



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:15 PM UTC

PDB ID : 4BER / pdb_00004ber
Title : Crystal structure of the Legionella pneumophila FIC domain-containing effector AnkX protein in complex with cytidine monophosphate
Authors : Campanacci, V.; Mukherjee, S.; Roy, C.R.; Cherfils, J.
Deposited on : 2013-03-12
Resolution : 2.60 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

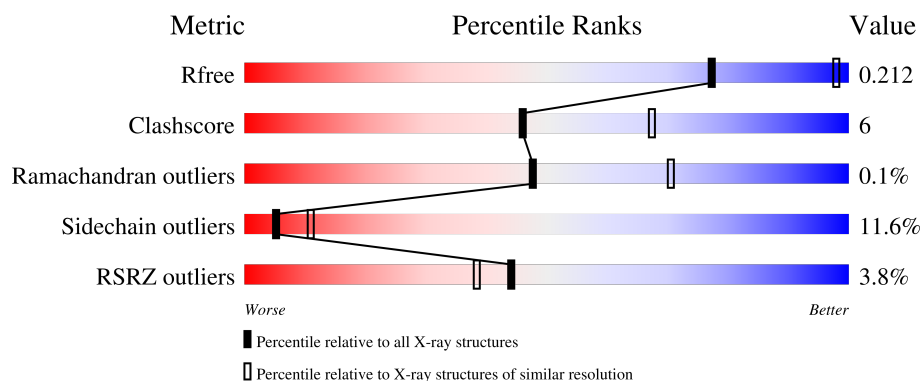
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	484	4% 74% 19% 5% .
1	B	484	3% 77% 17% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7755 atoms, of which 36 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.

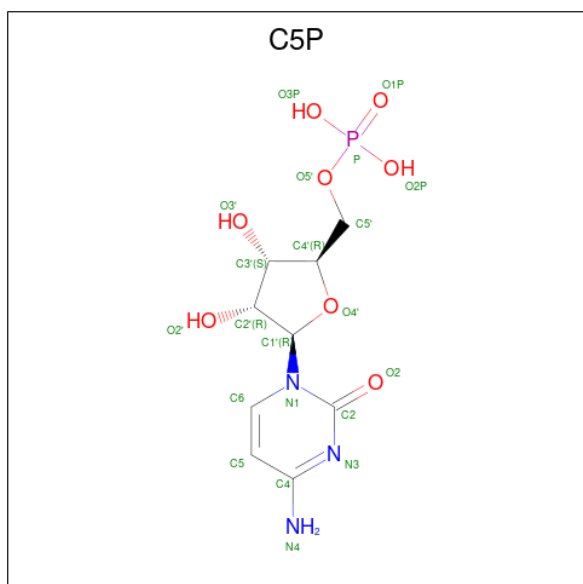
- Molecule 1 is a protein called PHOSPHOCHOLINE TRANSFERASE ANKX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3789	2429	633	710	17			
1	B	475	Total	C	N	O	S	0	0	0
			3789	2428	633	711	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q5ZXN6
A	247	PRO	LEU	engineered mutation	UNP Q5ZXN6
B	1	GLY	-	expression tag	UNP Q5ZXN6
B	247	PRO	LEU	engineered mutation	UNP Q5ZXN6

- Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	9	14	3	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			35	9	14	3	8	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	37	Total	O	0	0
			37	37		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	58.33Å 103.56Å 224.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.28 – 2.60 46.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.28-2.60) 99.7 (46.28-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.206 , 0.239 (Not available) , 0.212	Depositor DCC
R_{free} test set	2136 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7755	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, C5P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	3/3874 (0.1%)	1.42	25/5232 (0.5%)
1	B	0.85	4/3875 (0.1%)	1.43	19/5234 (0.4%)
All	All	0.84	7/7749 (0.1%)	1.43	44/10466 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	MET	SD-CE	-9.17	1.56	1.79
1	B	405	MET	SD-CE	-6.31	1.63	1.79
1	B	438	MET	SD-CE	-6.04	1.64	1.79
1	A	171	MET	SD-CE	-5.93	1.64	1.79
1	A	405	MET	SD-CE	-5.82	1.65	1.79
1	A	101	THR	CA-C	-5.24	1.49	1.52
1	B	171	MET	SD-CE	-5.06	1.66	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	LEU	N-CA-C	-7.84	97.86	109.15
1	B	429	LEU	N-CA-CB	7.77	121.66	110.16
1	A	228	LEU	N-CA-C	-7.75	98.00	109.15
1	B	350	GLN	CA-C-N	7.55	129.39	122.37
1	B	350	GLN	C-N-CA	7.55	129.39	122.37
1	B	348	ASN	N-CA-C	6.85	119.38	111.02
1	B	185	ALA	CA-C-N	6.55	129.53	120.49
1	B	185	ALA	C-N-CA	6.55	129.53	120.49
1	A	259	TYR	N-CA-C	-6.52	103.44	111.40
1	B	28	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	185	ALA	CA-C-N	6.33	129.23	120.49
1	A	185	ALA	C-N-CA	6.33	129.23	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ILE	N-CA-CB	6.29	117.38	110.53
1	A	28	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	88	VAL	CA-C-N	5.89	128.45	120.38
1	A	88	VAL	C-N-CA	5.89	128.45	120.38
1	B	437	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	259	TYR	N-CA-C	-5.72	103.80	112.04
1	A	204	GLU	N-CA-C	5.60	117.47	111.36
1	A	127	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	180	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	63	VAL	N-CA-CB	5.47	118.78	110.58
1	B	127	PHE	CA-CB-CG	5.46	119.25	113.80
1	A	348	ASN	CA-C-N	5.38	129.75	121.19
1	A	348	ASN	C-N-CA	5.38	129.75	121.19
1	A	180	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	383	GLU	CA-C-N	5.27	129.79	121.56
1	B	383	GLU	C-N-CA	5.27	129.79	121.56
1	A	256	ALA	N-CA-C	5.21	117.74	109.24
1	A	313	ASP	CA-C-N	5.16	127.62	120.29
1	A	313	ASP	C-N-CA	5.16	127.62	120.29
1	B	190	VAL	N-CA-CB	5.15	117.55	110.54
1	B	204	GLU	N-CA-C	5.14	117.79	111.82
1	B	256	ALA	N-CA-C	5.08	117.52	109.24
1	B	359	TYR	N-CA-C	5.07	119.60	113.41
1	A	239	PHE	N-CA-C	5.07	117.58	111.40
1	A	190	VAL	N-CA-CB	5.06	117.42	110.54
1	A	359	TYR	N-CA-C	5.05	119.57	113.41
1	A	126	VAL	N-CA-C	5.02	115.74	110.62
1	B	239	PHE	N-CA-C	5.01	117.51	111.40
1	A	367	LYS	CA-C-N	5.01	127.40	120.29
1	A	367	LYS	C-N-CA	5.01	127.40	120.29
1	A	383	GLU	CA-C-N	5.00	129.36	121.56
1	A	383	GLU	C-N-CA	5.00	129.36	121.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3789	0	3773	45	0
1	B	3789	0	3772	45	0
2	A	21	14	12	1	0
2	B	21	14	12	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	6	8	8	1	0
5	A	36	0	0	0	0
5	B	37	0	0	0	0
All	All	7719	36	7577	88	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 6.

