



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:11 AM UTC

PDB ID : 1PKG / pdb\_00001pkg  
Title : Structure of a c-Kit Kinase Product Complex  
Authors : Mol, C.D.; Lim, K.B.; Sridhar, V.; Zou, H.; Chien, E.Y.T.; Sang, B.-C.;  
Nowakowski, J.; Kassel, D.B.; Cronin, C.N.; McRee, D.E.  
Deposited on : 2003-06-05  
Resolution : 2.90 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

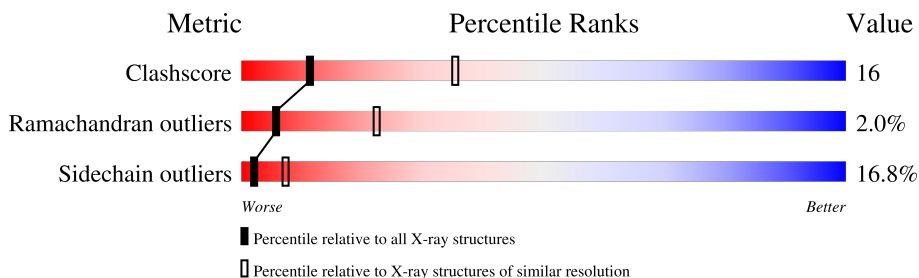
# 1 Overall quality at a glance

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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	 53% 28% 6% • 11%
1	B	329	 49% 29% 7% 15%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4619 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 c-kit protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	292	2328	1500	386	421	2	19	0	0	0
1	B	279	2232	1442	368	401	2	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	568	PTR	TYR	modified residue	UNP P10721
A	570	PTR	TYR	modified residue	UNP P10721
A	752	THR	-	SEE REMARK 999	UNP P10721
A	753	SER	-	SEE REMARK 999	UNP P10721

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

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
3	B	1	27	10	5	10	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total 3 3	0	0



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.67Å 116.46Å 60.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	97.1 (10.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.225 , 0.311	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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: PTR, ADP, MG

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	0.85	1/2349 (0.0%)	1.16	12/3172 (0.4%)
1	B	0.76	0/2251	1.04	3/3038 (0.1%)
All	All	0.80	1/4600 (0.0%)	1.10	15/6210 (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
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	821	SER	C-N	9.74	1.47	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	GLY	N-CA-C	10.52	126.89	114.16
1	A	802	HIS	N-CA-C	9.80	121.73	111.14
1	B	802	HIS	N-CA-C	8.50	121.31	111.11
1	A	829	ALA	N-CA-C	7.18	122.09	113.12
1	B	601	GLY	N-CA-C	6.83	119.08	110.96
1	A	833	VAL	N-CA-C	6.68	117.37	110.36
1	A	872	GLY	N-CA-C	-6.42	106.57	114.92
1	A	616	ALA	N-CA-C	6.36	118.09	111.03
1	A	821	SER	N-CA-C	-6.11	97.78	110.80
1	A	820	ASP	CA-C-N	5.88	132.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	ASP	C-N-CA	5.88	132.77	121.54
1	A	692	SER	N-CA-C	5.63	122.80	110.80
1	B	767	GLU	N-CA-C	-5.53	104.94	110.97
1	A	851	ASP	N-CA-C	-5.19	105.80	111.82
1	A	819	ASN	N-CA-C	5.04	116.46	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	820	ASP	Mainchain
1	A	821	SER	Mainchain
1	A	828	ASN	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	2328	0	2321	80	0
1	B	2232	0	2227	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	7	0
3	B	27	0	12	0	0
4	A	3	0	0	0	0
All	All	4619	0	4572	149	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 16.

