Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:51 AM EDT

PDB ID	:	3DKL / pdb_00003dkl
Title	:	Crystal structure of phosphorylated mimic form of human NAMPT complexed with benzamide and phosphoribosyl pyrophosphate
Authors	:	Ho, M.; Burgos, E.S.; Almo, S.C.; Schramm, V.L.
Deposited on	:	2008-06-25
Resolution	:	1.89 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:

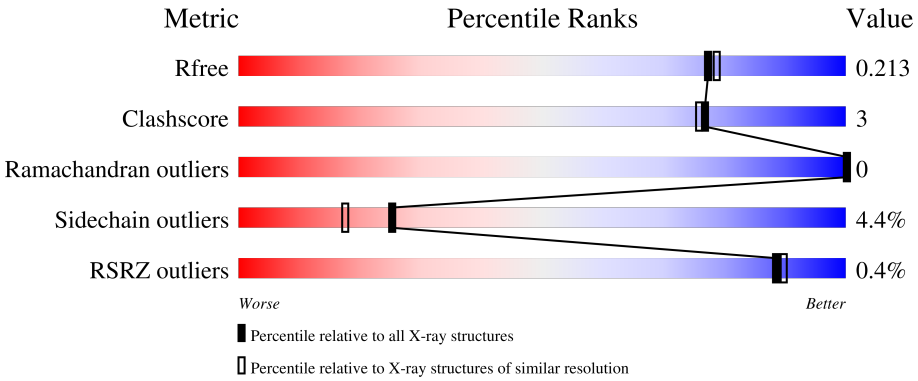
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	484	87% 8%
1	B	484	85% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7943 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.

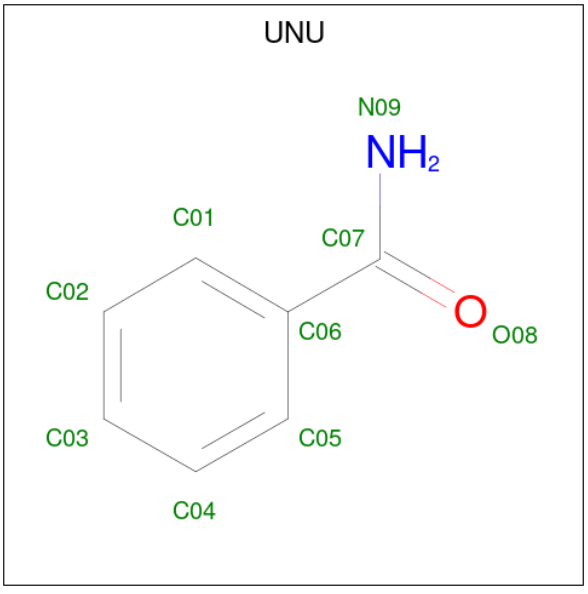
- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	3	0
			3729	2401	614	707	7			
1	B	464	Total	C	N	O	S	0	1	0
			3717	2392	613	705	7			

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

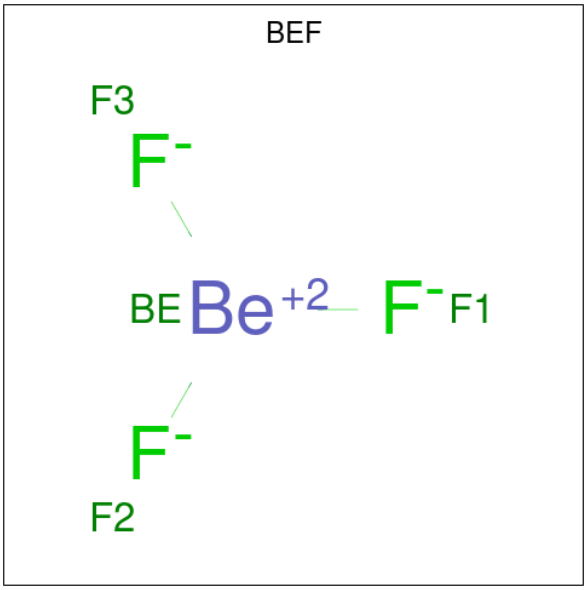
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is BENZAMIDE (CCD ID: UNU) (formula: C_7H_7NO).



