



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 AM GMT

PDB ID : 2FL2
Title : crystal structure of KSP in complex with inhibitor 19
Authors : Yan, Y.
Deposited on : 2006-01-05
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

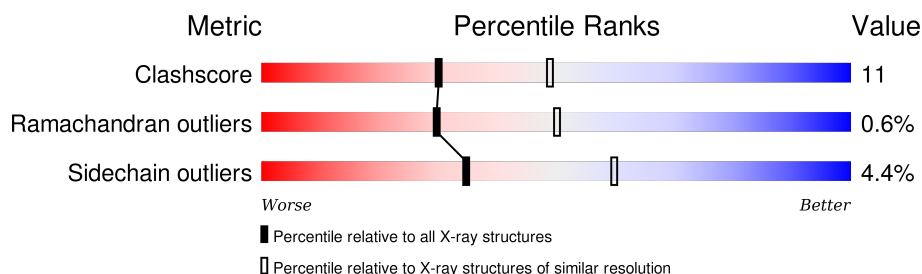
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5425 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.

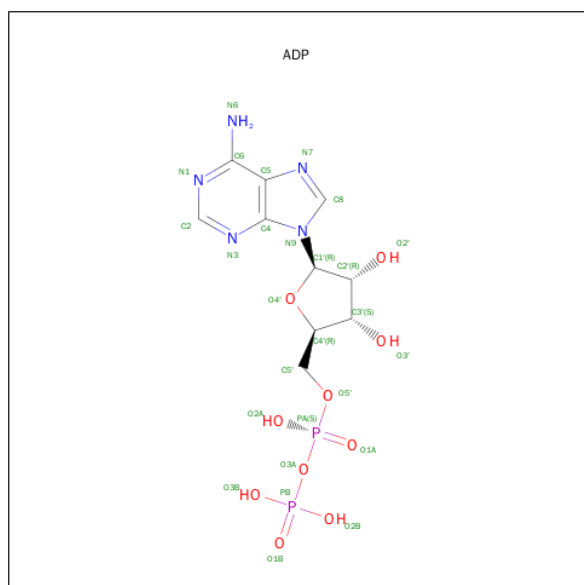
- Molecule 1 is a protein called Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			
1	B	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

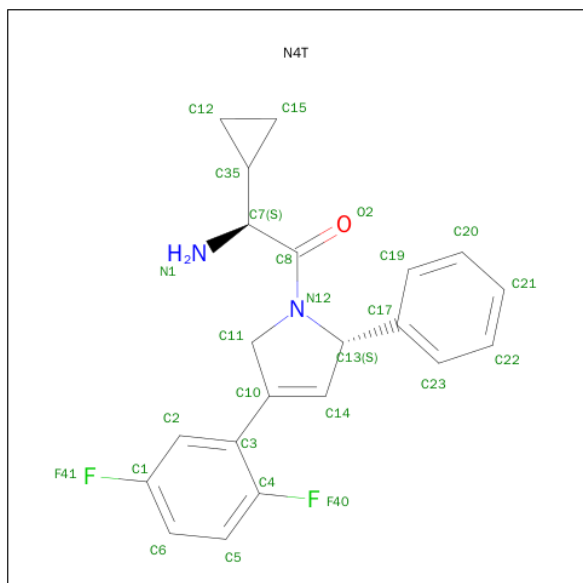
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- 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 (1S)-1-CYCLOPROPYL-2-[(2S)-4-(2,5-DIFLUOROPHENYL)-2-PHENYL-L-2,5-DIHYDRO-1H-PYRROL-1-YL]-2-OXOETHANAMINE (three-letter code: N4T) (formula: C₂₁H₂₀F₂N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	21	2	2	1		
4	B	1	Total	C	F	N	O	0	0
			26	21	2	2	1		

- Molecule 5 is water.

