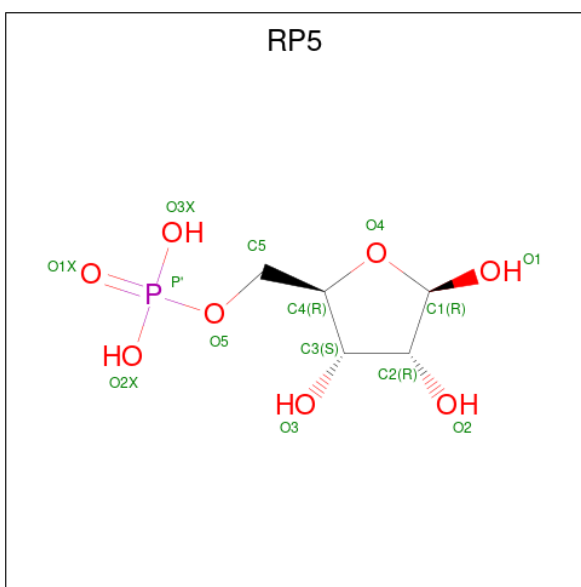
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 5	O 8	P 1	0	1
3	B	1	Total 14	C 5	O 8	P 1	0	1
3	C	1	Total 14	C 5	O 8	P 1	0	1
3	D	1	Total 14	C 5	O 8	P 1	0	1

- Molecule 4 is [(2 {R})-2,3,3-tris(oxidanyl)propyl] dihydrogen phosphate (three-letter code: HG3) (formula: $C_3H_9O_7P$).

HG3

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 11	C 3	O 7	P 1	0	1
4	B	1	Total 11	C 3	O 7	P 1	0	1
4	C	1	Total 11	C 3	O 7	P 1	0	1
4	D	1	Total 11	C 3	O 7	P 1	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
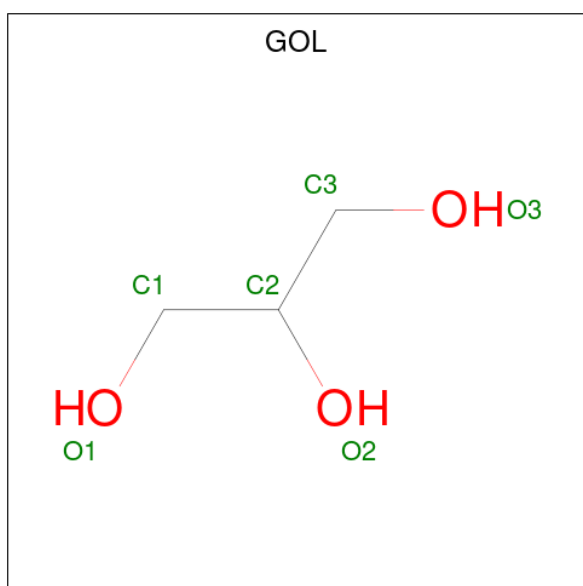
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

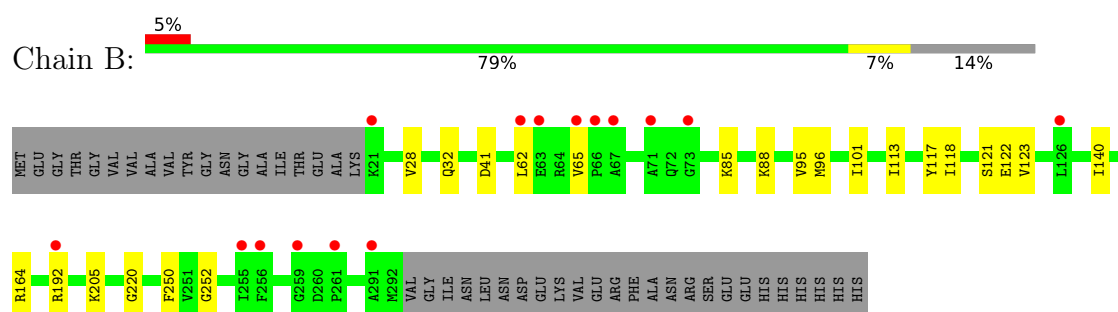| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total 135	O 135	0	0
6	B	139	Total 139	O 139	0	0
6	C	123	Total 123	O 123	0	0
6	D	119	Total 119	O 119	0	0

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.
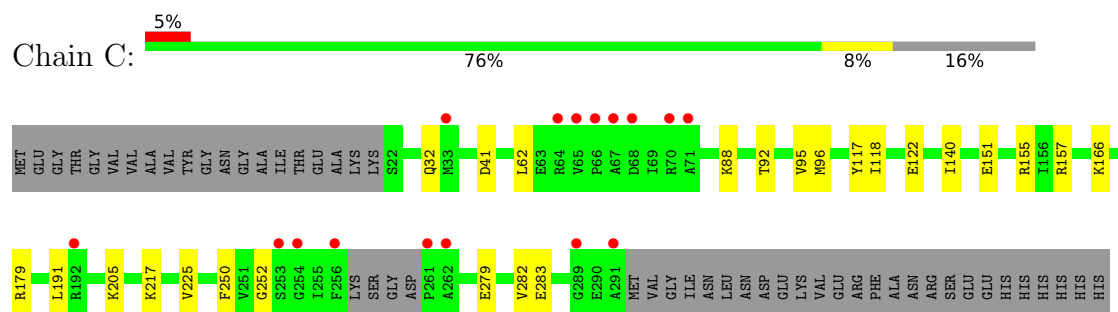
- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3
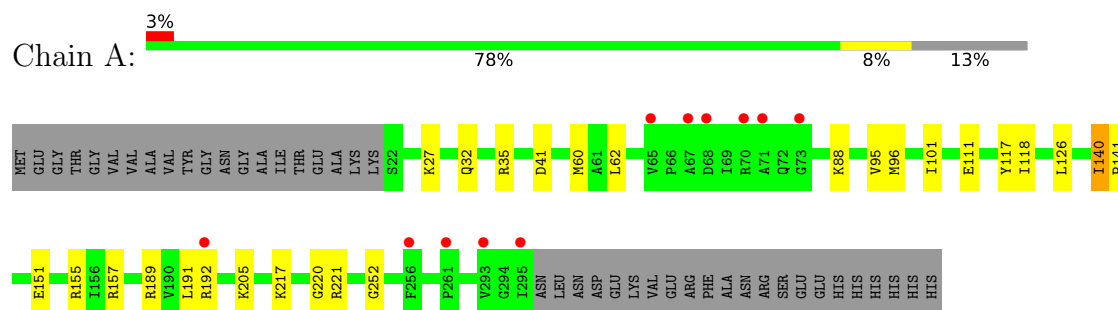
- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

