Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:09 PM GMT

PDB ID	:	1J1B
Title	:	Binary complex structure of human tau protein kinase I with AMPPNP
Authors	:	Aoki, M.; Yokota, T.; Sugiura, I.; Sasaki, C.; Hasegawa, T.; Okumura, C.; Kohno, T.; Sugio, S.; Matsuzaki, T.
Deposited on	:	2002-12-03
Resolution	:	1.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

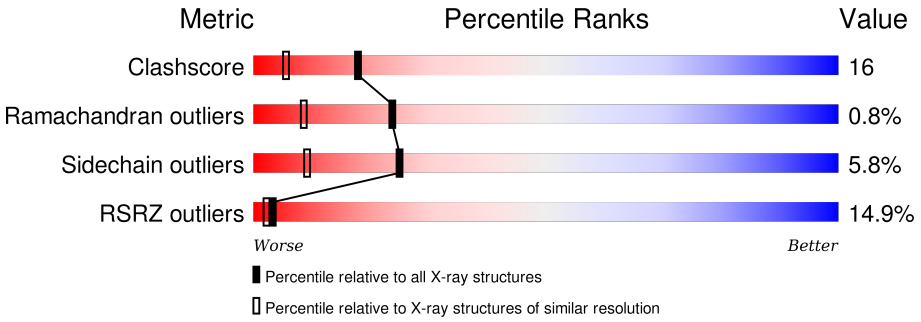
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	420	12% 65% 15% • 16%
1	B	420	14% 64% 20% • 13%

2 Entry composition

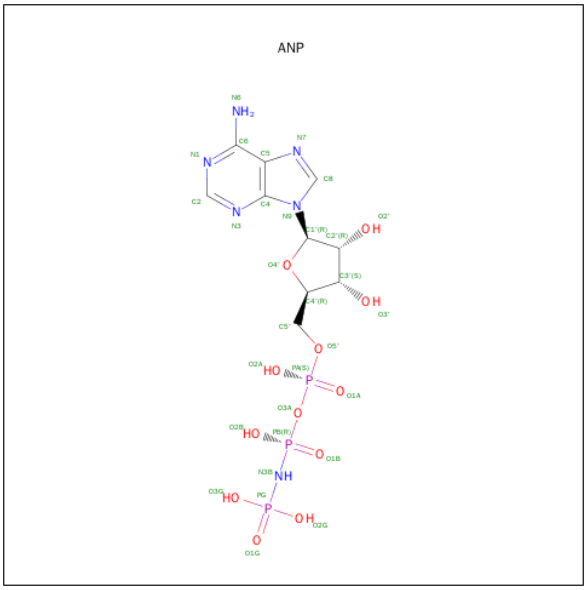
There are 3 unique types of molecules in this entry. The entry contains 6218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2828	1818	486	513	11			
1	B	364	Total	C	N	O	S	0	0	0
			2909	1867	501	529	12			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: 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.

