



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:14 PM UTC

PDB ID : 5JVL / pdb_00005jvl
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

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

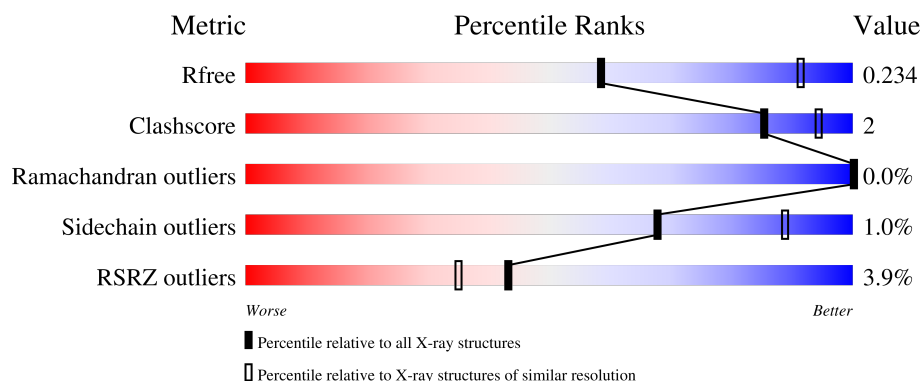
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	874	2% 92% 8%
1	B	874	5% 55% 41%
1	C	874	5% 92% 6%
1	D	874	2% 93% 6%

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	PEP	A	903	-	X	-	-
4	PEP	C	903	-	X	-	-
4	PEP	D	903	-	X	-	-

2 Entry composition [i](#)

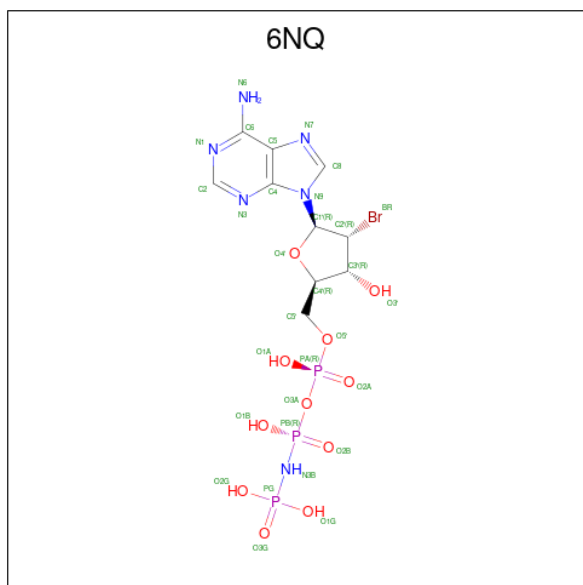
There are 4 unique types of molecules in this entry. The entry contains 23651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 6NQ) (formula: C₁₀H₁₆BrN₆O₁₁P₃).



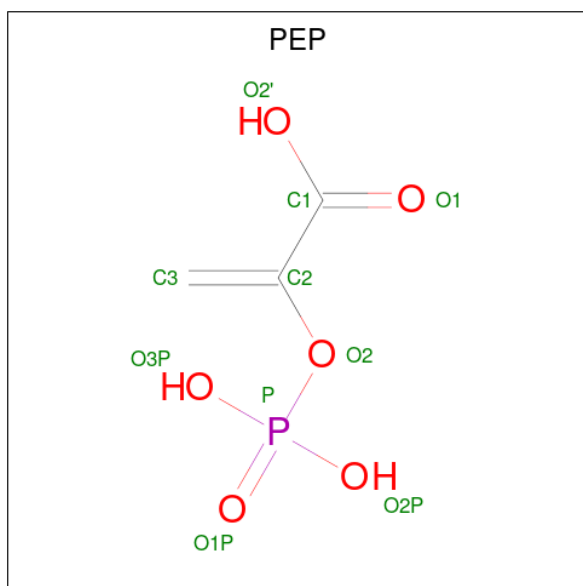
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	Br	C	N	O	P	0	0
			31	1	10	6	11	3		

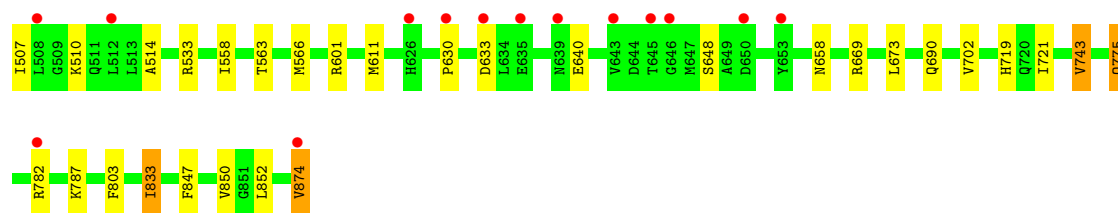
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