- Molecule 1: Pyridoxal 5'-phosphate synthase subunit PDX1.3

MET GLU GLY THR GLY VAL VAL ALA VAL TYR GLY ASN GLY ALA ILE THR GLU ALA LYS LYS SER P23 D41 L62 E63 R64 V65 P66 A67 D68 A71 Q72 G73 A76 K88 V95 I101 I109 I113 I118 D119 E120 S121 E122 L126 E129 I140

V143 E151 R155 M162 L191 R192 K204 K217 F250 V251 G252 I255 F256 LYS SER GLY ASP P261 L288 GLY GLU ALA MET VAL GLY ILE ASN LEU ASN ASP GLU LYS VAL GLU ARG PHE ALA ASN ARG SER GLU GLU HIS HIS HIS HIS HIS HIS
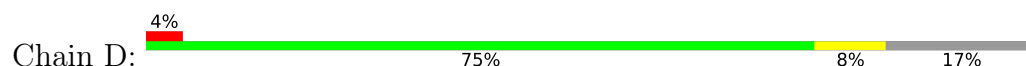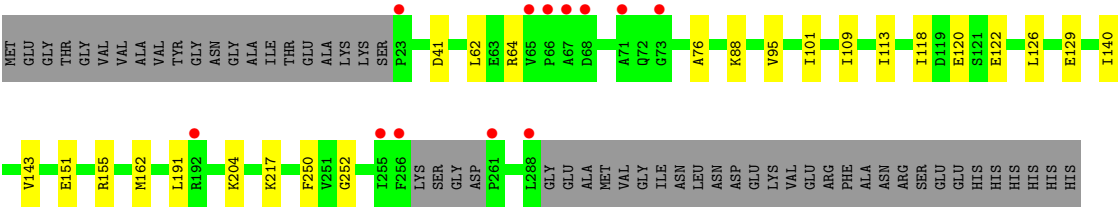
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	178.26Å 178.26Å 115.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.56 – 1.90 44.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.56-1.90) 99.4 (44.56-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.181 , 0.220 0.181 , 0.220	Depositor DCC
R_{free} test set	5462 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.007 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.004 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.013 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.005 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.003 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8862	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: K8P, HG3, GOL, RP5

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	0.37	0/2117	0.59	0/2853
1	B	0.36	0/2096	0.54	0/2826
1	C	0.35	0/2034	0.57	0/2743
1	D	0.37	0/2025	0.60	0/2729
All	All	0.36	0/8272	0.57	0/11151

There are no bond length outliers.

There are no bond angle outliers.

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	2090	0	2121	16	0
1	B	2069	0	2093	12	0
1	C	2008	0	2040	15	0
1	D	1999	0	2028	15	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	2	0
2	D	17	0	0	1	0
3	A	14	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	0	0	0
3	C	14	0	0	0	0
3	D	14	0	0	0	0
4	A	11	0	0	1	0
4	B	11	0	0	0	0
4	C	11	0	0	1	0
4	D	11	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	135	0	0	2	0
6	B	139	0	0	1	0
6	C	123	0	0	2	0
6	D	119	0	0	0	0
All	All	8862	0	8298	57	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 3.

