



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:50 PM GMT

PDB ID : 1VFZ
Title : Crystal Structure of the Kif1A Motor Domain Complexed With ADP-Mg-VO4
Authors : Nitta, R.; Kikkawa, M.; Okada, Y.; Hirokawa, N.
Deposited on : 2004-04-19
Resolution : 2.24 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) : 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

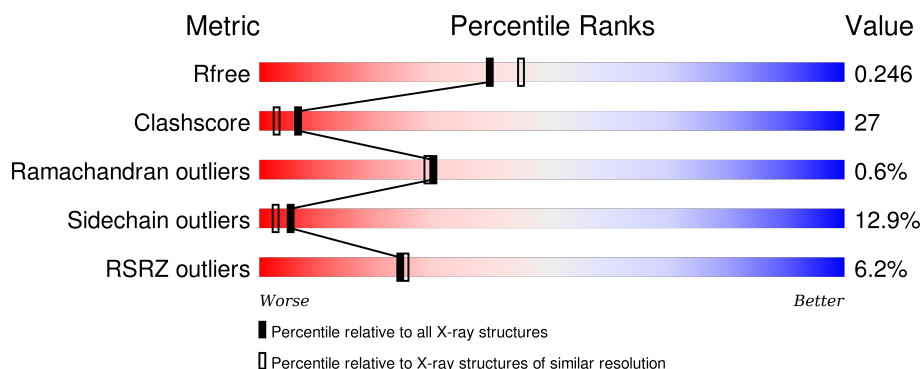
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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.

Mol	Chain	Length	Quality of chain
1	A	366	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VO4	A	400	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	A	500	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2848 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.

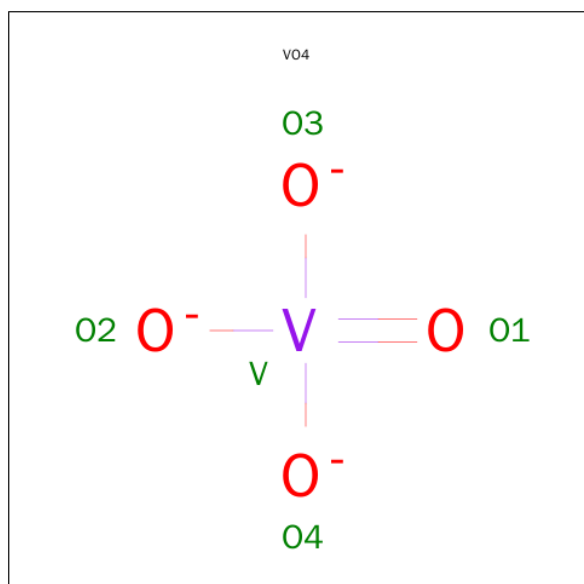
- Molecule 1 is a protein called PROTEIN (Fusion protein consisting of Kinesin-like protein KIF1A, Kinesin heavy chain isoform 5C and A HIS TAG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2641	1637	464	525	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	HIS	-	EXPRESSION TAG	UNP P28738
A	363	HIS	-	EXPRESSION TAG	UNP P28738
A	364	HIS	-	EXPRESSION TAG	UNP P28738
A	365	HIS	-	EXPRESSION TAG	UNP P28738
A	366	HIS	-	EXPRESSION TAG	UNP P28738

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O₄V).

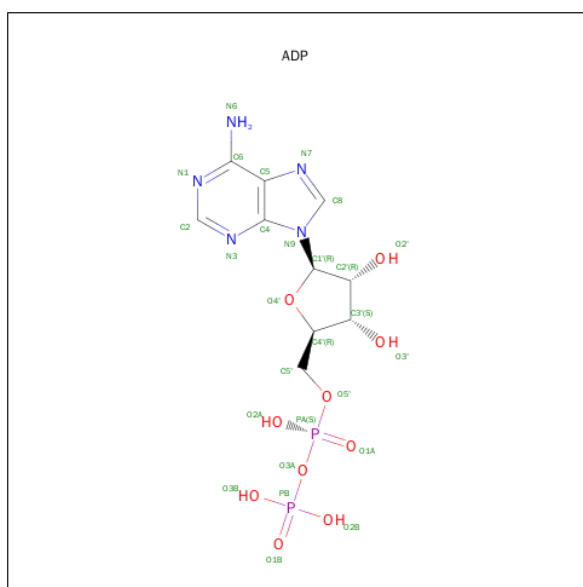


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	V	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