All (88) 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:103:GLU:OE1	1:A:103:GLU:N	1.88	1.05
1:B:14:LEU:HB2	1:B:249:MET:HE1	1.47	0.94
1:A:260:GLU:OE1	1:A:262:ASN:HB2	1.85	0.75
1:B:437:ASN:HB3	1:B:440:ILE:HG12	1.75	0.68
1:B:59:ILE:HG12	1:B:76:LEU:HD11	1.77	0.67
1:A:374:ASN:H	1:A:377:GLN:HE21	1.42	0.67
1:B:228:LEU:O	1:B:230:PRO:HD3	1.95	0.66
1:B:374:ASN:H	1:B:377:GLN:HE21	1.43	0.66
1:A:33:SER:HB3	1:A:34:LYS:HE2	1.78	0.66
1:B:245:ASN:HD21	1:B:256:ALA:H	1.44	0.66
1:A:228:LEU:O	1:A:230:PRO:HD3	1.95	0.66
1:A:245:ASN:HD21	1:A:256:ALA:H	1.44	0.66
1:A:336:LEU:O	1:A:340:THR:HG23	1.96	0.66
1:A:405:MET:HE2	1:A:443:LYS:HD2	1.77	0.65
1:B:405:MET:HE2	1:B:443:LYS:HD2	1.79	0.64
1:B:427:THR:OG1	1:B:429:LEU:HD12	1.96	0.64
1:A:217:ILE:O	1:A:221:HIS:HD2	1.80	0.64
1:B:217:ILE:O	1:B:221:HIS:HD2	1.79	0.64
1:A:59:ILE:HD11	1:A:246:ILE:HD13	1.83	0.60
1:A:427:THR:H	1:A:430:HIS:CD2	2.21	0.57
1:B:336:LEU:O	1:B:340:THR:HG23	2.06	0.56
1:B:405:MET:HE2	1:B:443:LYS:HZ2	1.70	0.56
1:B:427:THR:H	1:B:430:HIS:CD2	2.24	0.56
1:A:433:ALA:HB2	1:A:441:MET:HE1	1.89	0.54
1:A:102:ASP:N	1:A:103:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG22	1:B:4:ILE:HG12	1.91	0.51
1:A:263:VAL:HG11	1:A:388:PRO:HG3	1.93	0.51
1:A:405:MET:CE	1:A:443:LYS:HD2	2.40	0.51
1:A:188:LYS:HD3	1:A:189:ASN:H	1.75	0.51
1:B:467:THR:HG22	1:B:470:HIS:H	1.75	0.51
1:A:108:GLY:HA3	1:A:179:THR:HG21	1.93	0.51
1:B:108:GLY:HA3	1:B:179:THR:HG21	1.93	0.50
1:A:3:LYS:HE3	1:A:4:ILE:H	1.77	0.50
1:A:263:VAL:O	1:A:267:TYR:HB2	2.11	0.50
1:B:237:ARG:HA	1:B:241:ASN:HD22	1.77	0.49
1:B:263:VAL:O	1:B:267:TYR:HB2	2.12	0.49
1:B:220:LYS:HG2	1:B:224:MET:HE2	1.94	0.49
1:A:220:LYS:HG2	1:A:224:MET:HE2	1.95	0.49
1:A:405:MET:HE2	1:A:443:LYS:HZ2	1.77	0.48
1:B:282:ASN:O	1:B:286:ILE:HG12	2.14	0.48
1:A:245:ASN:ND2	1:A:256:ALA:H	2.11	0.48
1:A:188:LYS:HD3	1:A:189:ASN:N	2.28	0.48
1:A:174:TYR:CG	1:A:180:ASN:HB2	2.49	0.47
1:A:237:ARG:HA	1:A:241:ASN:HD22	1.79	0.47
1:A:29:GLY:HA2	1:A:32:TRP:CE2	2.49	0.47
1:A:134:GLU:HB2	1:A:184:LEU:HB3	1.96	0.47
