Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:59 PM GMT

PDB ID	:	1W2D
Title	:	HUMAN INOSITOL (1,4,5)-TRISPHOSPHATE 3-KINASE COMPLEXED WITH MN2+/ADP/INS(1,3,4,5)P4
Authors	:	Gonzalez, B.; Schell, M.J.; Irvine, R.F.; Williams, R.L.
Deposited on	:	2004-07-01
Resolution	:	1.94 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:

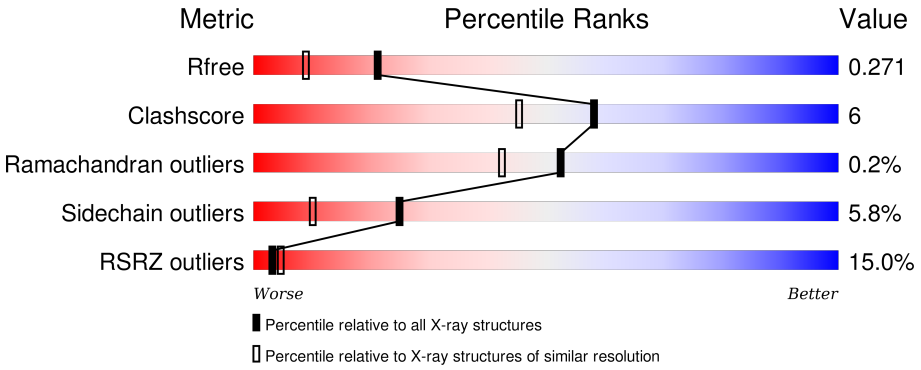
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.94 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))
R_{free}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	265	9%, 82%, 15%
1	B	265	20%, 78%, 14%, 6%

2 Entry composition

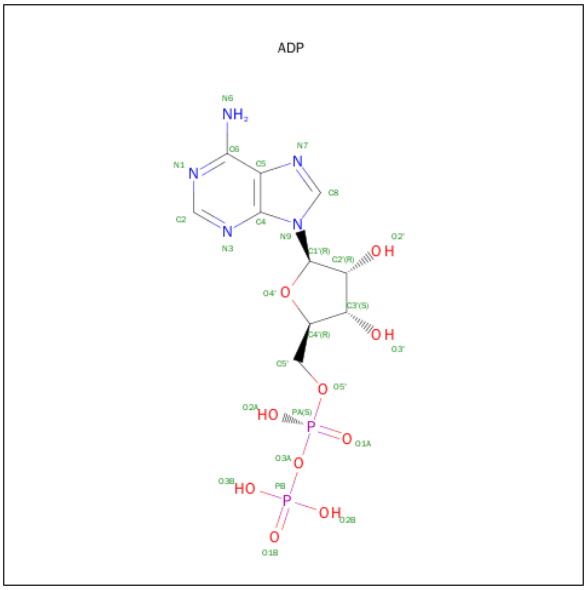
There are 6 unique types of molecules in this entry. The entry contains 4524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 INOSITOL-TRISPHOSPHATE 3-KINASE A.

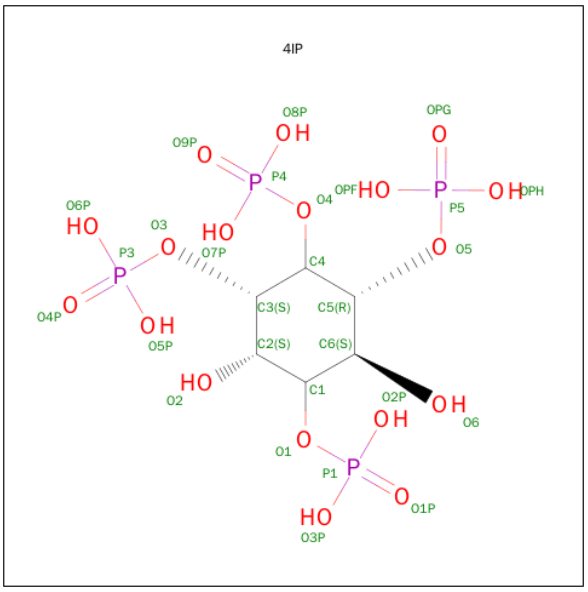
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2133	1334	388	399	12			
1	B	250	Total	C	N	O	S	0	0	0
			2005	1260	361	372	12			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is INOSITOL-(1,3,4,5)-TETRAKISPHOSPHATE (three-letter code: 4IP) (formula: $C_6H_{16}O_{18}P_4$).