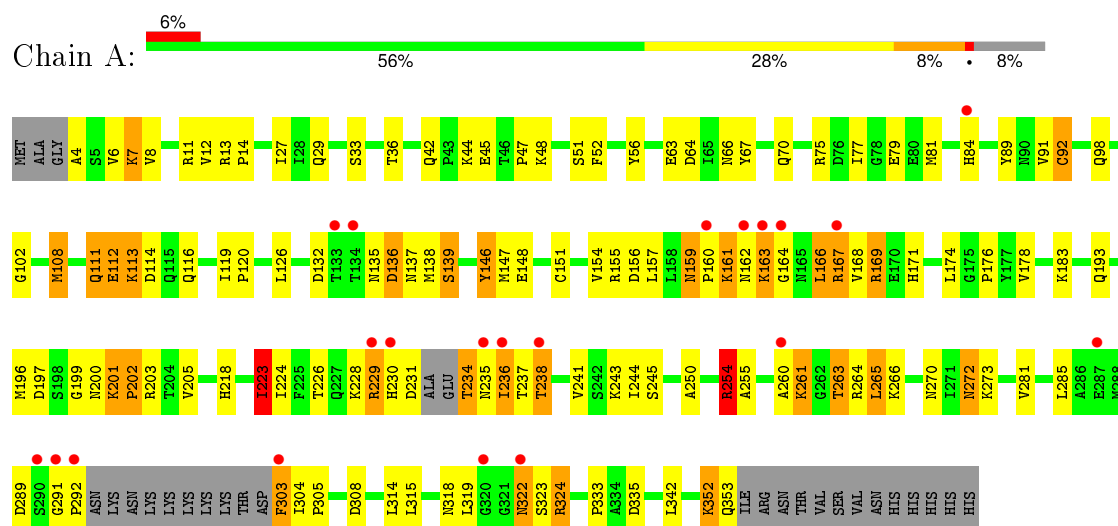
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	174	Total O 174 174	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 ($\text{RSRZ} > 2$). 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: PROTEIN (Fusion protein consisting of Kinesin-like protein KIF1A, Kinesin heavy chain isoform 5C and A HIS TAG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.47Å 51.80Å 156.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.36 – 2.24 49.20 – 2.23	Depositor EDS
% Data completeness (in resolution range)	94.2 (23.36-2.24) 93.8 (49.20-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.249 0.212 , 0.246	Depositor DCC
R_{free} test set	1609 reflections (11.18%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 69.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17094 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2848	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 7.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: VO4, MG, 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	0.47	0/2683	0.78	4/3622 (0.1%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	223	ILE	CB-CG1-CD1	-6.68	95.20	113.90
1	A	164	GLY	O-C-N	-6.41	112.44	122.70
1	A	254	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	202	PRO	N-CA-CB	5.55	109.96	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	PHE	Sidechain

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	2641	0	2593	143	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	27	0	12	2	0
5	A	174	0	0	13	0
All	All	2848	0	2605	144	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 27.

