



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:54 am BST

PDB ID : 1UMW
Title : Structure of a human Plk1 Polo-box domain/phosphopeptide complex
Authors : Rellos, P.; Elia, A.; Yaffe, M.B.; Smerdon, S.J.
Deposited on : 2003-08-29
Resolution : 1.90 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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

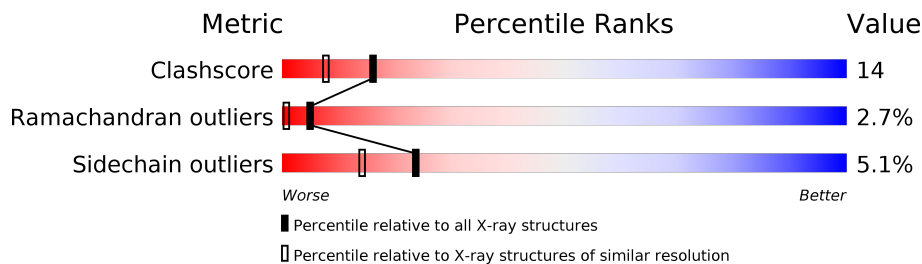
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 on 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	237	
1	B	237	
2	E	7	
2	F	7	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3983 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 SERINE/THREONINE-PROTEIN KINASE PLK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1798	1140	311	337	10	0	0	1
1	B	223	1798	1140	311	337	10	0	0	1

- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	E	7	56	33	8	13	1	1	0	0	0
2	F	7	56	33	8	13	1	1	0	0	0

- Molecule 3 is water.

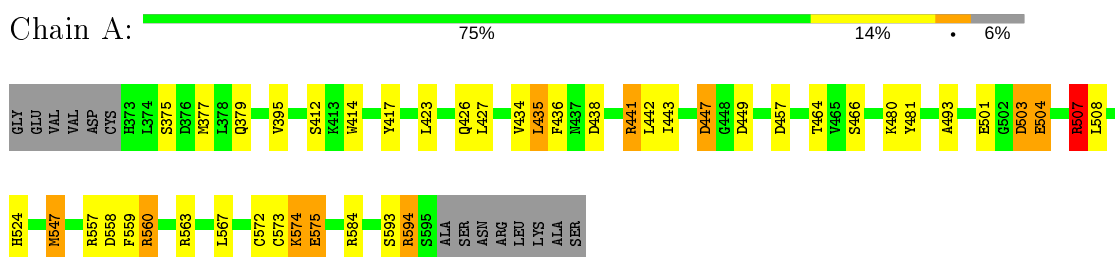
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	97	Total 97	O 97	0	0
3	E	11	Total 11	O 11	0	0
3	F	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

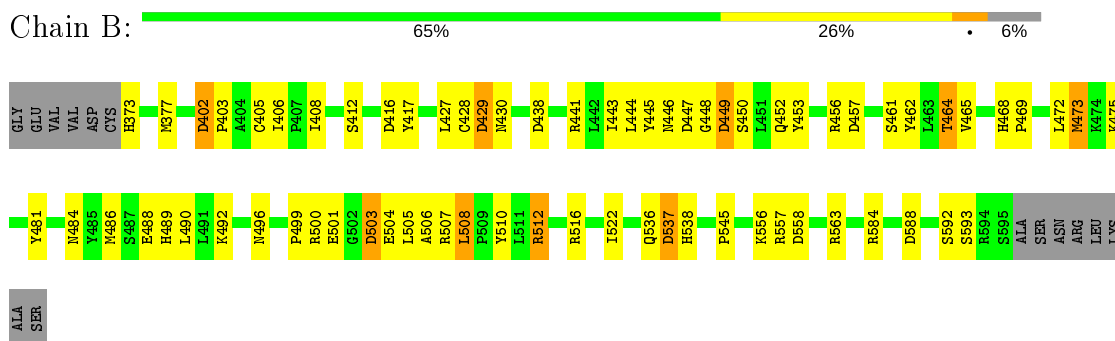
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: SERINE/THREONINE-PROTEIN KINASE PLK



