Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:01 AM EDT

PDB ID	:	1PKG
Title	:	Structure of a c-Kit Kinase Product Complex
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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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

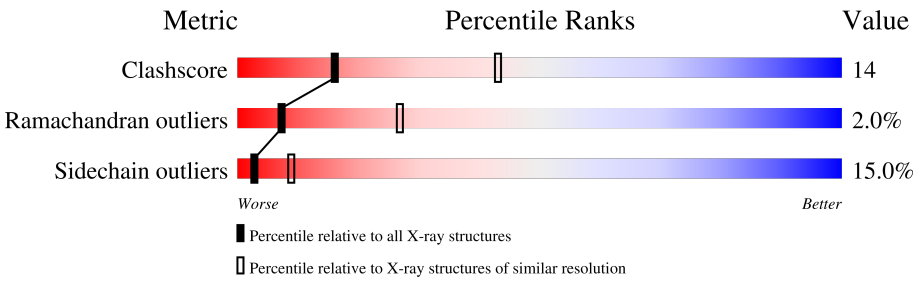
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	55% 27% 6% 11%
1	B	329	50% 28% 6% 15%

2 Entry composition (i)

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

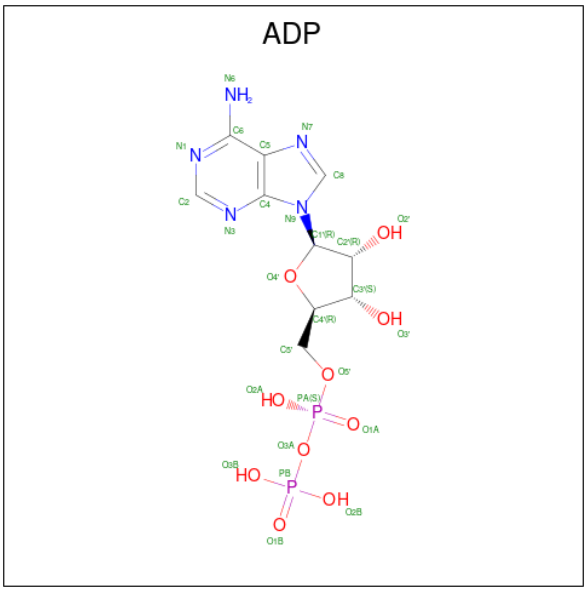
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is water.

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

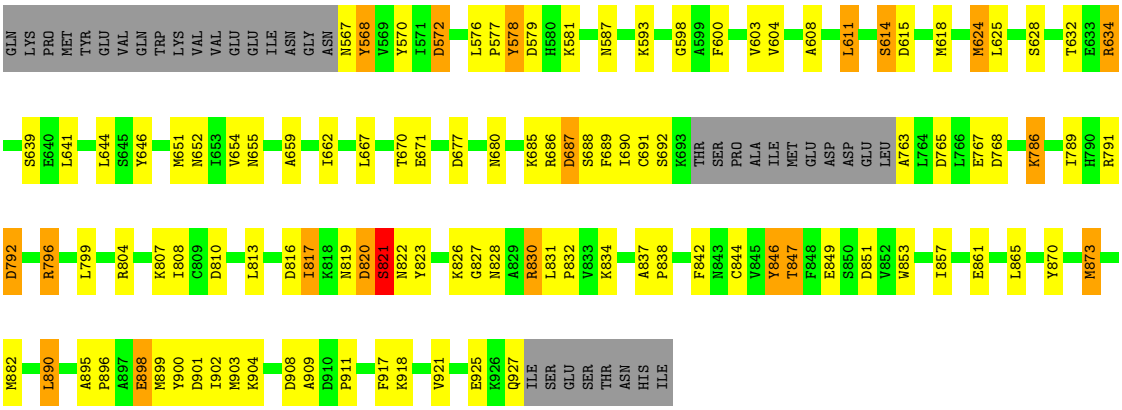
3 Residue-property plots (i)

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. 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.