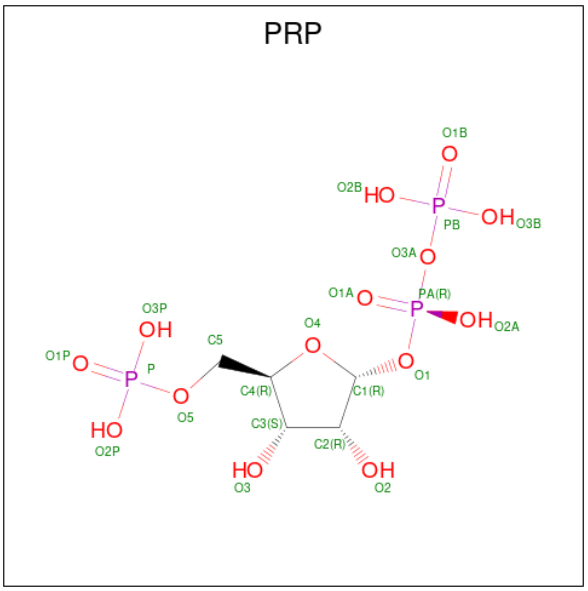
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 7 1 1	0	0
3	B	1	Total C N O 9 7 1 1	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Be F 4 1 3	0	0
4	B	1	Total Be F 4 1 3	0	0

- Molecule 5 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (CCD ID: PRP) (formula: $C_5H_{13}O_{14}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			22	5	14	3		
5	B	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 6 is water.

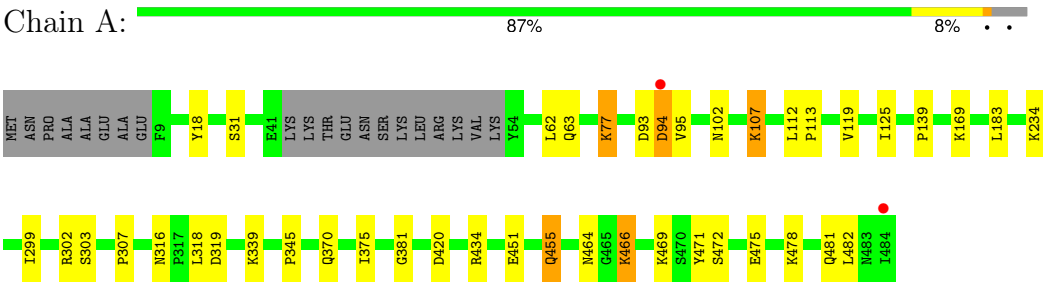
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total	O	0	0
			199	199		
6	B	224	Total	O	0	0
			224	224		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

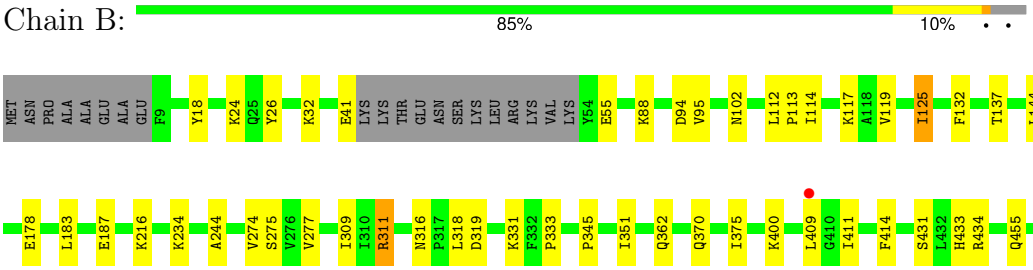
• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain A:



• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.13Å 106.59Å 83.24Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	28.56 – 1.89 28.56 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.6 (28.56-1.89) 96.5 (28.56-1.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.214 0.176 , 0.213	Depositor DCC
R_{free} test set	4084 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7943	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, UNU, MG, PRP

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	1.07	3/3826 (0.1%)	1.03	6/5184 (0.1%)
1	B	1.06	3/3808 (0.1%)	1.03	9/5161 (0.2%)
All	All	1.06	6/7634 (0.1%)	1.03	15/10345 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ILE	CA-CB	9.49	1.61	1.54
1	B	311	ARG	CD-NE	-6.12	1.37	1.46
1	B	125	ILE	CA-CB	5.71	1.58	1.54
1	A	119	VAL	CA-C	5.70	1.59	1.52
1	A	307	PRO	CA-C	5.38	1.59	1.52
1	B	274	VAL	CA-CB	5.01	1.61	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	ARG	NE-CZ-NH2	-10.35	109.89	119.20
1	A	302	ARG	NE-CZ-NH2	-6.83	113.06	119.20
1	A	94	ASP	N-CA-C	6.29	119.97	112.93
1	B	26	TYR	CA-C-N	-6.10	115.21	119.66
1	B	26	TYR	C-N-CA	-6.10	115.21	119.66
1	A	381	GLY	N-CA-C	-6.00	100.95	111.46
1	A	345	PRO	O-C-N	5.90	124.03	121.31
1	B	311	ARG	CA-C-N	-5.73	114.36	120.03
1	B	311	ARG	C-N-CA	-5.73	114.36	120.03
1	B	311	ARG	CG-CD-NE	-5.62	99.64	112.00
1	B	187	GLU	CA-CB-CG	-5.60	102.90	114.10
1	A	420	ASP	CA-C-N	5.45	125.80	119.47
1	A	420	ASP	C-N-CA	5.45	125.80	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	146	ASN	N-CA-C	5.15	119.28	112.89
1	B	311	ARG	NE-CZ-NH1	5.01	126.51	121.50