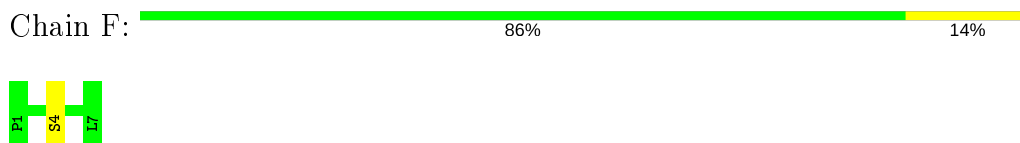
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE PLK



- Molecule 2: PEPTIDE



- Molecule 2: PEPTIDE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.35Å 79.52Å 61.99Å 90.00° 93.26° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.9 (15.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.230 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3983	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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: TPO

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	0.40	0/1835	0.74	3/2482 (0.1%)
1	B	0.33	0/1835	0.71	9/2482 (0.4%)
2	E	0.37	0/45	0.55	0/57
2	F	0.34	0/45	0.35	0/57
All	All	0.37	0/3760	0.72	12/5078 (0.2%)

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
2	F	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	537	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	457	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	438	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	416	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	429	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	503	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	503	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	449	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	438	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	588	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	574	LYS	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	4	SER	Mainchain

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	1798	0	1781	45	0
1	B	1798	0	1781	61	0
2	E	56	0	55	2	0
2	F	56	0	55	0	0
3	A	163	0	0	18	0
3	B	97	0	0	24	0
3	E	11	0	0	0	0
3	F	4	0	0	0	0
All	All	3983	0	3672	107	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 14.