All (149) 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:817:ILE:HG23	1:A:821:SER:HA	1.42	0.99
1:B:612:ILE:HB	1:B:618:MET:HE2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:PHE:CD1	1:B:865:LEU:HD11	2.11	0.85
1:A:817:ILE:CG2	1:A:821:SER:HA	2.10	0.81
1:B:626:LYS:HB3	1:B:627:PRO:HD2	1.63	0.81
1:B:578:TYR:HB3	1:B:662:ILE:HD11	1.68	0.75
1:A:817:ILE:HG23	1:A:821:SER:CA	2.18	0.72
1:B:689:PHE:HD1	1:B:865:LEU:HD11	1.53	0.71
1:B:612:ILE:CG2	1:B:613:LYS:H	2.03	0.70
1:B:578:TYR:O	1:B:580:HIS:HB2	1.91	0.69
1:A:600:PHE:CZ	1:A:813:LEU:HD21	2.30	0.67
1:B:578:TYR:O	1:B:580:HIS:N	2.28	0.67
1:A:670:THR:HG21	3:A:1480:ADP:HN61	1.59	0.67
1:A:602:LYS:HD2	1:A:624:MET:HE3	1.78	0.66
1:B:612:ILE:HG23	1:B:613:LYS:N	2.10	0.66
1:B:899:MET:HG2	1:B:927:GLN:OE1	1.96	0.66
1:B:586:ARG:NH2	1:B:665:PRO:O	2.28	0.65
1:A:789:ILE:HG12	1:A:817:ILE:HG13	1.77	0.64
1:B:774:TYR:HE2	1:B:925:GLU:HG2	1.62	0.64
1:B:612:ILE:HG23	1:B:613:LYS:H	1.62	0.63
1:A:655:ASN:HB2	1:A:671:GLU:OE2	1.97	0.63
1:B:660:CYS:HB2	1:B:667:LEU:HB2	1.81	0.62
1:B:588:ARG:HD2	1:B:609:TYR:O	1.99	0.62
1:B:612:ILE:CG2	1:B:613:LYS:N	2.62	0.62
1:B:586:ARG:NH1	1:B:662:ILE:O	2.33	0.62
1:B:612:ILE:HB	1:B:618:MET:CE	2.28	0.62
1:B:585:PRO:HG2	1:B:588:ARG:HG3	1.83	0.61
1:A:625:LEU:HD11	1:A:634:ARG:HG3	1.82	0.61
1:B:602:LYS:HD3	1:B:624:MET:HE2	1.83	0.60
1:A:890:LEU:H	1:A:890:LEU:HD12	1.65	0.59
1:A:600:PHE:HZ	1:A:813:LEU:HD21	1.67	0.59
1:A:568:PTR:N	1:A:568:PTR:HD1	2.17	0.59
1:B:681:PHE:CE2	1:B:685:LYS:HG3	2.38	0.59
1:B:916:THR:O	1:B:920:ILE:HG13	2.03	0.59
1:A:671:GLU:O	1:A:671:GLU:HG3	2.02	0.58
1:A:765:ASP:HB3	1:A:768:ASP:H	1.68	0.58
1:B:863:PHE:HB3	1:B:895:ALA:HB2	1.85	0.58
1:A:670:THR:HG21	3:A:1480:ADP:N6	2.18	0.57
1:A:899:MET:HE3	1:A:927:GLN:HE22	1.69	0.57
1:A:830:ARG:HA	1:B:569:VAL:O	2.04	0.57
1:B:860:TRP:CD1	1:B:892:PRO:HG3	2.39	0.57
1:A:670:THR:CG2	3:A:1480:ADP:N6	2.68	0.57
1:B:629:ALA:HB1	1:B:633:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:PHE:CE2	1:B:577:PRO:HD3	2.41	0.56
1:A:899:MET:HE3	1:A:927:GLN:OE1	2.05	0.56
1:B:608:ALA:O	1:B:617:ALA:HA	2.06	0.55
1:A:685:LYS:HZ1	1:A:763:ALA:N	2.04	0.55
1:B:646:TYR:HD1	1:B:646:TYR:N	2.04	0.55
1:B:928:ILE:HG22	1:B:928:ILE:O	2.05	0.55
1:A:821:SER:O	1:A:823:TYR:N	2.40	0.55
1:A:857:ILE:O	1:A:861:GLU:HG3	2.07	0.55
1:A:899:MET:HE3	1:A:927:GLN:NE2	2.22	0.55