1:A:282:ASN:O	1:A:286:ILE:HG12	2.15	0.47
1:A:44:ARG:NH1	2:A:1000:C5P:O2	2.47	0.47
1:A:467:THR:HG22	1:A:470:HIS:H	1.79	0.47
1:B:134:GLU:HB2	1:B:184:LEU:HB3	1.96	0.47
1:B:405:MET:CE	1:B:443:LYS:HD2	2.43	0.47
1:A:427:THR:H	1:A:430:HIS:HD2	1.60	0.46
1:B:29:GLY:HA2	1:B:32:TRP:CE2	2.50	0.46
1:B:174:TYR:CG	1:B:180:ASN:HB2	2.49	0.46
1:B:42:GLU:HG2	1:B:49:LEU:HD12	1.98	0.46
1:B:245:ASN:O	1:B:249:MET:HG3	2.15	0.46
1:A:259:TYR:H	4:A:3000:GOL:H12	1.81	0.46
1:A:211:LEU:HG	1:A:339:LYS:HE2	1.98	0.46
1:B:405:MET:HE1	1:B:440:ILE:HG22	1.98	0.46
1:A:42:GLU:HG2	1:A:49:LEU:HD12	1.97	0.45
1:B:10:GLY:O	1:B:249:MET:HE2	2.16	0.45
1:B:245:ASN:ND2	1:B:256:ALA:H	2.11	0.45
1:B:249:MET:HE3	1:B:255:PRO:HD3	1.99	0.44
1:A:101:THR:OG1	1:A:102:ASP:N	2.50	0.44
1:B:14:LEU:HB2	1:B:249:MET:CE	2.33	0.44
1:B:405:MET:CE	1:B:408:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HD11	1:A:246:ILE:CD1	2.47	0.43
1:B:309:THR:HG23	1:B:312:ARG:HH21	1.82	0.43
1:A:5:MET:HG3	1:B:5:MET:HE3	2.00	0.42
1:B:374:ASN:HD22	1:B:374:ASN:C	2.27	0.42
1:A:374:ASN:C	1:A:374:ASN:HD22	2.27	0.42
1:B:400:VAL:HG13	1:B:440:ILE:HD12	2.01	0.42
1:B:157:PRO:HA	1:B:160:ILE:HG23	2.02	0.41
1:A:344:LEU:O	1:A:347:LEU:HB2	2.20	0.41
1:B:254:PRO:HD3	1:B:340:THR:HG21	2.03	0.41
1:A:57:CYS:O	1:A:61:LEU:HD22	2.20	0.41
1:B:24:ARG:NH1	1:B:296:ILE:HD11	2.36	0.41
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.94	0.41
1:B:427:THR:H	1:B:430:HIS:HD2	1.65	0.41
1:A:332:ASN:HD22	1:A:333:PRO:HD2	1.86	0.41
1:A:157:PRO:HA	1:A:160:ILE:HG23	2.03	0.41
1:B:437:ASN:HB3	1:B:440:ILE:CG1	2.47	0.41
1:B:237:ARG:HA	1:B:241:ASN:HB2	2.03	0.41
1:B:332:ASN:HD22	1:B:333:PRO:HD2	1.85	0.40
1:A:59:ILE:O	1:A:63:VAL:HG13	2.21	0.40
1:A:254:PRO:HD2	1:A:280:ILE:HG23	2.02	0.40
1:B:254:PRO:HD2	1:B:280:ILE:HG23	2.02	0.40
1:B:127:PHE:CE1	1:B:228:LEU:HB2	2.57	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	471/484 (97%)	455 (97%)	16 (3%)	0	100	100
1	B	471/484 (97%)	455 (97%)	15 (3%)	1 (0%)	43	66
All	All	942/968 (97%)	910 (97%)	31 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	ASP