All (107) 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:B:507:ARG:HA	3:B:2049:HOH:O	1.34	1.28
1:A:447:ASP:CG	3:A:2054:HOH:O	1.77	1.22
1:A:447:ASP:OD1	3:A:2054:HOH:O	1.62	1.17
1:B:447:ASP:O	1:B:449:ASP:N	1.86	1.08
1:B:488:GLU:HB3	3:B:2040:HOH:O	1.49	1.07
1:B:507:ARG:HD3	3:B:2049:HOH:O	1.58	1.03
1:A:574:LYS:O	1:A:575:GLU:HB2	1.58	1.01
1:B:469:PRO:HA	3:B:2033:HOH:O	1.68	0.93
1:B:484:ASN:HB3	3:B:2036:HOH:O	1.78	0.83
1:A:507:ARG:HB3	3:A:2102:HOH:O	1.79	0.81
1:A:379:GLN:HG2	3:A:2007:HOH:O	1.81	0.81
1:A:395:VAL:HG23	3:A:2018:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ARG:NH1	3:B:2068:HOH:O	2.15	0.79
1:B:447:ASP:O	1:B:447:ASP:OD1	2.01	0.78
1:B:501:GLU:HB2	3:B:2044:HOH:O	1.84	0.76
1:B:500:ARG:HG2	1:B:501:GLU:H	1.51	0.72
1:B:429:ASP:O	1:B:430:ASN:HB2	1.87	0.72
1:A:507:ARG:NH2	3:A:2105:HOH:O	2.21	0.70
1:A:574:LYS:O	1:A:575:GLU:CB	2.31	0.70
1:A:559:PHE:O	1:A:560:ARG:HD3	1.92	0.68
1:A:503:ASP:O	1:A:504:GLU:HB2	1.96	0.66
1:A:449:ASP:OD2	1:A:464:THR:CG2	2.43	0.66
1:A:547:MET:CE	1:A:547:MET:HA	2.26	0.65
1:B:512:ARG:HD3	3:B:2057:HOH:O	1.96	0.65
1:A:480:LYS:HE3	3:A:2079:HOH:O	1.97	0.65
1:B:469:PRO:CD	3:B:2034:HOH:O	2.46	0.64
1:A:503:ASP:O	1:A:504:GLU:CB	2.47	0.63
1:A:574:LYS:O	1:A:575:GLU:OE1	2.18	0.62
1:A:441:ARG:CZ	3:A:2050:HOH:O	2.48	0.61
1:A:434:VAL:HG11	1:A:436:PHE:CZ	2.36	0.61
1:A:449:ASP:CG	1:A:464:THR:HG23	2.21	0.60
1:A:547:MET:HE3	1:A:547:MET:HA	1.82	0.60
1:B:469:PRO:HD2	3:B:2034:HOH:O	2.02	0.60
1:B:456:ARG:HG3	3:B:2032:HOH:O	2.00	0.59
1:B:449:ASP:OD1	1:B:464:THR:HG22	2.02	0.59
1:B:469:PRO:CA	3:B:2033:HOH:O	2.38	0.59
1:A:441:ARG:NH1	3:A:2050:HOH:O	2.37	0.58
1:B:473:MET:HE2	3:B:2034:HOH:O	2.02	0.58
1:B:489:HIS:CD2	3:B:2040:HOH:O	2.57	0.57
1:B:427:LEU:C	1:B:429:ASP:H	2.07	0.56
1:A:435:LEU:HD13	1:A:441:ARG:HH11	1.72	0.55
1:A:441:ARG:HB3	3:A:2041:HOH:O	2.07	0.54
1:A:593:SER:O	1:A:594:ARG:C	2.47	0.54
1:B:417:TYR:HE1	1:B:481:TYR:HE1	1.56	0.53
1:B:469:PRO:N	3:B:2034:HOH:O	2.41	0.53
1:A:442:LEU:C	1:A:443:ILE:HD12	2.29	0.53
1:A:481:TYR:HE1	3:A:2081:HOH:O	1.90	0.53
1:A:507:ARG:NH1	1:A:508:LEU:HD13	2.24	0.53
1:A:443:ILE:HD12	1:A:443:ILE:N	2.25	0.52
1:B:557:ARG:HG2	1:B:557:ARG:HH11	1.74	0.52
1:A:449:ASP:CG	1:A:464:THR:CG2	2.78	0.51
1:B:427:LEU:C	1:B:429:ASP:N	2.64	0.51
1:A:493:ALA:O	3:A:2089:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LEU:O	1:B:429:ASP:N	2.44	0.49
1:B:402:ASP:O	1:B:405:CYS:HB2	2.12	0.49
1:B:444:LEU:HG	3:B:2031:HOH:O	2.12	0.49
1:A:449:ASP:OD2	1:A:464:THR:HG23	2.12	0.49
1:B:503:ASP:H	1:B:507:ARG:HG3	1.77	0.48
1:B:507:ARG:O	1:B:508:LEU:HB2	2.12	0.48
1:A:567:LEU:HD22	1:A:572:CYS:HB3	1.95	0.48
1:B:445:TYR:C	1:B:447:ASP:H	2.17	0.48
1:B:408:ILE:HG12	1:B:500:ARG:HB3	1.96	0.47
1:B:503:ASP:O	1:B:505:LEU:N	2.48	0.47
1:B:484:ASN:CB	3:B:2036:HOH:O	2.52	0.47
1:B:405:CYS:SG	1:B:563:ARG:CZ	3.03	0.47
1:B:453:TYR:HB3	1:B:461:SER:OG	2.15	0.47
1:B:469:PRO:HB2	1:B:472:LEU:HB2	1.97	0.46
1:B:452:GLN:HE21	1:B:462:TYR:HE2	1.65	0.45
1:B:453:TYR:OH	1:B:475:LYS:NZ	2.46	0.45
1:A:464:THR:HG22	1:A:466:SER:H	1.81	0.45
1:A:501:GLU:CG	3:A:2099:HOH:O	2.64	0.45
1:B:449:ASP:O	1:B:465:VAL:HG23	2.17	0.45
1:B:496:ASN:CB	3:B:2042:HOH:O	2.65	0.45
1:A:594:ARG:CB	3:A:2162:HOH:O	2.66	0.44
1:A:414:TRP:CD1	2:E:4:SER:HB3	2.53	0.44
1:B:447:ASP:C	1:B:449:ASP:N	2.64	0.44
1:B:469:PRO:HB3	3:B:2033:HOH:O	2.16	0.44
1:B:429:ASP:O	1:B:430:ASN:CB	2.57	0.44
1:A:501:GLU:HG2	3:A:2099:HOH:O	2.17	0.43
1:B:496:ASN:N	3:B:2042:HOH:O	2.50	0.43
1:B:557:ARG:CG	1:B:557:ARG:HH11	2.30	0.43
1:B:469:PRO:CB	3:B:2033:HOH:O	2.65	0.43
1:B:496:ASN:HB3	3:B:2042:HOH:O	2.17	0.43
1:A:547:MET:HE2	1:A:547:MET:HA	2.00	0.43
1:B:377:MET:CE	1:B:545:PRO:HD3	2.49	0.43
1:B:443:ILE:HG21	1:B:508:LEU:HD23	1.99	0.42
2:E:5:TPO:HA	2:E:6:PRO:HD3	1.76	0.42
1:A:449:ASP:OD2	1:A:464:THR:HG21	2.18	0.42
1:B:445:TYR:HB2	1:B:450:SER:HB2	2.02	0.42
1:A:573:CYS:C	1:A:574:LYS:O	2.55	0.42
1:B:412:SER:HB2	1:B:492:LYS:HG3	2.02	0.42
1:B:522:ILE:HD12	1:B:522:ILE:N	2.35	0.42
1:A:377:MET:HG3	3:A:2008:HOH:O	2.19	0.42
1:B:516:ARG:HD3	3:B:2055:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ARG:CD	1:A:507:ARG:C	2.89	0.41
1:B:441:ARG:CD	1:B:510:TYR:CD1	3.04	0.41
1:A:426:GLN:HG2	1:A:427:LEU:O	2.20	0.41
1:A:573:CYS:HG	1:A:575:GLU:HB2	1.85	0.41
1:A:524:HIS:HD2	3:A:2151:HOH:O	2.04	0.41
1:B:403:PRO:O	1:B:406:ILE:HG13	2.20	0.41
1:A:507:ARG:HG2	3:A:2104:HOH:O	2.21	0.41
1:B:445:TYR:O	1:B:447:ASP:N	2.54	0.40
1:B:592:SER:OG	1:B:593:SER:N	2.55	0.40
1:B:373:HIS:CB	3:B:2046:HOH:O	2.70	0.40
1:B:537:ASP:O	1:B:538:HIS:HB2	2.20	0.40
1:B:486:MET:HG2	1:B:490:LEU:HD12	2.03	0.40
1:B:556:LYS:O	1:B:557:ARG:HB2	2.21	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	221/237 (93%)	208 (94%)	9 (4%)	4 (2%)	8	2
1	B	221/237 (93%)	199 (90%)	14 (6%)	8 (4%)	3	0
2	E	4/7 (57%)	4 (100%)	0	0	100	100
2	F	4/7 (57%)	4 (100%)	0	0	100	100
All	All	450/488 (92%)	415 (92%)	23 (5%)	12 (3%)	5	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	GLU
1	A	575	GLU