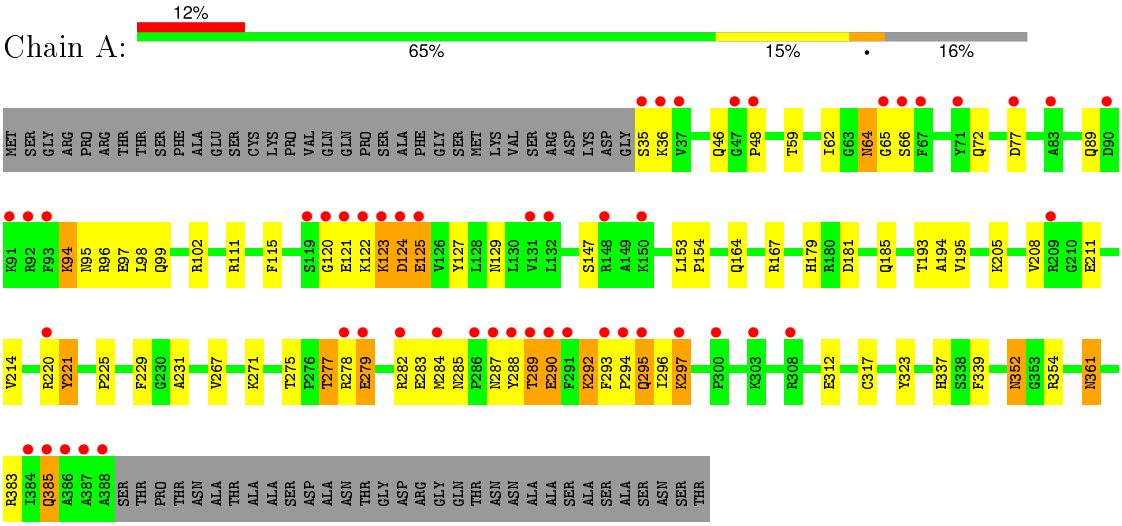
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	234	Total O 234 234	0	0
3	B	185	Total O 185 185	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

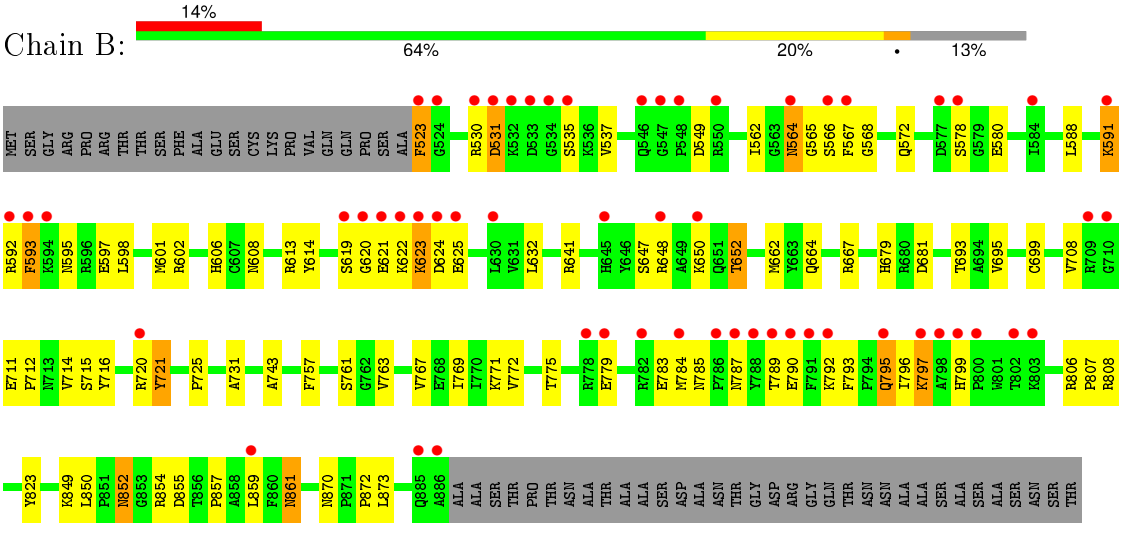
- Molecule 1: Glycogen synthase kinase-3 beta

Chain A:



- Molecule 1: Glycogen synthase kinase-3 beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.80Å 86.30Å 178.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 1.80 19.81 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.80-1.80) 89.6 (19.81-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.216 , 0.242 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 59.5	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 126063 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.36	0/2899	0.57	0/3944
1	B	0.36	0/2981	0.55	0/4050
All	All	0.36	0/5880	0.56	0/7994

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2828	0	2856	97	0
1	B	2909	0	2936	109	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	234	0	0	8	0
3	B	185	0	0	7	0
All	All	6218	0	5818	184	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 (184) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ASN:HD22	1:B:598:LEU:H	1.14	0.90
1:B:861:ASN:HD22	1:B:861:ASN:H	1.21	0.86
1:A:95:ASN:HD22	1:A:98:LEU:H	1.20	0.85
1:A:337:HIS:HD2	1:A:339:PHE:H	1.26	0.83
1:A:361:ASN:HD22	1:A:361:ASN:H	1.24	0.82
1:A:94:LYS:HE3	1:A:95:ASN:H	1.45	0.82
1:A:111:ARG:HD2	3:A:654:HOH:O	1.82	0.78
1:A:214:VAL:CG1	1:B:790:GLU:HB2	2.16	0.75
1:B:861:ASN:H	1:B:861:ASN:ND2	1.85	0.73
1:B:861:ASN:HD22	1:B:861:ASN:N	1.80	0.72
1:A:94:LYS:HG3	1:A:99:GLN:NE2	2.04	0.72
1:B:595:ASN:HD21	1:B:597:GLU:HB3	1.54	0.72
1:A:214:VAL:HG11	1:B:790:GLU:HB2	1.70	0.72
1:A:361:ASN:HD22	1:A:361:ASN:N	1.85	0.71
1:A:179:HIS:HD2	1:A:181:ASP:H	1.38	0.71
1:B:595:ASN:ND2	1:B:598:LEU:H	1.89	0.70
1:B:784:MET:HE1	1:B:823:TYR:HD1	1.57	0.69
1:B:807:PRO:O	1:B:808:ARG:HB2	1.92	0.69
1:A:214:VAL:HG11	1:B:790:GLU:CB	2.21	0.69