All (57) 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:88:LYS:HA	1:A:95:VAL:HG21	1.80	0.64
1:A:118:ILE:HG13	1:A:140:ILE:HD11	1.82	0.59
1:B:96:MET:HG2	1:B:117:TYR:HB2	1.84	0.59
1:A:41:ASP:HB2	1:A:252:GLY:HA2	1.85	0.59
1:B:88:LYS:HA	1:B:95:VAL:HG21	1.86	0.57
1:C:88:LYS:HA	1:C:95:VAL:HG21	1.86	0.57
1:A:35:ARG:HH12	1:A:221:ARG:NH1	2.03	0.56
4:A:403[B]:HG3:O1P	1:D:204:LYS:NZ	2.39	0.55
1:A:96:MET:HG2	1:A:117:TYR:HB2	1.88	0.54
1:B:85:LYS:HE3	1:B:113:ILE:HG23	1.88	0.54
1:D:88:LYS:HA	1:D:95:VAL:HG21	1.91	0.53
1:D:143:VAL:HG22	1:D:162:MET:HB3	1.90	0.52
1:B:28:VAL:O	1:B:32:GLN:HG2	2.10	0.52
1:D:41:ASP:HB2	1:D:252:GLY:HA2	1.92	0.51
1:C:205:LYS:HD2	6:C:618:HOH:O	2.10	0.51
1:B:192[A]:ARG:HD2	1:B:220:GLY:HA2	1.93	0.51
1:C:279:GLU:O	1:C:283:GLU:HG2	2.12	0.50
1:B:41:ASP:HB2	1:B:252:GLY:HA2	1.94	0.50
1:C:118:ILE:HG13	1:C:140:ILE:HD11	1.94	0.50
1:D:109:ILE:O	1:D:113:ILE:HG13	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:NH2	6:A:503:HOH:O	2.44	0.49
1:A:205[B]:LYS:HD2	6:A:617:HOH:O	2.13	0.48
4:C:403[B]:HG3:O1P	6:C:501:HOH:O	2.17	0.48
1:D:122:GLU:H	1:D:122:GLU:CD	2.18	0.47
1:C:282:VAL:HG22	1:D:109:ILE:HG23	1.95	0.47
1:D:151:GLU:O	1:D:155:ARG:HG2	2.14	0.47
1:A:27:LYS:HB3	1:A:141:PRO:HB3	1.96	0.47
1:C:32:GLN:HA	1:C:225:VAL:HG21	1.97	0.47
1:D:118:ILE:HG13	1:D:140:ILE:HD11	1.97	0.46
1:B:118:ILE:HG13	1:B:140:ILE:HD11	1.98	0.46
1:C:96:MET:HG2	1:C:117:TYR:HB2	1.97	0.46
1:C:191:LEU:HG	1:C:217:LYS:HB2	1.98	0.46
1:B:205:LYS:HD2	6:B:622:HOH:O	2.16	0.46
1:B:122:GLU:H	1:B:122:GLU:CD	2.19	0.45
1:D:126[A]:LEU:HD21	1:D:129:GLU:HA	1.97	0.45
1:A:192[B]:ARG:HD3	1:A:220:GLY:CA	2.46	0.44
1:A:32:GLN:OE1	1:A:35:ARG:NH2	2.45	0.44
1:C:179:ARG:NH2	1:D:129:GLU:OE1	2.40	0.44
1:A:191:LEU:HG	1:A:217:LYS:HB2	2.00	0.44
1:B:101:ILE:HD11	1:B:122:GLU:HG3	2.00	0.44
1:C:157:ARG:HA	1:C:157:ARG:HD2	1.79	0.43
1:A:151:GLU:O	1:A:155:ARG:HG2	2.18	0.43
1:C:151:GLU:O	1:C:155:ARG:HG2	2.18	0.43
1:A:111:GLU:HG3	1:A:140:ILE:HG23	2.00	0.43
1:A:41:ASP:HA	1:A:60:MET:HB3	2.01	0.42
1:D:250:PHE:HB3	2:D:401:K8P:O'	2.18	0.42
1:B:121:SER:OG	1:B:123:VAL:HG22	2.19	0.42
1:D:64:ARG:HH11	1:D:76:ALA:HB2	1.84	0.42
1:B:164:ARG:HG2	1:B:250:PHE:CE1	2.55	0.42
1:D:101:ILE:HG12	1:D:120:GLU:HG2	2.02	0.41
1:A:101:ILE:HB	1:A:126[A]:LEU:HD23	2.01	0.41
1:C:122:GLU:H	1:C:122:GLU:CD	2.23	0.41
1:A:157:ARG:HA	1:A:157:ARG:HD2	1.89	0.41
1:C:41:ASP:HB2	1:C:252:GLY:HA2	2.02	0.41
1:C:250:PHE:HB3	2:C:401:K8P:O'	2.20	0.41
1:C:166:LYS:NZ	2:C:401:K8P:O3C	2.55	0.40
1:D:191:LEU:HG	1:D:217:LYS:HB2	2.03	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	276/316 (87%)	274 (99%)	2 (1%)	0	100	100
1	B	273/316 (86%)	270 (99%)	3 (1%)	0	100	100
1	C	264/316 (84%)	259 (98%)	5 (2%)	0	100	100
1	D	261/316 (83%)	257 (98%)	4 (2%)	0	100	100
All	All	1074/1264 (85%)	1060 (99%)	14 (1%)	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	215/246 (87%)	213 (99%)	2 (1%)	75	77
1	B	213/246 (87%)	211 (99%)	2 (1%)	75	77
1	C	205/246 (83%)	203 (99%)	2 (1%)	73	74
1	D	205/246 (83%)	204 (100%)	1 (0%)	86	88
All	All	838/984 (85%)	831 (99%)	7 (1%)	79	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	140	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	LEU
1	B	65	VAL
1	C	62	LEU
1	C	92	THR
1	D	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	82	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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	HG3	C	403[B]	-	10,10,10	0.86	0	12,14,14	0.69	0
3	RP5	C	402[A]	-	14,14,14	0.58	0	20,21,21	0.77	0
3	RP5	D	402[A]	-	14,14,14	0.62	0	20,21,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	RP5	A	402[A]	-	14,14,14	0.62	0	20,21,21	0.74	0
2	K8P	A	401	1	14,16,16	0.73	0	15,22,22	1.30	2 (13%)
5	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.35	0
2	K8P	C	401	1	14,16,16	0.77	0	15,22,22	1.32	2 (13%)
5	GOL	A	404	-	5,5,5	0.29	0	5,5,5	0.53	0
4	HG3	D	403[B]	-	10,10,10	0.87	0	12,14,14	0.64	0
4	HG3	B	403[B]	-	10,10,10	0.91	0	12,14,14	0.63	0
2	K8P	D	401	1	14,16,16	0.74	0	15,22,22	1.31	2 (13%)
4	HG3	A	403[B]	-	10,10,10	0.89	0	12,14,14	0.70	0
2	K8P	B	401	1	14,16,16	0.71	0	15,22,22	1.35	2 (13%)
3	RP5	B	402[A]	-	14,14,14	0.61	0	20,21,21	0.89	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	HG3	C	403[B]	-	-	0/10/10/10	-
3	RP5	C	402[A]	-	-	2/6/22/22	0/1/1/1
3	RP5	D	402[A]	-	-	5/6/22/22	0/1/1/1
3	RP5	A	402[A]	-	-	4/6/22/22	0/1/1/1
2	K8P	A	401	1	-	9/17/20/20	-
5	GOL	B	404	-	-	4/4/4/4	-
2	K8P	C	401	1	-	9/17/20/20	-
5	GOL	A	404	-	-	0/4/4/4	-
4	HG3	D	403[B]	-	-	1/10/10/10	-
4	HG3	B	403[B]	-	-	0/10/10/10	-
2	K8P	D	401	1	-	9/17/20/20	-
4	HG3	A	403[B]	-	-	1/10/10/10	-
2	K8P	B	401	1	-	9/17/20/20	-
3	RP5	B	402[A]	-	-	2/6/22/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	K8P	C1-C2-N2	2.97	115.14	108.85
2	D	401	K8P	C1-C2-N2	2.74	114.64	108.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	K8P	C1-C2-N2	2.72	114.60	108.85
2	A	401	K8P	P-O4P-C3'	2.60	125.46	118.30
2	B	401	K8P	P-O4P-C3'	2.59	125.44	118.30
2	C	401	K8P	P-O4P-C3'	2.59	125.42	118.30
2	D	401	K8P	P-O4P-C3'	2.57	125.39	118.30
2	A	401	K8P	C1-C2-N2	2.30	113.71	108.85