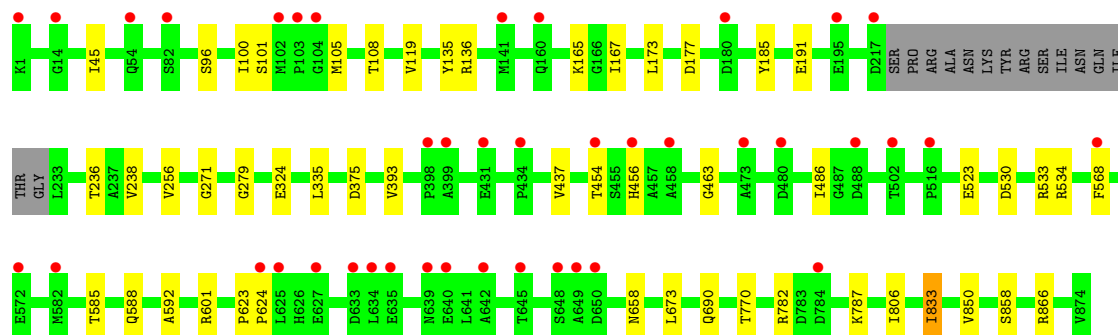
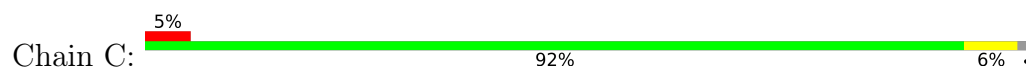
- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



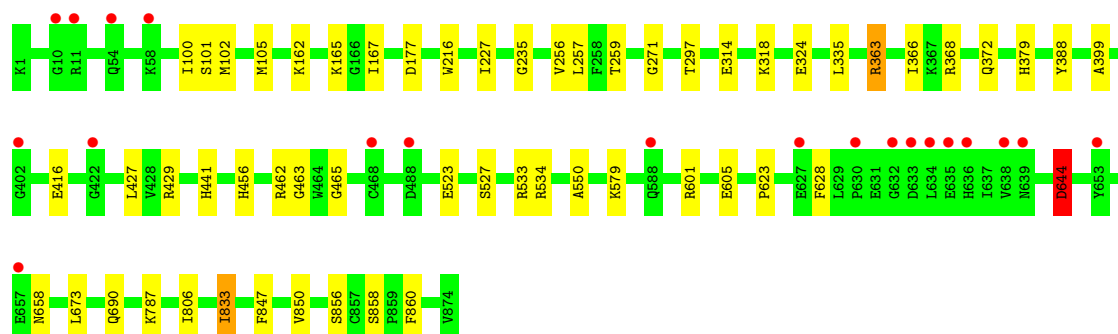
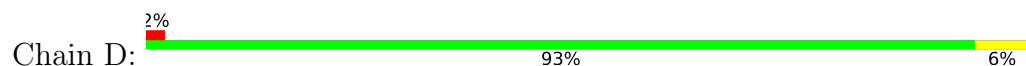
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		
4	C	1	Total	C	O	P	0	0
			10	3	6	1		
4	D	1	Total	C	O	P	0	0
			10	3	6	1		



- Molecule 1: Pyruvate, phosphate dikinase, chloroplastic



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.5 (19.79-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: PEP, MG, 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	1.18	17/6733 (0.3%)	0.84	4/9101 (0.0%)
1	B	1.16	9/3883 (0.2%)	0.86	0/5265
1	C	1.16	7/6557 (0.1%)	0.81	1/8879 (0.0%)
1	D	1.16	9/6752 (0.1%)	0.81	5/9130 (0.1%)
All	All	1.17	42/23925 (0.2%)	0.83	10/32375 (0.0%)

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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	514	ALA	CA-C	9.18	1.62	1.52
1	A	454	THR	CA-CB	7.75	1.64	1.53
1	D	806	ILE	C-O	-7.37	1.16	1.24
1	B	633	ASP	CA-C	6.62	1.60	1.52
1	D	534	ARG	C-O	-6.61	1.15	1.23
1	A	443	ALA	C-O	-6.59	1.15	1.23
1	A	19	LYS	C-O	-6.58	1.16	1.24
1	C	806	ILE	C-O	-6.40	1.17	1.24
1	A	169	LEU	N-CA	6.33	1.53	1.45
1	B	533	ARG	C-O	-6.27	1.15	1.23
1	D	533	ARG	C-O	-6.25	1.16	1.23
1	B	775	GLN	C-O	-6.20	1.17	1.24
1	B	507	ILE	C-O	-6.14	1.17	1.24
1	B	719	HIS	C-O	-5.93	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	VAL	C-O	-5.83	1.17	1.24
1	A	515	PRO	CA-C	5.82	1.57	1.52
1	B	339	THR	C-O	-5.79	1.17	1.23
1	A	271	GLY	C-O	-5.77	1.17	1.23
1	A	521	ASP	C-O	-5.75	1.16	1.24
1	A	862	VAL	C-O	-5.75	1.19	1.24
1	C	533	ARG	C-O	-5.66	1.17	1.23
1	B	514	ALA	CA-C	5.63	1.57	1.52
1	B	702	VAL	C-O	-5.51	1.17	1.24
1	C	271	GLY	C-O	-5.49	1.17	1.23
1	D	297	THR	C-O	-5.48	1.17	1.24
1	D	416	GLU	CD-OE1	5.47	1.35	1.25
1	C	592	ALA	C-O	-5.45	1.17	1.24
1	C	191	GLU	C-O	-5.44	1.17	1.24
1	A	560	LEU	C-O	-5.41	1.17	1.24
1	A	281	ASP	N-CA	5.39	1.53	1.46
1	A	533	ARG	C-O	-5.38	1.17	1.23
1	C	534	ARG	C-O	-5.36	1.17	1.24
1	A	766	PHE	CA-C	-5.34	1.46	1.52
1	A	514	ALA	C-N	5.31	1.39	1.33
1	D	856	SER	C-O	5.20	1.29	1.24
1	C	624	PRO	CA-C	5.15	1.58	1.53
1	D	271	GLY	C-O	-5.12	1.17	1.23
1	D	605	GLU	C-O	-5.07	1.18	1.24
1	A	623	PRO	C-O	5.06	1.30	1.24
1	B	510	LYS	C-O	-5.05	1.17	1.23
1	A	597	LEU	C-O	-5.03	1.19	1.24
1	D	550	ALA	C-O	-5.01	1.18	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	GLU	N-CA-CB	6.32	119.23	110.07
1	D	363	ARG	CG-CD-NE	6.11	125.45	112.00
1	D	523	GLU	CA-CB-CG	5.91	125.91	114.10
1	C	523	GLU	CA-CB-CG	5.78	125.66	114.10
1	D	628	PHE	N-CA-C	5.68	119.95	113.19
1	A	170	ASP	CA-C-N	5.51	128.42	120.38
1	A	170	ASP	C-N-CA	5.51	128.42	120.38
1	A	233	LEU	N-CA-C	5.19	117.87	110.24
1	D	363	ARG	CB-CG-CD	-5.18	99.39	111.30
1	D	644	ASP	N-CA-CB	5.16	118.81	110.40