1:B:689:PHE:HB2	1:B:764:LEU:HB3	1.89	0.55
1:A:654:VAL:HG22	1:A:670:THR:HG23	1.89	0.54
1:B:646:TYR:N	1:B:646:TYR:CD1	2.75	0.54
1:A:899:MET:CE	1:A:902:ILE:HD12	2.36	0.54
1:A:792:ASP:HB2	1:A:813:LEU:HD12	1.88	0.54
1:A:578:TYR:CE2	1:A:641:LEU:HD21	2.43	0.53
1:A:900:TYR:CE2	1:A:904:LYS:HD2	2.44	0.53
1:B:853:TRP:CE3	1:B:907:TRP:HA	2.44	0.53
1:B:900:TYR:CE2	1:B:904:LYS:HD2	2.45	0.52
1:B:834:LYS:HG2	1:B:870:TYR:HD1	1.74	0.51
1:A:579:ASP:CG	1:A:581:LYS:HG2	2.35	0.51
1:A:899:MET:HE2	1:A:902:ILE:HD12	1.92	0.51
1:A:917:PHE:O	1:A:921:VAL:HG23	2.11	0.51
1:B:898:GLU:HA	1:B:901:ASP:HB2	1.92	0.51
1:A:572:ASP:OD1	1:A:572:ASP:C	2.53	0.50
1:A:834:LYS:HD3	1:A:870:TYR:HD1	1.75	0.50
1:A:577:PRO:O	1:A:578:TYR:CB	2.59	0.50
1:A:652:ASN:O	1:A:807:LYS:HA	2.11	0.50
1:B:572:ASP:OD2	1:B:573:PRO:HD2	2.12	0.50
1:A:646:TYR:CZ	1:A:786:LYS:HD3	2.47	0.49
1:B:791:ARG:HD3	1:B:813:LEU:O	2.12	0.49
1:B:769:LEU:HD22	1:B:862:LEU:HG	1.94	0.49
1:A:900:TYR:HA	1:A:903:MET:HE3	1.95	0.49
1:A:831:LEU:HB3	1:A:832:PRO:HD2	1.94	0.48
1:A:834:LYS:NZ	1:A:873:MET:O	2.39	0.48
1:A:846:TYR:CD1	1:A:846:TYR:N	2.81	0.48
1:B:580:HIS:HB3	1:B:583:GLU:H	1.76	0.48
1:B:600:PHE:CZ	1:B:813:LEU:HD21	2.47	0.48
1:B:774:TYR:CE2	1:B:925:GLU:HG2	2.45	0.48
1:B:630:HIS:O	1:B:633:GLU:HG2	2.13	0.48
1:B:770:LEU:HD22	1:B:899:MET:HE3	1.95	0.47
1:B:891:SER:HB2	1:B:900:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LEU:HB3	1:A:832:PRO:CD	2.44	0.47
1:A:608:ALA:HB1	1:A:611:LEU:HB2	1.97	0.47
1:A:799:LEU:HD13	3:A:1480:ADP:C6	2.50	0.47
1:A:836:MET:HE1	1:B:571:ILE:HD11	1.95	0.47
1:A:689:PHE:CD2	1:A:865:LEU:HD21	2.50	0.47
1:A:899:MET:CE	1:A:927:GLN:HE22	2.26	0.47
1:B:651:MET:O	1:B:807:LYS:HE3	2.15	0.47
1:A:902:ILE:O	1:A:903:MET:C	2.58	0.47
1:B:645:SER:C	1:B:646:TYR:HD1	2.22	0.47
1:B:765:ASP:CG	1:B:766:LEU:H	2.22	0.47
1:A:899:MET:HE3	1:A:927:GLN:CD	2.39	0.46
1:B:913:LYS:HE3	1:B:913:LYS:HB2	1.54	0.46
1:A:641:LEU:HD11	1:A:659:ALA:HB2	1.97	0.46
1:B:882:MET:O	1:B:887:PHE:HB3	2.14	0.46
1:A:654:VAL:CG2	1:A:670:THR:HG23	2.46	0.46
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.71	0.45
1:B:924:ILE:O	1:B:927:GLN:HB2	2.16	0.45
1:A:671:GLU:OE2	1:A:807:LYS:HD2	2.16	0.45
1:B:600:PHE:HZ	1:B:813:LEU:HD21	1.81	0.45
1:B:842:PHE:HE1	1:B:884:LYS:HB2	1.81	0.45
1:B:578:TYR:O	1:B:580:HIS:CB	2.62	0.45