All (144) 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:138:MET:CE	1:A:229:ARG:HA	1.78	1.13
1:A:304:ILE:HG23	1:A:305:PRO:HD2	1.31	1.12
1:A:138:MET:HE1	1:A:229:ARG:HA	1.13	1.07
1:A:223:ILE:HG23	1:A:244:ILE:HB	1.35	1.07
1:A:324:ARG:HH11	1:A:324:ARG:HG2	1.18	1.06
1:A:234:THR:N	1:A:235:ASN:HA	1.68	1.05
1:A:304:ILE:CG2	1:A:305:PRO:HD2	2.00	0.92
1:A:171:HIS:HD2	1:A:174:LEU:H	1.20	0.88
1:A:324:ARG:NH1	1:A:324:ARG:HG2	1.87	0.88
4:A:500:ADP:H5'2	5:A:589:HOH:O	1.75	0.85
1:A:108:MET:SD	1:A:119:ILE:HD12	2.18	0.84
1:A:273:LYS:HD2	1:A:308:ASP:O	1.78	0.83
1:A:171:HIS:CD2	1:A:174:LEU:H	1.98	0.81
1:A:138:MET:HE3	1:A:229:ARG:CB	2.11	0.80
1:A:138:MET:CE	1:A:229:ARG:CA	2.60	0.78
1:A:138:MET:HE3	1:A:229:ARG:CG	2.15	0.77
1:A:108:MET:HG2	1:A:200:ASN:HD21	1.50	0.77
1:A:226:THR:HG23	1:A:241:VAL:HG22	1.68	0.76
1:A:167:ARG:HH11	1:A:167:ARG:HB3	1.51	0.75
1:A:11:ARG:HH12	1:A:70:GLN:HE22	1.34	0.74
1:A:254:ARG:HD3	5:A:670:HOH:O	1.88	0.74
1:A:151:CYS:HB3	1:A:266:LYS:HE2	1.69	0.73
1:A:138:MET:HE3	1:A:229:ARG:HG3	1.71	0.73
1:A:315:LEU:HA	5:A:658:HOH:O	1.87	0.73
1:A:228:LYS:HZ3	1:A:228:LYS:HB2	1.54	0.72
1:A:167:ARG:HB3	1:A:167:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:OE2	1:A:203:ARG:HD2	1.91	0.70
1:A:281:VAL:HG11	1:A:319:LEU:HD13	1.73	0.70
1:A:48:LYS:HD2	5:A:667:HOH:O	1.90	0.70
1:A:147:MET:CE	1:A:314:LEU:CD2	2.70	0.69
1:A:218:HIS:HD2	1:A:250:ALA:H	1.38	0.69
1:A:108:MET:CE	1:A:196:MET:HB2	2.24	0.67
1:A:116:GLN:NE2	5:A:605:HOH:O	2.27	0.67
1:A:223:ILE:CG2	1:A:244:ILE:HB	2.19	0.67
1:A:11:ARG:HH12	1:A:70:GLN:NE2	1.92	0.66
1:A:112:GLU:HG3	1:A:113:LYS:N	2.11	0.66
1:A:138:MET:CE	1:A:138:MET:HA	2.23	0.66
1:A:266:LYS:HE3	1:A:270:ASN:OD1	1.96	0.66
1:A:159:ASN:HD22	1:A:160:PRO:N	1.93	0.66
1:A:218:HIS:CD2	1:A:250:ALA:H	2.14	0.66
1:A:303:PHE:CD1	1:A:303:PHE:O	2.49	0.65
1:A:255:ALA:O	1:A:272:ASN:HB2	1.95	0.65
1:A:113:LYS:O	1:A:114:ASP:HB2	1.96	0.65
1:A:84:HIS:NE2	1:A:89:TYR:HB2	2.12	0.65
1:A:6:VAL:O	1:A:7:LYS:HD2	1.97	0.65
1:A:272:ASN:HD22	1:A:272:ASN:C	2.01	0.64
1:A:111:GLN:HB2	5:A:584:HOH:O	1.96	0.64
1:A:147:MET:HE2	1:A:314:LEU:CD2	2.28	0.64
1:A:159:ASN:C	1:A:159:ASN:HD22	2.02	0.63
1:A:228:LYS:NZ	1:A:228:LYS:HB2	2.13	0.63
1:A:147:MET:HE1	1:A:314:LEU:CD2	2.29	0.63
1:A:135:ASN:OD1	1:A:137:ASN:HB2	1.98	0.62
1:A:4:ALA:O	1:A:324:ARG:HD3	1.99	0.62
1:A:171:HIS:HD2	1:A:174:LEU:N	1.94	0.61
1:A:236:ILE:N	1:A:236:ILE:HD12	2.15	0.61
1:A:304:ILE:CG2	1:A:305:PRO:CD	2.77	0.61
1:A:42:GLN:O	1:A:45:GLU:HB2	2.01	0.60
1:A:266:LYS:O	1:A:266:LYS:HG3	1.99	0.60
1:A:137:ASN:HB3	1:A:230:HIS:O	2.01	0.59