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	K8P	C1'-C2'-C3'-O4P
2	A	401	K8P	O'-C2'-C3'-O4P
2	A	401	K8P	C3'-O4P-P-O1P
2	A	401	K8P	C3'-O4P-P-O3P
2	B	401	K8P	C1'-C2'-C3'-O4P
2	B	401	K8P	O'-C2'-C3'-O4P
2	B	401	K8P	C3'-O4P-P-O1P
2	B	401	K8P	C3'-O4P-P-O3P
2	C	401	K8P	C1'-C2'-C3'-O4P
2	C	401	K8P	O'-C2'-C3'-O4P
2	C	401	K8P	C3'-O4P-P-O2P
2	C	401	K8P	C3'-O4P-P-O1P
2	C	401	K8P	C3'-O4P-P-O3P
2	D	401	K8P	C1'-C2'-C3'-O4P
2	D	401	K8P	O'-C2'-C3'-O4P
2	D	401	K8P	C3'-O4P-P-O2P
2	D	401	K8P	C3'-O4P-P-O1P
2	D	401	K8P	C3'-O4P-P-O3P
3	A	402[A]	RP5	C5-O5-P'-O1X
3	A	402[A]	RP5	C5-O5-P'-O2X
3	A	402[A]	RP5	C5-O5-P'-O3X
3	B	402[A]	RP5	C5-O5-P'-O2X
3	B	402[A]	RP5	C5-O5-P'-O3X
3	C	402[A]	RP5	C5-O5-P'-O1X
3	D	402[A]	RP5	C5-O5-P'-O1X
3	D	402[A]	RP5	C5-O5-P'-O2X
3	D	402[A]	RP5	C5-O5-P'-O3X
5	B	404	GOL	O1-C1-C2-O2
5	B	404	GOL	O1-C1-C2-C3
2	A	401	K8P	C3'-O4P-P-O2P
2	B	401	K8P	C3'-O4P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	402[A]	RP5	C3-C4-C5-O5
2	A	401	K8P	C2'-C3'-O4P-P
2	D	401	K8P	C2'-C3'-O4P-P
2	A	401	K8P	C1-C2-N2-C1'
2	B	401	K8P	C1-C2-N2-C1'
2	C	401	K8P	C1-C2-N2-C1'
2	D	401	K8P	C1-C2-N2-C1'
3	C	402[A]	RP5	C5-O5-P'-O2X
2	B	401	K8P	C2'-C3'-O4P-P
2	C	401	K8P	C2'-C3'-O4P-P
2	A	401	K8P	C3-C2-N2-C1'
2	A	401	K8P	N2-C2-C3-O3C
2	B	401	K8P	C3-C2-N2-C1'
2	B	401	K8P	N2-C2-C3-O3C
2	C	401	K8P	C3-C2-N2-C1'
2	C	401	K8P	N2-C2-C3-O3C
2	D	401	K8P	C3-C2-N2-C1'
2	D	401	K8P	N2-C2-C3-O3C
3	D	402[A]	RP5	O4-C4-C5-O5
5	B	404	GOL	O2-C2-C3-O3
5	B	404	GOL	C1-C2-C3-O3
4	D	403[B]	HG3	O1-C1-C2-C3
3	A	402[A]	RP5	C3-C4-C5-O5
4	A	403[B]	HG3	C3-O4P-P-O3P

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403[B]	HG3	1	0
2	C	401	K8P	2	0
2	D	401	K8P	1	0
4	A	403[B]	HG3	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 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 K8P A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand K8P C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand K8P D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand K8P B 401