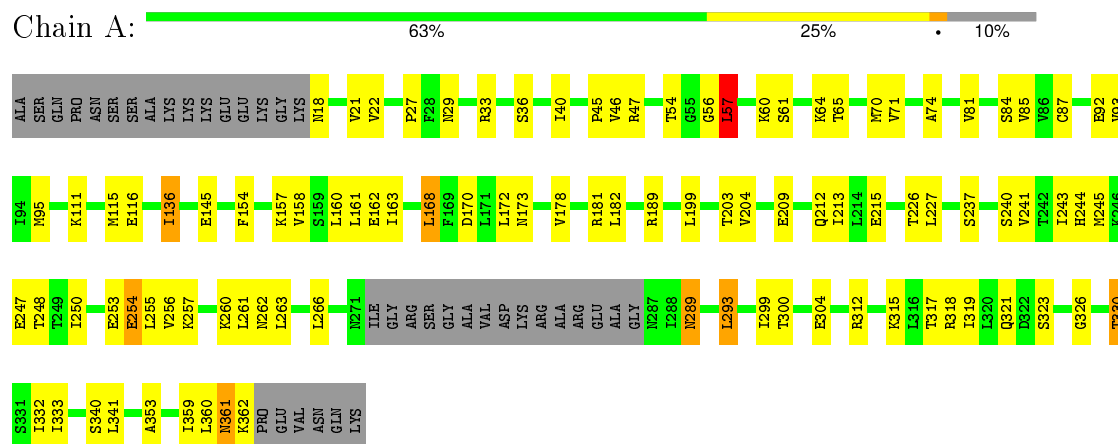
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	64	Total	O	0	0
			64	64		

3 Residue-property plots [i](#)

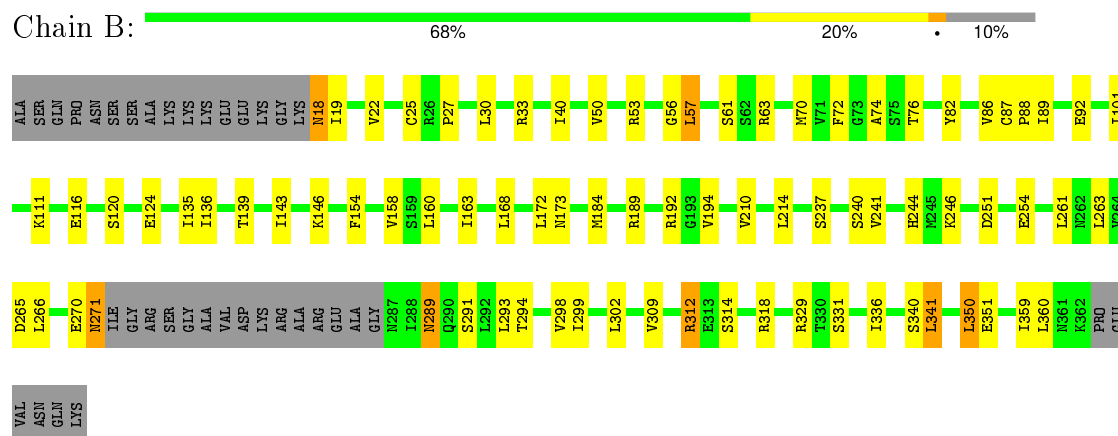
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Kinesin-like protein KIF11



- Molecule 1: Kinesin-like protein KIF11



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.80 Å 79.50 Å 159.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	53.0 (50.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: MG, N4T, ADP

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	0.66	1/2632 (0.0%)	0.69	0/3559
1	B	0.66	1/2632 (0.0%)	0.68	0/3559
All	All	0.66	2/5264 (0.0%)	0.69	0/7118

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	ILE	CA-C	5.54	1.67	1.52
1	B	120	SER	CA-C	-5.38	1.39	1.52

There are no bond angle outliers.

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	2594	0	2618	64	0
1	B	2594	0	2618	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	26	0	17	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	26	0	17	2	0
5	A	65	0	0	3	0
5	B	64	0	0	6	0
All	All	5425	0	5294	118	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 11.