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	32	0
1	B	3819	0	3678	20	0
1	C	6442	0	6337	31	0
1	D	6632	0	6587	28	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
All	All	23651	0	23189	105	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 (105) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:105:MET:HE1	1:C:236:THR:CB	2.21	0.71
1:D:102:MET:HB3	1:D:105:MET:HE1	1.76	0.68
1:A:787:LYS:NZ	1:D:658:ASN:O	2.27	0.68
1:C:96:SER:HB3	1:C:105:MET:HE2	1.77	0.67
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:A:433:SER:OG	1:A:631:GLU:OE1	2.26	0.53
1:C:105:MET:HE1	1:C:236:THR:OG1	2.08	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: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
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:363:ARG:O	1:D:366:ILE:HG13	2.13	0.49
1:D:463:GLY:HA2	1:D:858:SER:HB2	1.94	0.48
1:A:102:MET:HE1	1:A:225:ARG:HG3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:GLN:CD	1:B:782:ARG:HB2	2.41	0.46
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:B:317:TYR:CB	1:B:321:MET:HE3	2.46	0.45
1:D:102:MET:HB3	1:D:105:MET:CE	2.42	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:A:257:LEU:C	1:A:257:LEU:HD12	2.42	0.45
1:C:105:MET:HE1	1:C:236:THR:HG21	1.99	0.45
1:C:623:PRO:HD2	1:C:673:LEU:HD12	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: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:388:TYR:CD1	1:A:388:TYR:C	2.95	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:D:257:LEU:C	1:D:257:LEU:HD12	2.43	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:A:547:ALA:O	1:A:611:MET:HE2	2.19	0.42
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:VAL:O	1:A:850:VAL:HG12	2.19	0.41
1:C:585:THR:HG1	1:C:588:GLN:H	1.68	0.41
1:D:216:TRP:CE2	1:D:235:GLY:HA2	2.55	0.41
1:B:259:THR:HG21	1:B:314:GLU:CD	2.46	0.41
1:C:105:MET:HE1	1:C:236:THR:CG2	2.50	0.41
1:C:119:VAL:HG21	1:C:135:TYR:CG	2.55	0.41
1:A:273:PHE:CZ	1:A:299:MET:HE1	2.56	0.41
1:A:669:ARG:HA	1:A:673:LEU:HD13	2.03	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: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:259:THR:OG1	1:D:314:GLU:OE2	2.37	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:D:388:TYR:CD1	1:D:388:TYR:C	2.99	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	72
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%)	691 (99%)	10 (1%)	59	85
1	B	378/715 (53%)	373 (99%)	5 (1%)	61	86
1	C	671/715 (94%)	668 (100%)	3 (0%)	84	94
1	D	702/715 (98%)	694 (99%)	8 (1%)	65	88
All	All	2452/2860 (86%)	2426 (99%)	26 (1%)	68	88

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	339	THR
1	A	455	SER
1	A	527	SER
1	A	631	GLU
1	A	657	GLU
1	A	833	ILE
1	B	320	MET
1	B	462	ARG
1	B	743	VAL
1	B	833	ILE
1	B	874	VAL
1	C	335	LEU
1	C	375	ASP
1	C	833	ILE
1	D	227	ILE
1	D	335	LEU
1	D	372[A]	GLN

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Mol	Chain	Res	Type
1	D	372[B]	GLN
1	D	441	HIS
1	D	527	SER
1	D	644	ASP
1	D	833	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	76	GLN
1	A	228	ASN
1	A	391	HIS
1	A	626	HIS
1	B	379	HIS
1	B	698	GLN
1	C	168	HIS
1	C	813	GLN
1	D	56	ASN
1	D	210	ASN
1	D	228	ASN
1	D	376	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 ⓘ