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	412/422 (98%)	361 (88%)	51 (12%)	4	9
1	B	413/422 (98%)	368 (89%)	45 (11%)	6	13
All	All	825/844 (98%)	729 (88%)	96 (12%)	5	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	20	GLU
1	A	28	ASP
1	A	34	LYS
1	A	42	GLU
1	A	53	LEU
1	A	59	ILE
1	A	61	LEU
1	A	63	VAL
1	A	72	LEU
1	A	82	LYS
1	A	88	VAL
1	A	98	GLU
1	A	143	PHE
1	A	149	LYS
1	A	160	ILE
1	A	163	LEU
1	A	166	GLN
1	A	173	LYS
1	A	186	VAL
1	A	188	LYS
1	A	190	VAL

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Mol	Chain	Res	Type
1	A	203	LYS
1	A	211	LEU
1	A	215	LEU
1	A	229	HIS
1	A	240	VAL
1	A	288	GLU
1	A	291	LYS
1	A	296	ILE
1	A	315	LEU
1	A	334	GLU
1	A	336	LEU
1	A	338	LEU
1	A	340	THR
1	A	341	GLN
1	A	347	LEU
1	A	349	GLU
1	A	360	LEU
1	A	368	LEU
1	A	371	SER
1	A	374	ASN
1	A	384	GLN
1	A	414	LYS
1	A	415	LYS
1	A	437	ASN
1	A	449	LEU
1	A	451	GLN
1	A	452	GLU
1	A	455	ILE
1	A	467	THR
1	B	20	GLU
1	B	28	ASP
1	B	42	GLU
1	B	53	LEU
1	B	59	ILE
1	B	72	LEU
1	B	82	LYS
1	B	90	GLU
1	B	103	GLU
1	B	160	ILE
1	B	163	LEU
1	B	166	GLN
1	B	186	VAL

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Mol	Chain	Res	Type
1	B	190	VAL
1	B	211	LEU
1	B	215	LEU
1	B	229	HIS
1	B	240	VAL
1	B	266	LEU
1	B	288	GLU
1	B	291	LYS
1	B	296	ILE
1	B	297	THR
1	B	305	LEU
1	B	327	ASP
1	B	331	LEU
1	B	336	LEU
1	B	338	LEU
1	B	340	THR
1	B	341	GLN
1	B	347	LEU
1	B	351	TYR
1	B	360	LEU
1	B	368	LEU
1	B	371	SER
1	B	374	ASN
1	B	384	GLN
1	B	401	ILE
1	B	415	LYS
1	B	429	LEU
1	B	435	CYS
1	B	441	MET
1	B	449	LEU
1	B	455	ILE
1	B	467	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	92	GLN
1	A	159	GLN
1	A	178	ASN
1	A	199	GLN
1	A	221	HIS

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	242	ASN
1	A	245	ASN
1	A	251	GLN
1	A	308	GLN
1	A	332	ASN
1	A	374	ASN
1	A	377	GLN
1	A	380	GLN
1	A	430	HIS
1	A	437	ASN
1	A	463	ASN
1	A	464	HIS
1	B	159	GLN
1	B	178	ASN
1	B	199	GLN
1	B	221	HIS
1	B	241	ASN
1	B	242	ASN
1	B	245	ASN
1	B	251	GLN
1	B	262	ASN
1	B	308	GLN
1	B	332	ASN
1	B	374	ASN
1	B	377	GLN
1	B	380	GLN
1	B	430	HIS
1	B	437	ASN

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

7 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
3	PO4	A	2000	-	4,4,4	1.35	1 (25%)	6,6,6	0.44	0
2	C5P	B	1000	-	22,22,22	0.32	0	32,33,33	0.44	0
3	PO4	B	2000	-	4,4,4	1.30	1 (25%)	6,6,6	0.50	0
2	C5P	A	1000	-	22,22,22	0.22	0	32,33,33	0.48	0
3	PO4	A	2001	-	4,4,4	1.42	1 (25%)	6,6,6	0.45	0
4	GOL	A	3000	-	5,5,5	0.15	0	5,5,5	0.45	0
3	PO4	B	2001	-	4,4,4	1.24	1 (25%)	6,6,6	0.41	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
2	C5P	A	1000	-	-	3/10/26/26	0/2/2/2
4	GOL	A	3000	-	-	2/4/4/4	-
2	C5P	B	1000	-	-	3/10/26/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	PO4	P-O1	2.70	1.56	1.50
3	A	2000	PO4	P-O1	2.53	1.56	1.50
3	B	2000	PO4	P-O1	2.43	1.56	1.50
3	B	2001	PO4	P-O1	2.29	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

