



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:23 PM UTC

PDB ID : 1MQB / pdb_00001mqb
Title : Crystal Structure of Ephrin A2 (ephA2) Receptor Protein Kinase
Authors : Nowakowski, J.; Cronin, C.N.; McRee, D.E.; Knuth, M.W.; Nelson, C.; Pavletich, N.; Rogers, J.; Sang, B.C.; Scheibe, D.N.; Swanson, R.V.; Thompson, D.A.
Deposited on : 2002-09-16
Resolution : 2.30 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)	:	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

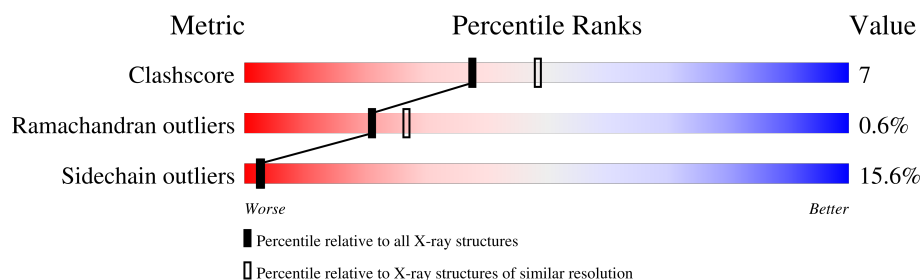
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4349 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 Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2101	1349	360	374	18			
1	B	265	Total	C	N	O	S	0	0	0
			2120	1362	365	375	18			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	568	MET	-	cloning artifact	UNP P29317
A	569	SER	-	cloning artifact	UNP P29317
A	570	TYR	-	cloning artifact	UNP P29317
A	571	TYR	-	cloning artifact	UNP P29317
A	572	HIS	-	cloning artifact	UNP P29317
A	573	HIS	-	cloning artifact	UNP P29317
A	574	HIS	-	cloning artifact	UNP P29317
A	575	HIS	-	cloning artifact	UNP P29317
A	576	HIS	-	cloning artifact	UNP P29317
A	577	HIS	-	cloning artifact	UNP P29317
A	578	ASP	-	cloning artifact	UNP P29317
A	579	TYR	-	cloning artifact	UNP P29317
A	580	ASP	-	cloning artifact	UNP P29317
A	581	ILE	-	cloning artifact	UNP P29317
A	582	PRO	-	cloning artifact	UNP P29317
A	583	THR	-	cloning artifact	UNP P29317
A	584	THR	-	cloning artifact	UNP P29317
A	585	GLU	-	cloning artifact	UNP P29317
A	586	ASN	-	cloning artifact	UNP P29317
A	587	LEU	-	cloning artifact	UNP P29317
A	588	TYR	-	cloning artifact	UNP P29317
A	589	PHE	-	cloning artifact	UNP P29317
A	590	GLN	-	cloning artifact	UNP P29317
A	591	GLY	-	cloning artifact	UNP P29317
A	592	ALA	-	cloning artifact	UNP P29317

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Chain	Residue	Modelled	Actual	Comment	Reference
A	593	MET	-	cloning artifact	UNP P29317
A	594	GLY	-	cloning artifact	UNP P29317
A	595	SER	-	cloning artifact	UNP P29317
B	568	MET	-	cloning artifact	UNP P29317
B	569	SER	-	cloning artifact	UNP P29317
B	570	TYR	-	cloning artifact	UNP P29317
B	571	TYR	-	cloning artifact	UNP P29317
B	572	HIS	-	cloning artifact	UNP P29317
B	573	HIS	-	cloning artifact	UNP P29317
B	574	HIS	-	cloning artifact	UNP P29317
B	575	HIS	-	cloning artifact	UNP P29317
B	576	HIS	-	cloning artifact	UNP P29317
B	577	HIS	-	cloning artifact	UNP P29317
B	578	ASP	-	cloning artifact	UNP P29317
B	579	TYR	-	cloning artifact	UNP P29317
B	580	ASP	-	cloning artifact	UNP P29317
B	581	ILE	-	cloning artifact	UNP P29317
B	582	PRO	-	cloning artifact	UNP P29317
B	583	THR	-	cloning artifact	UNP P29317
B	584	THR	-	cloning artifact	UNP P29317
B	585	GLU	-	cloning artifact	UNP P29317
B	586	ASN	-	cloning artifact	UNP P29317
B	587	LEU	-	cloning artifact	UNP P29317
B	588	TYR	-	cloning artifact	UNP P29317
B	589	PHE	-	cloning artifact	UNP P29317
B	590	GLN	-	cloning artifact	UNP P29317
B	591	GLY	-	cloning artifact	UNP P29317
B	592	ALA	-	cloning artifact	UNP P29317
B	593	MET	-	cloning artifact	UNP P29317
B	594	GLY	-	cloning artifact	UNP P29317
B	595	SER	-	cloning artifact	UNP P29317