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
2	6NQ	D	901	3	31,33,33	2.54	8 (25%)	41,52,52	1.34	7 (17%)
4	PEP	D	903	3	9,9,9	1.74	2 (22%)	11,13,13	2.89	7 (63%)
4	PEP	C	903	3	9,9,9	1.80	2 (22%)	11,13,13	1.92	5 (45%)
4	PEP	A	903	3	9,9,9	1.92	2 (22%)	11,13,13	2.01	5 (45%)
2	6NQ	A	901	3	31,33,33	2.03	8 (25%)	41,52,52	1.69	7 (17%)
2	6NQ	C	901	3	31,33,33	2.66	6 (19%)	41,52,52	0.95	2 (4%)
4	PEP	B	901	3	9,9,9	1.47	3 (33%)	11,13,13	2.43	6 (54%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6NQ	D	901	3	-	4/18/38/38	0/3/3/3
4	PEP	D	903	3	-	6/9/9/9	-
4	PEP	C	903	3	-	6/9/9/9	-
4	PEP	A	903	3	-	6/9/9/9	-
2	6NQ	A	901	3	-	2/18/38/38	0/3/3/3
2	6NQ	C	901	3	-	5/18/38/38	0/3/3/3
4	PEP	B	901	3	-	2/9/9/9	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	6NQ	PB-O3A	10.34	1.71	1.59
2	D	901	6NQ	PB-O3A	10.23	1.71	1.59
2	C	901	6NQ	PB-O2B	6.40	1.55	1.46
2	A	901	6NQ	PA-O3A	-6.21	1.52	1.59
2	C	901	6NQ	PG-O3G	5.83	1.55	1.46
2	D	901	6NQ	PB-O2B	5.13	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	PEP	O1-C1	4.58	1.33	1.22
2	D	901	6NQ	PG-O3G	4.34	1.52	1.46
4	C	903	PEP	C2-C1	-3.89	1.45	1.49
2	A	901	6NQ	PG-O3G	3.83	1.52	1.46
2	A	901	6NQ	PB-O2B	3.68	1.51	1.46
4	D	903	PEP	C2-C1	-3.64	1.45	1.49
2	A	901	6NQ	PB-O3A	3.64	1.63	1.59
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	D	901	6NQ	PA-O3A	3.27	1.63	1.59
2	A	901	6NQ	PB-O1B	-3.25	1.48	1.56
2	A	901	6NQ	PB-N3B	3.22	1.71	1.63
2	D	901	6NQ	PB-N3B	2.97	1.71	1.63
4	C	903	PEP	O2-C2	2.83	1.46	1.39
2	D	901	6NQ	PB-O1B	-2.77	1.49	1.56
2	A	901	6NQ	PG-O1G	-2.76	1.49	1.56
4	A	903	PEP	C2-C1	-2.66	1.46	1.49
4	B	901	PEP	C2-C1	-2.48	1.46	1.49
2	D	901	6NQ	BR-C2'	2.36	2.02	1.96
4	B	901	PEP	O1-C1	2.35	1.28	1.22
4	D	903	PEP	O2-C2	2.31	1.45	1.39
2	C	901	6NQ	PA-O3A	2.20	1.61	1.59
4	B	901	PEP	P-O1P	2.05	1.56	1.50
2	D	901	6NQ	PA-O1A	-2.02	1.46	1.55

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	6NQ	O1G-PG-O3G	-6.68	96.70	113.45
2	A	901	6NQ	O2B-PB-N3B	-5.08	104.28	111.77
4	D	903	PEP	O1-C1-C2	-4.80	114.55	121.79
4	B	901	PEP	O1-C1-C2	-4.39	115.16	121.79
4	D	903	PEP	O2P-P-O2	4.34	117.94	105.32
4	B	901	PEP	O2P-P-O2	-4.10	93.37	105.32
2	D	901	6NQ	O2G-PG-O3G	-3.76	104.03	113.45
2	D	901	6NQ	O5'-PA-O2A	-3.47	95.19	108.94
2	A	901	6NQ	O3A-PB-N3B	3.37	115.93	106.59
4	A	903	PEP	O2-C2-C3	-3.37	118.42	124.85
4	A	903	PEP	O2P-P-O2	-3.34	95.59	105.32
2	D	901	6NQ	O3G-PG-N3B	3.28	116.59	111.77
4	D	903	PEP	O2-C2-C3	-3.22	118.70	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	PEP	O3P-P-O1P	3.17	123.19	110.83
4	D	903	PEP	O3P-P-O2P	-3.15	95.98	107.80
4	D	903	PEP	O3P-P-O1P	3.15	123.10	110.83
2	C	901	6NQ	O1G-PG-O3G	-3.06	105.78	113.45
4	C	903	PEP	O3P-P-O2P	2.97	118.93	107.80
2	D	901	6NQ	O1B-PB-O2B	-2.95	103.54	109.87
4	D	903	PEP	O3P-P-O2	-2.92	96.81	105.32
4	B	901	PEP	O2-P-O1P	2.92	118.82	109.47
2	C	901	6NQ	O5'-PA-O2A	2.86	120.27	108.94
4	C	903	PEP	O2P-P-O1P	-2.70	100.31	110.83
2	A	901	6NQ	O1B-PB-O3A	2.70	113.64	104.64
4	A	903	PEP	O1-C1-C2	-2.70	117.72	121.79
2	A	901	6NQ	O1G-PG-O2G	2.67	114.77	107.59
4	D	903	PEP	O2'-C1-C2	2.66	118.45	113.91
2	A	901	6NQ	O5'-PA-O2A	-2.61	98.60	108.94
4	B	901	PEP	O2'-C1-C2	2.57	118.30	113.91
4	C	903	PEP	O3P-P-O2	-2.55	97.89	105.32
4	A	903	PEP	O2'-C1-O1	2.55	129.97	123.90
4	C	903	PEP	O2-C2-C3	-2.43	120.21	124.85
4	B	901	PEP	O2P-P-O1P	2.41	120.21	110.83
2	A	901	6NQ	O1A-PA-O2A	2.36	123.42	112.44
4	B	901	PEP	O2-C2-C3	-2.28	120.50	124.85
2	D	901	6NQ	O1G-PG-O3G	2.19	118.93	113.45
2	D	901	6NQ	O1G-PG-O2G	-2.16	101.79	107.59
4	A	903	PEP	O2P-P-O1P	2.14	119.19	110.83
2	D	901	6NQ	O1A-PA-O5'	2.09	117.04	107.57