All (118) 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:299:ILE:HG23	1:A:359:ILE:HD11	1.32	1.11
1:B:40:ILE:HD13	1:B:340:SER:HA	1.33	1.09
1:B:18:ASN:HB2	1:B:360:LEU:HD12	1.45	0.99
1:A:116:GLU:HB3	4:A:604:N4T:H14	1.48	0.95
1:A:56:GLY:O	1:A:57:LEU:HB2	1.71	0.88
1:A:21:VAL:HG22	1:A:332:ILE:HB	1.57	0.87
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.63	0.80
1:A:323:SER:O	1:A:330:THR:HG21	1.89	0.72
1:A:54:THR:HG21	1:A:64:LYS:HD3	1.70	0.72
1:B:124:GLU:OE1	5:B:607:HOH:O	2.08	0.71
1:B:341:LEU:O	1:B:341:LEU:HG	1.95	0.66
1:A:326:GLY:O	1:A:361:ASN:HB2	1.96	0.65
1:A:18:ASN:HB2	1:A:360:LEU:HD12	1.78	0.65
1:B:116:GLU:HB3	4:B:605:N4T:H14	1.79	0.65
1:B:40:ILE:CD1	1:B:340:SER:HA	2.20	0.64
1:A:40:ILE:HD13	1:A:340:SER:HA	1.79	0.63
1:B:92:GLU:OE2	1:B:329:ARG:HD2	1.99	0.63
1:A:361:ASN:O	1:A:362:LYS:HB2	1.99	0.62
1:B:312:ARG:HA	1:B:318:ARG:HG3	1.82	0.61
1:B:351:GLU:HA	5:B:638:HOH:O	2.02	0.60
1:A:178:VAL:HG23	1:A:227:LEU:HD23	1.84	0.59
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.85	0.59
1:B:237:SER:OG	1:B:265:ASP:HB3	2.03	0.58
1:B:139:THR:O	1:B:143:ILE:HG13	2.03	0.58
1:B:160:LEU:HB3	1:B:172:LEU:HG	1.85	0.57
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.69	0.56
1:A:45:PRO:HA	1:A:71:VAL:HG23	1.86	0.56
1:A:312:ARG:HA	1:A:318:ARG:HG2	1.87	0.56
1:A:312:ARG:HA	1:A:318:ARG:CG	2.37	0.55
1:B:63:ARG:HD2	5:B:615:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:HE3	1:B:266:LEU:O	2.07	0.55
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.90	0.54
1:A:115:MET:CE	1:A:263:LEU:HB3	2.37	0.54
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.89	0.54
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.89	0.54
1:A:57:LEU:HB3	1:A:60:LYS:O	2.08	0.53
1:A:315:LYS:O	1:A:319:ILE:HG13	2.08	0.53
1:B:19:ILE:HD12	1:B:359:ILE:HB	1.91	0.52
1:A:81:VAL:O	1:A:85:VAL:HG22	2.10	0.51
1:B:57:LEU:HD12	1:B:57:LEU:H	1.74	0.51
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.41	0.51
1:A:317:THR:O	1:A:321:GLN:HB3	2.12	0.51
1:B:184:MET:HE3	1:B:318:ARG:HH21	1.76	0.50
1:B:146:LYS:HE3	5:B:618:HOH:O	2.11	0.50
1:A:300:THR:O	1:A:304:GLU:HG3	2.12	0.50
1:B:18:ASN:HD22	1:B:360:LEU:HD11	1.77	0.50
1:A:27:PRO:HB3	1:A:74:ALA:HB1	1.93	0.49
1:A:116:GLU:HB3	4:A:604:N4T:C14	2.32	0.49
1:A:158:VAL:HA	1:A:240:SER:O	2.13	0.49
1:B:163:ILE:HG12	1:B:168:LEU:HD23	1.94	0.49
1:B:251:ASP:HB2	5:B:665:HOH:O	2.13	0.48
1:B:312:ARG:HA	1:B:318:ARG:CG	2.42	0.48
1:A:181:ARG:HD2	5:A:661:HOH:O	2.12	0.48
1:A:241:VAL:O	1:A:241:VAL:HG13	2.14	0.48
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.95	0.48
1:A:70:MET:HE1	1:A:84:SER:HB3	1.96	0.48
1:B:86:VAL:HG21	1:B:135:ILE:HG12	1.96	0.48
1:A:209:GLU:O	1:A:213:ILE:HG13	2.14	0.48
1:A:92:GLU:HA	1:A:95:MET:CE	2.44	0.47
1:A:93:VAL:HG21	1:A:261:LEU:HB2	1.96	0.47
1:A:57:LEU:CB	1:A:60:LYS:O	2.63	0.47