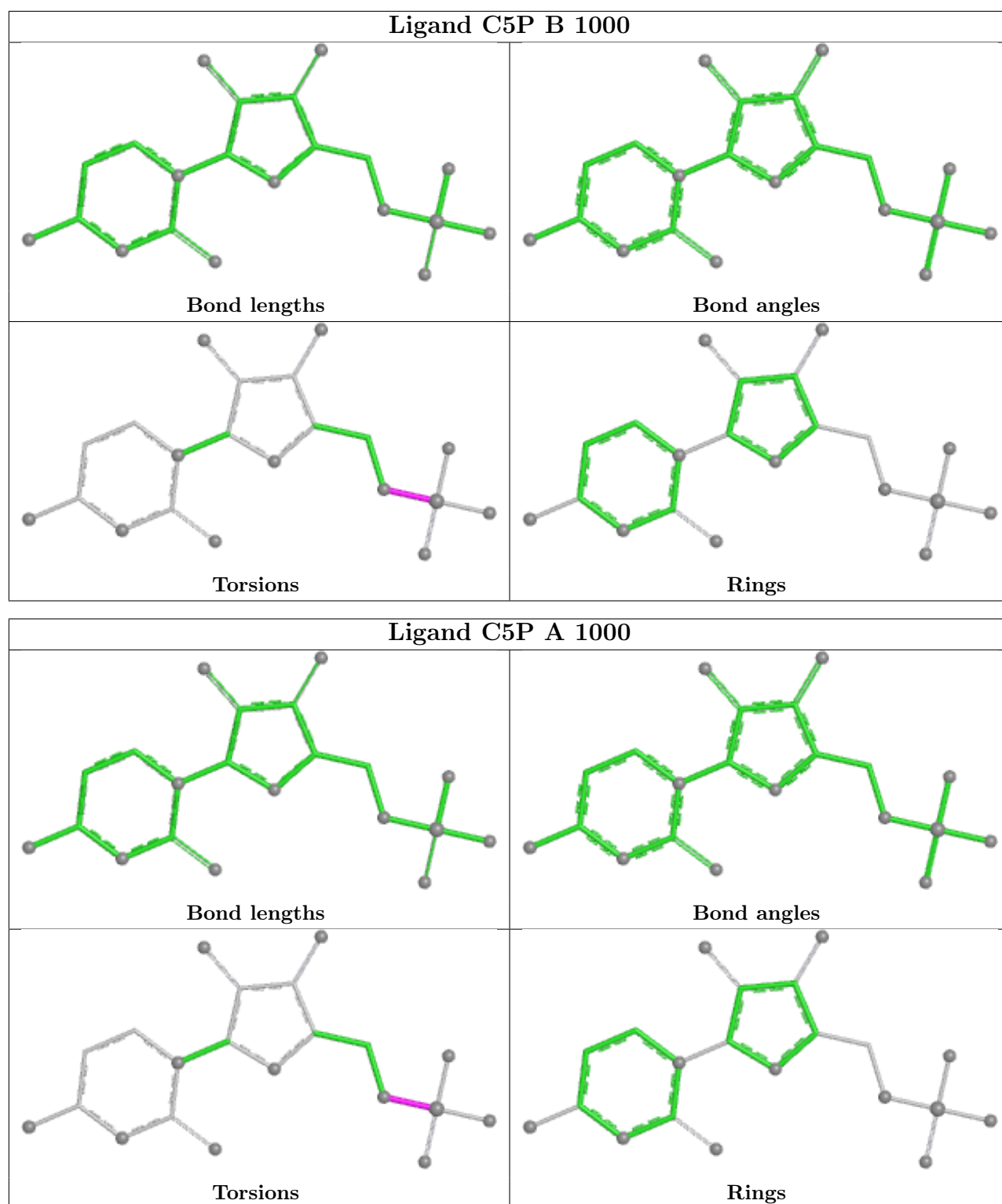
Mol	Chain	Res	Type	Atoms
2	A	1000	C5P	C5'-O5'-P-O3P
2	A	1000	C5P	C5'-O5'-P-O2P
2	B	1000	C5P	C5'-O5'-P-O3P
4	A	3000	GOL	O1-C1-C2-O2
4	A	3000	GOL	O1-C1-C2-C3
2	A	1000	C5P	C5'-O5'-P-O1P
2	B	1000	C5P	C5'-O5'-P-O1P
2	B	1000	C5P	C5'-O5'-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	C5P	1	0
4	A	3000	GOL	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 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 ⓘ