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	6NQ	PG-N3B-PB-O2B
2	A	901	6NQ	C5'-O5'-PA-O3A
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
2	D	901	6NQ	PB-N3B-PG-O3G
4	A	903	PEP	O1-C1-C2-C3
4	A	903	PEP	O2'-C1-C2-C3
4	A	903	PEP	O2'-C1-C2-O2
4	A	903	PEP	C1-C2-O2-P

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Mol	Chain	Res	Type	Atoms
4	A	903	PEP	C3-C2-O2-P
4	B	901	PEP	C1-C2-O2-P
4	B	901	PEP	C3-C2-O2-P
4	C	903	PEP	O2'-C1-C2-C3
4	C	903	PEP	O2'-C1-C2-O2
4	C	903	PEP	C3-C2-O2-P
4	D	903	PEP	O1-C1-C2-C3
4	D	903	PEP	O1-C1-C2-O2
4	D	903	PEP	O2'-C1-C2-C3
4	D	903	PEP	O2'-C1-C2-O2
4	D	903	PEP	C1-C2-O2-P
4	D	903	PEP	C3-C2-O2-P
2	D	901	6NQ	PB-O3A-PA-O2A
4	A	903	PEP	O1-C1-C2-O2
4	C	903	PEP	O1-C1-C2-O2
2	D	901	6NQ	C5'-O5'-PA-O2A
2	D	901	6NQ	C5'-O5'-PA-O3A
4	C	903	PEP	O1-C1-C2-C3
4	C	903	PEP	C1-C2-O2-P
2	C	901	6NQ	PB-O3A-PA-O2A

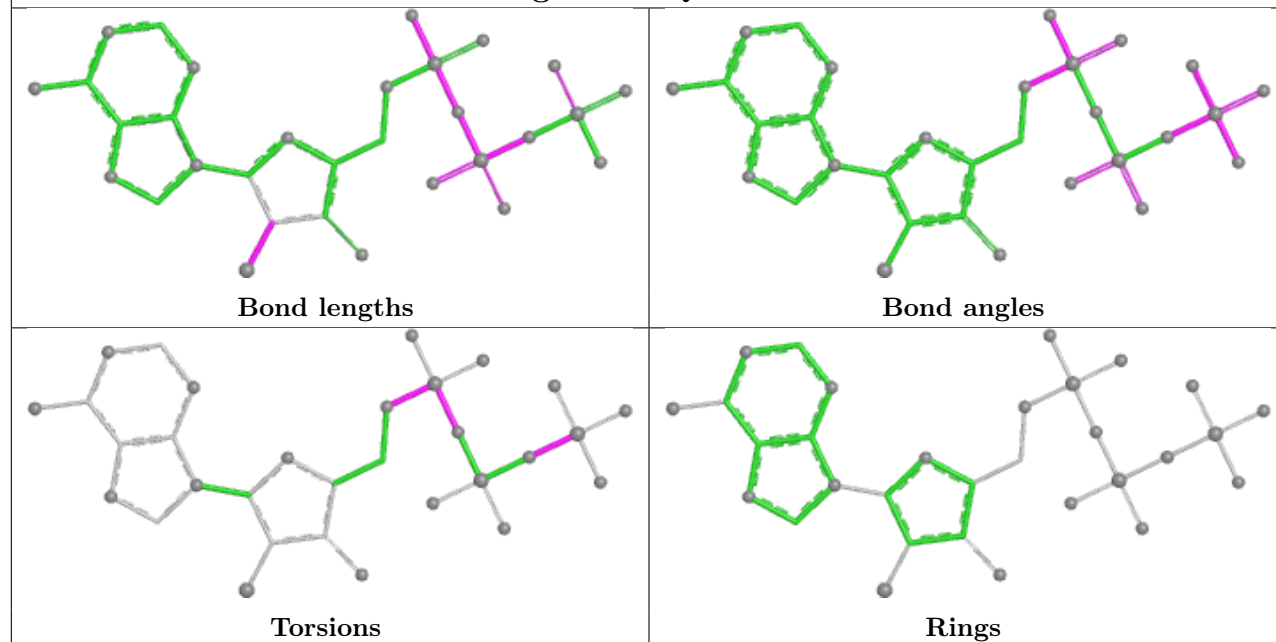
There are no ring outliers.