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	3729	0	3711	20	0
1	B	3717	0	3692	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	7	0	0
3	B	9	0	7	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	B	44	0	14	1	0
6	A	199	0	0	1	0
6	B	224	0	0	2	0
All	All	7943	0	7431	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (44) 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:469:LYS:HE2	6:A:645:HOH:O	1.59	1.02
1:B:484:ILE:H	1:B:484:ILE:HD13	1.30	0.96
1:A:316:ASN:HD22	1:A:319:ASP:H	1.28	0.78
1:B:316:ASN:HD22	1:B:319:ASP:H	1.37	0.70
1:B:431:SER:OG	1:B:433:HIS:HE1	1.76	0.67
1:A:63:GLN:HE22	1:A:471:TYR:H	1.44	0.63
1:B:311:ARG:NH2	5:B:504:PRP:O2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ILE:H	1:B:484:ILE:CD1	2.08	0.60
1:A:478:LYS:HA	1:A:481:GLN:HE21	1.67	0.59
1:A:169:LYS:HG2	1:A:482:LEU:HD11	1.85	0.58
1:A:113:PRO:HA	1:A:464:ASN:HD22	1.70	0.55
1:A:472:SER:OG	1:A:475:GLU:HG3	2.07	0.54
1:B:333:PRO:HD2	1:B:345:PRO:HG3	1.91	0.52
1:B:484:ILE:HD13	1:B:484:ILE:N	2.13	0.52
1:A:31:SER:HB2	1:A:139:PRO:HB3	1.91	0.51
1:A:478:LYS:HG3	1:A:481:GLN:NE2	2.26	0.49
1:A:316:ASN:ND2	1:A:319:ASP:H	2.04	0.49
1:A:107:LYS:HA	1:A:107:LYS:HE3	1.95	0.49
1:A:112:LEU:O	1:A:464:ASN:HA	2.14	0.48
1:B:88:LYS:O	1:B:88:LYS:HD2	2.14	0.47
1:B:244:ALA:HA	1:B:275:SER:O	2.15	0.47
1:B:311:ARG:HG3	1:B:351:ILE:HG23	1.96	0.47
1:B:277:VAL:HA	1:B:311:ARG:HB3	1.97	0.47
1:B:175:TYR:HB3	1:B:375:ILE:HG13	1.98	0.46
1:A:77:LYS:HA	1:A:77:LYS:HD2	1.40	0.46
1:A:31:SER:O	1:A:139:PRO:HA	2.17	0.45
1:A:478:LYS:HG3	1:A:481:GLN:HE22	1.82	0.45
1:B:117:LYS:O	1:B:132:PHE:HA	2.18	0.43
1:B:362:GLN:NE2	6:B:650:HOH:O	2.51	0.43
1:B:414:PHE:N	1:B:414:PHE:CD2	2.86	0.43
1:B:275:SER:HA	1:B:309:ILE:O	2.19	0.43
1:A:291:TRP:CE3	1:A:299:ILE:HD11	2.55	0.42
1:A:455:GLN:HE21	1:A:455:GLN:HB2	1.59	0.42
1:B:114:ILE:HD11	1:B:144:LEU:HG	2.02	0.41
1:B:137:THR:OG1	1:B:464:ASN:ND2	2.48	0.41
1:B:434:ARG:HA	1:B:434:ARG:HD3	1.88	0.41
1:B:331:LYS:HD2	1:B:331:LYS:HA	1.88	0.41
1:B:112:LEU:O	1:B:464:ASN:HA	2.21	0.41
1:B:113:PRO:HA	1:B:464:ASN:HD22	1.86	0.41
1:A:93:ASP:OD2	1:A:94:ASP:N	2.54	0.41
1:B:400:LYS:NZ	6:B:637:HOH:O	2.49	0.41
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.35	0.40
1:A:466:LYS:HA	1:A:466:LYS:HD2	1.87	0.40
1:B:119:VAL:HG21	1:B:125:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/484 (96%)	449 (97%)	14 (3%)	0	100	100
1	B	461/484 (95%)	449 (97%)	12 (3%)	0	100	100
All	All	924/968 (96%)	898 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/425 (97%)	393 (96%)	18 (4%)	25	17
1	B	409/425 (96%)	391 (96%)	18 (4%)	25	17
All	All	820/850 (96%)	784 (96%)	36 (4%)	25	17

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	62	LEU
1	A	77	LYS
1	A	95	VAL
1	A	102	ASN
1	A	107	LYS
1	A	183	LEU
1	A	234	LYS

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Mol	Chain	Res	Type
1	A	255	LYS
1	A	303	SER
1	A	318	LEU
1	A	339	LYS
1	A	370	GLN
1	A	375	ILE
1	A	434	ARG
1	A	451	GLU
1	A	455	GLN
1	A	466	LYS
1	B	18	TYR
1	B	24	LYS
1	B	32	LYS
1	B	41	GLU
1	B	55	GLU
1	B	94	ASP
1	B	95	VAL
1	B	102	ASN
1	B	178	GLU
1	B	183	LEU
1	B	216	LYS
1	B	234	LYS
1	B	318	LEU
1	B	370	GLN
1	B	409	LEU
1	B	411	ILE
1	B	455	GLN
1	B	484	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	102	ASN
1	A	268	GLN
1	A	305	GLN
1	A	316	ASN
1	A	370	GLN
1	A	412	ASN
1	A	455	GLN
1	A	464	ASN
1	A	481	GLN