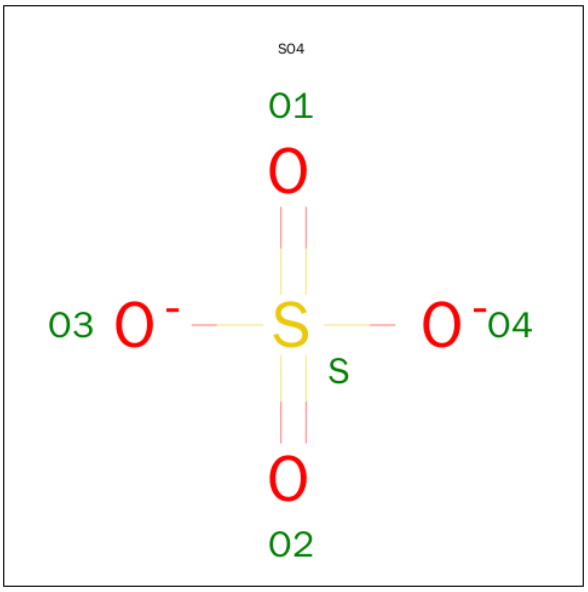


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			28	6	18	4		
3	B	1	Total	C	O	P	0	0
			28	6	18	4		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

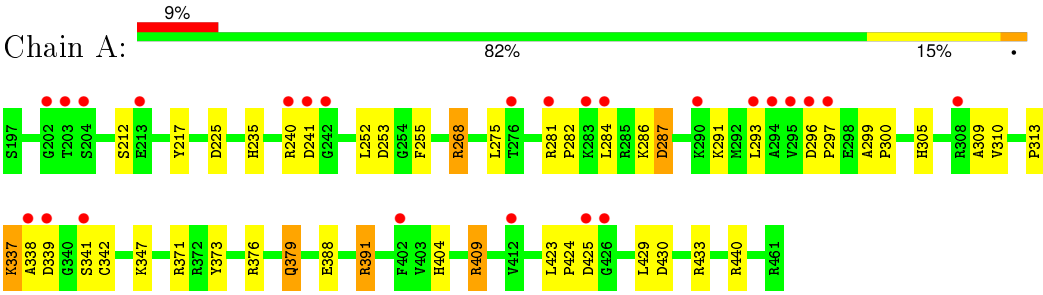
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	129	Total O 129 129	0	0
6	B	130	Total O 130 130	0	0

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.

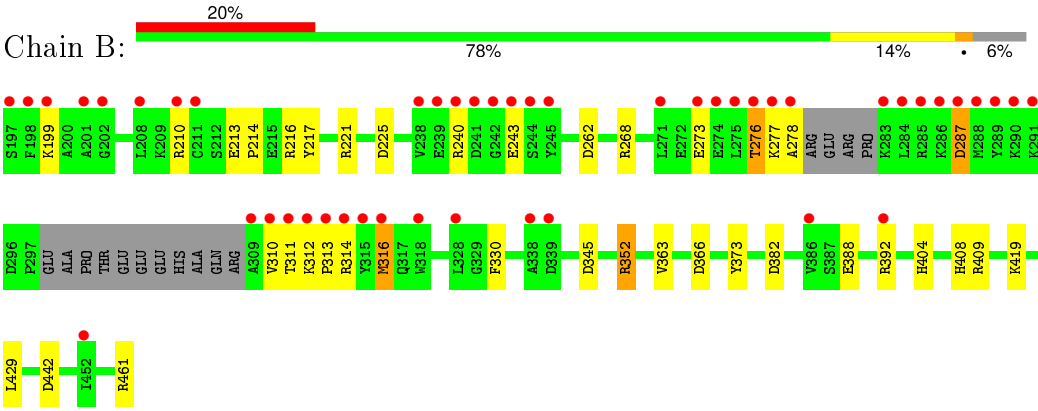
- Molecule 1: INOSITOL-TRISPHOSPHATE 3-KINASE A

Chain A:



- Molecule 1: INOSITOL-TRISPHOSPHATE 3-KINASE A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	72.05Å 97.41Å 190.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 1.94 47.71 – 1.94	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.80-1.94) 95.0 (47.71-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.267 0.229 , 0.271	Depositor DCC
R_{free} test set	2409 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 47570 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4524	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: MN, 4IP, SO4, 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	0.92	0/2173	1.03	11/2924 (0.4%)
1	B	0.91	2/2040 (0.1%)	1.00	7/2741 (0.3%)
All	All	0.92	2/4213 (0.0%)	1.01	18/5665 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	VAL	CB-CG1	-6.73	1.38	1.52
1	B	330	PHE	CD2-CE2	-5.77	1.27	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	253	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	268	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	287	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	241	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	262	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	382	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	352	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	225	ASP	CB-CG-OD2	5.41	123.16	118.30
1	A	319	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	268	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	371	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	442	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	409	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	268	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	425	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	430	ASP	CB-CG-OD2	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	ASP	CB-CG-OD2	5.04	122.83	118.30