4 monomers are involved in 6 short contacts:

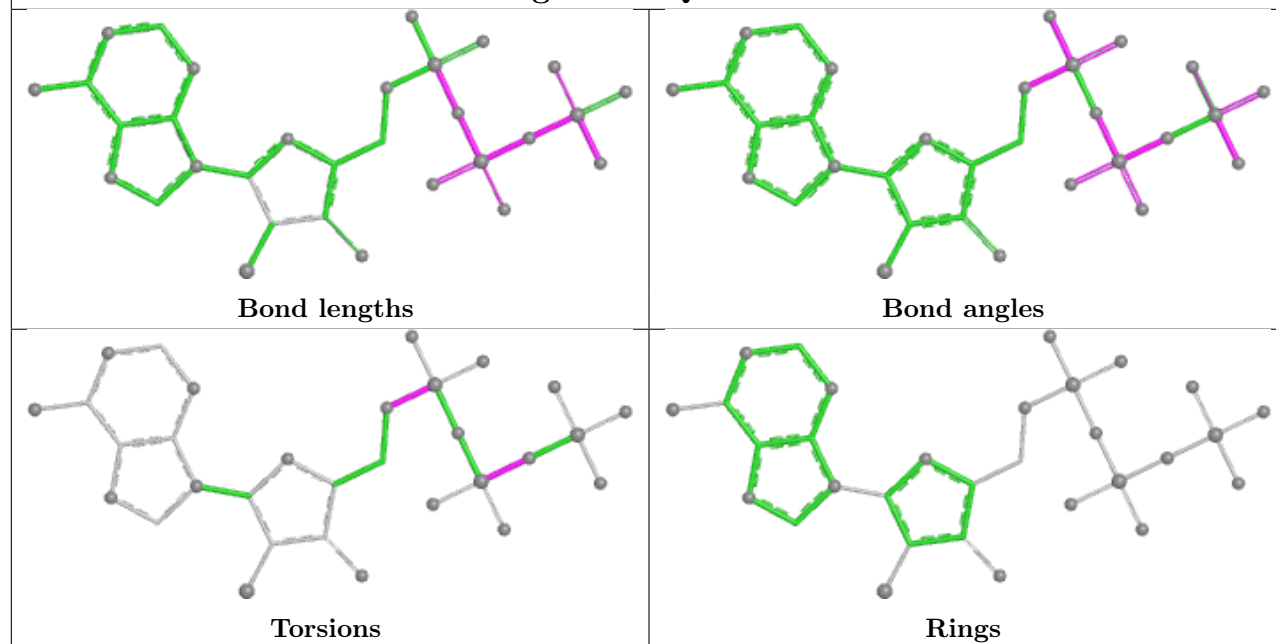
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	903	PEP	1	0
4	C	903	PEP	1	0
2	A	901	6NQ	2	0
2	C	901	6NQ	2	0

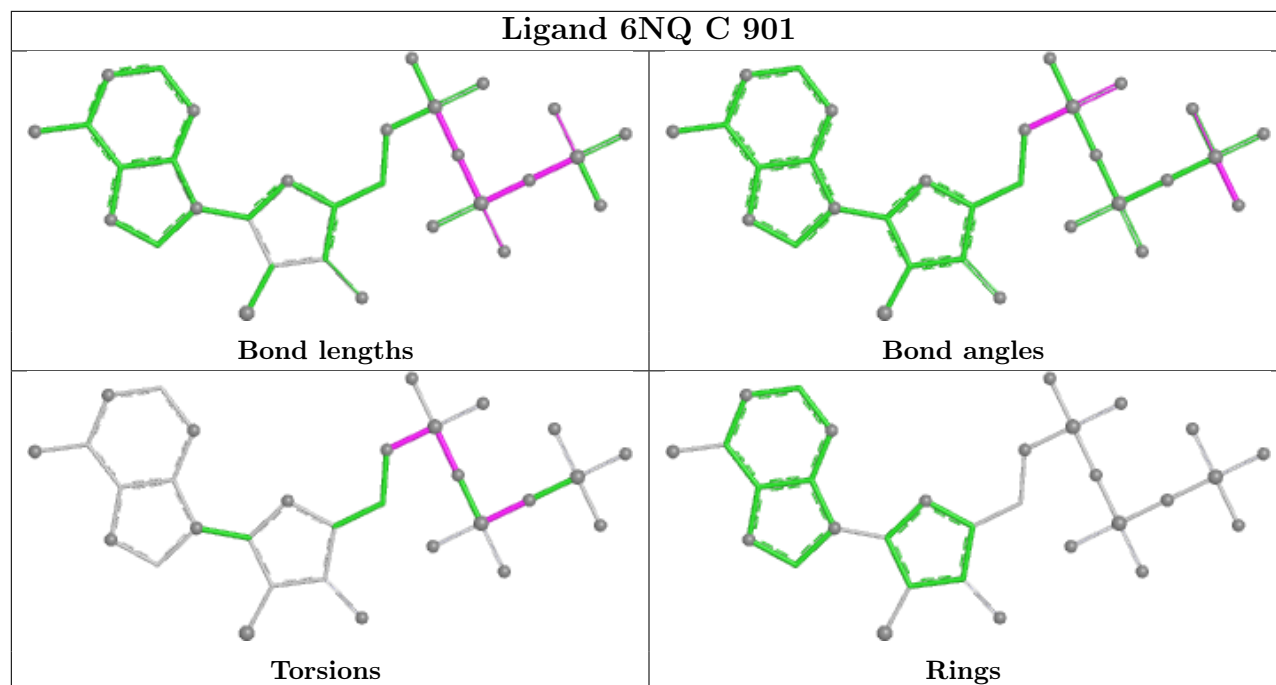
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 6NQ D 901