1:B:679:HIS:HD2	1:B:681:ASP:H	1.40	0.69
1:A:46:GLN:HG3	3:A:473:HOH:O	1.93	0.69
1:A:123:LYS:HB3	1:A:125:GLU:HG2	1.74	0.69
3:A:649:HOH:O	1:B:790:GLU:HG3	1.93	0.68
1:A:277:THR:HG22	1:A:279:GLU:N	2.08	0.68
1:A:285:ASN:ND2	1:A:287:ASN:HD22	1.92	0.67
1:A:95:ASN:HD21	1:A:97:GLU:HB3	1.61	0.66
1:A:277:THR:HG22	1:A:279:GLU:H	1.59	0.66
1:B:664:GLN:HE22	1:B:695:VAL:HA	1.61	0.66
1:A:385:GLN:O	1:A:385:GLN:HG3	1.95	0.66
1:A:290:GLU:HG2	3:A:617:HOH:O	1.96	0.65
1:A:361:ASN:H	1:A:361:ASN:ND2	1.94	0.65
1:B:771:LYS:O	1:B:799:HIS:HB2	1.96	0.64
1:B:592:ARG:HG3	1:B:593:PHE:CE1	2.33	0.64
1:B:667:ARG:HH12	1:B:861:ASN:HD21	1.46	0.64
1:B:797:LYS:H	1:B:797:LYS:HD3	1.62	0.64
1:B:622:LYS:HB2	1:B:625:GLU:OE2	1.99	0.63
1:B:806:ARG:NH1	3:B:417:HOH:O	2.31	0.63
1:B:523:PHE:N	1:B:523:PHE:CD1	2.67	0.63
1:A:220:ARG:HD3	1:B:720:ARG:HD3	1.79	0.63
1:A:279:GLU:O	1:A:283:GLU:HG2	1.99	0.63
1:A:65:GLY:HA3	2:A:430:ANP:O1B	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:HG2	1:A:383:ARG:HH11	1.64	0.62
1:B:523:PHE:N	1:B:523:PHE:HD1	1.96	0.62
1:A:352:ASN:ND2	1:A:354:ARG:H	1.98	0.62
1:A:267:VAL:HG11	1:B:566:SER:HB2	1.81	0.61
1:A:337:HIS:CD2	1:A:339:PHE:H	2.14	0.61
1:A:297:LYS:HD3	1:A:297:LYS:H	1.64	0.61
1:A:122:LYS:HB3	1:A:125:GLU:OE2	2.01	0.60
1:A:220:ARG:O	1:A:221:TYR:HB2	2.01	0.60
1:B:784:MET:HE3	1:B:823:TYR:CA	2.32	0.60
1:A:288:TYR:OH	1:B:715:SER:OG	2.20	0.60
1:B:725:PRO:HG2	1:B:784:MET:HE2	1.83	0.60
1:B:852:ASN:C	1:B:852:ASN:HD22	2.05	0.60
1:B:620:GLY:C	1:B:622:LYS:H	2.05	0.60
1:A:288:TYR:HE2	1:B:716:TYR:HD2	1.48	0.60
1:A:284:MET:HE1	1:A:323:TYR:HD1	1.66	0.60
1:B:667:ARG:HH12	1:B:861:ASN:ND2	2.00	0.60
1:B:852:ASN:HD21	1:B:854:ARG:HB3	1.67	0.59
1:A:94:LYS:HE2	1:A:98:LEU:HD23	1.84	0.59
1:A:290:GLU:HB2	1:B:714:VAL:CG1	2.32	0.59
1:A:94:LYS:CE	1:A:95:ASN:H	2.13	0.58
1:B:720:ARG:O	1:B:721:TYR:HB2	2.02	0.58
1:B:852:ASN:ND2	1:B:854:ARG:H	2.01	0.58
1:A:62:ILE:HG21	1:A:72:GLN:HB2	1.86	0.58
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.17	0.58
1:A:290:GLU:HB2	1:B:714:VAL:HG13	1.87	0.57