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	27	Total	O	0	0
			27	27		

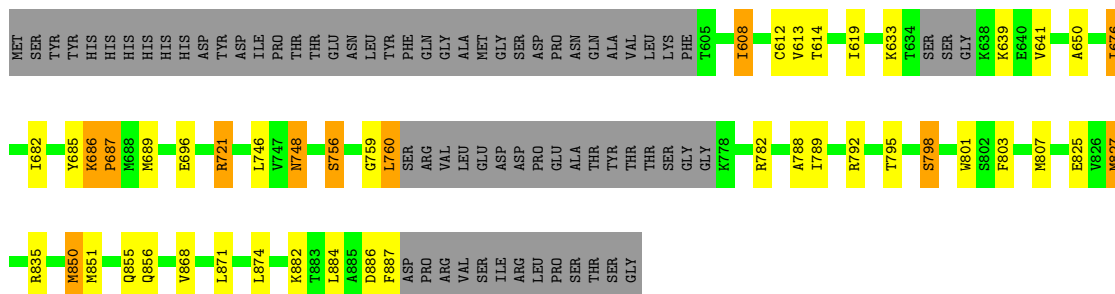
3 Residue-property plots [i](#)

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.

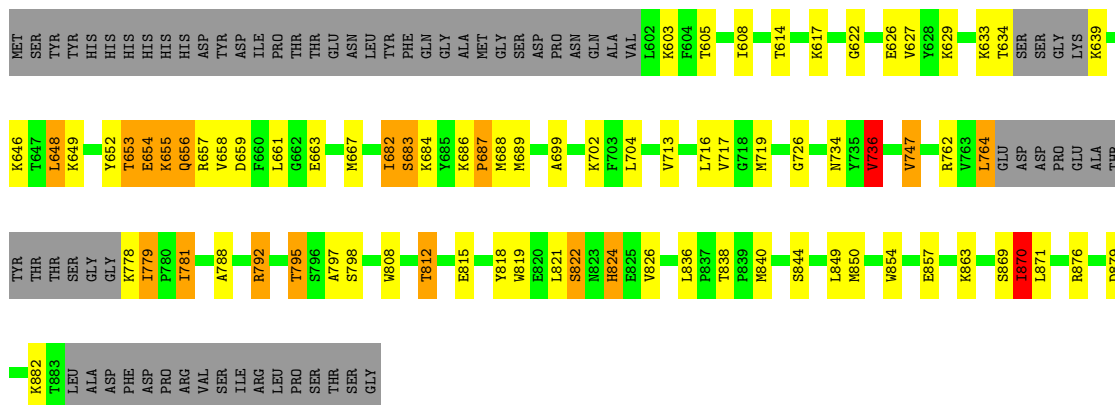
- Molecule 1: Ephrin type-A receptor 2

Chain A: 



- Molecule 1: Ephrin type-A receptor 2

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.13Å 72.13Å 241.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	93.7 (40.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.236 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4349	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP

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	1.01	0/2145	1.07	2/2888 (0.1%)
1	B	0.97	2/2164 (0.1%)	1.12	9/2913 (0.3%)
All	All	0.99	2/4309 (0.0%)	1.10	11/5801 (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	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	870	ILE	CA-CB	7.74	1.65	1.54
1	B	699	ALA	CA-C	-5.75	1.45	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	687	PRO	N-CA-CB	-6.95	95.96	103.25
1	B	736	VAL	CB-CA-C	-6.93	101.42	110.84
1	B	687	PRO	N-CD-CG	-6.79	93.02	103.20
1	A	650	ALA	N-CA-C	-5.92	101.90	110.24
1	B	797	ALA	CA-C-N	5.77	127.94	120.44
1	B	797	ALA	C-N-CA	5.77	127.94	120.44
1	A	687	PRO	N-CD-CG	-5.68	94.67	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	747	VAL	CB-CA-C	-5.49	102.37	110.82
1	B	726	GLY	N-CA-C	-5.31	105.97	112.77
1	B	683	SER	N-CA-C	-5.20	102.31	110.17
1	B	822	SER	N-CA-C	-5.09	103.96	110.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	686	LYS	Peptide
1	B	654	GLU	Peptide
1	B	686	LYS	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	2101	0	2133	28	0
1	B	2120	0	2162	31	0
2	A	31	0	13	1	0
2	B	31	0	13	2	0
3	A	39	0	0	0	0
3	B	27	0	0	0	0
All	All	4349	0	4321	60	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 7.

All (60) 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:807:MET:HE2	1:A:850:MET:HB3	1.39	0.99
1:A:682:ILE:HD12	1:A:689:MET:HE3	1.49	0.95
1:A:807:MET:HE2	1:A:850:MET:CB	2.06	0.84
1:A:748:ASN:C	1:A:748:ASN:HD22	1.86	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:THR:HG22	1:B:798:SER:H	1.51	0.75
1:B:808:TRP:O	1:B:812:THR:HB	1.93	0.68
1:B:849:LEU:HD22	1:B:870:ILE:CD1	2.25	0.65
1:A:789:ILE:HG21	1:A:827:MET:HE1	1.79	0.65
1:A:807:MET:CE	1:A:850:MET:CB	2.74	0.64
1:B:812:THR:CG2	1:B:815:GLU:HB3	2.28	0.64
1:B:655:LYS:O	1:B:658:VAL:HG22	1.99	0.63
1:A:807:MET:HE1	1:A:850:MET:N	2.16	0.61
1:B:608:ILE:O	1:B:682:ILE:CG2	2.50	0.59
1:B:704:LEU:HD21	1:B:719:MET:HE1	1.83	0.59
1:A:676:ILE:HD13	1:A:756:SER:CB	2.33	0.57
1:A:807:MET:CE	1:A:850:MET:HB3	2.24	0.57
1:B:608:ILE:O	1:B:682:ILE:HG23	2.05	0.56
1:A:608:ILE:HD11	1:A:613:VAL:HG23	1.87	0.56
1:B:812:THR:HG21	1:B:815:GLU:HB3	1.88	0.55
1:A:788:ALA:O	1:A:792:ARG:HA	2.06	0.55
1:B:736:VAL:HG22	1:B:764:LEU:HG	1.89	0.55
1:B:812:THR:HG23	1:B:815:GLU:CB	2.37	0.55
1:A:803:PHE:O	1:A:807:MET:HG3	2.08	0.54
1:B:648:LEU:HD13	1:B:652:TYR:CD1	2.43	0.53
1:A:807:MET:HE2	1:A:850:MET:CA	2.38	0.53
1:A:807:MET:CE	1:A:850:MET:CA	2.86	0.53
1:B:713:VAL:O	1:B:717:VAL:HG23	2.08	0.52
1:B:812:THR:HG23	1:B:815:GLU:HB3	1.91	0.52
1:B:653:THR:OG1	1:B:656:GLN:HG2	2.10	0.52
1:A:608:ILE:HD11	1:A:613:VAL:CG2	2.40	0.51
1:A:760:LEU:HD22	1:A:760:LEU:N	2.27	0.50
1:A:795:THR:H	1:A:798:SER:HB2	1.77	0.50
1:B:716:LEU:HA	1:B:719:MET:HE2	1.94	0.50
1:B:822:SER:O	1:B:826:VAL:HG23	2.14	0.48
1:A:612:CYS:HB3	1:A:633:LYS:O	2.14	0.46
1:B:683:SER:O	1:B:684:LYS:HB2	2.15	0.46
1:B:850:MET:HG2	1:B:854:TRP:CH2	2.51	0.45
1:B:779:ILE:HG22	1:B:781:ILE:HD12	1.98	0.45
1:B:788:ALA:O	1:B:792:ARG:HA	2.15	0.45
1:A:721:ARG:HH11	1:A:868:VAL:HG13	1.81	0.45
1:A:759:GLY:HA2	1:A:760:LEU:HD22	1.98	0.45
1:B:818:TYR:O	1:B:819:TRP:C	2.60	0.45
1:B:818:TYR:CD1	1:B:836:LEU:HD21	2.52	0.44
1:B:622:GLY:HA2	2:B:1001:ANP:O1B	2.18	0.43
1:A:807:MET:HE2	1:A:850:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:VAL:HG21	2:B:1001:ANP:H5'1	2.01	0.42
1:A:676:ILE:HD13	1:A:756:SER:HB2	2.01	0.42
1:A:789:ILE:HG21	1:A:827:MET:CE	2.46	0.41
1:A:835:ARG:HG3	1:A:851:MET:HE1	2.03	0.41
1:A:676:ILE:HD13	1:A:756:SER:CA	2.50	0.41
1:B:656:GLN:OE1	1:B:656:GLN:HA	2.20	0.41
1:B:824:HIS:ND1	1:B:824:HIS:C	2.78	0.41
1:B:646:LYS:O	1:B:689:MET:HA	2.21	0.41
1:A:748:ASN:C	1:A:748:ASN:ND2	2.61	0.41
1:B:658:VAL:HG23	1:B:659:ASP:N	2.36	0.41
1:B:717:VAL:HG13	1:B:871:LEU:HD22	2.02	0.41
2:A:1000:ANP:O5'	2:A:1000:ANP:H8	2.20	0.40
1:B:795:THR:O	1:B:798:SER:HB3	2.20	0.40
1:A:788:ALA:HB2	1:A:798:SER:OG	2.21	0.40
1:A:801:TRP:CD1	1:A:801:TRP:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/333 (77%)	248 (96%)	8 (3%)	1 (0%)	30	38
1	B	259/333 (78%)	244 (94%)	13 (5%)	2 (1%)	16	20
All	All	516/666 (78%)	492 (95%)	21 (4%)	3 (1%)	21	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	687	PRO
1	B	687	PRO
1	B	653	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/287 (79%)	199 (88%)	27 (12%)	5	6
1	B	229/287 (80%)	185 (81%)	44 (19%)	1	1
All	All	455/574 (79%)	384 (84%)	71 (16%)	2	3