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	475/484 (98%)	0.25	20 (4%) 40 35	37, 62, 101, 123	1 (0%)
1	B	475/484 (98%)	0.17	16 (3%) 48 42	39, 62, 103, 136	1 (0%)
All	All	950/968 (98%)	0.21	36 (3%) 44 38	37, 62, 102, 136	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	479	GLU	5.3
1	A	331	LEU	4.9
1	B	85	GLY	4.8
1	A	86	LYS	3.9
1	B	91	LEU	3.9
1	B	331	LEU	3.8
1	A	143	PHE	3.8
1	A	477	THR	3.4
1	A	147	PHE	3.4
1	A	328	PHE	3.3
1	B	328	PHE	3.2
1	B	94	LYS	3.1
1	A	470	HIS	3.0
1	A	88	VAL	2.8
1	B	470	HIS	2.8
1	B	92	GLN	2.6
1	A	4	ILE	2.6
1	A	85	GLY	2.5
1	A	262	ASN	2.5
1	B	327	ASP	2.4
1	A	305	LEU	2.4
1	B	440	ILE	2.4
1	A	91	LEU	2.3
1	A	449	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	LYS	2.3
1	B	95	ASN	2.2
1	B	93	GLU	2.2
1	A	146	ARG	2.2
1	A	145	PRO	2.2
1	B	453	ASP	2.2
1	B	478	PRO	2.1
1	A	93	GLU	2.1
1	B	297	THR	2.1
1	B	330	ASP	2.1
1	A	95	ASN	2.1
1	A	16	ALA	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

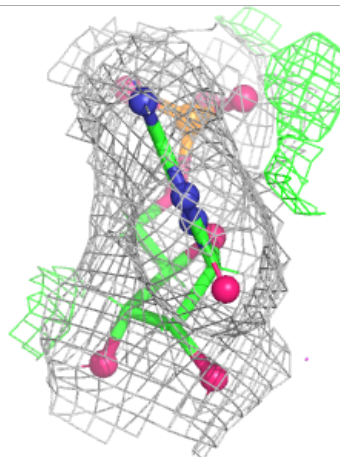
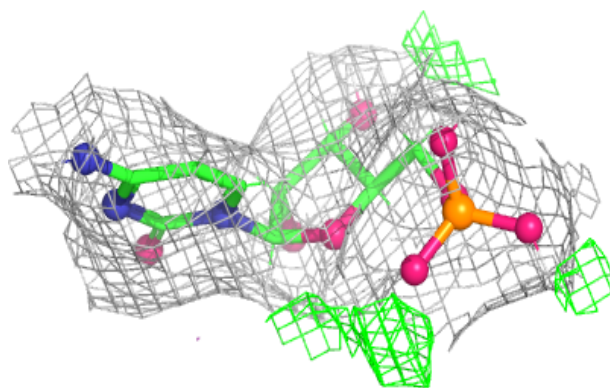
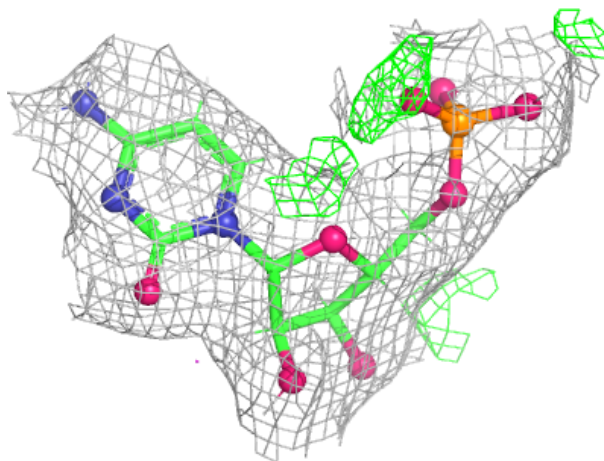
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