1:A:94:LYS:HE3	1:A:95:ASN:N	2.19	0.57
1:B:772:VAL:HA	1:B:799:HIS:HB3	1.86	0.57
1:A:284:MET:CE	1:A:323:TYR:HD1	2.18	0.57
1:B:578:SER:OG	1:B:580:GLU:HB2	2.06	0.56
1:A:167:ARG:HH12	1:A:361:ASN:HD21	1.52	0.56
1:B:784:MET:HE3	1:B:823:TYR:CB	2.36	0.56
1:A:214:VAL:HG13	1:B:790:GLU:HB2	1.88	0.56
1:A:290:GLU:CB	1:B:714:VAL:HG11	2.36	0.56
1:A:275:THR:OG1	1:A:295:GLN:HA	2.06	0.55
1:B:806:ARG:HG2	1:B:806:ARG:HH11	1.72	0.55
1:A:167:ARG:HH12	1:A:361:ASN:ND2	2.06	0.54
1:B:784:MET:CE	1:B:823:TYR:HD1	2.19	0.54
1:A:352:ASN:HD21	1:A:354:ARG:HB2	1.72	0.54
1:A:277:THR:CG2	1:A:279:GLU:H	2.21	0.54
1:A:290:GLU:HB3	1:B:714:VAL:HG11	1.89	0.53
1:B:849:LYS:HE3	1:B:855:ASP:OD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:SER:OG	1:B:763:VAL:HG22	2.07	0.53
1:A:96:ARG:NH1	1:A:205:LYS:HD2	2.23	0.53
1:B:721:TYR:N	3:B:345:HOH:O	2.26	0.53
1:A:123:LYS:HG2	1:A:124:ASP:H	1.72	0.53
1:A:352:ASN:C	1:A:352:ASN:HD22	2.10	0.53
1:A:64:ASN:HD22	1:A:65:GLY:H	1.57	0.52
1:A:48:PRO:HA	3:A:522:HOH:O	2.10	0.52
1:A:220:ARG:CZ	1:B:720:ARG:CZ	2.88	0.52
1:A:164:GLN:HE22	1:A:195:VAL:HA	1.75	0.52
1:A:66:SER:HB2	1:B:767:VAL:HG11	1.91	0.52
1:B:595:ASN:ND2	1:B:597:GLU:HB3	2.25	0.51
1:A:120:GLY:HA3	1:A:127:TYR:HE1	1.74	0.51
1:B:620:GLY:O	1:B:622:LYS:N	2.43	0.51
1:B:641:ARG:HD3	3:B:281:HOH:O	2.10	0.51
1:A:383:ARG:HG2	1:A:383:ARG:NH1	2.25	0.51
1:A:225:PRO:HG2	1:A:284:MET:HE2	1.93	0.51
1:B:580:GLU:CD	1:B:613:ARG:HH12	2.15	0.50
1:B:598:LEU:O	1:B:602:ARG:HG3	2.12	0.50
1:B:592:ARG:HG3	1:B:593:PHE:CD1	2.47	0.50
1:A:288:TYR:HD2	1:B:716:TYR:HE2	1.58	0.50
1:B:530:ARG:HA	1:B:535:SER:O	2.12	0.50
1:B:792:LYS:O	1:B:792:LYS:HG2	2.12	0.50
1:A:292:LYS:HG2	1:A:292:LYS:O	2.12	0.50
1:A:220:ARG:O	1:A:221:TYR:CB	2.60	0.49
1:B:785:ASN:HD21	1:B:787:ASN:HD22	1.60	0.49
1:B:784:MET:HE3	1:B:823:TYR:HB3	1.94	0.49
1:A:285:ASN:HD21	1:A:287:ASN:HD22	1.57	0.49
1:B:725:PRO:HG2	1:B:784:MET:CE	2.43	0.49
1:B:870:ASN:OD1	1:B:872:PRO:HD2	2.13	0.49
1:B:861:ASN:N	1:B:861:ASN:ND2	2.49	0.49
1:A:214:VAL:HG11	1:B:790:GLU:HB3	1.93	0.49