1:B:89:ILE:HD12	1:B:101:ILE:HD11	1.95	0.47
1:A:341:LEU:HD12	1:A:341:LEU:H	1.79	0.47
1:B:241:VAL:HG13	1:B:261:LEU:HB3	1.97	0.47
1:B:291:SER:HA	1:B:314:SER:HB2	1.97	0.46
1:B:270:GLU:O	1:B:271:ASN:HB3	2.14	0.46
1:B:210:VAL:O	1:B:214:LEU:HG	2.16	0.46
1:B:82:TYR:CD2	1:B:86:VAL:HB	2.51	0.46
1:A:181:ARG:HB2	5:A:624:HOH:O	2.14	0.46
1:B:57:LEU:O	1:B:61:SER:HB3	2.17	0.46
1:A:247:GLU:O	1:A:254:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HA	1:B:240:SER:O	2.16	0.45
1:A:22:VAL:HG22	1:A:333:ILE:HG12	1.99	0.45
1:A:18:ASN:CB	1:A:360:LEU:HD12	2.45	0.45
1:B:189:ARG:HD3	5:B:622:HOH:O	2.17	0.45
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.46	0.45
1:B:246:LYS:HD3	1:B:254:GLU:OE2	2.17	0.45
1:A:92:GLU:HG2	1:A:95:MET:HE3	1.97	0.45
1:B:184:MET:CG	1:B:194:VAL:HG21	2.47	0.44
1:B:336:ILE:HG21	1:B:350:LEU:CD1	2.47	0.44
1:A:21:VAL:HG11	1:A:353:ALA:HB1	1.98	0.44
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.47	0.44
1:A:154:PHE:HA	1:A:244:HIS:O	2.16	0.44
1:A:162:GLU:HG2	1:A:237:SER:HA	1.98	0.44
1:B:30:LEU:HD23	1:B:33:ARG:HD3	2.00	0.44
1:A:111:LYS:HE3	1:A:266:LEU:O	2.17	0.44
1:A:245:MET:O	1:A:256:VAL:HA	2.16	0.43
1:A:163:ILE:HD11	1:A:319:ILE:HD12	2.00	0.43
1:A:29:ASN:O	1:A:33:ARG:HG2	2.19	0.43
1:A:243:ILE:HG22	1:A:245:MET:HG3	2.00	0.43
1:B:294:THR:O	1:B:298:VAL:HG23	2.18	0.43
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.49	0.43
1:B:298:VAL:HG13	1:B:309:VAL:CG1	2.49	0.43
1:A:157:LYS:HE2	1:A:203:THR:OG1	2.18	0.43
1:A:289:ASN:O	1:A:293:LEU:HB2	2.19	0.43
1:A:247:GLU:HB3	1:A:255:LEU:HB2	2.01	0.42
1:B:18:ASN:HD22	1:B:360:LEU:CD1	2.32	0.42
1:B:53:ARG:HB2	1:B:63:ARG:NH1	2.34	0.42
1:A:160:LEU:HB3	1:A:172:LEU:HG	2.02	0.42
1:A:92:GLU:HA	1:A:95:MET:HE2	2.01	0.42
1:A:212:GLN:HB2	5:A:643:HOH:O	2.19	0.42
1:B:154:PHE:HA	1:B:244:HIS:O	2.19	0.42
1:A:257:LYS:HB2	1:A:257:LYS:HE3	1.92	0.42
1:B:25:CYS:O	1:B:74:ALA:HA	2.19	0.42
1:B:192:ARG:HB3	1:B:192:ARG:NH1	2.35	0.42
1:A:163:ILE:HG12	1:A:168:LEU:HD12	2.02	0.41
1:A:116:GLU:CB	4:A:604:N4T:H14	2.34	0.41
1:A:215:GLU:HG2	4:A:604:N4T:C12	2.50	0.41
1:B:116:GLU:HB3	4:B:605:N4T:C14	2.49	0.41
1:A:204:VAL:HG22	1:A:213:ILE:CD1	2.50	0.41
1:A:46:VAL:HG13	1:A:47:ARG:HG3	2.03	0.41
1:A:248:THR:HA	1:A:253:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:VAL:O	1:B:50:VAL:HG13	2.22	0.40
1:A:57:LEU:O	1:A:61:SER:HB3	2.21	0.40
1:B:27:PRO:HB3	1:B:74:ALA:HB1	2.02	0.40
1:B:289:ASN:HD22	1:B:289:ASN:C	2.25	0.40
1:A:45:PRO:HA	1:A:71:VAL:CG2	2.51	0.40
1:B:72:PHE:HB3	1:B:76:THR:HG21	2.02	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	326/367 (89%)	314 (96%)	9 (3%)	3 (1%)	21	37
1	B	326/367 (89%)	317 (97%)	8 (2%)	1 (0%)	46	68
All	All	652/734 (89%)	631 (97%)	17 (3%)	4 (1%)	30	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	189	ARG
1	A	36	SER
1	B	56	GLY

