



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:06 pm BST

PDB ID : 5JVL  
Title : C4-type pyruvate phosphate dikinase: nucleotide binding domain with bound ATP analogue  
Authors : Minges, A.; Hoepfner, A.; Groth, G.  
Deposited on : 2016-05-11  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

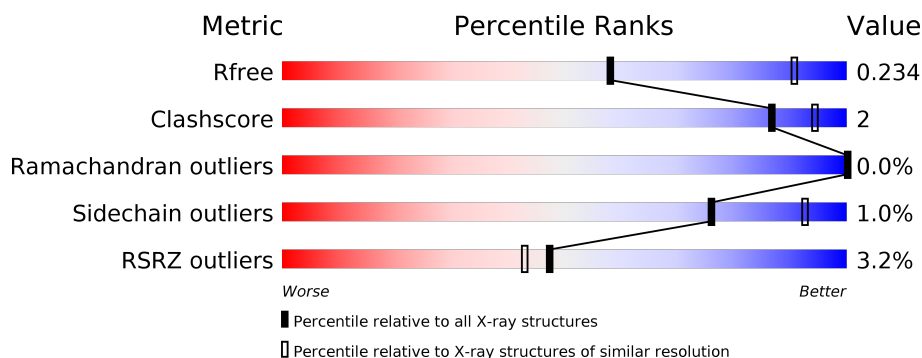
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	874	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	874	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>41%</div> </div> </div>
1	C	874	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	D	874	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

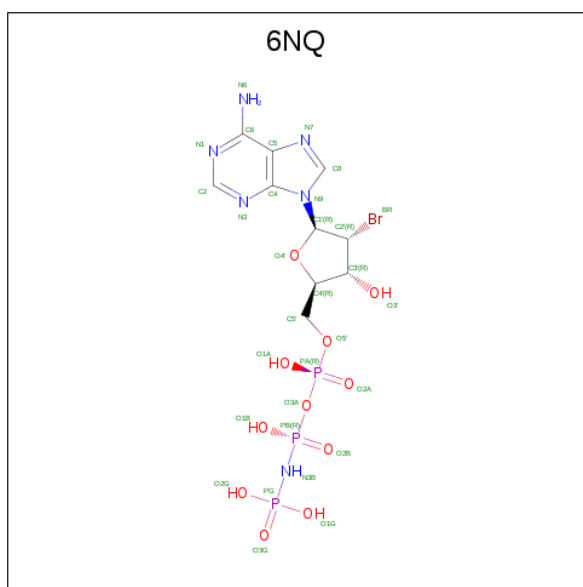
There are 4 unique types of molecules in this entry. The entry contains 23651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, phosphate dikinase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	874	Total	C	N	O	S	0	0	0
			6618	4157	1144	1269	48			
1	B	520	Total	C	N	O	S	0	0	0
			3819	2403	671	719	26			
1	C	859	Total	C	N	O	S	0	0	0
			6442	4056	1110	1231	45			
1	D	874	Total	C	N	O	S	0	2	0
			6632	4173	1141	1270	48			

- Molecule 2 is 2'-Bromo-2'-deoxyadenosine 5'-[beta,gamma-imide]triphosphoric acid (three-letter code: 6NQ) (formula: C<sub>10</sub>H<sub>16</sub>BrN<sub>6</sub>O<sub>11</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O P	0	0
			31	1	10	6	11 3		
2	C	1	Total	Br	C	N	O P	0	0
			31	1	10	6	11 3		

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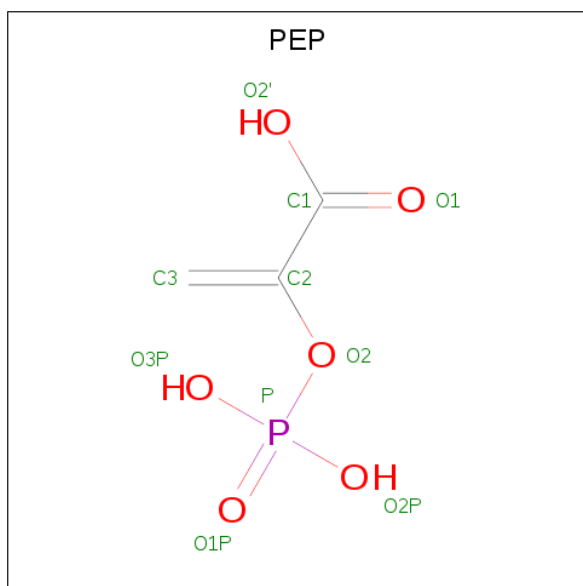
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	Br	C	N	O	P	0	0
			31	1	10	6	11	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

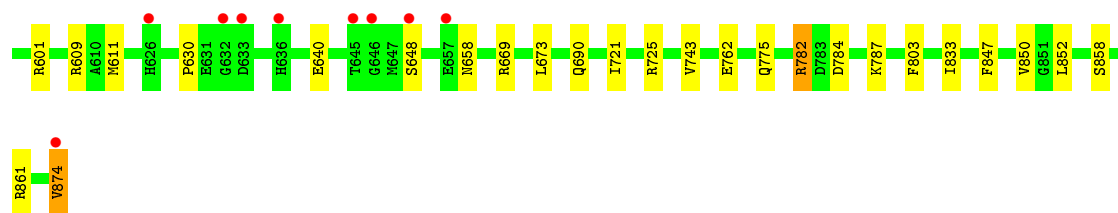
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C<sub>3</sub>H<sub>5</sub>O<sub>6</sub>P).