Bond lengths

Bond angles

Torsions

Rings
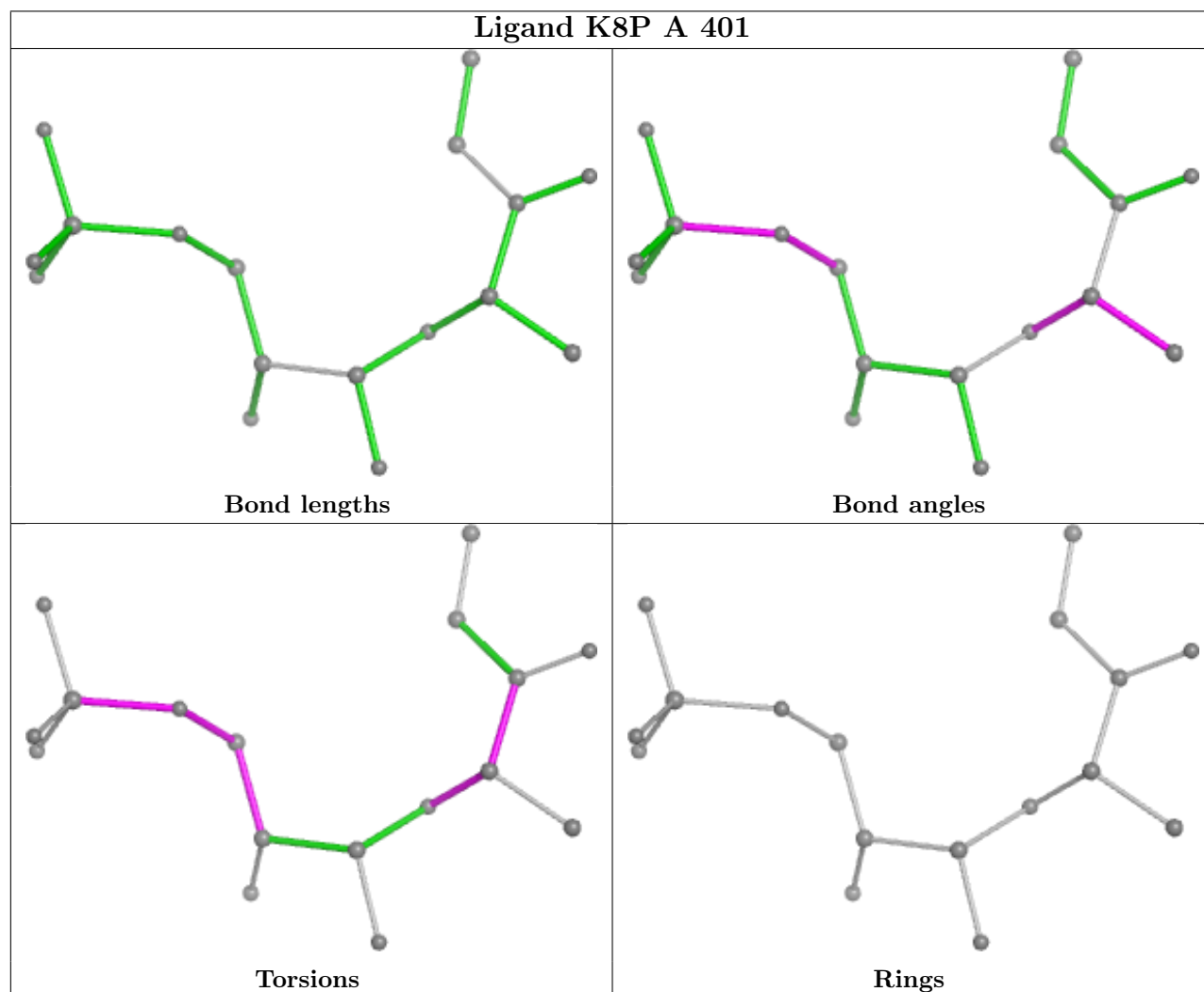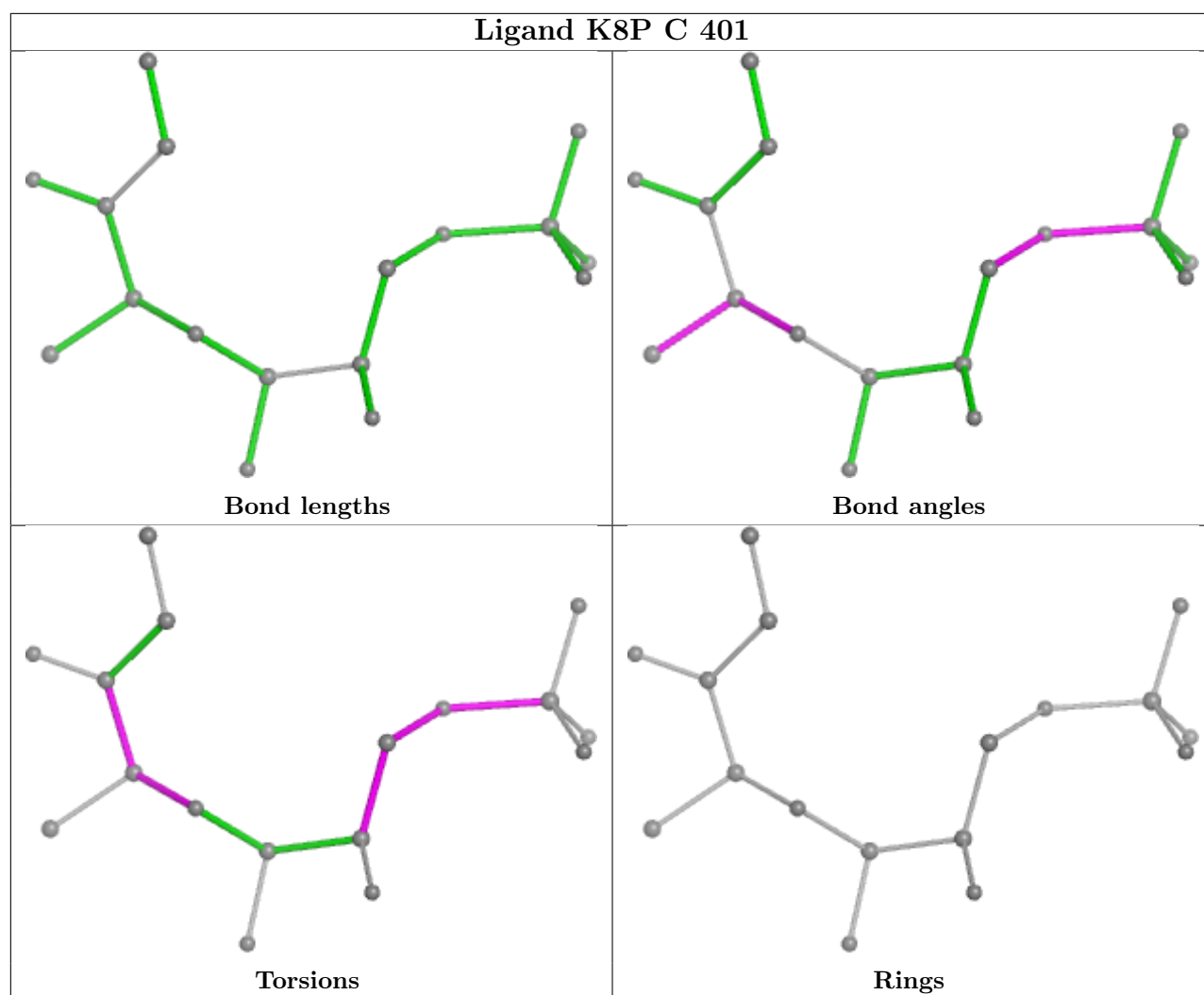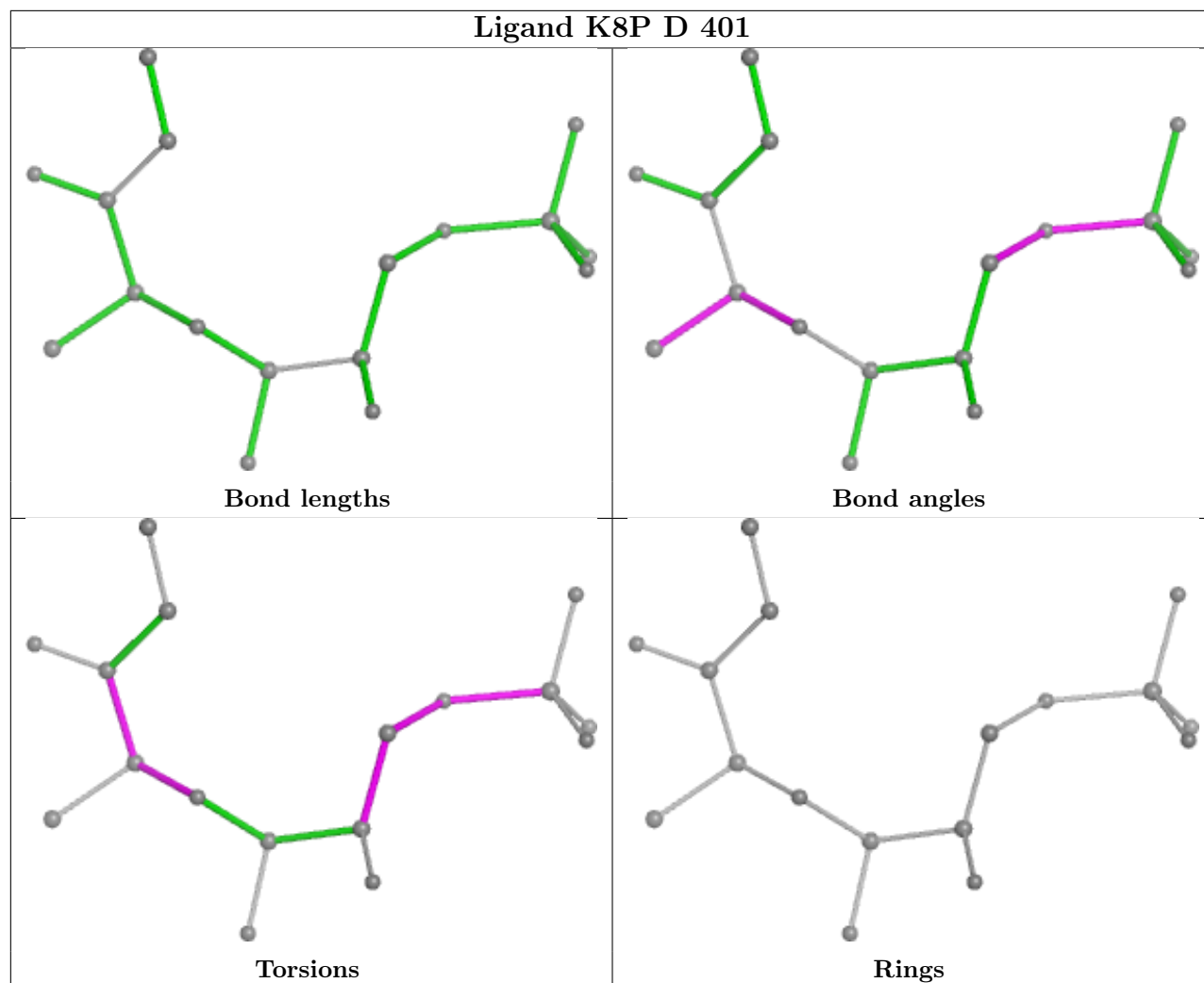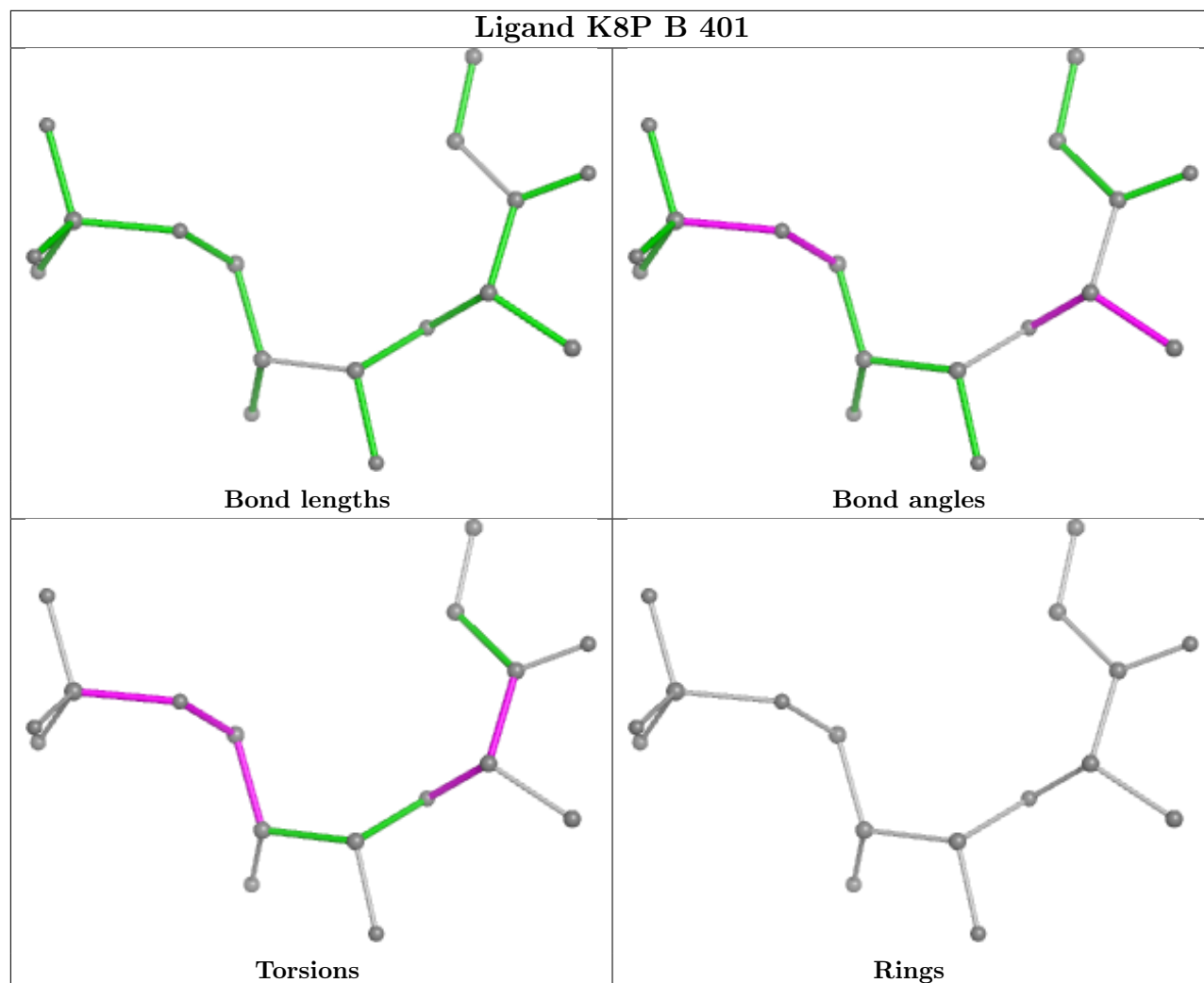
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	274/316 (86%)	-0.19	11 (4%)	43	44	12, 27, 59, 76	4 (1%)
1	B	272/316 (86%)	-0.12	15 (5%)	32	33	15, 30, 60, 86	3 (1%)
1	C	266/316 (84%)	-0.01	16 (6%)	29	30	12, 33, 64, 88	2 (0%)
1	D	262/316 (82%)	-0.03	12 (4%)	38	39	13, 30, 61, 78	3 (1%)
All	All	1074/1264 (84%)	-0.09	54 (5%)	35	36	12, 30, 62, 88	12 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	261	PRO	8.2
1	C	256	PHE	5.2
1	D	67	ALA	5.1
1	B	65	VAL	5.1
1	A	67	ALA	5.1
1	B	67	ALA	4.9
1	D	66	PRO	4.8
1	D	261	PRO	4.8
1	B	256	PHE	4.2
1	D	65	VAL	4.1
1	C	65	VAL	4.0
1	C	67	ALA	4.0
1	A	65	VAL	3.7
1	C	71	ALA	3.7
1	A	295	ILE	3.6
1	A	293	VAL	3.6
1	D	71	ALA	3.5
1	C	66	PRO	3.4
1	D	73	GLY	3.3
1	D	255	ILE	3.3
1	B	192[A]	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	262	ALA	3.1
1	A	68	ASP	3.1
1	C	291	ALA	3.0
1	D	256	PHE	3.0
1	B	259	GLY	2.9
1	C	289	GLY	2.9
1	A	256	PHE	2.8