1:A:277:THR:CG2	1:A:278:ARG:N	2.75	0.49
1:A:312:GLU:OE2	1:A:312:GLU:HA	2.13	0.48
1:A:179:HIS:CD2	1:A:181:ASP:H	2.27	0.48
1:B:562:ILE:HG21	1:B:572:GLN:HB2	1.95	0.48
1:B:720:ARG:HA	3:B:345:HOH:O	2.13	0.48
1:B:852:ASN:HD22	1:B:854:ARG:H	1.61	0.48
1:A:229:PHE:O	1:A:288:TYR:CE1	2.65	0.48
1:A:290:GLU:CB	1:B:714:VAL:CG1	2.92	0.48
1:B:720:ARG:O	1:B:721:TYR:CB	2.61	0.47
1:A:289:THR:HG21	1:B:712:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:O	1:A:102:ARG:HG3	2.15	0.46
1:B:567:PHE:N	1:B:567:PHE:CD2	2.84	0.46
1:B:784:MET:HE3	1:B:823:TYR:HA	1.98	0.46
1:B:679:HIS:HD2	1:B:681:ASP:N	2.11	0.46
1:A:221:TYR:N	3:A:452:HOH:O	2.35	0.46
1:A:288:TYR:CE2	1:B:716:TYR:HD2	2.30	0.46
1:B:601:MET:HE1	1:B:632:LEU:CD2	2.46	0.46
1:A:185:GLN:NE2	3:A:431:HOH:O	2.33	0.46
1:B:797:LYS:H	1:B:797:LYS:CD	2.28	0.45
1:A:288:TYR:HE2	1:B:716:TYR:CD2	2.32	0.45
1:B:662:MET:HE1	1:B:743:ALA:O	2.16	0.45
1:B:564:ASN:HD22	1:B:565:GLY:H	1.65	0.45
1:B:620:GLY:C	1:B:622:LYS:N	2.70	0.45
1:B:693:THR:O	1:B:857:PRO:HG3	2.16	0.45
1:A:94:LYS:HG3	1:A:99:GLN:HE21	1.80	0.45
1:B:715:SER:HB3	1:B:731:ALA:O	2.17	0.45
1:A:284:MET:HE3	1:A:323:TYR:CA	2.46	0.45
1:B:852:ASN:C	1:B:852:ASN:ND2	2.70	0.45
1:A:89:GLN:HA	1:A:89:GLN:NE2	2.30	0.45
1:A:294:PRO:HB2	1:A:296:ILE:CD1	2.47	0.45
1:A:267:VAL:O	1:A:271:LYS:HG3	2.16	0.44
1:A:288:TYR:HE1	3:A:642:HOH:O	2.01	0.44
1:A:95:ASN:ND2	1:A:98:LEU:H	2.00	0.44
1:B:850:LEU:HD13	3:B:286:HOH:O	2.17	0.44
1:A:284:MET:HE3	1:A:323:TYR:CB	2.48	0.43
1:B:757:PHE:CE2	1:B:769:ILE:HA	2.53	0.43
1:B:531:ASP:OD2	1:B:537:VAL:HG21	2.18	0.43
1:B:679:HIS:HE1	1:B:699:CYS:O	2.02	0.43
1:A:267:VAL:CG1	1:B:566:SER:HB2	2.48	0.43
1:B:679:HIS:CD2	1:B:681:ASP:H	2.28	0.43
1:A:352:ASN:C	1:A:352:ASN:ND2	2.71	0.43
1:B:779:GLU:O	1:B:783:GLU:HG2	2.19	0.42
1:A:153:LEU:HD12	1:A:154:PRO:HD2	2.01	0.42
1:A:95:ASN:ND2	1:A:97:GLU:HB3	2.30	0.42
1:B:652:THR:HG21	3:B:417:HOH:O	2.18	0.42
1:B:588:LEU:HD11	1:B:625:GLU:HB2	2.01	0.42
1:A:193:THR:O	1:A:194:ALA:HB3	2.19	0.42