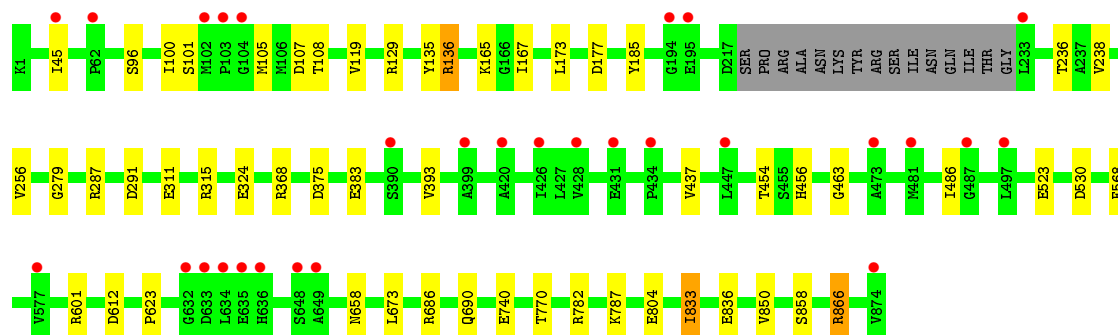
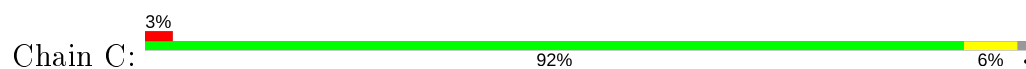


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		
4	C	1	Total	C	O	P	0	0
			10	3	6	1		
4	D	1	Total	C	O	P	0	0
			10	3	6	1		

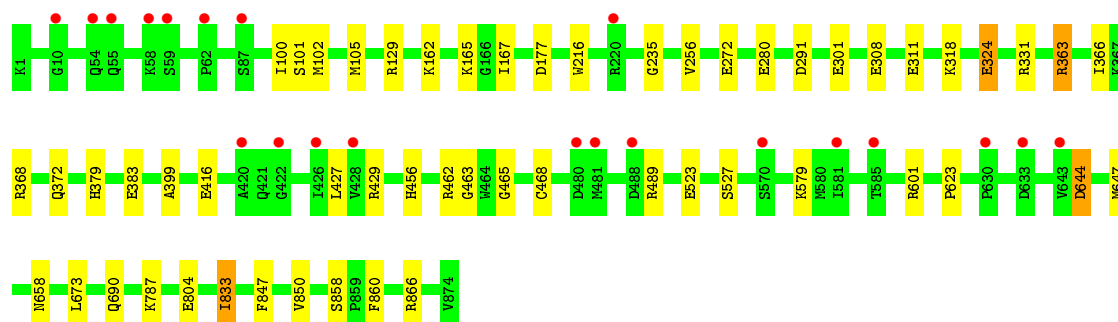
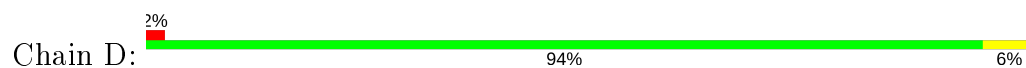




- Molecule 1: Pyruvate, phosphate dikinase, chloroplastic



- Molecule 1: Pyruvate, phosphate dikinase, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.98Å 108.45Å 152.76Å 106.22° 101.81° 98.32°	Depositor
Resolution (Å)	19.79 – 2.90 19.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.79-2.90) 98.6 (19.79-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.211 , 0.232 0.212 , 0.234	Depositor DCC
$R_{free}$ test set	1875 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PEP, 6NQ

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	0.90	5/6733 (0.1%)	0.77	8/9101 (0.1%)
1	B	0.87	2/3883 (0.1%)	0.78	7/5265 (0.1%)
1	C	0.90	8/6557 (0.1%)	0.76	12/8879 (0.1%)
1	D	0.91	9/6752 (0.1%)	0.76	12/9130 (0.1%)
All	All	0.90	24/23925 (0.1%)	0.77	39/32375 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	416	GLU	CD-OE1	9.17	1.35	1.25
1	D	804	GLU	CD-OE1	7.24	1.33	1.25
1	C	804	GLU	CD-OE2	7.16	1.33	1.25
1	A	311	GLU	CD-OE2	7.09	1.33	1.25
1	C	804	GLU	CG-CD	7.04	1.62	1.51
1	D	523	GLU	CG-CD	6.71	1.62	1.51
1	D	308	GLU	CD-OE1	-6.49	1.18	1.25
1	A	740	GLU	CD-OE1	6.36	1.32	1.25
1	C	836	GLU	CD-OE1	-6.35	1.18	1.25
1	D	324	GLU	CD-OE1	6.27	1.32	1.25
1	B	762	GLU	CG-CD	-5.83	1.43	1.51
1	C	523	GLU	CG-CD	5.70	1.60	1.51
1	B	858	SER	CB-OG	-5.57	1.35	1.42
1	C	311	GLU	CD-OE1	5.49	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	383	GLU	CD-OE2	5.48	1.31	1.25
1	A	411	SER	CB-OG	-5.41	1.35	1.42
1	A	383	GLU	CD-OE1	5.40	1.31	1.25
1	D	301	GLU	CD-OE2	5.39	1.31	1.25
1	D	280	GLU	CD-OE2	5.38	1.31	1.25
1	D	468	CYS	CB-SG	-5.35	1.73	1.81
1	A	682	GLU	CD-OE2	5.26	1.31	1.25
1	C	740	GLU	CD-OE1	5.22	1.31	1.25
1	D	383	GLU	CD-OE2	5.13	1.31	1.25
1	C	740	GLU	CD-OE2	5.04	1.31	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	GLU	OE1-CD-OE2	8.17	133.10	123.30
1	C	107	ASP	CB-CG-OD1	7.40	124.96	118.30
1	D	291	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	D	129	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	782	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	784	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	129	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	291	ASP	CB-CG-OD1	6.76	124.38	118.30
1	C	315	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	363	ARG	CG-CD-NE	6.50	125.45	111.80
1	B	782	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	647	MET	CG-SD-CE	6.24	110.19	100.20
1	A	368	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	804	GLU	OE1-CD-OE2	-6.12	115.96	123.30
1	D	866	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	534	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	291	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	D	331	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	523	GLU	CA-CB-CG	5.69	125.91	113.40
1	C	523	GLU	CA-CB-CG	5.57	125.66	113.40
1	B	609	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	647	MET	CG-SD-CE	5.53	109.05	100.20
1	C	368	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	D	489	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	866	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	272	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	D	489	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	107	ASP	CB-CG-OD2	-5.32	113.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	612	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	291	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	725	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	866	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	287	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	866	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	686	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	861	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	11	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	480	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	A	331	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	513	LEU	Peptide

## 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	6618	0	6579	29	0
1	B	3819	0	3678	19	0
1	C	6442	0	6337	29	0
1	D	6632	0	6587	26	0
2	A	31	0	0	2	0
2	C	31	0	0	2	0
2	D	31	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	0	0
4	C	10	0	2	1	0
4	D	10	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23651	0	23189	97	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 2.