1:B:595:LEU:HD21	1:B:672:TYR:HE2	1.81	0.45
1:B:789:ILE:HG23	1:B:791:ARG:HG3	1.98	0.44
1:A:598:GLY:HA3	3:A:1480:ADP:O3B	2.16	0.44
1:A:837:ALA:HB2	1:A:853:TRP:CB	2.47	0.44
1:A:847:THR:HB	1:A:849:GLU:OE2	2.16	0.44
1:A:895:ALA:HA	1:A:896:PRO:HD3	1.86	0.44
1:B:578:TYR:C	1:B:580:HIS:N	2.75	0.44
1:B:584:PHE:CE2	1:B:611:LEU:HA	2.53	0.44
1:A:686:ARG:C	1:A:688:SER:H	2.24	0.44
1:B:584:PHE:CD2	1:B:585:PRO:HD2	2.53	0.43
1:B:776:VAL:HG22	1:B:798:ILE:HD12	2.00	0.43
1:B:773:SER:O	1:B:855:TYR:OH	2.26	0.43
1:A:838:PRO:HD3	1:A:853:TRP:CH2	2.54	0.43
1:B:611:LEU:HB3	1:B:618:MET:HE3	2.00	0.43
1:B:626:LYS:HB3	1:B:627:PRO:CD	2.41	0.43
1:B:842:PHE:CE1	1:B:884:LYS:HB2	2.52	0.43
1:A:909:ALA:O	1:A:911:PRO:HD3	2.18	0.43
1:A:568:PTR:N	1:A:568:PTR:CD1	2.78	0.43
1:A:577:PRO:O	1:A:578:TYR:HB3	2.19	0.43
1:A:899:MET:HE2	1:A:899:MET:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:PHE:CE2	1:B:577:PRO:CD	3.02	0.43
1:B:801:THR:OG1	1:B:802:HIS:N	2.51	0.43
1:A:576:LEU:HD22	1:A:577:PRO:HD2	2.01	0.42
1:A:792:ASP:OD2	1:A:796:ARG:NH1	2.51	0.42
1:B:773:SER:HB3	1:B:859:LEU:HD21	2.01	0.42
1:A:900:TYR:CZ	1:A:904:LYS:HD2	2.55	0.42
1:A:652:ASN:O	1:A:808:ILE:N	2.51	0.42
1:A:611:LEU:HD23	1:A:618:MET:SD	2.60	0.41
1:A:804:ARG:HH11	1:A:804:ARG:HA	1.85	0.41
1:A:659:ALA:HA	1:A:667:LEU:O	2.20	0.41
1:A:615:ASP:OD1	1:A:615:ASP:N	2.54	0.41
1:A:677:ASP:O	1:A:678:LEU:C	2.62	0.41
1:A:670:THR:HG22	3:A:1480:ADP:N6	2.34	0.41
1:A:817:ILE:CG2	1:A:817:ILE:O	2.67	0.41
1:B:618:MET:HE1	1:B:657:LEU:HD13	2.02	0.41
1:A:603:VAL:HG21	3:A:1480:ADP:C8	2.56	0.40
1:A:651:MET:HE3	1:A:651:MET:HB2	1.85	0.40
1:B:855:TYR:CE2	1:B:859:LEU:HD11	2.55	0.40
1:B:576:LEU:HD12	1:B:662:ILE:HG21	2.04	0.40
1:A:650:HIS:O	1:A:651:MET:C	2.63	0.40
1:A:789:ILE:HD12	1:A:791:ARG:HG2	2.03	0.40
1:A:898:GLU:H	1:A:898:GLU:HG2	1.51	0.40
1:B:572:ASP:OD2	1:B:574:THR:HG23	2.22	0.40
1:B:860:TRP:CZ3	1:B:867:SER:HB2	2.56	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	286/329 (87%)	256 (90%)	24 (8%)	6 (2%)	<b>5</b> <b>21</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	271/329 (82%)	245 (90%)	21 (8%)	5 (2%)	6	25
All	All	557/658 (85%)	501 (90%)	45 (8%)	11 (2%)	6	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	TYR
1	A	692	SER
1	A	822	ASN
1	B	579	ASP
1	B	617	ALA
1	B	928	ILE
1	A	821	SER
1	B	810	ASP
1	A	614	SER
1	A	830	ARG
1	B	792	ASP