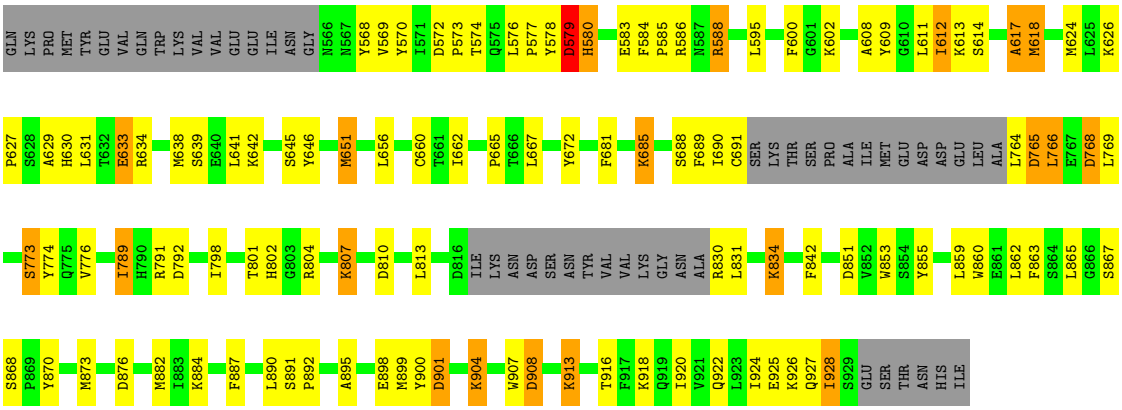
• Molecule 1: c-kit protein

Chain A: 55% 27% 6% 11%



• Molecule 1: c-kit protein

Chain B: 50% 28% 6% 15%



4 Data and refinement statistics (i)

Xtriage (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, α, β, γ	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.	Xtriage
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å^2)	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: ADP, PTR, 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	0.64	1/2349 (0.0%)	0.91	10/3172 (0.3%)
1	B	0.59	0/2251	0.86	7/3038 (0.2%)
All	All	0.62	1/4600 (0.0%)	0.89	17/6210 (0.3%)

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	5.77	1.47	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	876	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	851	ASP	CB-CG-OD2	7.82	125.34	118.30
1	B	901	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	792	ASP	CB-CG-OD2	7.33	124.89	118.30
1	A	810	ASP	CB-CG-OD2	7.12	124.71	118.30
1	B	851	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	677	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	572	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	816	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	768	ASP	CB-CG-OD2	6.12	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	908	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	579	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	901	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	765	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	687	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	827	GLY	N-CA-C	5.52	126.89	113.10
1	B	908	ASP	CB-CG-OD2	5.50	123.25	118.30

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 (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	2328	0	2321	69	0
1	B	2232	0	2227	67	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	133	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 (133) 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:899:MET:HE1	1:A:902:ILE:HD12	1.42	1.02

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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: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:B:612:ILE:HB	1:B:618:MET:HE1	1.76	0.68
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: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: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: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
1:A:842:PHE:CE2	1:B:577:PRO:HD3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:899:MET:HE1	1:A:902:ILE:CD1	2.27	0.52
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: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: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:604:VAL:HB	1:A:624:MET:HE1	1.93	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:899:MET:CE	1:A:927:GLN:HE22	2.26	0.49
1:A:831:LEU:HB3	1:A:832:PRO:HD2	1.94	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:891:SER:HB2	1:B:900:TYR:CD2	2.50	0.47
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:689:PHE:CD2	1:A:865:LEU:HD21	2.50	0.47
1:B:651:MET:O	1:B:807:LYS:HE3	2.15	0.47
1:A:579:ASP:CG	1:A:581:LYS:HG2	2.35	0.47
1:B:913:LYS:HE3	1:B:913:LYS:HB2	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HD11	1:A:659:ALA:HB2	1.97	0.46
1:A:572:ASP:OD1	1:A:572:ASP:C	2.53	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:A:834:LYS:NZ	1:A:873:MET:O	2.39	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:584:PHE:CE2	1:B:611:LEU:HA	2.53	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: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: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:902:ILE:O	1:A:903:MET:C	2.58	0.42
1:B:645:SER:C	1:B:646:TYR:HD1	2.22	0.42
1:B:765:ASP:CG	1:B:766:LEU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:603:VAL:HG21	3:A:1480:ADP:C8	2.56	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: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%)	7 26
1	B	271/329 (82%)	245 (90%)	21 (8%)	5 (2%)	8 29
All	All	557/658 (85%)	501 (90%)	45 (8%)	11 (2%)	7 27

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

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Mol	Chain	Res	Type
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%)	215 (86%)	34 (14%)	3 11
1	B	239/285 (84%)	200 (84%)	39 (16%)	2 7
All	All	488/570 (86%)	415 (85%)	73 (15%)	3 9

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	ASN
1	A	587	ASN
1	A	593	LYS
1	A	611	LEU
1	A	614	SER
1	A	624	MET
1	A	628	SER
1	A	632	THR
1	A	634	ARG
1	A	639	SER
1	A	651	MET
1	A	662	ILE
1	A	680	ASN
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	796	ARG