1:B:595:ASN:HD22	1:B:598:LEU:N	1.97	0.42
1:A:279:GLU:OE1	1:A:282:ARG:HD3	2.20	0.42
1:A:231:ALA:HB2	1:A:285:ASN:HB2	2.02	0.41
1:B:775:THR:OG1	1:B:795:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:LEU:HB2	1:B:852:ASN:ND2	2.35	0.41
1:B:622:LYS:HD2	1:B:625:GLU:OE2	2.21	0.41
1:B:708:VAL:O	1:B:711:GLU:HB2	2.21	0.41
1:B:648:ARG:C	1:B:650:LYS:H	2.23	0.41
1:A:120:GLY:O	1:A:125:GLU:HG3	2.20	0.41
1:B:606:HIS:HE1	1:B:608:ASN:HD22	1.69	0.41
1:A:94:LYS:HD2	1:A:94:LYS:HA	1.56	0.41
1:B:784:MET:CE	1:B:823:TYR:CD1	3.02	0.41
1:A:122:LYS:HB3	1:A:125:GLU:CD	2.40	0.41
1:B:622:LYS:HB2	1:B:625:GLU:CD	2.41	0.41
1:A:288:TYR:CE2	1:B:716:TYR:CD2	3.07	0.41
1:A:59:THR:HA	1:A:72:GLN:O	2.21	0.41
1:B:623:LYS:HG2	1:B:624:ASP:H	1.85	0.41
1:B:568:GLY:HA2	3:B:220:HOH:O	2.20	0.41
1:B:873:LEU:HD23	1:B:873:LEU:HA	1.84	0.41
1:A:115:PHE:HA	1:A:129:ASN:O	2.21	0.41
1:B:565:GLY:HA3	2:B:930:ANP:O1B	2.20	0.40
1:B:857:PRO:O	1:B:859:LEU:HG	2.22	0.40
1:A:208:VAL:HB	1:A:211:GLU:CD	2.41	0.40
1:B:795:GLN:H	1:B:795:GLN:HG2	1.69	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	352/420 (84%)	331 (94%)	19 (5%)	2 (1%)	30 14
1	B	362/420 (86%)	339 (94%)	19 (5%)	4 (1%)	17 5
All	All	714/840 (85%)	670 (94%)	38 (5%)	6 (1%)	24 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	621	GLU
1	A	221	TYR
1	B	721	TYR
1	B	623	LYS
1	A	123	LYS
1	B	549	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	313/364 (86%)	292 (93%)	21 (7%)	20 6
1	B	323/364 (89%)	307 (95%)	16 (5%)	30 13
All	All	636/728 (87%)	599 (94%)	37 (6%)	25 9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	36	LYS
1	A	64	ASN
1	A	77	ASP
1	A	94	LYS
1	A	121	GLU
1	A	124	ASP
1	A	125	GLU
1	A	147	SER
1	A	277	THR
1	A	279	GLU
1	A	289	THR
1	A	290	GLU
1	A	292	LYS
1	A	293	PHE
1	A	295	GLN
1	A	297	LYS
1	A	317	CYS

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Mol	Chain	Res	Type
1	A	352	ASN
1	A	361	ASN
1	A	385	GLN
1	B	523	PHE
1	B	531	ASP
1	B	564	ASN
1	B	591	LYS
1	B	593	PHE
1	B	614	TYR
1	B	619	SER
1	B	647	SER
1	B	652	THR
1	B	789	THR
1	B	793	PHE