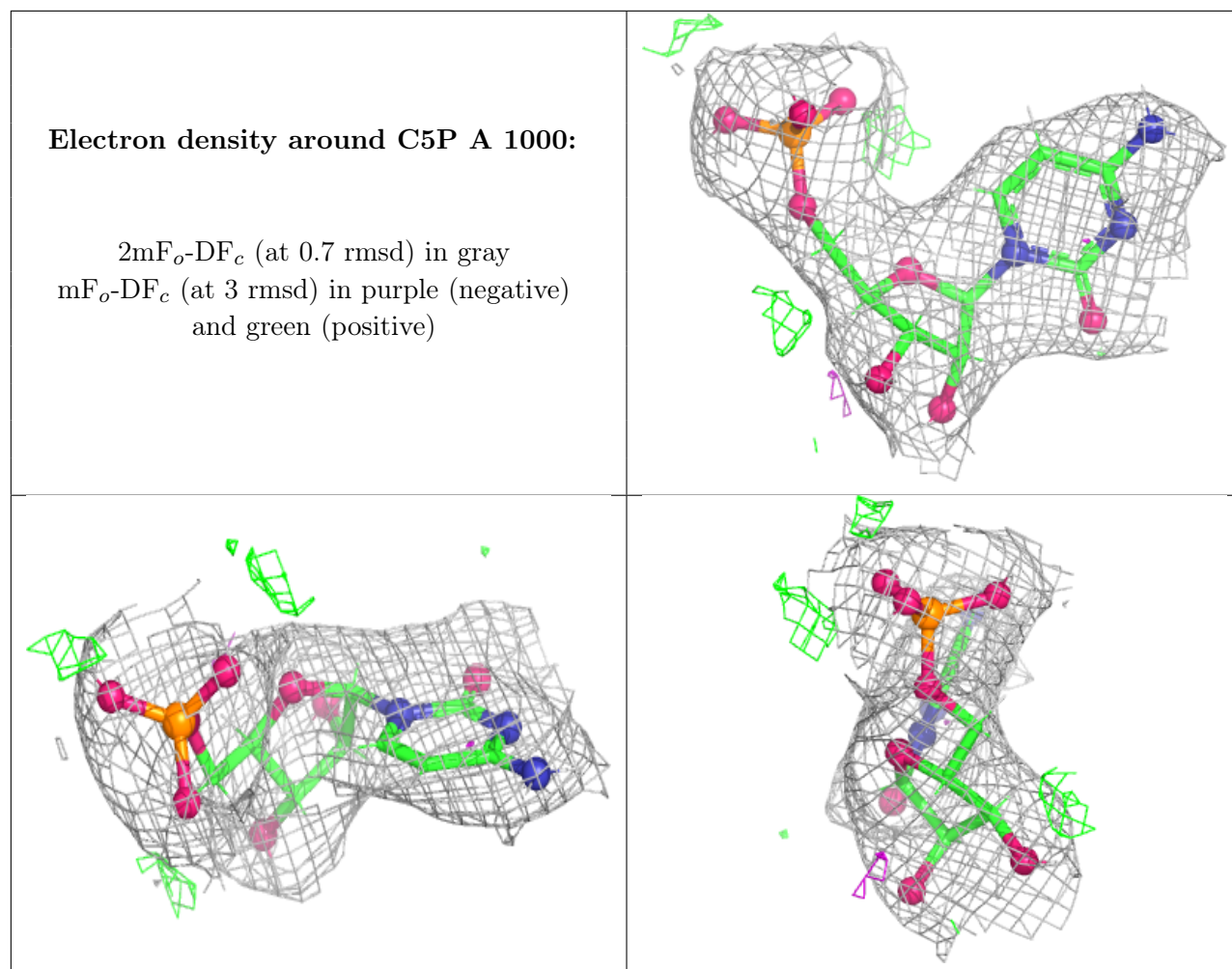
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	3000	6/6	0.79	0.21	36,48,55,55	0
3	PO4	A	2000	5/5	0.81	0.20	120,120,121,122	0
3	PO4	B	2000	5/5	0.82	0.15	125,125,125,125	0
3	PO4	A	2001	5/5	0.85	0.14	113,113,115,115	0
2	C5P	B	1000	21/21	0.92	0.07	57,62,65,65	0
3	PO4	B	2001	5/5	0.93	0.15	81,81,82,83	0
2	C5P	A	1000	21/21	0.95	0.07	57,59,64,66	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 C5P B 1000:

$2mF_o-DF_c$ (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.