All (97) 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:274:LEU:HD11	1:A:282:VAL:CG2	1.97	0.93
1:D:318:LYS:O	1:D:368:ARG:NH1	2.06	0.89
1:C:437:VAL:HG11	1:C:568:PHE:HB3	1.63	0.81
1:A:274:LEU:HD11	1:A:282:VAL:HG22	1.62	0.78
1:A:641:LEU:O	1:A:645:THR:HG22	1.84	0.78
1:A:129:ARG:NH1	1:A:173:LEU:O	2.20	0.75
1:A:1:LYS:N	1:A:4:VAL:O	2.23	0.71
1:A:275:ILE:O	1:A:287:ARG:NH2	2.24	0.71
1:A:787:LYS:NZ	1:D:658:ASN:O	2.27	0.68
1:C:601:ARG:NH1	1:C:690:GLN:OE1	2.28	0.67
1:B:601:ARG:NH1	1:B:690:GLN:OE1	2.29	0.65
1:C:463:GLY:HA2	1:C:858:SER:HB2	1.82	0.61
1:A:420:ALA:O	1:B:601:ARG:NH2	2.35	0.60
1:A:95:ARG:NH2	2:A:901:6NQ:O2A	2.31	0.59
1:D:601:ARG:NH1	1:D:690:GLN:OE1	2.32	0.59
1:B:787:LYS:NZ	1:C:658:ASN:O	2.36	0.58
1:C:108:THR:OG1	2:C:901:6NQ:O1A	2.14	0.57
1:B:721:ILE:HG12	1:B:743:VAL:HG11	1.87	0.56
1:D:165:LYS:HE2	1:D:177:ASP:OD1	2.06	0.55
1:B:658:ASN:O	1:C:787:LYS:NZ	2.40	0.54
1:A:601:ARG:NH1	1:A:690:GLN:OE1	2.36	0.53
1:C:105:MET:HE1	1:C:236:THR:HG21	1.90	0.53
1:A:165:LYS:HE2	1:A:177:ASP:OD1	2.09	0.52
1:A:274:LEU:CD2	1:A:289:PRO:HA	2.39	0.52
1:B:259:THR:HG21	1:B:314:GLU:OE2	2.09	0.52
1:D:379:HIS:CD2	1:D:860[B]:PHE:CE1	2.97	0.52
1:D:456:HIS:HE2	4:D:903:PEP:P	2.32	0.52
1:C:165:LYS:HE2	1:C:177:ASP:OD1	2.09	0.52
1:D:579:LYS:HE2	1:D:644:ASP:O	2.10	0.51
1:D:102:MET:HB3	1:D:105:MET:HE1	1.93	0.50
1:B:630:PRO:HB3	1:B:640:GLU:OE1	2.11	0.50
1:C:393:VAL:CG1	1:C:486:ILE:HD12	2.41	0.50
1:B:363:ARG:HB3	1:B:874:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:VAL:HG23	1:B:852:LEU:HD13	1.93	0.50
1:D:100:ILE:HD12	1:D:101:SER:O	2.12	0.50
1:D:623:PRO:HD2	1:D:673:LEU:HD12	1.93	0.49
1:C:393:VAL:HG12	1:C:486:ILE:CD1	2.43	0.49
1:D:102:MET:HG2	1:D:105:MET:HE1	1.95	0.49
1:D:363:ARG:O	1:D:366:ILE:HG13	2.13	0.49
1:D:102:MET:HB3	1:D:105:MET:CE	2.42	0.48
1:D:463:GLY:HA2	1:D:858:SER:HB2	1.94	0.48
1:C:105:MET:HE3	1:C:105:MET:HB3	1.63	0.48
1:C:393:VAL:HG12	1:C:486:ILE:HD12	1.96	0.48
1:C:454:THR:HG22	1:C:782:ARG:HD3	1.95	0.47
1:C:96:SER:HB3	1:C:105:MET:CE	2.44	0.47
1:A:274:LEU:CD1	1:A:282:VAL:CG2	2.84	0.46
1:A:590:LYS:NZ	1:A:594:ASP:OD2	2.48	0.46
1:C:456:HIS:NE2	4:C:903:PEP:O1P	2.33	0.45
1:C:279:GLY:HA3	2:C:901:6NQ:O3'	2.16	0.45
1:A:274:LEU:HD21	1:A:289:PRO:HA	1.97	0.45
1:C:623:PRO:HD2	1:C:673:LEU:HD12	1.98	0.44
1:B:557:GLY:HA2	1:B:611:MET:HE2	1.98	0.44
1:C:100:ILE:HG22	1:C:101:SER:N	2.33	0.44
1:D:256:VAL:HG12	1:D:324:GLU:HG2	1.99	0.44
1:D:379:HIS:CD2	1:D:860[B]:PHE:CZ	3.06	0.44
1:A:433:SER:OG	1:A:631:GLU:OE1	2.26	0.44
1:D:850:VAL:O	1:D:850:VAL:HG12	2.17	0.44
1:A:25:LYS:NZ	2:A:901:6NQ:O1G	2.47	0.43
1:A:645:THR:HG23	1:A:647:MET:H	1.83	0.43
1:C:256:VAL:HG12	1:C:324:GLU:HG2	2.00	0.43
1:B:259:THR:CG2	1:B:314:GLU:OE2	2.66	0.43
1:D:162:LYS:HG2	1:D:167:ILE:HD11	2.01	0.43
1:C:136:ARG:HG2	1:C:185:TYR:CE2	2.53	0.43
1:A:282:VAL:O	1:A:285:GLY:HA2	2.19	0.43
1:B:669:ARG:HA	1:B:673:LEU:HD13	2.01	0.43
1:C:850:VAL:O	1:C:850:VAL:HG12	2.18	0.42
1:D:102:MET:HG2	1:D:105:MET:CE	2.49	0.42
1:B:833:ILE:CD1	1:B:847:PHE:CZ	3.02	0.42
1:C:770:THR:CG2	1:C:833:ILE:HD11	2.50	0.42
1:A:291:ASP:OD1	1:A:292:LEU:N	2.52	0.42
1:B:558:ILE:HG12	1:B:611:MET:HG3	2.00	0.42
1:D:399:ALA:O	1:D:462:ARG:HD3	2.20	0.42
1:A:429:ARG:O	1:A:448:THR:HA	2.19	0.42
1:D:427:LEU:CD2	1:D:429:ARG:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:O	1:D:787:LYS:NZ	2.50	0.42
1:C:45:ILE:HB	1:C:238:VAL:CG1	2.50	0.41
1:B:775:GLN:CD	1:B:782:ARG:HB2	2.41	0.41
1:C:530:ASP:OD1	1:C:866:ARG:HD2	2.21	0.41
1:C:167:ILE:HD13	1:C:173:LEU:HD23	2.03	0.41
1:D:833:ILE:HD12	1:D:847:PHE:CZ	2.56	0.41
1:A:563:THR:HA	1:A:566:MET:SD	2.60	0.41
1:A:850:VAL:O	1:A:850:VAL:HG12	2.19	0.41
1:D:216:TRP:CE2	1:D:235:GLY:HA2	2.55	0.41
1:C:105:MET:HE2	1:C:236:THR:OG1	2.21	0.41
1:C:119:VAL:HG21	1:C:135:TYR:CG	2.55	0.41
1:C:105:MET:HE1	1:C:236:THR:CB	2.50	0.41
1:B:775:GLN:HG3	1:B:803:PHE:HE1	1.85	0.41
1:D:833:ILE:CD1	1:D:847:PHE:CZ	3.04	0.41
1:A:669:ARG:HA	1:A:673:LEU:HD13	2.03	0.41
1:B:320:MET:HG3	1:B:342:ARG:NH2	2.36	0.41
1:C:454:THR:HG22	1:C:454:THR:O	2.21	0.41
1:D:465:GLY:HA3	1:D:860[B]:PHE:CD1	2.56	0.41
1:A:119:VAL:HG21	1:A:135:TYR:CG	2.56	0.40
1:A:601:ARG:NH2	1:B:420:ALA:O	2.54	0.40
1:A:257:LEU:C	1:A:257:LEU:HD12	2.42	0.40
1:A:388:TYR:CD1	1:A:388:TYR:C	2.95	0.40
1:B:563:THR:HA	1:B:566:MET:SD	2.62	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	872/874 (100%)	858 (98%)	14 (2%)	0	100	100
1	B	510/874 (58%)	498 (98%)	11 (2%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	855/874 (98%)	842 (98%)	13 (2%)	0	100	100
1	D	874/874 (100%)	860 (98%)	14 (2%)	0	100	100
All	All	3111/3496 (89%)	3058 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	648	SER