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Mol	Chain	Res	Type
1	B	448	GLY
1	B	504	GLU
1	A	594	ARG
1	B	446	ASN
1	B	506	ALA
1	B	428	CYS
1	A	507	ARG
1	B	468	HIS
1	B	508	LEU
1	B	499	PRO

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	199/213 (93%)	184 (92%)	15 (8%)	13	5
1	B	199/213 (93%)	193 (97%)	6 (3%)	41	33
2	E	6/6 (100%)	6 (100%)	0	100	100
2	F	6/6 (100%)	6 (100%)	0	100	100
All	All	410/438 (94%)	389 (95%)	21 (5%)	24	14

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	SER
1	A	412	SER
1	A	417	TYR
1	A	423	LEU
1	A	435	LEU
1	A	441	ARG
1	A	447	ASP
1	A	457	ASP
1	A	507	ARG
1	A	547	MET
1	A	557	ARG

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Mol	Chain	Res	Type
1	A	558	ASP
1	A	560	ARG
1	A	563	ARG
1	A	584	ARG
1	B	464	THR
1	B	473	MET
1	B	512	ARG
1	B	536	GLN
1	B	558	ASP
1	B	584	ARG

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	468	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	TPO	F	5	2	8,10,11	1.89	2 (25%)	10,14,16	1.29	1 (10%)
2	TPO	E	5	2	8,10,11	1.74	2 (25%)	10,14,16	1.32	1 (10%)

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	TPO	F	5	2	-	1/9/11/13	-
2	TPO	E	5	2	-	0/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	TPO	O-C	3.45	1.33	1.19
2	E	5	TPO	O-C	3.33	1.33	1.19
2	F	5	TPO	P-O1P	3.28	1.61	1.50
2	E	5	TPO	P-O1P	2.91	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	5	TPO	O3P-P-O2P	2.80	118.35	107.64
2	E	5	TPO	OG1-P-O1P	-2.13	101.16	109.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	5	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	5	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.