### 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	249/285 (87%)	212 (85%)	37 (15%)	3	10
1	B	239/285 (84%)	194 (81%)	45 (19%)	1	5
All	All	488/570 (86%)	406 (83%)	82 (17%)	2	7

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	ASN
1	A	587	ASN
1	A	602	LYS
1	A	604	VAL
1	A	611	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	614	SER
1	A	628	SER
1	A	632	THR
1	A	635	GLU
1	A	639	SER
1	A	651	MET
1	A	662	ILE
1	A	670	THR
1	A	686	ARG
1	A	687	ASP
1	A	688	SER
1	A	690	ILE
1	A	691	CYS
1	A	767	GLU
1	A	786	LYS
1	A	798	ILE
1	A	802	HIS
1	A	817	ILE
1	A	819	ASN
1	A	820	ASP
1	A	824	VAL
1	A	826	LYS
1	A	844	CYS
1	A	846	TYR
1	A	847	THR
1	A	873	MET
1	A	882	MET
1	A	890	LEU
1	A	898	GLU
1	A	918	LYS
1	A	925	GLU
1	A	927	GLN
1	B	569	VAL
1	B	579	ASP
1	B	580	HIS
1	B	588	ARG
1	B	602	LYS
1	B	612	ILE
1	B	613	LYS
1	B	614	SER
1	B	618	MET
1	B	623	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	624	MET
1	B	631	LEU
1	B	633	GLU
1	B	634	ARG
1	B	638	MET
1	B	641	LEU
1	B	642	LYS
1	B	651	MET
1	B	653	ILE
1	B	656	LEU
1	B	685	LYS
1	B	690	ILE
1	B	691	CYS
1	B	766	LEU
1	B	768	ASP
1	B	773	SER
1	B	786	LYS
1	B	789	ILE
1	B	804	ARG
1	B	807	LYS
1	B	830	ARG
1	B	831	LEU
1	B	834	LYS
1	B	868	SER
1	B	873	MET
1	B	878	LYS
1	B	890	LEU
1	B	893	GLU
1	B	898	GLU
1	B	904	LYS
1	B	913	LYS
1	B	918	LYS
1	B	920	ILE
1	B	922	GLN
1	B	926	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	580	HIS
1	A	587	ASN
1	A	655	ASN