### 5.3.2 Protein sidechains ⓘ

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	701/715 (98%)	688 (98%)	13 (2%)	57	84
1	B	378/715 (53%)	374 (99%)	4 (1%)	73	92
1	C	671/715 (94%)	668 (100%)	3 (0%)	91	97
1	D	702/715 (98%)	696 (99%)	6 (1%)	78	93
All	All	2452/2860 (86%)	2426 (99%)	26 (1%)	76	92

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	70	GLU
1	A	129	ARG
1	A	335	LEU
1	A	388	TYR
1	A	455	SER
1	A	462	ARG
1	A	527	SER
1	A	589	ARG
1	A	631	GLU
1	A	644	ASP

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Mol	Chain	Res	Type
1	A	657	GLU
1	A	833	ILE
1	B	320	MET
1	B	388	TYR
1	B	462	ARG
1	B	874	VAL
1	C	136	ARG
1	C	375	ASP
1	C	833	ILE
1	D	311	GLU
1	D	372[A]	GLN
1	D	372[B]	GLN
1	D	527	SER
1	D	644	ASP
1	D	833	ILE

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

Mol	Chain	Res	Type
1	A	813	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	PEP	C	903	3	6,9,9	1.32	1 (16%)	8,13,13	2.18	5 (62%)
4	PEP	B	901	3	6,9,9	1.18	0	8,13,13	2.10	4 (50%)
2	6NQ	C	901	3	28,33,33	2.81	6 (21%)	27,52,52	1.46	3 (11%)
4	PEP	D	903	3	6,9,9	1.23	1 (16%)	8,13,13	2.66	5 (62%)
2	6NQ	A	901	3	28,33,33	1.84	8 (28%)	27,52,52	2.36	9 (33%)
4	PEP	A	903	3	6,9,9	1.01	0	8,13,13	1.90	3 (37%)
2	6NQ	D	901	3	28,33,33	2.60	6 (21%)	27,52,52	1.88	9 (33%)