Ligand 6NQ A 901





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	874/874 (100%)	0.04	18 (2%) 63 54	24, 42, 79, 109	0
1	B	520/874 (59%)	0.18	43 (8%) 17 14	24, 43, 97, 133	0
1	C	859/874 (98%)	0.18	41 (4%) 35 28	20, 46, 87, 127	0
1	D	874/874 (100%)	-0.00	20 (2%) 61 52	16, 41, 71, 122	2 (0%)
All	All	3127/3496 (89%)	0.09	122 (3%) 43 35	16, 43, 86, 133	2 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	633	ASP	5.9
1	B	323	ILE	4.6
1	D	633	ASP	4.3
1	A	284	ALA	4.1
1	C	635	GLU	4.0
1	A	515	PRO	3.9
1	B	645	THR	3.9
1	B	646	GLY	3.8
1	C	633	ASP	3.8
1	D	635	GLU	3.7
1	B	453	MET	3.6
1	C	399	ALA	3.6
1	B	495	ASP	3.5
1	D	634	LEU	3.4
1	B	457	ALA	3.4
1	B	469	VAL	3.4
1	B	388	TYR	3.3
1	A	168	HIS	3.2
1	A	280	GLU	3.2
1	B	635	GLU	3.2
1	C	103	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	54	GLN	3.1
1	D	488	ASP	3.1
1	A	1	LYS	3.1
1	D	639	ASN	3.0
1	C	54	GLN	3.0
1	D	422	GLY	3.0
1	B	393	VAL	3.0
1	C	639	ASN	3.0
1	A	517	ALA	3.0
1	B	653	TYR	3.0
1	B	427	LEU	3.0
1	B	650	ASP	3.0
1	A	282	VAL	3.0
1	C	456	HIS	3.0
1	C	473	ALA	3.0
1	B	501	GLY	2.9
1	B	456	HIS	2.9
1	B	468	CYS	2.9
1	C	458	ALA	2.8
1	C	650	ASP	2.8
1	B	386	SER	2.8
1	B	390	SER	2.8
1	D	630	PRO	2.8
1	A	283	VAL	2.8
1	C	104	GLY	2.8
1	C	180	ASP	2.8
1	D	653	TYR	2.7
1	A	646	GLY	2.7
1	B	454	THR	2.6
1	A	520	ASN	2.6
1	C	1	LYS	2.6
1	B	392	VAL	2.6
1	C	625	LEU	2.6
1	C	648	SER	2.5
1	D	588	GLN	2.5
1	B	455	SER	2.5
1	D	638	VAL	2.5
1	C	195	GLU	2.5
1	C	454	THR	2.5
1	A	167	ILE	2.5
1	D	10	GLY	2.5
1	C	649	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	627	GLU	2.5
1	B	412	ALA	2.5
1	B	397	LEU	2.4
1	C	434	PRO	2.4
1	B	782	ARG	2.4
1	B	387	ALA	2.4
1	B	639	ASN	2.4
1	C	102	MET	2.4
1	B	385	PRO	2.4
1	C	141	MET	2.4
1	C	582	MET	2.4
1	B	630	PRO	2.4
1	B	459	VAL	2.4
1	D	11	ARG	2.3
1	B	410	PHE	2.3
1	C	784	ASP	2.3
1	A	635	GLU	2.3
1	C	642	ALA	2.3
1	B	381	GLN	2.3
1	C	645	THR	2.3
1	D	632	GLY	2.3
1	B	512	LEU	2.3
1	A	514	ALA	2.3
1	A	141	MET	2.3
1	C	431	GLU	2.3
1	B	407	GLN	2.3
1	C	82	SER	2.3
1	B	317	TYR	2.3
1	D	58	LYS	2.2
1	B	643	VAL	2.2
1	D	468	CYS	2.2
1	B	508	LEU	2.2
1	B	500	ASN	2.2
1	B	874	VAL	2.2
1	C	398	PRO	2.2
1	C	634	LEU	2.2
1	C	572	GLU	2.2
1	C	217	ASP	2.1
1	D	402	GLY	2.1
1	C	640	GLU	2.1
1	C	14	GLY	2.1
1	D	627	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	657	GLU	2.1
1	B	626	HIS	2.1
1	A	226	SER	2.1
1	C	568	PHE	2.1
1	B	316	HIS	2.0
1	C	160	GLN	2.0
1	D	636	HIS	2.0
1	C	516	PRO	2.0
1	C	502	THR	2.0
1	C	480	ASP	2.0
1	C	488	ASP	2.0
1	A	586	PRO	2.0
1	C	624	PRO	2.0
1	B	306	LEU	2.0
1	A	285	GLY	2.0
1	A	297	THR	2.0
1	B	425	ALA	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(Å ²)	Q<0.9
3	MG	C	902	1/1	0.89	0.09	34,34,34,34	0
2	6NQ	C	901	31/31	0.91	0.09	24,37,56,63	0
2	6NQ	D	901	31/31	0.92	0.09	21,27,34,63	0
3	MG	D	902	1/1	0.94	0.06	30,30,30,30	0
2	6NQ	A	901	31/31	0.95	0.07	19,28,34,55	0
3	MG	A	902	1/1	0.96	0.05	33,33,33,33	0