1	B	795	GLN
1	B	796	ILE
1	B	797	LYS
1	B	852	ASN
1	B	861	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	89	GLN
1	A	95	ASN
1	A	99	GLN
1	A	108	ASN
1	A	164	GLN
1	A	179	HIS
1	A	265	GLN
1	A	285	ASN
1	A	295	GLN
1	A	337	HIS
1	A	352	ASN
1	A	361	ASN
1	B	546	GLN
1	B	552	GLN
1	B	564	ASN
1	B	589	GLN
1	B	595	ASN
1	B	608	ASN

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Mol	Chain	Res	Type
1	B	664	GLN
1	B	679	HIS
1	B	765	GLN
1	B	787	ASN
1	B	795	GLN
1	B	852	ASN
1	B	861	ASN
1	B	881	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

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	A	430	-	27,33,33	2.80	5 (18%)	30,52,52	1.79	5 (16%)
2	ANP	B	930	-	27,33,33	2.69	5 (18%)	30,52,52	1.63	4 (13%)

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	A	430	-	-	0/12/38/38	0/3/3/3
2	ANP	B	930	-	-	0/12/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	930	ANP	PG-O3G	2.86	1.64	1.56
2	A	430	ANP	PG-O3G	2.94	1.64	1.56
2	A	430	ANP	C5-C4	3.92	1.49	1.40
2	B	930	ANP	C5-C4	4.16	1.49	1.40
2	B	930	ANP	PG-O1G	5.00	1.51	1.46
2	A	430	ANP	PG-O1G	6.03	1.53	1.46
2	B	930	ANP	PB-O1B	6.44	1.53	1.46
2	A	430	ANP	PB-O1B	6.99	1.54	1.46
2	A	430	ANP	C4-N3	9.37	1.49	1.35
2	B	930	ANP	C4-N3	9.44	1.49	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	430	ANP	C2'-C1'-N9	-5.26	106.25	114.29
2	B	930	ANP	C2'-C1'-N9	-4.52	107.38	114.29
2	A	430	ANP	N3-C2-N1	-3.50	126.22	128.89
2	B	930	ANP	N3-C2-N1	-2.88	126.69	128.89
2	A	430	ANP	O3'-C3'-C4'	2.06	117.22	111.05
2	B	930	ANP	O2B-PB-O3A	2.06	114.44	105.09
2	A	430	ANP	O2B-PB-O3A	2.08	114.53	105.09
2	B	930	ANP	C4-C5-N7	4.11	113.26	109.48
2	A	430	ANP	C4-C5-N7	4.54	113.65	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	430	ANP	1	0
2	B	930	ANP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	354/420 (84%)	0.80	50 (14%) 4 3	15, 28, 71, 94	0
1	B	364/420 (86%)	0.86	57 (15%) 3 2	17, 32, 83, 94	0
All	All	718/840 (85%)	0.83	107 (14%) 3 2	15, 30, 78, 94	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	TYR	16.3