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	PEP	C	903	3	-	3/5/9/9	-
4	PEP	B	901	3	-	2/5/9/9	-
2	6NQ	C	901	3	-	5/14/38/38	0/3/3/3
4	PEP	D	903	3	-	2/5/9/9	-
2	6NQ	A	901	3	-	3/14/38/38	0/3/3/3
4	PEP	A	903	3	-	2/5/9/9	-
2	6NQ	D	901	3	-	4/14/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	6NQ	PB-O3A	10.21	1.71	1.59
2	D	901	6NQ	PB-O3A	10.10	1.71	1.59
2	C	901	6NQ	PB-O2B	6.12	1.55	1.46
2	C	901	6NQ	PG-O3G	5.58	1.55	1.46
2	D	901	6NQ	PB-O2B	4.91	1.54	1.46
2	D	901	6NQ	PG-O3G	4.16	1.52	1.46
2	A	901	6NQ	PG-O3G	3.67	1.52	1.46
2	A	901	6NQ	PB-O3A	3.59	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	6NQ	PB-O2B	3.53	1.51	1.46
2	A	901	6NQ	PG-N3B	3.51	1.72	1.63
2	C	901	6NQ	PB-N3B	3.44	1.72	1.63
2	C	901	6NQ	PG-N3B	3.34	1.72	1.63
2	C	901	6NQ	C1'-C2'	3.30	1.59	1.52
2	A	901	6NQ	PB-N3B	3.22	1.71	1.63
2	A	901	6NQ	PB-O1B	-3.19	1.48	1.56
2	D	901	6NQ	PB-N3B	2.97	1.71	1.63
4	C	903	PEP	O2-C2	2.77	1.46	1.39
2	D	901	6NQ	PB-O1B	-2.71	1.49	1.56
2	A	901	6NQ	PG-O1G	-2.71	1.49	1.56
2	D	901	6NQ	BR-C2'	2.34	2.02	1.96
4	D	903	PEP	O2-C2	2.27	1.45	1.39
2	A	901	6NQ	C4-N3	-2.07	1.32	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	6NQ	O1G-PG-O3G	-6.66	96.70	113.45
2	A	901	6NQ	PA-O3A-PB	-5.29	113.98	132.62
2	A	901	6NQ	O2B-PB-N3B	-5.08	104.28	111.77
2	D	901	6NQ	PA-O3A-PB	-4.20	117.83	132.62
4	D	903	PEP	O2P-P-O2	4.16	117.94	105.25
2	C	901	6NQ	PA-O3A-PB	-3.90	118.87	132.62
4	B	901	PEP	O2P-P-O2	-3.90	93.37	105.25
2	D	901	6NQ	O2G-PG-O3G	-3.75	104.03	113.45
2	D	901	6NQ	O5'-PA-O2A	-3.55	95.19	109.07
2	A	901	6NQ	O3A-PB-N3B	3.37	115.93	106.59
4	A	903	PEP	O2-C2-C3	-3.31	118.42	124.79
2	D	901	6NQ	O3G-PG-N3B	3.28	116.59	111.77
4	C	903	PEP	O3P-P-O1P	3.20	123.19	110.68
4	D	903	PEP	O3P-P-O1P	3.17	123.10	110.68
4	A	903	PEP	O2P-P-O2	-3.17	95.59	105.25
4	D	903	PEP	O2-C2-C3	-3.16	118.70	124.79
2	C	901	6NQ	O1G-PG-O3G	-3.05	105.78	113.45
4	D	903	PEP	O3P-P-O2P	-3.05	95.98	107.64
2	D	901	6NQ	O1B-PB-O2B	-3.04	103.54	109.92
4	C	903	PEP	O3P-P-O2P	2.95	118.93	107.64
2	C	901	6NQ	O5'-PA-O2A	2.87	120.27	109.07
4	D	903	PEP	O3P-P-O2	-2.77	96.81	105.25
2	A	901	6NQ	O1B-PB-O3A	2.70	113.64	104.64
2	A	901	6NQ	O5'-PA-O2A	-2.68	98.60	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	6NQ	O2G-PG-O1G	2.68	114.77	107.64
4	B	901	PEP	O2-P-O1P	2.67	118.82	109.32
4	C	903	PEP	O2P-P-O1P	-2.65	100.31	110.68
4	B	901	PEP	O2P-P-O1P	2.43	120.21	110.68
4	C	903	PEP	O3P-P-O2	-2.42	97.89	105.25
4	C	903	PEP	O2-C2-C3	-2.38	120.21	124.79
2	D	901	6NQ	C5-C6-N6	2.35	123.92	120.35
2	A	901	6NQ	O1A-PA-O2A	2.26	123.42	112.24
4	B	901	PEP	O2-C2-C3	-2.23	120.50	124.79
2	A	901	6NQ	C5-C6-N6	2.21	123.71	120.35
2	D	901	6NQ	O2G-PG-O1G	-2.20	101.79	107.64
2	D	901	6NQ	O1G-PG-O3G	2.18	118.93	113.45
4	A	903	PEP	O2P-P-O1P	2.17	119.19	110.68
2	D	901	6NQ	O1A-PA-O5'	2.00	117.04	107.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

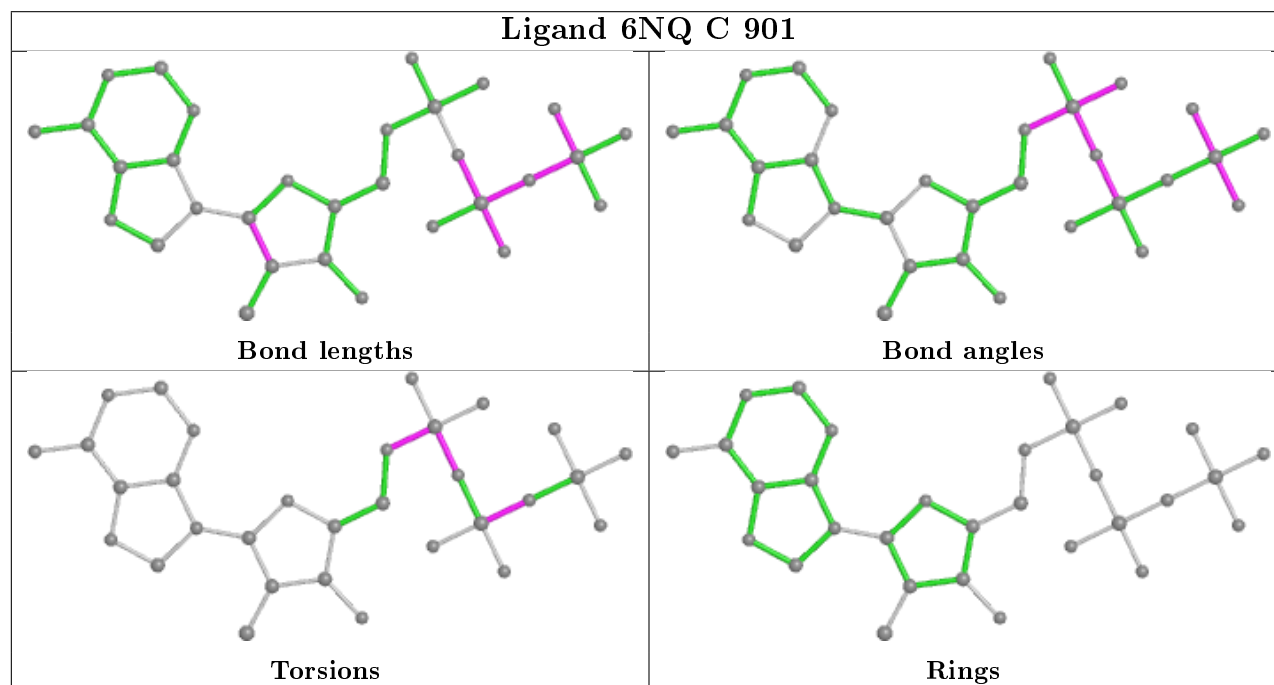
Mol	Chain	Res	Type	Atoms
4	C	903	PEP	C3-C2-O2-P
4	B	901	PEP	C1-C2-O2-P
4	B	901	PEP	C3-C2-O2-P
2	C	901	6NQ	PG-N3B-PB-O2B
2	C	901	6NQ	C5'-O5'-PA-O1A
2	C	901	6NQ	C5'-O5'-PA-O2A
2	C	901	6NQ	C5'-O5'-PA-O3A
4	D	903	PEP	C1-C2-O2-P
4	D	903	PEP	C3-C2-O2-P
2	A	901	6NQ	PG-N3B-PB-O2B
2	A	901	6NQ	C5'-O5'-PA-O3A
4	A	903	PEP	C1-C2-O2-P
4	A	903	PEP	C3-C2-O2-P
2	D	901	6NQ	PB-N3B-PG-O3G
2	D	901	6NQ	PB-O3A-PA-O2A
2	D	901	6NQ	C5'-O5'-PA-O3A
4	C	903	PEP	C1-C2-O2-P
2	C	901	6NQ	PB-O3A-PA-O2A
2	A	901	6NQ	C5'-O5'-PA-O2A
2	D	901	6NQ	C5'-O5'-PA-O2A
4	C	903	PEP	C2-O2-P-O3P