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Mol	Chain	Res	Type
1	B	81	GLN
1	B	316	ASN
1	B	352	GLN
1	B	362	GLN
1	B	412	ASN
1	B	433	HIS
1	B	439	ASN
1	B	455	GLN
1	B	464	ASN
1	B	481	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	UNU	A	504	-	9,9,9	1.59	1 (11%)	11,11,11	1.27	2 (18%)
5	PRP	B	503	2	20,22,22	1.00	1 (5%)	32,35,35	1.26	2 (6%)
4	BEF	B	506	1	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BEF	A	505	1	0,3,3	-	-	-		
3	UNU	B	505	-	9,9,9	1.69	3 (33%)	11,11,11	0.81	0
5	PRP	B	504	2	20,22,22	1.04	1 (5%)	32,35,35	1.14	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PRP	B	504	2	-	1/16/33/33	0/1/1/1
3	UNU	B	505	-	-	0/4/4/4	0/1/1/1
3	UNU	A	504	-	-	0/4/4/4	0/1/1/1
5	PRP	B	503	2	-	1/16/33/33	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	PRP	PA-O3A	3.36	1.63	1.59
3	B	505	UNU	C01-C06	2.66	1.43	1.39
5	B	503	PRP	PA-O3A	2.65	1.62	1.59
3	A	504	UNU	C01-C06	2.40	1.43	1.39
3	B	505	UNU	C03-C04	2.33	1.43	1.38
3	B	505	UNU	C04-C05	2.15	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	503	PRP	O5-P-O1P	-2.96	98.44	106.44
5	B	504	PRP	C1-C2-C3	2.75	105.71	102.29
3	A	504	UNU	O08-C07-C06	2.65	122.83	119.60
3	A	504	UNU	O08-C07-N09	-2.31	119.28	122.62
5	B	504	PRP	O3P-P-O5	-2.12	101.15	106.67
5	B	504	PRP	O4-C1-C2	-2.05	102.38	104.98
5	B	503	PRP	O3P-P-O2P	2.02	115.37	107.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	PRP	C4-C5-O5-P

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Mol	Chain	Res	Type	Atoms
5	B	504	PRP	C4-C5-O5-P

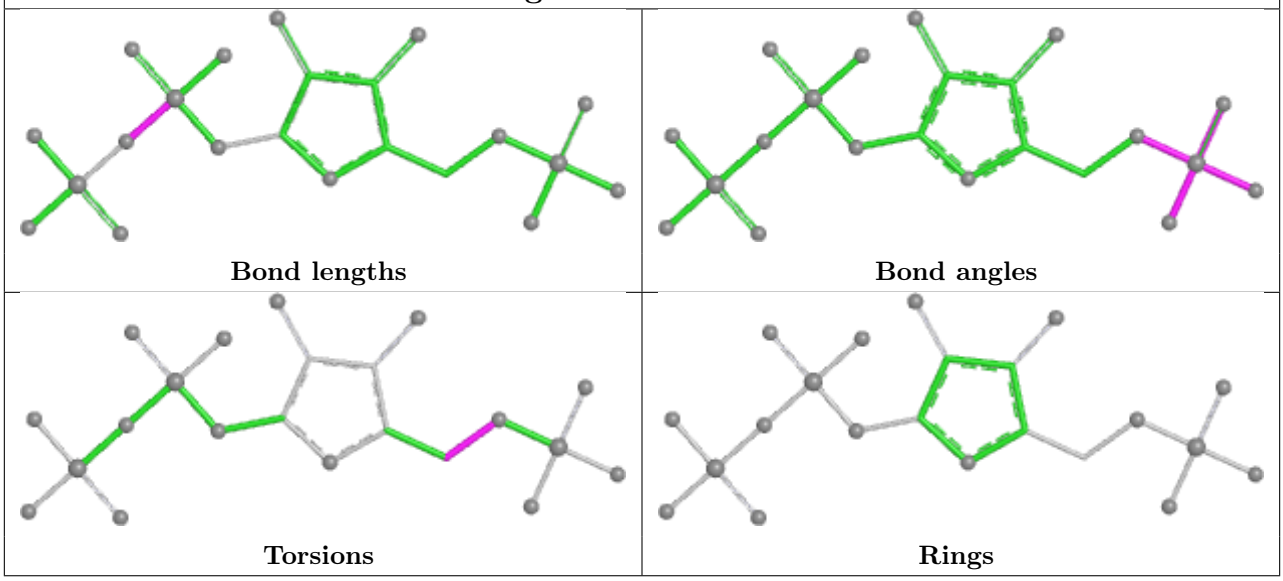
There are no ring outliers.