1	A	388	ALA	14.3
1	B	523	PHE	11.7
1	B	620	GLY	11.5
1	A	120	GLY	10.5
1	B	788	TYR	10.2
1	A	122	LYS	10.0
1	B	533	ASP	9.4
1	A	387	ALA	9.3
1	A	289	THR	9.0
1	B	789	THR	8.7
1	B	621	GLU	8.6
1	B	531	ASP	8.4
1	A	121	GLU	8.2
1	B	624	ASP	7.9
1	B	593	PHE	7.8
1	B	534	GLY	7.8
1	A	35	SER	7.7
1	A	287	ASN	7.4
1	A	308	ARG	7.1
1	A	386	ALA	7.0
1	B	886	ALA	7.0
1	A	93	PHE	6.9
1	A	92	ARG	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	790	GLU	6.1
1	A	286	PRO	6.1
1	B	592	ARG	6.0
1	A	385	GLN	5.9
1	B	622	LYS	5.8
1	B	623	LYS	5.8
1	B	532	LYS	5.8
1	B	786	PRO	5.7
1	B	567	PHE	5.7
1	A	123	LYS	5.7
1	A	384	ILE	5.5
1	B	530	ARG	5.4
1	B	798	ALA	5.2
1	A	124	ASP	5.2
1	A	91	LYS	5.0
1	B	650	LYS	4.9
1	B	791	PHE	4.9
1	A	291	PHE	4.8
1	A	282	ARG	4.6
1	B	787	ASN	4.6
1	B	778	ARG	4.5
1	A	297	LYS	4.5
1	A	290	GLU	4.2
1	B	782	ARG	4.2
1	B	619	SER	4.1
1	B	547	GLY	4.1
1	B	591	LYS	3.8
1	B	800	PRO	3.8
1	A	65	GLY	3.8
1	B	524	GLY	3.7
1	B	797	LYS	3.6
1	B	594	LYS	3.6
1	A	278	ARG	3.6
1	A	67	PHE	3.5
1	A	119	SER	3.5
1	A	209	ARG	3.5
1	B	799	HIS	3.5
1	A	47	GLY	3.4
1	B	885	GLN	3.4
1	A	36	LYS	3.4
1	A	279	GLU	3.4
1	B	648	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	284	MET	3.3
1	B	720	ARG	3.3
1	A	150	LYS	3.3
1	B	564	ASN	3.3
1	B	535	SER	3.2
1	A	303	LYS	3.2
1	B	795	GLN	3.2
1	B	709	ARG	3.1
1	A	48	PRO	3.0
1	B	546	GLN	3.0
1	B	803	LYS	3.0
1	A	77	ASP	2.9
1	A	294	PRO	2.8
1	A	148	ARG	2.8
1	B	630	LEU	2.8
1	B	566	SER	2.8
1	A	293	PHE	2.8
1	B	578	SER	2.8
1	A	66	SER	2.8
1	B	550	ARG	2.7
1	A	90	ASP	2.6
1	B	802	THR	2.6
1	B	792	LYS	2.6
1	A	83	ALA	2.5
1	B	548	PRO	2.5
1	A	37	VAL	2.5
1	B	784	MET	2.4
1	B	779	GLU	2.4
1	A	131	VAL	2.3
1	B	577	ASP	2.2
1	A	125	GLU	2.2
1	A	300	PRO	2.2
1	A	132	LEU	2.2
1	B	625	GLU	2.1
1	A	295	GLN	2.1
1	A	220	ARG	2.1
1	B	859	LEU	2.1
1	B	710	GLY	2.1
1	B	584	ILE	2.1
1	A	71	TYR	2.0
1	B	645	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ANP	B	930	31/31	0.91	0.12	-0.34	24,30,48,49	0
2	ANP	A	430	31/31	0.90	0.12	-0.37	23,33,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.