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Mol	Chain	Res	Type
1	A	922	GLN
1	B	580	HIS
1	B	652	ASN
1	B	655	ASN
1	B	680	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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
1	PTR	B	570	1	15,16,17	1.84	1 (6%)	17,22,24	1.24	3 (17%)
1	PTR	B	568	1,2	15,16,17	2.06	1 (6%)	17,22,24	0.97	1 (5%)
1	PTR	A	570	1	15,16,17	1.77	1 (6%)	17,22,24	0.79	1 (5%)
1	PTR	A	568	1,2	15,16,17	2.13	1 (6%)	17,22,24	0.79	1 (5%)

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
1	PTR	B	570	1	-	0/10/11/13	0/1/1/1
1	PTR	B	568	1,2	-	0/10/11/13	0/1/1/1
1	PTR	A	570	1	-	2/10/11/13	0/1/1/1
1	PTR	A	568	1,2	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	568	PTR	OH-CZ	-8.08	1.22	1.40
1	B	568	PTR	OH-CZ	-7.50	1.23	1.40
1	B	570	PTR	OH-CZ	-6.72	1.25	1.40
1	A	570	PTR	OH-CZ	-6.13	1.26	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	PTR	O3P-P-OH	3.14	114.61	105.32
1	B	568	PTR	O2P-P-OH	2.93	113.99	105.32
1	B	570	PTR	P-OH-CZ	2.71	133.52	123.88
1	B	570	PTR	OH-CZ-CE1	2.23	125.91	119.22
1	A	570	PTR	O2P-P-OH	2.16	111.71	105.32
1	A	568	PTR	O2P-P-OH	2.03	111.31	105.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	570	PTR	N-CA-CB-CG
1	A	570	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	568	PTR	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ADP	A	1480	2	28,29,29	1.03	3 (10%)	43,45,45	1.67	7 (16%)
3	ADP	B	1486	2	28,29,29	1.21	4 (14%)	43,45,45	1.74	10 (23%)

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
3	ADP	A	1480	2	-	2/16/32/32	0/3/3/3
3	ADP	B	1486	2	-	3/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1486	ADP	C2-N1	2.86	1.39	1.33
3	B	1486	ADP	C2-N3	2.69	1.38	1.33
3	A	1480	ADP	C2-N1	2.64	1.38	1.33
3	A	1480	ADP	C2-N3	2.60	1.38	1.33
3	B	1486	ADP	C5-N7	-2.54	1.34	1.39
3	A	1480	ADP	C8-N7	2.09	1.35	1.31
3	B	1486	ADP	PA-O3A	-2.01	1.57	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	ADP	N3-C2-N1	-5.22	120.68	128.58
3	B	1486	ADP	N3-C2-N1	-4.84	121.26	128.58
3	B	1486	ADP	C5-C4-N3	-4.49	120.54	126.72
3	A	1480	ADP	C5-C4-N3	-4.17	120.97	126.72
3	A	1480	ADP	N9-C8-N7	-3.58	108.85	113.94
3	B	1486	ADP	C5-N7-C8	3.37	108.74	103.45
3	A	1480	ADP	C2-N3-C4	3.35	120.02	111.83
3	B	1486	ADP	N9-C8-N7	-3.29	109.27	113.94
3	A	1480	ADP	C5-N7-C8	2.96	108.11	103.45
3	B	1486	ADP	N3-C4-N9	2.91	132.12	127.17
3	B	1486	ADP	C2-N3-C4	2.88	118.88	111.83
3	B	1486	ADP	O4'-C1'-N9	2.80	113.47	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	ADP	N3-C4-N9	2.61	131.60	127.17
3	B	1486	ADP	C2'-C1'-N9	-2.53	107.02	113.30
3	A	1480	ADP	C4-C5-N7	-2.26	108.00	110.58
3	B	1486	ADP	C6-C5-C4	2.19	120.17	117.18
3	B	1486	ADP	C4-C5-N7	-2.14	108.14	110.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