1	D	23	PRO	2.8
1	C	253	SER	2.8
1	B	261	PRO	2.7
1	D	68	ASP	2.7
1	B	21	LYS	2.7
1	C	192[A]	ARG	2.7
1	B	73	GLY	2.6
1	D	288	LEU	2.6
1	B	71	ALA	2.5
1	B	66	PRO	2.4
1	C	68	ASP	2.4
1	A	73	GLY	2.4
1	C	70	ARG	2.3
1	C	33	MET	2.3
1	A	261	PRO	2.3
1	B	126[A]	LEU	2.3
1	B	291	ALA	2.2
1	A	70	ARG	2.2
1	B	62	LEU	2.2
1	B	255	ILE	2.2
1	C	64	ARG	2.2
1	B	63	GLU	2.1
1	A	192[A]	ARG	2.1
1	A	71	ALA	2.1
1	D	192[A]	ARG	2.1
1	C	254	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
5	GOL	A	404	6/6	0.81	0.17	52,61,61,65	0
5	GOL	B	404	6/6	0.86	0.15	57,63,67,67	0
2	K8P	D	401	17/17	0.92	0.11	34,51,58,60	0
2	K8P	C	401	17/17	0.93	0.11	32,49,57,62	0
2	K8P	A	401	17/17	0.94	0.11	28,46,58,59	0
2	K8P	B	401	17/17	0.94	0.10	29,41,57,61	0
3	RP5	C	402[A]	14/14	0.96	0.09	29,37,43,45	14
4	HG3	C	403[B]	11/11	0.96	0.07	29,34,42,45	11
3	RP5	A	402[A]	14/14	0.96	0.09	20,39,48,48	14
3	RP5	B	402[A]	14/14	0.96	0.09	24,33,40,41	14
4	HG3	D	403[B]	11/11	0.97	0.07	28,37,45,47	11
4	HG3	B	403[B]	11/11	0.97	0.08	24,33,40,41	11
3	RP5	D	402[A]	14/14	0.97	0.08	28,40,45,47	14
4	HG3	A	403[B]	11/11	0.98	0.06	24,31,48,48	11