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	608	ILE
1	A	614	THR
1	A	619	ILE
1	A	639	LYS
1	A	641	VAL
1	A	676	ILE
1	A	685	TYR
1	A	686	LYS
1	A	696	GLU
1	A	721	ARG
1	A	746	LEU
1	A	748	ASN
1	A	756	SER
1	A	760	LEU
1	A	782	ARG
1	A	798	SER
1	A	825	GLU
1	A	827	MET
1	A	850	MET
1	A	855	GLN
1	A	856	GLN
1	A	871	LEU
1	A	874	LEU
1	A	882	LYS
1	A	884	LEU
1	A	886	ASP
1	A	887	PHE

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Mol	Chain	Res	Type
1	B	603	LYS
1	B	605	THR
1	B	614	THR
1	B	617	LYS
1	B	626	GLU
1	B	629	LYS
1	B	633	LYS
1	B	634	THR
1	B	639	LYS
1	B	648	LEU
1	B	649	LYS
1	B	654	GLU
1	B	655	LYS
1	B	656	GLN
1	B	657	ARG
1	B	661	LEU
1	B	663	GLU
1	B	667	MET
1	B	682	ILE
1	B	688	MET
1	B	702	LYS
1	B	734	ASN
1	B	736	VAL
1	B	747	VAL
1	B	762	ARG
1	B	764	LEU
1	B	778	LYS
1	B	779	ILE
1	B	781	ILE
1	B	792	ARG
1	B	795	THR
1	B	812	THR
1	B	821	LEU
1	B	824	HIS
1	B	838	THR
1	B	840	MET
1	B	844	SER
1	B	857	GLU
1	B	863	LYS
1	B	869	SER
1	B	870	ILE
1	B	876	ARG