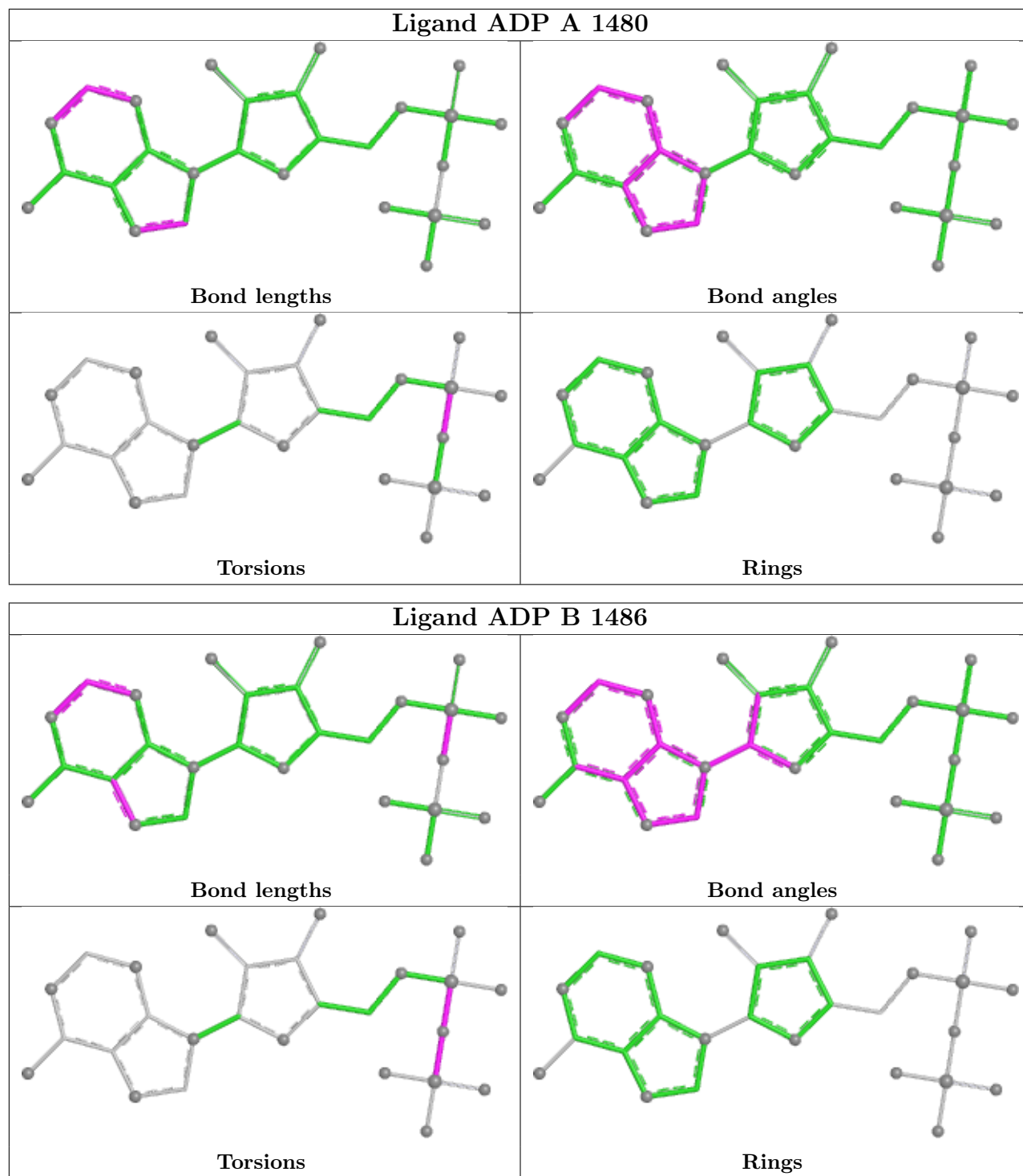
Mol	Chain	Res	Type	Atoms
3	B	1486	ADP	PA-O3A-PB-O3B
3	A	1480	ADP	PB-O3A-PA-O2A
3	B	1486	ADP	PB-O3A-PA-O1A
3	B	1486	ADP	PA-O3A-PB-O2B
3	A	1480	ADP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1480	ADP	7	0

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.