1 monomer is involved in 1 short contact:

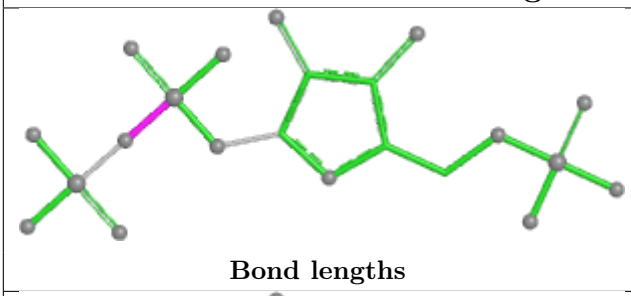
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	PRP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

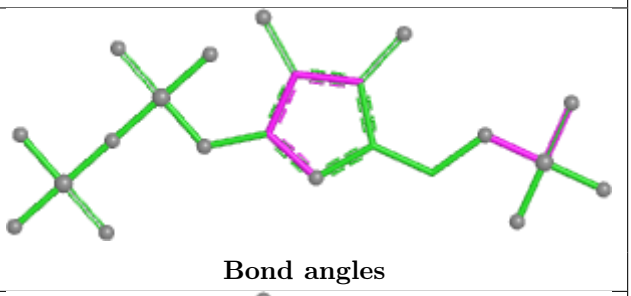
Ligand PRP B 503



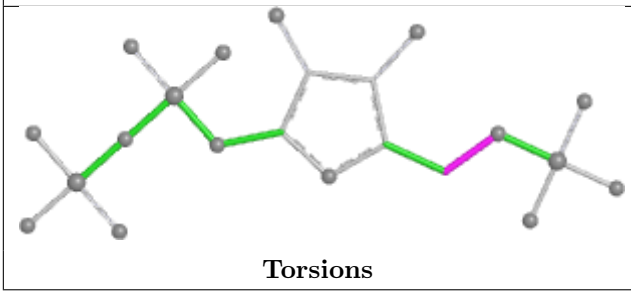
Ligand PRP B 504



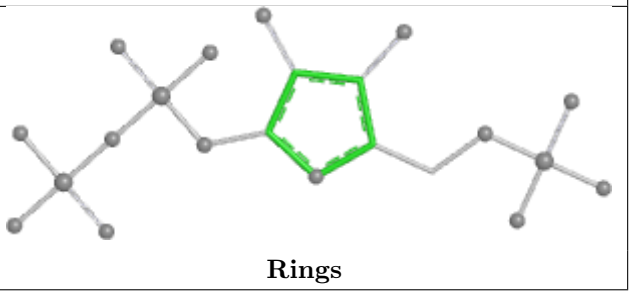
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	464/484 (95%)	-0.43	2 (0%)	88	90	13, 22, 34, 51	3 (0%)
1	B	464/484 (95%)	-0.43	2 (0%)	88	90	13, 22, 34, 49	1 (0%)
All	All	928/968 (95%)	-0.43	4 (0%)	88	90	13, 22, 34, 51	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	ILE	4.7
1	B	484	ILE	3.7
1	B	409	LEU	2.6
1	A	94	ASP	2.1

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

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

6.3 Carbohydrates

There are no 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, 95^{th} 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	UNU	A	504	9/9	0.95	0.06	15,18,18,20	0