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Mol	Chain	Res	Type
1	B	879	ASP
1	B	882	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	HIS
1	A	669	GLN
1	A	673	HIS
1	A	674	ASN
1	A	697	ASN
1	A	732	ASN
1	A	748	ASN
1	A	855	GLN
1	B	852	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	B	1001	-	33,33,33	1.47	6 (18%)	45,52,52	1.91	12 (26%)
2	ANP	A	1000	-	33,33,33	1.29	4 (12%)	45,52,52	2.05	12 (26%)

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	ANP	B	1001	-	-	7/18/38/38	0/3/3/3
2	ANP	A	1000	-	-	7/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ANP	PB-O3A	4.68	1.64	1.59
2	B	1001	ANP	PB-O3A	3.79	1.63	1.59
2	B	1001	ANP	PA-O3A	3.65	1.63	1.59
2	B	1001	ANP	C8-N7	2.57	1.36	1.31
2	B	1001	ANP	C2-N1	2.49	1.38	1.33
2	B	1001	ANP	PG-O1G	2.49	1.50	1.46
2	A	1000	ANP	C8-N7	2.45	1.36	1.31
2	A	1000	ANP	C2-N1	2.26	1.38	1.33
2	A	1000	ANP	PB-O1B	2.19	1.49	1.46
2	B	1001	ANP	C2-N3	2.13	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ANP	N3-C2-N1	-6.53	118.70	128.58
2	B	1001	ANP	N3-C2-N1	-5.78	119.84	128.58
2	A	1000	ANP	N9-C8-N7	-4.24	107.92	113.94
2	A	1000	ANP	O1B-PB-N3B	-4.18	105.62	111.77
2	B	1001	ANP	C5-C4-N3	-4.10	121.07	126.72
2	A	1000	ANP	C5-C4-N3	-4.06	121.13	126.72
2	B	1001	ANP	O2A-PA-O3A	3.98	118.04	107.27
2	A	1000	ANP	C5-N7-C8	3.88	109.55	103.45
2	B	1001	ANP	C5-N7-C8	3.61	109.13	103.45
2	A	1000	ANP	C2-N3-C4	3.59	120.60	111.83
2	A	1000	ANP	O2A-PA-O3A	3.50	116.74	107.27
2	A	1000	ANP	C4-C5-N7	-3.39	106.70	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ANP	N9-C8-N7	-3.33	109.21	113.94
2	B	1001	ANP	C4-C5-N7	-3.21	106.91	110.58
2	B	1001	ANP	C2-N3-C4	3.01	119.19	111.83
2	B	1001	ANP	C2-N1-C6	2.72	123.19	118.73
2	B	1001	ANP	O4'-C1'-N9	2.55	112.98	108.09
2	A	1000	ANP	C5-C4-N9	2.25	108.26	105.81
2	A	1000	ANP	C2-N1-C6	2.14	122.25	118.73
2	B	1001	ANP	N3-C4-N9	2.14	130.81	127.17
2	B	1001	ANP	C5-C4-N9	2.12	108.12	105.81
2	B	1001	ANP	O1B-PB-N3B	-2.04	108.76	111.77
2	A	1000	ANP	O4'-C1'-N9	2.04	112.01	108.09
2	A	1000	ANP	N3-C4-N9	2.02	130.60	127.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	ANP	PB-N3B-PG-O1G
2	A	1000	ANP	PA-O3A-PB-O1B
2	A	1000	ANP	PA-O3A-PB-O2B
2	A	1000	ANP	C5'-O5'-PA-O1A
2	A	1000	ANP	C5'-O5'-PA-O3A
2	B	1001	ANP	PG-N3B-PB-O1B
2	B	1001	ANP	O4'-C4'-C5'-O5'
2	B	1001	ANP	C3'-C4'-C5'-O5'
2	B	1001	ANP	PB-O3A-PA-O1A
2	B	1001	ANP	C5'-O5'-PA-O1A
2	A	1000	ANP	PB-O3A-PA-O2A
2	B	1001	ANP	PB-O3A-PA-O2A
2	B	1001	ANP	PA-O3A-PB-O1B
2	A	1000	ANP	PB-O3A-PA-O1A