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Mol	Chain	Res	Type
1	A	817	ILE
1	A	819	ASN
1	A	820	ASP
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	B	579	ASP
1	B	580	HIS
1	B	588	ARG
1	B	602	LYS
1	B	612	ILE
1	B	614	SER
1	B	618	MET
1	B	624	MET
1	B	631	LEU
1	B	633	GLU
1	B	634	ARG
1	B	638	MET
1	B	639	SER
1	B	641	LEU
1	B	642	LYS
1	B	651	MET
1	B	656	LEU
1	B	685	LYS
1	B	688	SER
1	B	690	ILE
1	B	691	CYS
1	B	766	LEU
1	B	768	ASP
1	B	773	SER
1	B	789	ILE
1	B	804	ARG
1	B	807	LYS
1	B	830	ARG
1	B	831	LEU

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Mol	Chain	Res	Type
1	B	834	LYS
1	B	868	SER
1	B	873	MET
1	B	890	LEU
1	B	904	LYS
1	B	908	ASP
1	B	913	LYS
1	B	918	LYS
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:

Mol	Chain	Res	Type
1	A	580	HIS
1	A	587	ASN
1	A	649	ASN
1	A	652	ASN
1	A	680	ASN
1	A	819	ASN
1	A	894	HIS
1	A	922	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)

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	A	568	2,1	15,16,17	2.12	1 (6%)	19,22,24	0.75	0
1	PTR	B	570	1	15,16,17	1.86	2 (13%)	19,22,24	1.30	4 (21%)
1	PTR	A	570	1	15,16,17	1.80	2 (13%)	19,22,24	0.78	1 (5%)
1	PTR	B	568	2,1	15,16,17	2.04	1 (6%)	19,22,24	0.97	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	A	568	2,1	-	0/10/11/13	0/1/1/1
1	PTR	B	570	1	-	0/10/11/13	0/1/1/1
1	PTR	A	570	1	-	2/10/11/13	0/1/1/1
1	PTR	B	568	2,1	-	0/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	568	PTR	OH-CZ	-8.00	1.22	1.40
1	B	568	PTR	OH-CZ	-7.43	1.23	1.40
1	B	570	PTR	OH-CZ	-6.66	1.25	1.40
1	A	570	PTR	OH-CZ	-6.07	1.26	1.40
1	A	570	PTR	P-OH	2.56	1.63	1.59
1	B	570	PTR	P-OH	2.10	1.62	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	570	PTR	P-OH-CZ	3.05	133.52	123.75
1	B	570	PTR	O3P-P-OH	3.00	114.61	105.24
1	B	568	PTR	O2P-P-OH	2.80	113.99	105.24
1	B	570	PTR	OH-CZ-CE1	2.25	125.91	119.23
1	B	570	PTR	CB-CA-C	-2.23	107.28	111.47
1	A	570	PTR	O2P-P-OH	2.07	111.71	105.24

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 monosaccharides 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	24,29,29	1.17	2 (8%)	29,45,45	1.37	2 (6%)
3	ADP	B	1486	2	24,29,29	1.23	2 (8%)	29,45,45	1.48	3 (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
3	ADP	A	1480	2	-	2/12/32/32	0/3/3/3
3	ADP	B	1486	2	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1486	ADP	C2-N3	4.11	1.38	1.32
3	A	1480	ADP	C2-N3	4.00	1.38	1.32
3	B	1486	ADP	C2-N1	2.74	1.39	1.33
3	A	1480	ADP	C2-N1	2.54	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1480	ADP	N3-C2-N1	-5.12	120.68	128.68
3	B	1486	ADP	N3-C2-N1	-4.74	121.26	128.68
3	B	1486	ADP	PA-O3A-PB	-4.14	118.63	132.83
3	A	1480	ADP	PA-O3A-PB	-2.97	122.62	132.83
3	B	1486	ADP	C3'-C2'-C1'	2.22	104.32	100.98

There are no chirality outliers.

All (6) 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
3	B	1486	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