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	293/321 (91%)	278 (95%)	15 (5%)	29	52
1	B	293/321 (91%)	282 (96%)	11 (4%)	40	67
All	All	586/642 (91%)	560 (96%)	26 (4%)	35	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	65	THR
1	A	87	CYS
1	A	145	GLU
1	A	161	LEU
1	A	168	LEU
1	A	173	ASN
1	A	199	LEU
1	A	226	THR
1	A	250	ILE
1	A	254	GLU
1	A	289	ASN
1	A	293	LEU
1	A	330	THR
1	A	361	ASN
1	B	18	ASN
1	B	57	LEU
1	B	173	ASN
1	B	271	ASN
1	B	289	ASN
1	B	293	LEU
1	B	302	LEU
1	B	312	ARG
1	B	331	SER
1	B	341	LEU
1	B	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	262	ASN
1	A	289	ASN
1	A	342	ASN
1	A	361	ASN
1	B	18	ASN
1	B	141	HIS
1	B	142	GLN
1	B	173	ASN
1	B	262	ASN
1	B	289	ASN
1	B	290	GLN
1	B	342	ASN
1	B	358	ASN
1	B	361	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	601	2	22,29,29	1.71	5 (22%)	27,45,45	2.78	3 (11%)
4	N4T	A	604	-	26,29,29	2.74	9 (34%)	34,42,42	1.94	11 (32%)
3	ADP	B	600	2	22,29,29	1.69	7 (31%)	27,45,45	2.97	4 (14%)
4	N4T	B	605	-	26,29,29	2.68	8 (30%)	34,42,42	1.92	13 (38%)