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	2133	0	2113	33	0
1	B	2005	0	1996	29	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	28	0	8	0	0
3	B	28	0	8	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	129	0	0	4	0
6	B	130	0	0	3	0
All	All	4524	0	4149	50	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 6.

All (50) 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:338:ALA:C	1:B:294:ALA:HB1	1.98	0.82
1:A:338:ALA:HB1	1:B:294:ALA:HB1	1.71	0.72
1:A:339:ASP:HB3	1:B:295:VAL:HA	1.71	0.72
1:A:338:ALA:O	1:B:294:ALA:CB	2.38	0.72
1:A:338:ALA:CA	1:B:294:ALA:HB1	2.20	0.72
1:A:338:ALA:CB	1:B:294:ALA:HB1	2.25	0.66
1:A:376:ARG:HH11	1:A:379:GLN:HE22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:HB2	6:A:2036:HOH:O	1.99	0.63
1:A:338:ALA:O	1:B:294:ALA:HB3	1.99	0.62
1:A:338:ALA:O	1:B:294:ALA:HB1	1.99	0.62
1:B:221:ARG:NH2	6:B:2009:HOH:O	2.35	0.58
1:B:419:LYS:NZ	3:B:1463:4IP:O9P	2.32	0.58
1:A:341:SER:HB2	1:B:345:ASP:HA	1.85	0.57
1:A:339:ASP:HB2	1:B:295:VAL:HG22	1.86	0.57
1:A:293:LEU:HD13	1:A:305:HIS:HE1	1.69	0.56
1:A:284:LEU:HB3	1:A:309:ALA:HB1	1.88	0.55
1:B:316:MET:HE3	1:B:316:MET:HA	1.88	0.55
1:A:338:ALA:C	1:B:294:ALA:CB	2.71	0.55
1:B:423:LEU:HD11	1:B:429:LEU:HG	1.88	0.54
1:B:373:TYR:OH	1:B:404:HIS:HD2	1.91	0.53
1:B:388:GLU:O	1:B:392:ARG:HG2	2.08	0.53
1:A:299:ALA:HB3	1:A:300:PRO:HD3	1.91	0.52
1:A:338:ALA:HB1	1:B:294:ALA:CB	2.39	0.52
1:A:293:LEU:CD1	1:A:305:HIS:HE1	2.22	0.52
1:B:366:ASP:OD2	1:B:408:HIS:HD2	1.92	0.51
1:A:255:PHE:CE1	1:A:409:ARG:HG2	2.45	0.51
1:B:419:LYS:CE	3:B:1463:4IP:O9P	2.59	0.51
1:A:337:LYS:HB2	1:A:341:SER:O	2.13	0.48
1:B:409:ARG:NE	6:B:2088:HOH:O	2.45	0.48
1:A:287:ASP:O	1:A:291:LYS:HD2	2.13	0.48
1:A:376:ARG:NH1	1:A:379:GLN:HE22	2.12	0.47
1:A:336:LYS:HG3	1:A:342:CYS:SG	2.55	0.47
1:A:275:LEU:CD1	1:A:313:PRO:HB3	2.45	0.46
1:A:388:GLU:OE2	1:A:391:ARG:HD3	2.17	0.45
1:A:235:HIS:HE1	6:A:2017:HOH:O	1.99	0.45
1:B:419:LYS:HE3	3:B:1463:4IP:O9P	2.17	0.45
1:B:404:HIS:HE1	6:B:2068:HOH:O	2.00	0.44
1:A:282:PRO:HD2	6:A:2033:HOH:O	2.16	0.44
1:B:373:TYR:OH	1:B:404:HIS:CD2	2.71	0.43
1:B:311:THR:OG1	1:B:314:ARG:HB2	2.17	0.43
1:A:373:TYR:OH	1:A:404:HIS:HD2	2.01	0.43
1:B:312:LYS:HB3	1:B:313:PRO:HD3	1.99	0.43
1:A:424:PRO:HD3	1:A:440:ARG:NH1	2.34	0.42
1:B:273:GLU:O	1:B:276:THR:HB	2.20	0.42
1:A:296:ASP:HB3	1:A:299:ALA:HB2	2.02	0.42
1:B:277:LYS:O	1:B:278:ALA:HB2	2.20	0.41
1:B:213:GLU:N	1:B:214:PRO:CD	2.83	0.41
1:A:275:LEU:HD12	1:A:313:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:HD11	1:A:429:LEU:HG	2.01	0.41
1:A:319:ARG:HD2	6:A:2066:HOH:O	2.20	0.41