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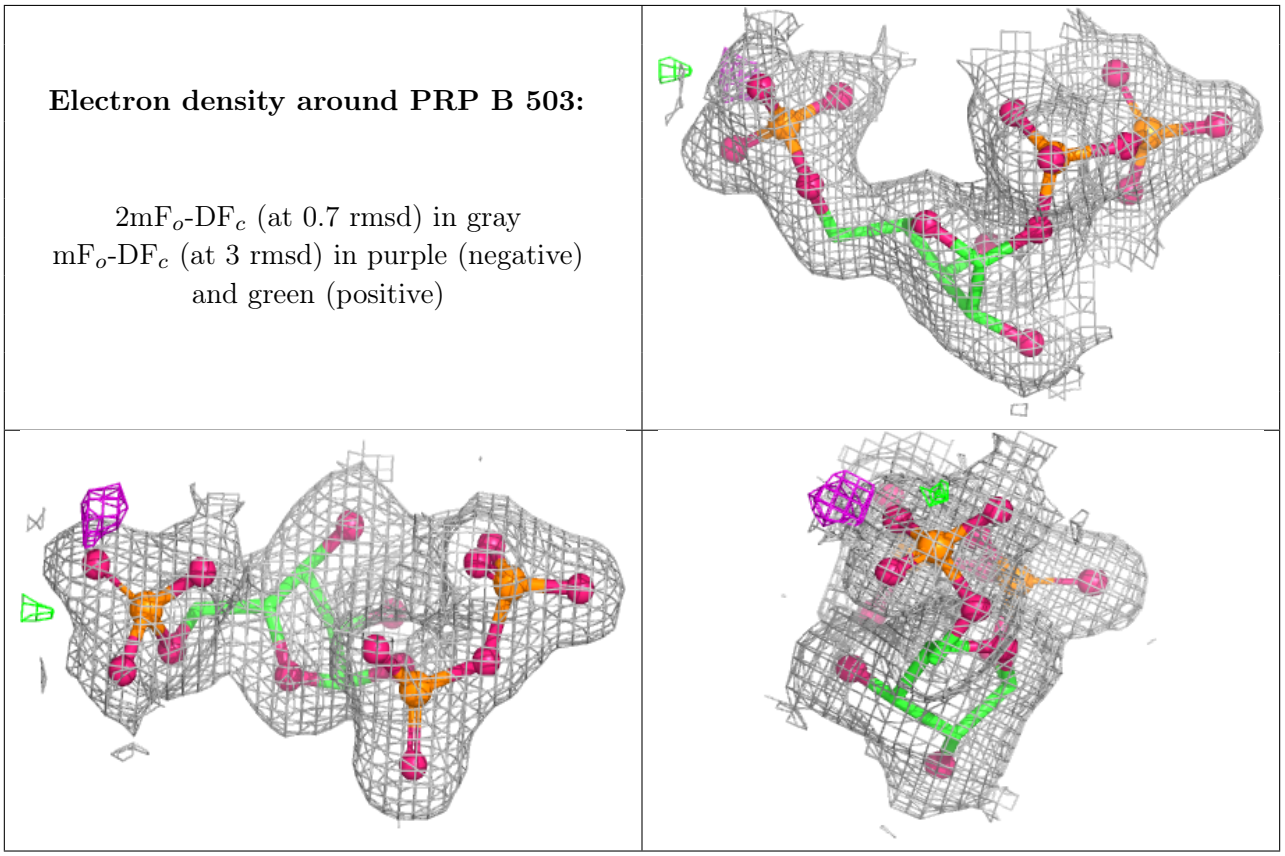
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BEF	A	505	4/4	0.95	0.07	20,21,21,24	0
4	BEF	B	506	4/4	0.95	0.07	18,20,23,24	0
3	UNU	B	505	9/9	0.96	0.05	17,18,20,20	0
2	MG	A	502	1/1	0.98	0.03	23,23,23,23	0
2	MG	B	501	1/1	0.99	0.02	21,21,21,21	0
2	MG	B	502	1/1	0.99	0.03	20,20,20,20	0
2	MG	A	501	1/1	0.99	0.03	22,22,22,22	0
5	PRP	B	503	22/22	0.99	0.04	14,19,22,24	0
5	PRP	B	504	22/22	0.99	0.04	17,19,21,23	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.