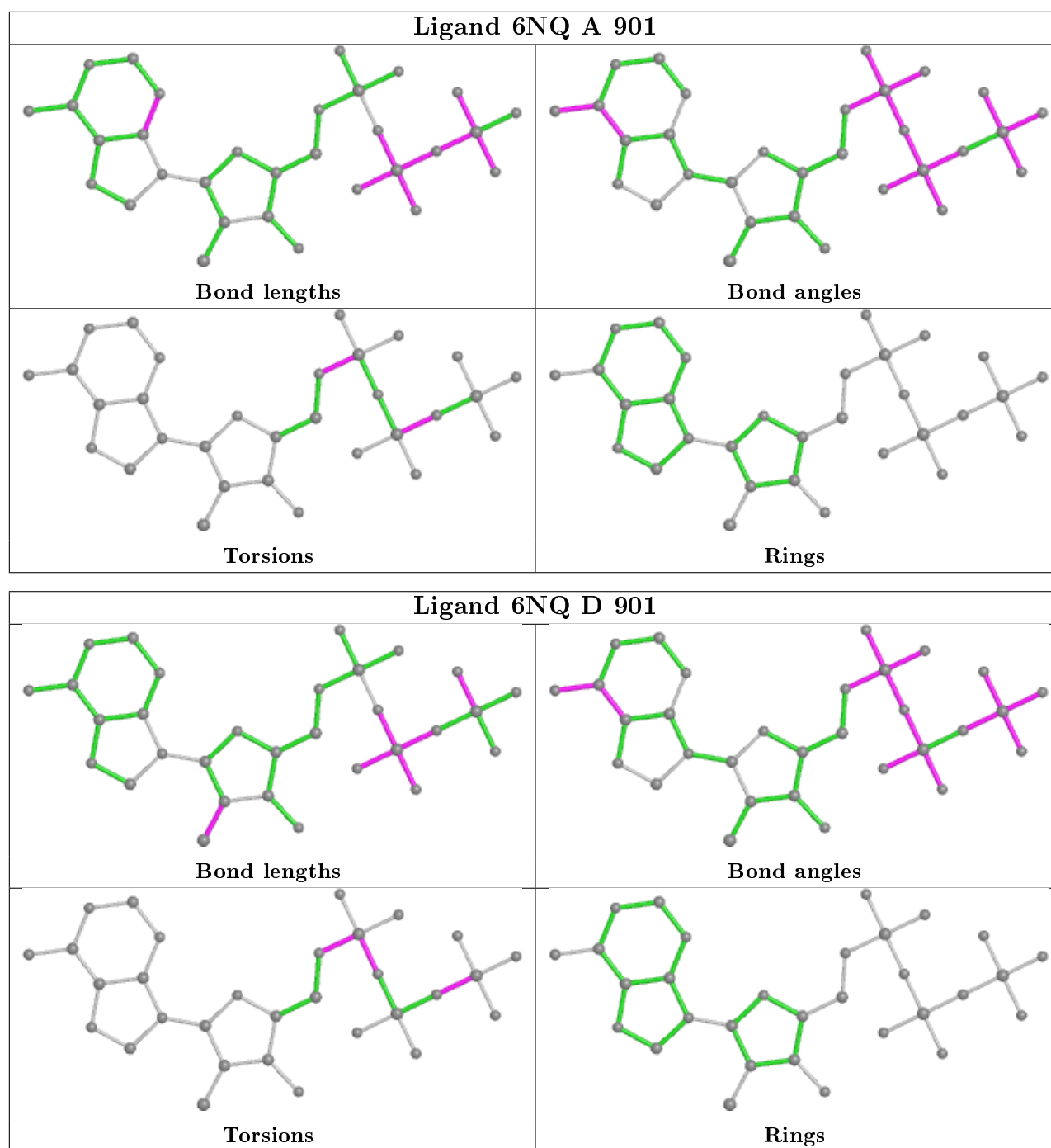
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	903	PEP	1	0
2	C	901	6NQ	2	0
4	D	903	PEP	1	0
2	A	901	6NQ	2	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	874/874 (100%)	-0.19	18 (2%) 63 61	24, 42, 79, 109	0
1	B	520/874 (59%)	-0.08	32 (6%) 20 16	24, 43, 97, 133	0
1	C	859/874 (98%)	-0.09	29 (3%) 45 40	20, 46, 87, 127	0
1	D	874/874 (100%)	-0.24	21 (2%) 59 56	21, 41, 71, 122	0
All	All	3127/3496 (89%)	-0.16	100 (3%) 47 43	20, 43, 86, 133	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	635	GLU	5.5
1	C	104	GLY	4.9
1	C	103	PRO	4.5
1	A	285	GLY	4.4
1	A	632	GLY	4.3
1	B	457	ALA	4.3
1	A	284	ALA	4.2
1	C	473	ALA	4.2
1	D	422	GLY	4.2
1	D	420	ALA	3.9
1	C	428	VAL	3.7
1	B	399	ALA	3.6
1	B	874	VAL	3.6
1	B	414	ASP	3.5
1	C	102	MET	3.5
1	B	387	ALA	3.5
1	B	411	SER	3.4
1	C	481	MET	3.3
1	B	636	HIS	3.3
1	B	386	SER	3.3
1	B	646	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	634	LEU	3.2
1	B	456	HIS	3.0
1	D	58	LYS	2.9
1	D	87	SER	2.9
1	D	54	GLN	2.9
1	B	633	ASP	2.9
1	B	632	GLY	2.9
1	D	59	SER	2.9
1	B	494	GLY	2.9
1	C	399	ALA	2.9
1	B	420	ALA	2.8
1	C	636	HIS	2.8
1	A	58	LYS	2.8
1	B	418	TRP	2.7
1	C	447	LEU	2.7
1	A	648	SER	2.7
1	C	497	LEU	2.7
1	C	632	GLY	2.7
1	C	390	SER	2.6
1	B	460	VAL	2.6
1	D	480	ASP	2.6
1	B	359	LEU	2.6
1	B	388	TYR	2.6
1	A	126	SER	2.6
1	A	635	GLU	2.6
1	D	55	GLN	2.6
1	D	481	MET	2.5
1	B	390	SER	2.5
1	D	488	ASP	2.5
1	C	487	GLY	2.5
1	D	10	GLY	2.5
1	C	426	ILE	2.5
1	B	309	ASN	2.5
1	B	645	THR	2.4
1	D	426	ILE	2.4
1	C	62	PRO	2.4
1	D	633	ASP	2.4
1	C	233	LEU	2.4
1	A	386	SER	2.4
1	C	577	VAL	2.3
1	C	420	ALA	2.3
1	B	648	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	874	VAL	2.3
1	B	464	TRP	2.3
1	A	57	GLY	2.3
1	B	412	ALA	2.3
1	B	455	SER	2.2
1	A	84	GLY	2.2
1	A	515	PRO	2.2
1	C	649	ALA	2.2
1	D	581	ILE	2.2
1	B	398	PRO	2.2
1	A	194	GLY	2.2
1	C	45	ILE	2.2
1	A	518	MET	2.2
1	B	385	PRO	2.2
1	D	643	VAL	2.2
1	C	194	GLY	2.2
1	B	626	HIS	2.2
1	D	62	PRO	2.1
1	A	283	VAL	2.1
1	A	634	LEU	2.1
1	B	417	THR	2.1
1	C	431	GLU	2.1
1	C	648	SER	2.1
1	C	195	GLU	2.1
1	C	633	ASP	2.1
1	A	631	GLU	2.1
1	B	657	GLU	2.1
1	B	454	THR	2.0
1	D	585	THR	2.0
1	C	434	PRO	2.0
1	D	630	PRO	2.0
1	A	447	LEU	2.0
1	B	461	ALA	2.0
1	A	587	GLU	2.0
1	D	570	SER	2.0
1	D	220	ARG	2.0
1	D	428	VAL	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