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	263/265 (99%)	254 (97%)	9 (3%)	0	100 100
1	B	244/265 (92%)	238 (98%)	5 (2%)	1 (0%)	39 26
All	All	507/530 (96%)	492 (97%)	14 (3%)	1 (0%)	52 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	THR

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	229/229 (100%)	215 (94%)	14 (6%)	23 9
1	B	216/229 (94%)	204 (94%)	12 (6%)	26 11
All	All	445/458 (97%)	419 (94%)	26 (6%)	25 10

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

Mol	Chain	Res	Type
1	A	212	SER
1	A	217	TYR
1	A	240	ARG
1	A	252	LEU
1	A	268	ARG
1	A	281	ARG
1	A	286	LYS
1	A	310	VAL
1	A	336	LYS
1	A	337	LYS
1	A	347	LYS
1	A	379	GLN
1	A	391	ARG
1	A	433	ARG
1	B	199	LYS
1	B	210	ARG
1	B	216	ARG
1	B	217	TYR
1	B	240	ARG
1	B	243	GLU
1	B	287	ASP
1	B	295	VAL
1	B	310	VAL
1	B	316	MET
1	B	352	ARG
1	B	461	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	HIS
1	A	379	GLN
1	A	404	HIS
1	A	406	HIS
1	A	427	GLN
1	B	404	HIS
1	B	408	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
2	ADP	A	1462	-	22,29,29	1.21	2 (9%)	27,45,45	2.40	3 (11%)
3	4IP	A	1463	4	28,28,28	1.12	2 (7%)	38,46,46	1.49	5 (13%)
5	SO4	A	1465	-	4,4,4	0.44	0	6,6,6	0.20	0
5	SO4	A	1466	-	4,4,4	0.62	0	6,6,6	0.20	0
2	ADP	B	1462	4	22,29,29	1.05	2 (9%)	27,45,45	2.94	7 (25%)
3	4IP	B	1463	-	28,28,28	1.17	3 (10%)	38,46,46	1.30	4 (10%)
5	SO4	B	1465	-	4,4,4	0.31	0	6,6,6	0.46	0