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.
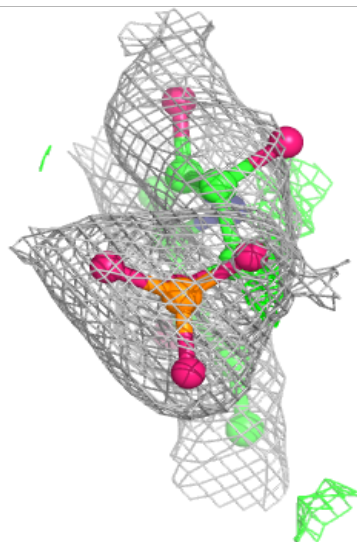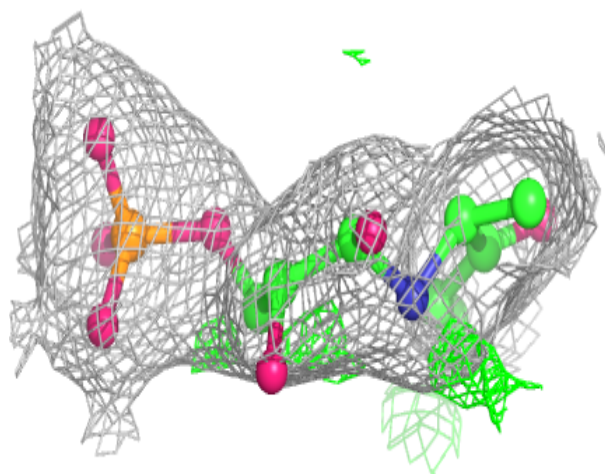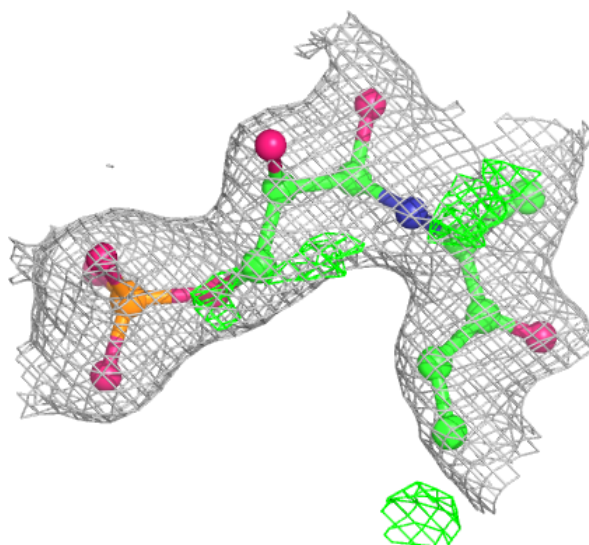
Electron density around K8P D 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
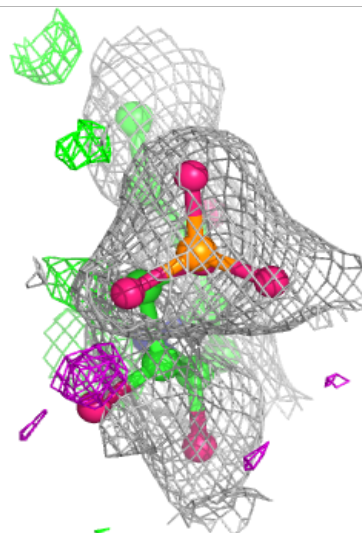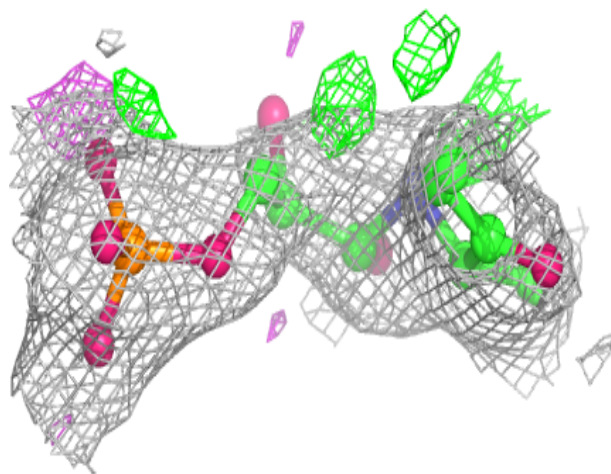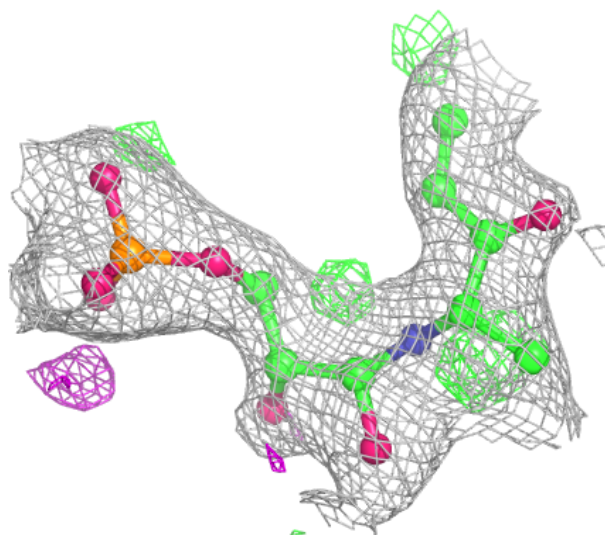and green (positive)
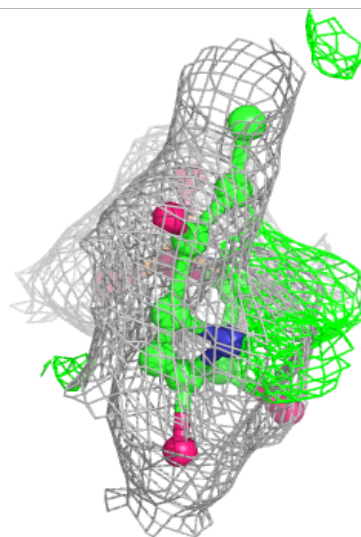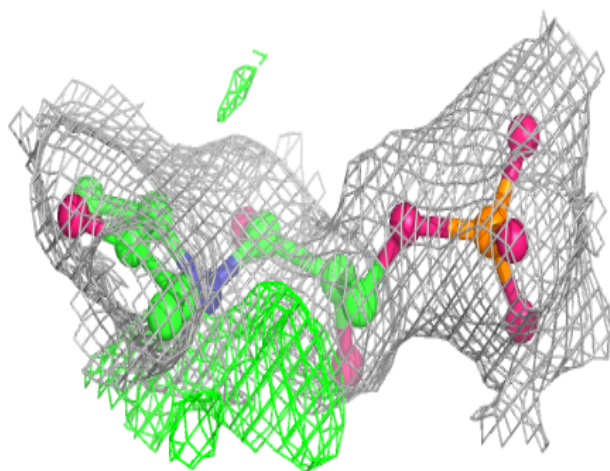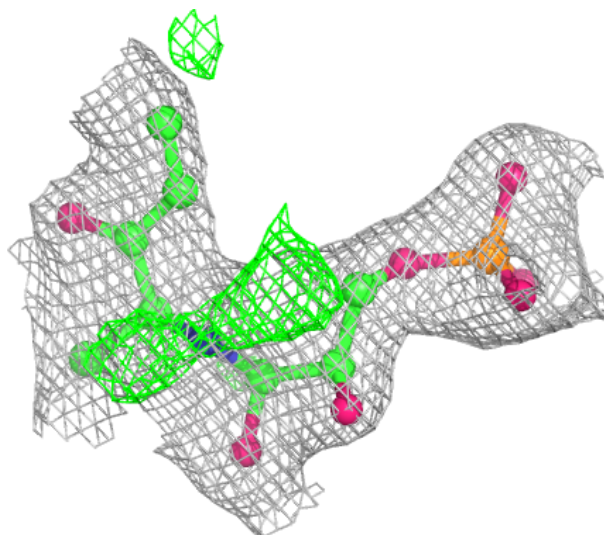
Electron density around K8P C 401:

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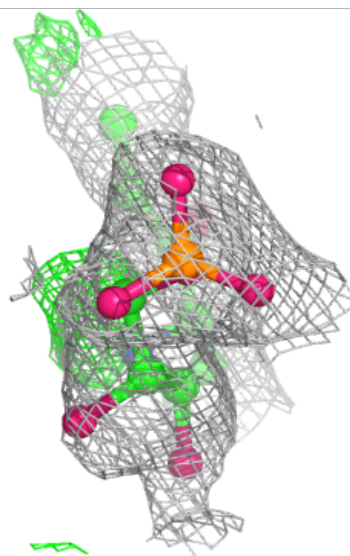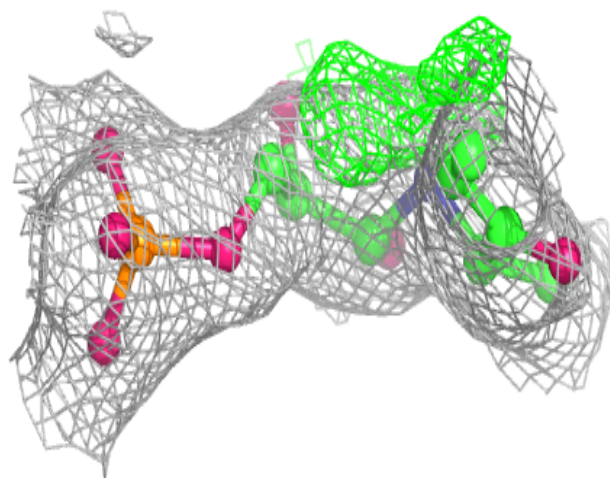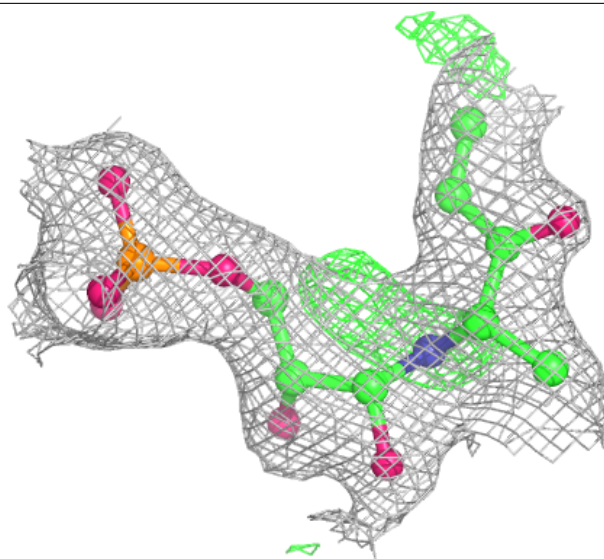and green (positive)

Electron density around K8P A 401:

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 K8P B 401:

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 ⓘ

There are no such residues in this entry.