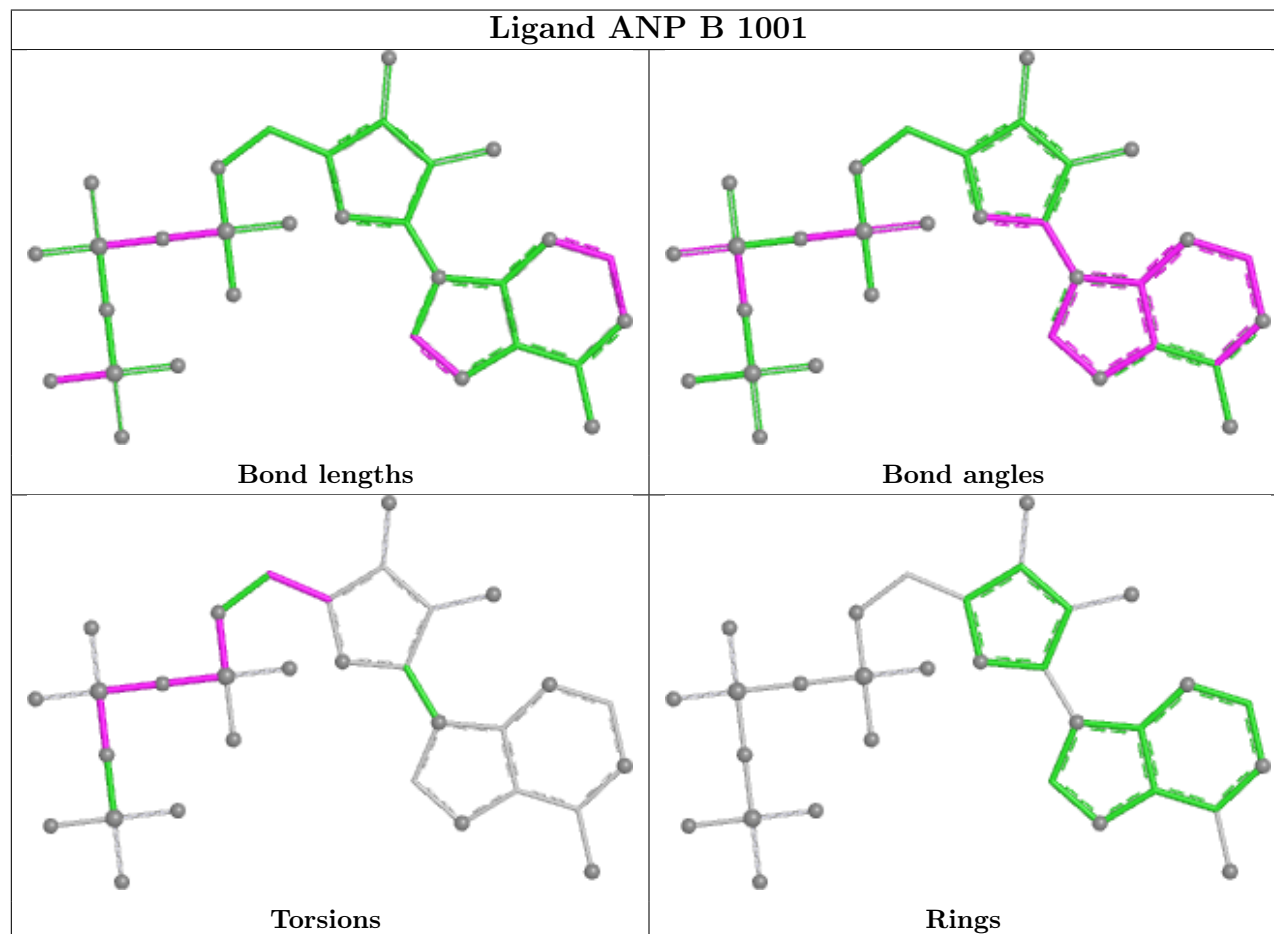
There are no ring outliers.