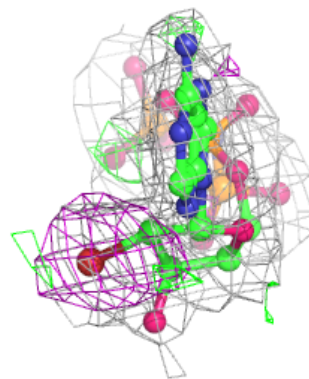
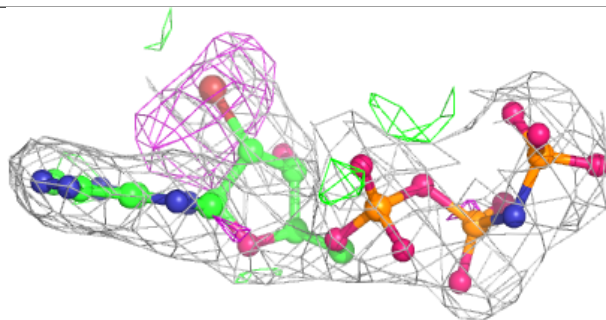
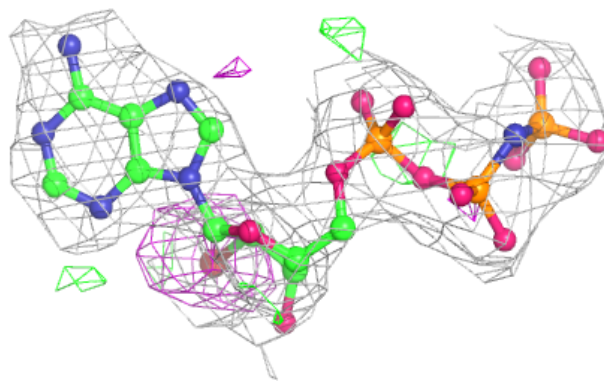
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	D	902	1/1	0.75	0.11	30,30,30,30	0
3	MG	A	902	1/1	0.86	0.07	33,33,33,33	0
3	MG	C	902	1/1	0.88	0.14	34,34,34,34	0
3	MG	A	904	1/1	0.92	0.10	23,23,23,23	0
2	6NQ	C	901	31/31	0.92	0.15	24,37,56,63	0
2	6NQ	D	901	31/31	0.94	0.15	21,27,34,63	0
2	6NQ	A	901	31/31	0.95	0.13	19,28,34,55	0
3	MG	C	904	1/1	0.96	0.07	20,20,20,20	0
4	PEP	B	901	10/10	0.97	0.11	12,13,20,21	0
4	PEP	D	903	10/10	0.98	0.09	22,24,26,27	0
3	MG	B	902	1/1	0.98	0.05	25,25,25,25	0
4	PEP	A	903	10/10	0.98	0.10	10,12,18,19	0
4	PEP	C	903	10/10	0.98	0.10	24,26,31,34	0
3	MG	D	904	1/1	0.99	0.06	11,11,11,11	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.