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	ADP	A	1462	-	-	0/12/32/32	0/3/3/3
3	4IP	A	1463	4	-	0/20/44/44	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	1465	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1466	-	-	0/0/0/0	0/0/0/0
2	ADP	B	1462	4	-	0/12/32/32	0/3/3/3
3	4IP	B	1463	-	-	0/20/44/44	0/1/1/1
5	SO4	B	1465	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1463	4IP	P5-OPH	-2.16	1.46	1.54
3	A	1463	4IP	P5-OPH	-2.11	1.47	1.54
3	B	1463	4IP	P5-OPG	2.11	1.58	1.51
2	B	1462	ADP	C2-N1	2.18	1.38	1.33
3	A	1463	4IP	P4-O9P	2.19	1.58	1.51
3	B	1463	4IP	P1-O1P	2.23	1.58	1.51
2	A	1462	ADP	C2-N3	2.39	1.36	1.32
2	B	1462	ADP	C2-N3	3.26	1.38	1.32
2	A	1462	ADP	C2-N1	3.27	1.40	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1462	ADP	N3-C2-N1	-13.35	118.67	128.89
2	A	1462	ADP	N3-C2-N1	-10.87	120.57	128.89
3	B	1463	4IP	P1-O1-C1	-3.58	112.98	121.56
3	A	1463	4IP	O6P-P3-O4P	-3.00	100.91	110.58
2	B	1462	ADP	C1'-N9-C4	-2.77	122.77	126.94
3	A	1463	4IP	P1-O1-C1	-2.65	115.22	121.56
3	B	1463	4IP	O6P-P3-O4P	-2.35	103.02	110.58
2	B	1462	ADP	C4-C5-N7	-2.22	107.44	109.48
3	B	1463	4IP	O4-P4-O9P	-2.14	101.77	107.11
2	A	1462	ADP	C4-C5-N7	-2.14	107.51	109.48
2	B	1462	ADP	O3A-PA-O5'	2.20	108.78	102.94
2	B	1462	ADP	C4'-O4'-C1'	2.28	112.22	109.72
2	B	1462	ADP	O4'-C4'-C5'	2.28	117.47	109.32
3	A	1463	4IP	O3P-P1-O2P	2.60	117.29	107.38
2	B	1462	ADP	C2-N1-C6	2.61	123.43	118.77
3	A	1463	4IP	O5P-P3-O4P	2.66	119.15	110.58
3	B	1463	4IP	O5P-P3-O4P	2.72	119.32	110.58
2	A	1462	ADP	C4'-O4'-C1'	3.13	113.16	109.72
3	A	1463	4IP	P4-O4-C4	3.43	129.78	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1463	4IP	3	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	265/265 (100%)	0.80	25 (9%)	11	16	15, 29, 48, 53	0
1	B	250/265 (94%)	1.30	52 (20%)	1	1	14, 30, 52, 59	0
All	All	515/530 (97%)	1.04	77 (14%)	3	5	14, 30, 51, 59	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	LEU	9.3
1	B	310	VAL	8.1
1	B	311	THR	7.5
1	B	313	PRO	7.2
1	B	309	ALA	7.0
1	B	338	ALA	6.9
1	B	278	ALA	6.8
1	B	283	LYS	6.6
1	A	294	ALA	6.3
1	B	288	MET	6.1
1	B	286	LYS	5.9
1	B	295	VAL	5.9
1	B	287	ASP	5.8
1	B	276	THR	5.5
1	A	338	ALA	5.5
1	B	312	LYS	4.8
1	B	289	TYR	4.7
1	B	242	GLY	4.7
1	B	285	ARG	4.6
1	B	238	VAL	4.5
1	B	277	LYS	4.4
1	B	315	TYR	4.3
1	A	241	ASP	4.3
1	B	290	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	4.2
1	A	293	LEU	4.1
1	B	294	ALA	4.1
1	B	293	LEU	4.1
1	B	198	PHE	4.0
1	A	295	VAL	3.9
1	A	213	GLU	3.7
1	B	245	TYR	3.7
1	B	202	GLY	3.6
1	A	204	SER	3.5
1	B	292	MET	3.4
1	A	202	GLY	3.4
1	B	316	MET	3.4
1	B	239	GLU	3.3
1	B	244	SER	3.3
1	B	243	GLU	3.3
1	B	291	LYS	3.2
1	B	273	GLU	3.2
1	B	425	ASP	3.1
1	A	290	LYS	3.1
1	B	211	CYS	3.1
1	B	241	ASP	3.0
1	A	339	ASP	3.0
1	A	240	ARG	2.9
1	A	296	ASP	2.8
1	B	314	ARG	2.8
1	A	425	ASP	2.7
1	A	281	ARG	2.7
1	A	283	LYS	2.6
1	A	203	THR	2.6
1	A	426	GLY	2.6
1	B	274	GLU	2.5
1	B	210	ARG	2.4
1	B	201	ALA	2.4
1	B	339	ASP	2.3
1	A	297	PRO	2.3
1	A	284	LEU	2.3
1	A	276	THR	2.3
1	B	208	LEU	2.3
1	B	452	ILE	2.3
1	A	402	PHE	2.2
1	B	199	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	240	ARG	2.2
1	B	271	LEU	2.2
1	B	318	TRP	2.1
1	A	412	VAL	2.1
1	A	341	SER	2.1
1	A	308	ARG	2.1
1	B	328	LEU	2.1
1	B	386	VAL	2.1
1	A	242	GLY	2.1
1	B	197	SER	2.1
1	B	392	ARG	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
3	4IP	B	1463	28/28	0.73	0.28	0.40	55,62,65,66	28
2	ADP	B	1462	27/27	0.94	0.14	-0.09	28,36,50,52	0
3	4IP	A	1463	28/28	0.90	0.11	-0.95	51,55,63,65	0
2	ADP	A	1462	27/27	0.95	0.10	-1.30	25,31,46,47	0
5	SO4	A	1465	5/5	0.93	0.19	-	35,37,37,37	5
4	MN	B	1464	1/1	0.95	0.21	-	42,42,42,42	1
4	MN	A	1464	1/1	0.89	0.12	-	51,51,51,51	1
5	SO4	B	1465	5/5	0.89	0.19	-	35,35,37,38	5
5	SO4	A	1466	5/5	0.94	0.17	-	34,34,36,36	5

6.5 Other polymers (i)

There are no such residues in this entry.