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	601	2	-	0/12/32/32	0/3/3/3
4	N4T	A	604	-	-	0/20/34/34	0/3/4/4
3	ADP	B	600	2	-	0/12/32/32	0/3/3/3
4	N4T	B	605	-	-	0/20/34/34	0/3/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	N4T	C35-C7	-10.12	1.36	1.53
4	B	605	N4T	C35-C7	-8.92	1.38	1.53
4	A	604	N4T	C17-C13	-3.20	1.49	1.52
3	A	601	ADP	C5-N7	-2.29	1.31	1.39
3	B	600	ADP	C5-N7	-2.21	1.31	1.39
3	B	600	ADP	PB-O3B	-2.00	1.47	1.54
3	B	600	ADP	C5'-C4'	2.00	1.58	1.51
4	A	604	N4T	C14-C10	2.03	1.37	1.34
3	B	600	ADP	C2-N1	2.04	1.37	1.33
4	B	605	N4T	C6-C1	2.06	1.41	1.37
4	A	604	N4T	C20-C19	2.16	1.43	1.38
3	A	601	ADP	C4-N3	2.22	1.38	1.35
4	B	605	N4T	C21-C20	2.22	1.43	1.38
3	A	601	ADP	C5'-C4'	2.40	1.59	1.51
4	A	604	N4T	C6-C1	2.43	1.41	1.37
4	A	604	N4T	C11-C10	2.91	1.55	1.50
3	B	600	ADP	C4-N3	2.99	1.40	1.35
4	A	604	N4T	C3-C4	3.08	1.43	1.38
4	B	605	N4T	C14-C10	3.09	1.39	1.34
3	A	601	ADP	C2-N3	3.17	1.37	1.32
4	B	605	N4T	C11-C10	3.25	1.55	1.50
3	B	600	ADP	C2-N3	3.44	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	ADP	O4'-C1'	3.61	1.45	1.41
4	A	604	N4T	C23-C17	3.66	1.45	1.39
4	B	605	N4T	C3-C4	4.02	1.44	1.38
4	B	605	N4T	C19-C17	4.08	1.45	1.39
4	A	604	N4T	C19-C17	4.26	1.46	1.39
3	A	601	ADP	O4'-C1'	4.41	1.46	1.41
4	B	605	N4T	C23-C17	4.72	1.46	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	ADP	N3-C2-N1	-14.37	117.89	128.89
3	A	601	ADP	N3-C2-N1	-13.35	118.67	128.89
4	A	604	N4T	O2-C8-C7	-4.54	111.20	120.12
4	B	605	N4T	O2-C8-C7	-3.69	112.88	120.12
4	A	604	N4T	C11-C10-C14	-3.03	103.83	111.41
4	B	605	N4T	C6-C5-C4	-3.00	115.73	119.00
4	A	604	N4T	F41-C1-C2	-2.72	114.59	118.22
4	A	604	N4T	C23-C17-C13	-2.60	116.21	120.70
4	B	605	N4T	C12-C35-C15	-2.39	58.24	59.88
4	B	605	N4T	C20-C19-C17	-2.18	117.75	120.64
4	B	605	N4T	C11-C10-C14	-2.10	106.15	111.41
4	B	605	N4T	C23-C17-C13	-2.09	117.08	120.70
4	A	604	N4T	C6-C5-C4	-2.07	116.74	119.00
4	B	605	N4T	F40-C4-C5	-2.06	113.79	118.47
3	A	601	ADP	C4'-O4'-C1'	2.04	111.96	109.72
4	B	605	N4T	C5-C4-C3	2.05	125.59	123.20
4	B	605	N4T	C22-C21-C20	2.05	123.52	119.93
3	B	600	ADP	C2-N1-C6	2.09	122.50	118.77
4	B	605	N4T	C7-C8-N12	2.10	124.13	118.62
4	A	604	N4T	C4-C3-C10	2.15	124.41	123.20
3	B	600	ADP	C4'-O4'-C1'	2.19	112.13	109.72
4	A	604	N4T	C11-C10-C3	2.21	125.24	120.89
4	A	604	N4T	C35-C7-N1	2.38	124.78	112.13
4	A	604	N4T	C35-C7-C8	2.38	115.97	110.86
4	B	605	N4T	C8-C7-N1	2.46	114.01	108.84
4	A	604	N4T	O2-C8-N12	2.63	125.92	121.41
3	A	601	ADP	O3A-PA-O5'	2.88	110.58	102.94
3	B	600	ADP	O3A-PA-O5'	2.93	110.70	102.94
4	B	605	N4T	C35-C7-C8	3.32	117.98	110.86
4	B	605	N4T	C12-C35-C7	4.91	128.06	119.40
4	A	604	N4T	C12-C35-C7	4.92	128.09	119.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	N4T	4	0
4	B	605	N4T	2	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.