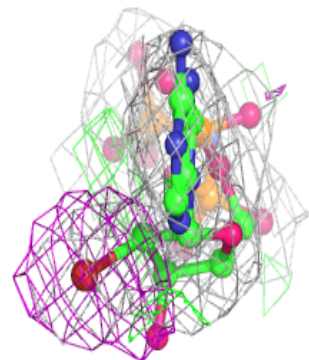
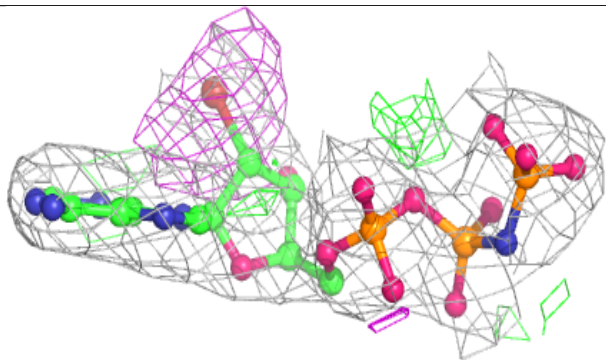
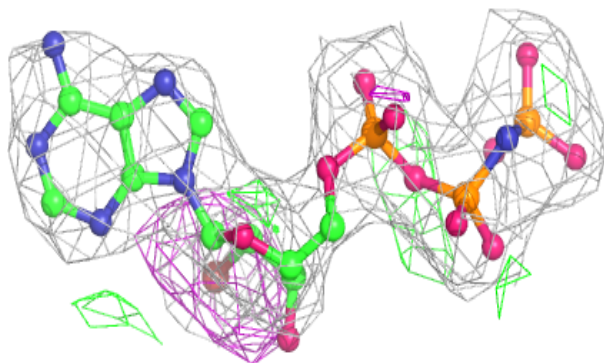


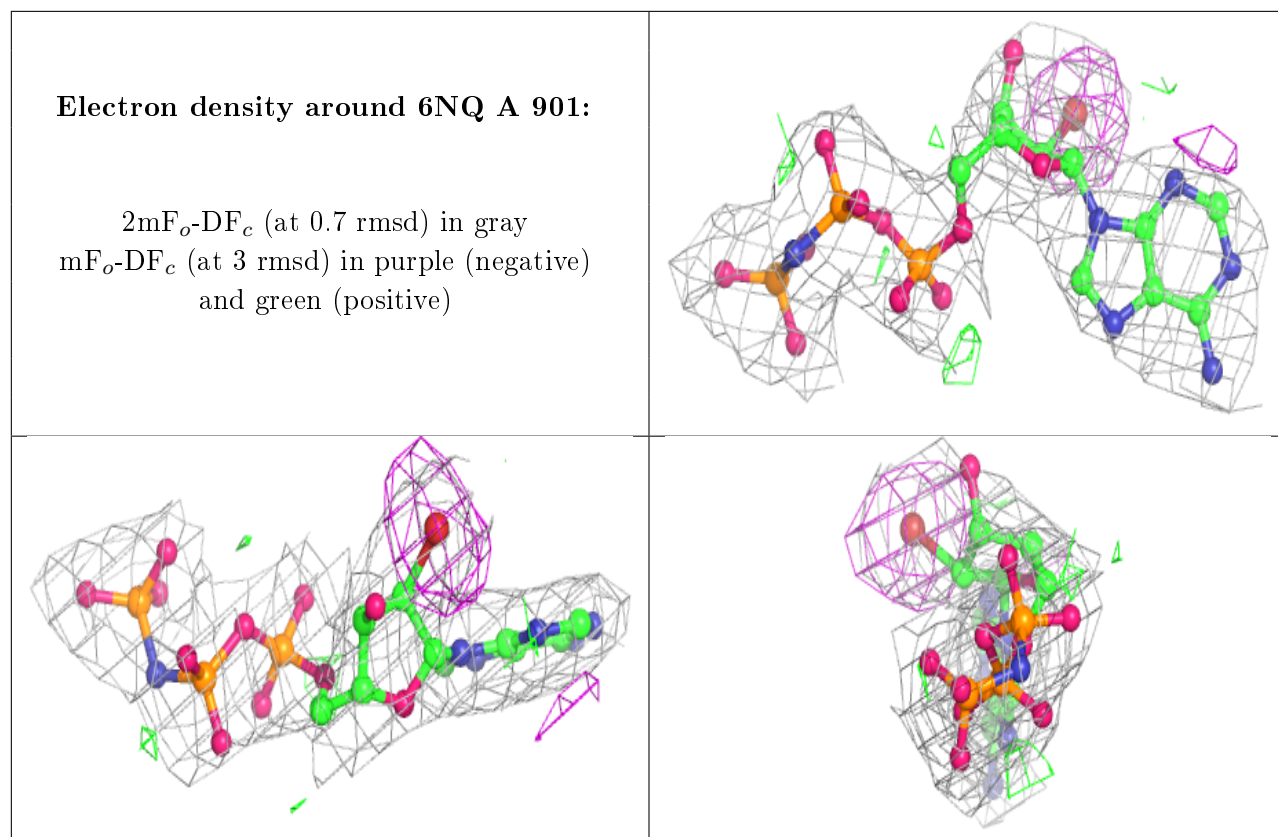
**Electron density around 6NQ C 901:**

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

**Electron density around 6NQ D 901:**

$2mF_o-DF_c$  (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.