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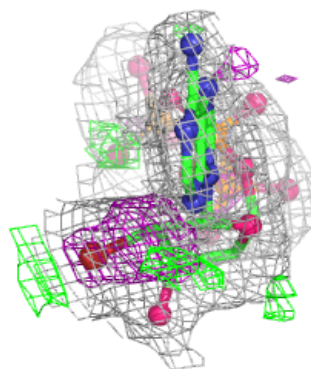
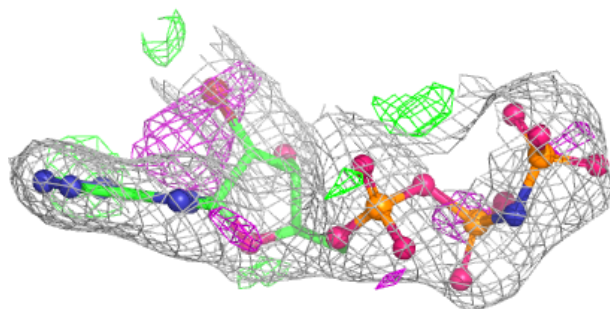
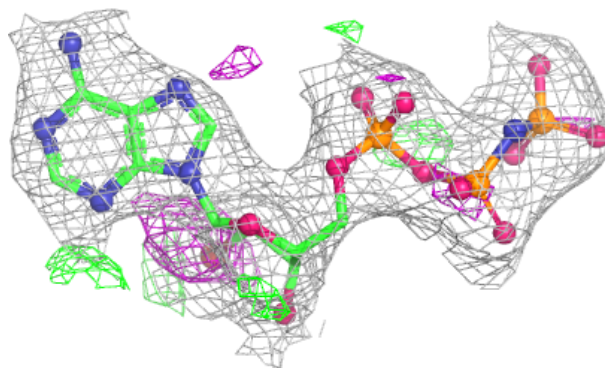
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEP	B	901	10/10	0.96	0.08	12,13,20,21	0
4	PEP	A	903	10/10	0.97	0.07	10,12,18,19	0
3	MG	A	904	1/1	0.97	0.09	23,23,23,23	0
4	PEP	C	903	10/10	0.97	0.09	24,26,31,34	0
4	PEP	D	903	10/10	0.97	0.08	22,24,26,27	0
3	MG	C	904	1/1	0.99	0.03	20,20,20,20	0
3	MG	B	902	1/1	0.99	0.07	25,25,25,25	0
3	MG	D	904	1/1	1.00	0.03	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.

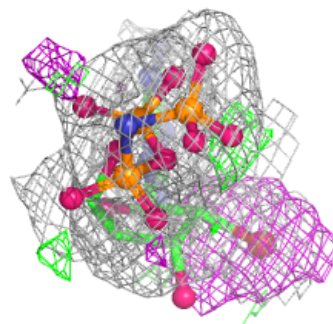
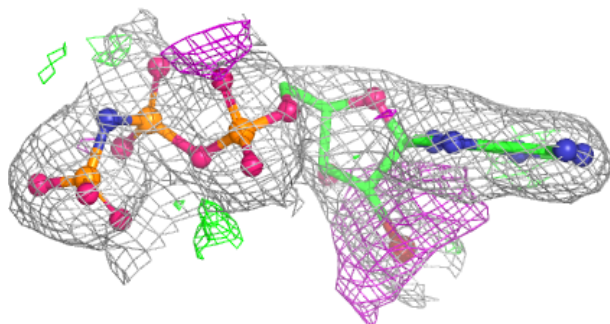
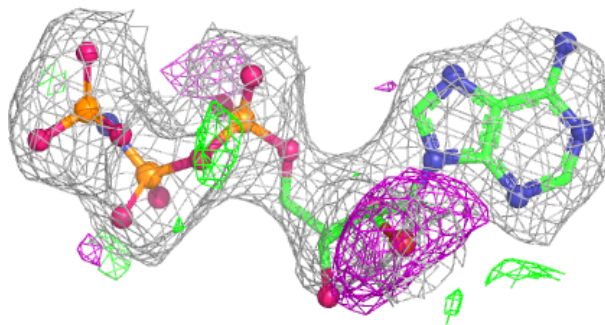
Electron density around 6NQ C 901:

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

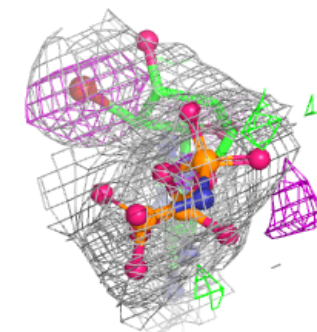
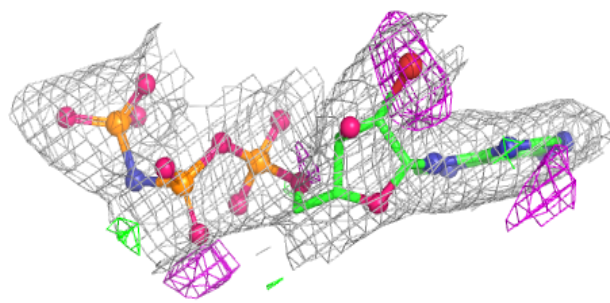
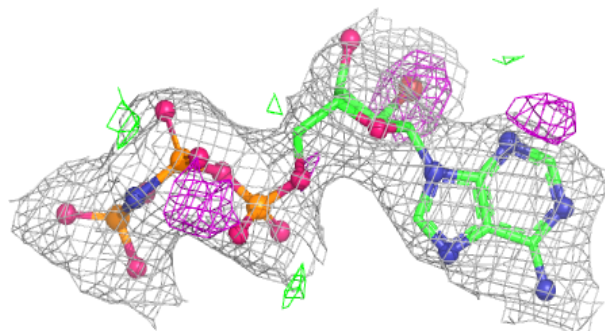


Electron density around 6NQ D 901:

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

**Electron density around 6NQ A 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.