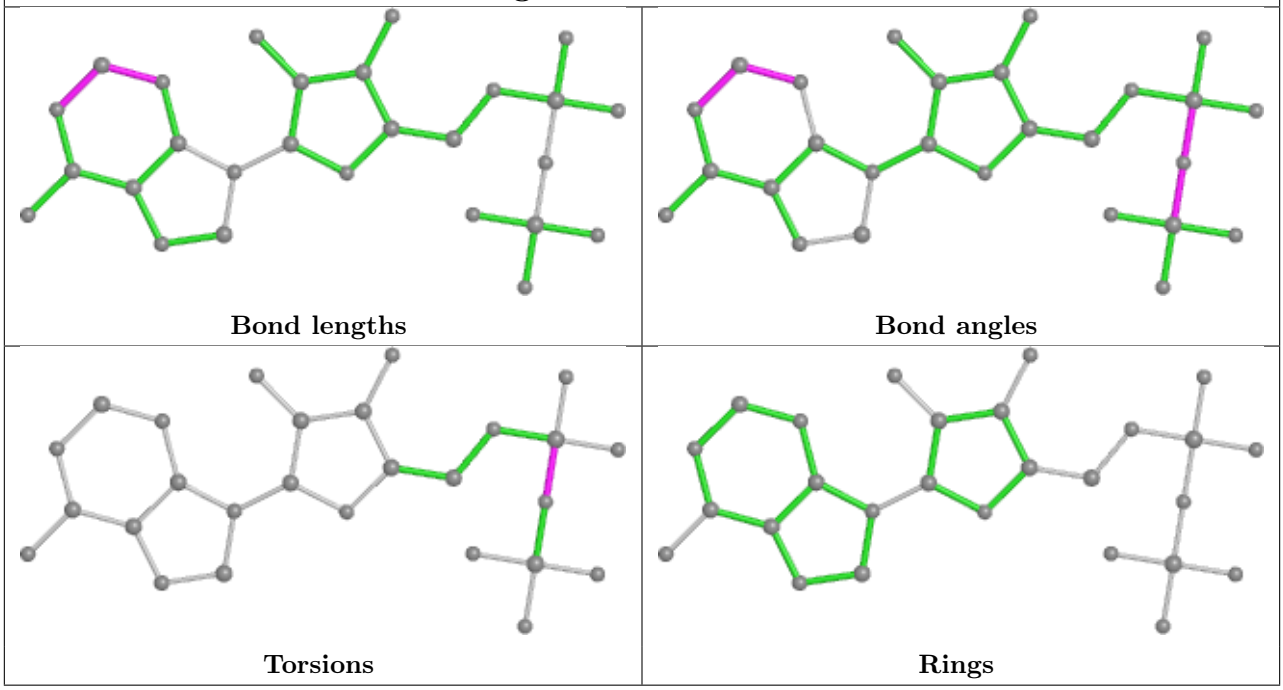
1 monomer is involved in 7 short contacts:

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

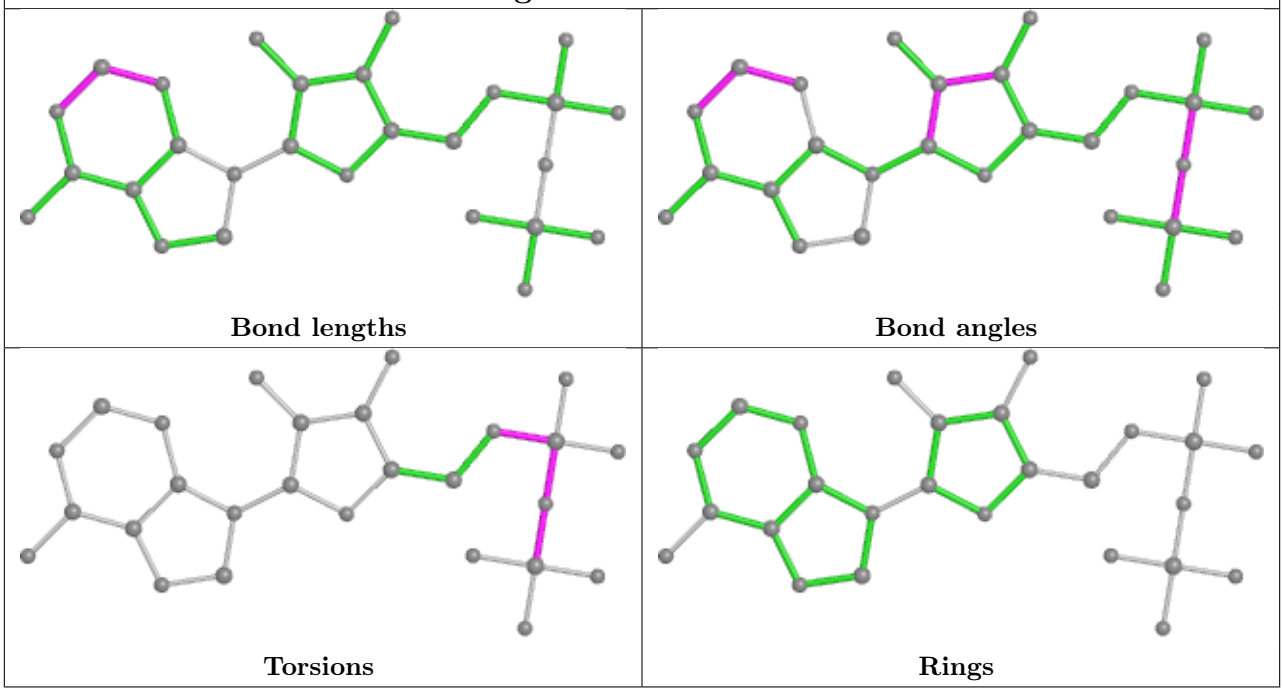
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ADP A 1480



Ligand ADP B 1486



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 (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.