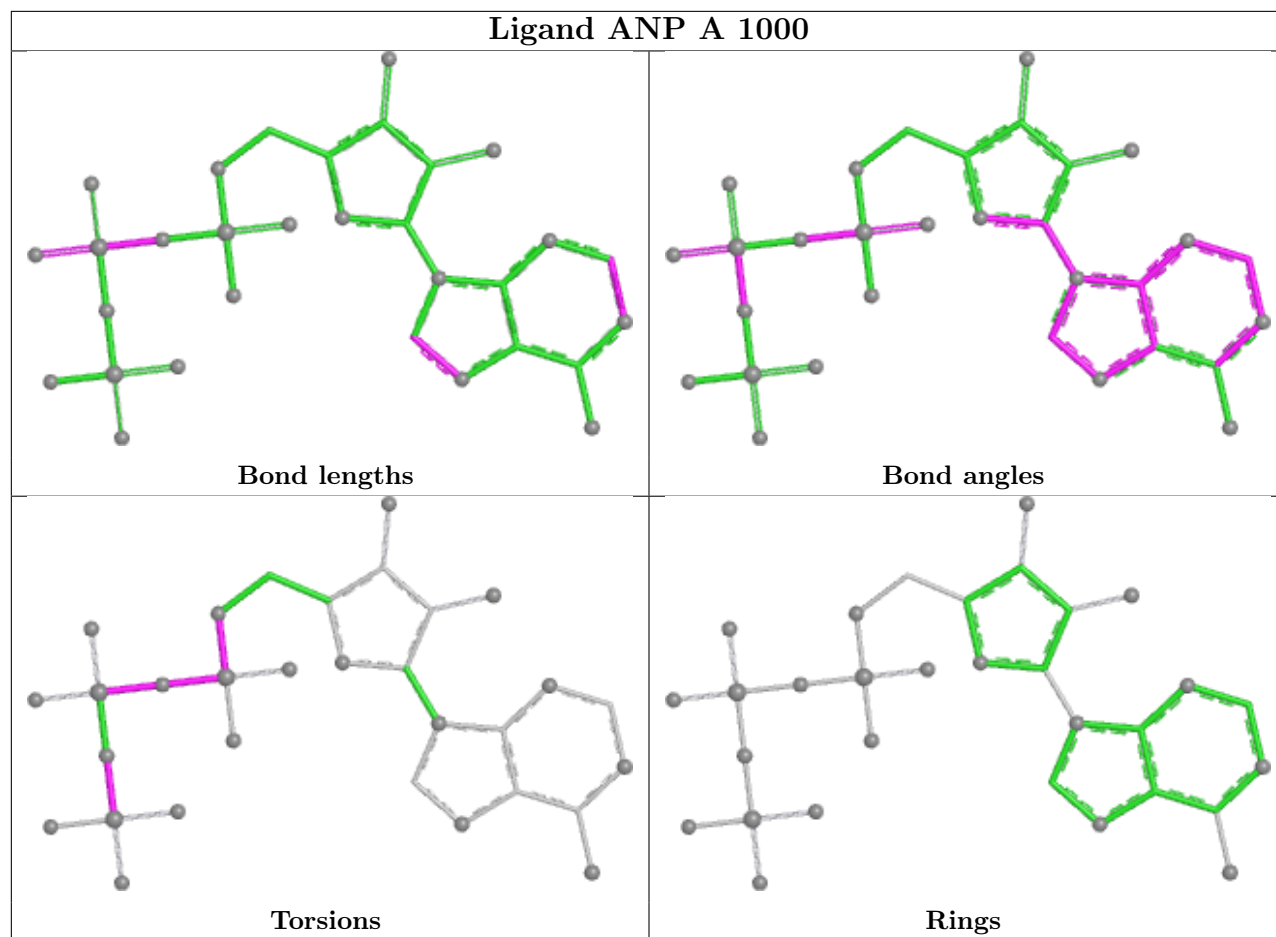
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	ANP	2	0
2	A	1000	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [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

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.