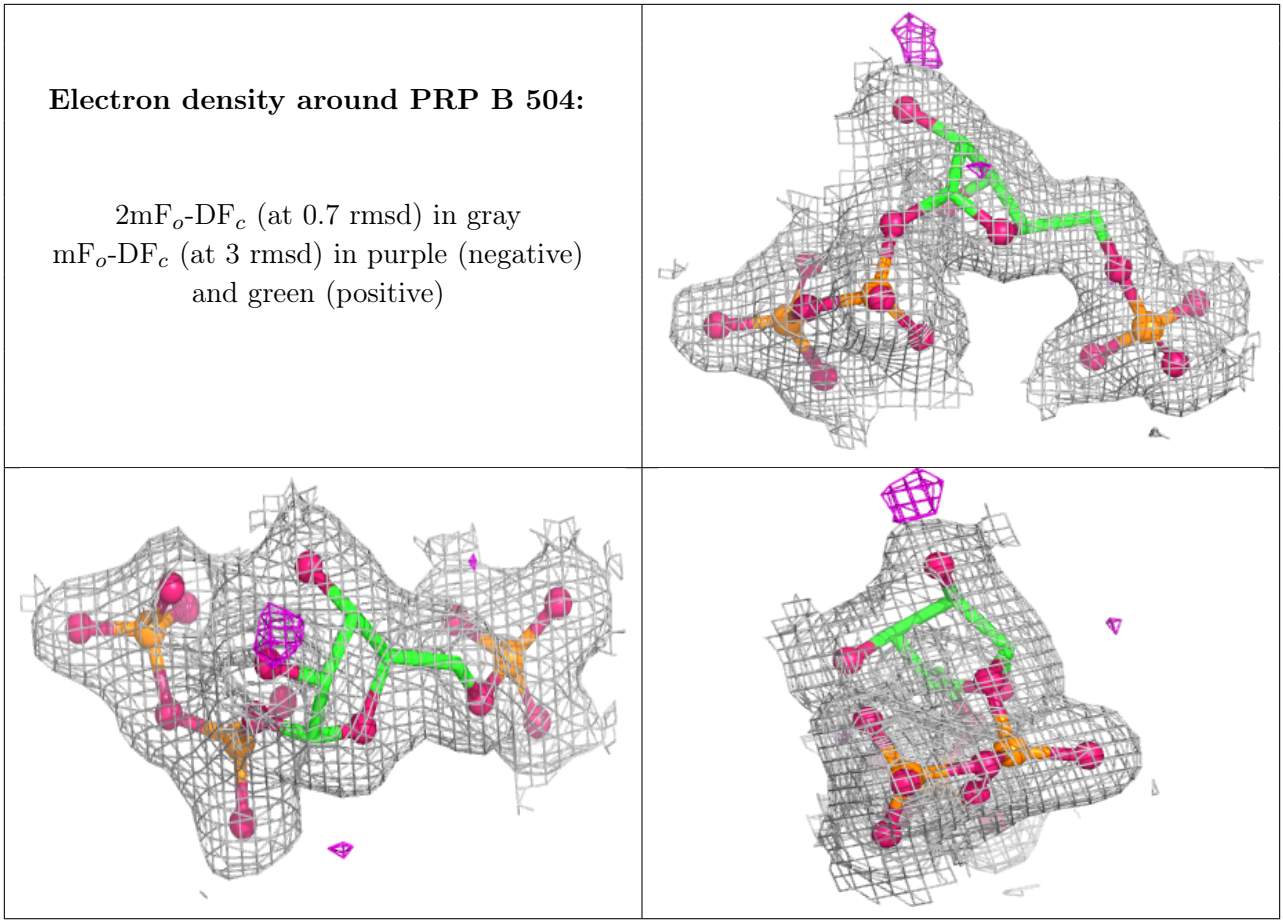
Electron density around PRP B 503:

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



Electron density around PRP B 504:

$2mF_o$-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.