1:A:183:LYS:HD2	1:A:224:ILE:HD12	1.85	0.59
1:A:42:GLN:HB3	5:A:663:HOH:O	2.03	0.58
1:A:84:HIS:CD2	1:A:89:TYR:HB2	2.38	0.58
1:A:139:SER:HB3	1:A:228:LYS:HZ3	1.68	0.58
1:A:108:MET:HG2	1:A:200:ASN:ND2	2.19	0.58
1:A:11:ARG:HD3	5:A:583:HOH:O	2.04	0.58
1:A:138:MET:HE3	1:A:229:ARG:CA	2.30	0.58
1:A:92:CYS:SG	1:A:318:ASN:HB3	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:O	1:A:234:THR:OG1	2.21	0.57
1:A:147:MET:CE	1:A:314:LEU:HD21	2.35	0.57
1:A:155:ARG:HG3	1:A:163:LYS:HB3	1.87	0.57
1:A:234:THR:N	1:A:235:ASN:CA	2.53	0.57
1:A:352:LYS:CD	1:A:353:GLN:H	2.17	0.57
1:A:322:ASN:N	5:A:675:HOH:O	2.23	0.56
1:A:159:ASN:C	1:A:159:ASN:ND2	2.58	0.56
1:A:42:GLN:OE1	1:A:45:GLU:OE2	2.25	0.55
1:A:201:LYS:HG3	1:A:202:PRO:N	2.21	0.55
1:A:119:ILE:HB	1:A:120:PRO:HD3	1.87	0.55
1:A:92:CYS:SG	1:A:245:SER:HB2	2.46	0.55
1:A:137:ASN:O	1:A:138:MET:CE	2.56	0.54
1:A:112:GLU:CG	1:A:113:LYS:N	2.70	0.54
1:A:303:PHE:CG	1:A:303:PHE:O	2.60	0.54
1:A:51:SER:O	1:A:352:LYS:NZ	2.39	0.54
1:A:289:ASP:O	1:A:292:PRO:HD2	2.08	0.54
1:A:324:ARG:NH1	1:A:324:ARG:CG	2.60	0.53
1:A:137:ASN:O	1:A:138:MET:HE2	2.09	0.53
1:A:75:ARG:HG2	1:A:79:GLU:OE2	2.08	0.52
1:A:289:ASP:C	1:A:292:PRO:HD2	2.30	0.52
1:A:102:GLY:N	4:A:500:ADP:O2B	2.33	0.52
1:A:154:VAL:O	1:A:166:LEU:HB2	2.09	0.52
1:A:155:ARG:HG3	1:A:163:LYS:CB	2.40	0.52
1:A:171:HIS:CD2	1:A:174:LEU:HB2	2.46	0.51
1:A:352:LYS:CG	1:A:353:GLN:H	2.23	0.51
1:A:11:ARG:HH22	1:A:70:GLN:HE21	1.58	0.50
1:A:291:GLY:N	1:A:292:PRO:CD	2.75	0.50
1:A:136:ASP:HB2	5:A:586:HOH:O	2.11	0.49
1:A:226:THR:HG23	1:A:241:VAL:CG2	2.40	0.49
1:A:303:PHE:O	1:A:304:ILE:HG13	2.12	0.49
1:A:265:LEU:HD13	1:A:265:LEU:N	2.29	0.48
1:A:147:MET:HE1	1:A:314:LEU:HD22	1.95	0.48
1:A:167:ARG:HD2	5:A:553:HOH:O	2.13	0.47
1:A:228:LYS:HA	1:A:238:THR:O	2.14	0.47
1:A:77:ILE:O	1:A:81:MET:HG2	2.14	0.47
1:A:352:LYS:O	1:A:353:GLN:C	2.53	0.47
1:A:169:ARG:O	1:A:176:PRO:HA	2.14	0.47
1:A:231:ASP:O	1:A:234:THR:HG23	2.14	0.47
1:A:33:SER:HB2	1:A:52:PHE:O	2.15	0.47
1:A:64:ASP:HB3	1:A:67:TYR:HB2	1.97	0.46
1:A:11:ARG:HG3	1:A:56:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HA	1:A:324:ARG:O	2.15	0.46
1:A:138:MET:CE	1:A:229:ARG:CB	2.88	0.46
1:A:44:LYS:NZ	5:A:665:HOH:O	2.34	0.46
1:A:29:GLN:HB2	1:A:36:THR:OG1	2.16	0.46
1:A:84:HIS:CE1	1:A:324:ARG:HG3	2.51	0.46
1:A:322:ASN:HA	1:A:322:ASN:HD22	1.58	0.46
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.79	0.46
1:A:159:ASN:HD22	1:A:160:PRO:CD	2.29	0.45
1:A:291:GLY:N	1:A:292:PRO:HD3	2.31	0.45
1:A:138:MET:HE1	1:A:138:MET:HA	1.98	0.45
1:A:108:MET:HE2	1:A:196:MET:HB2	1.99	0.45
1:A:27:ILE:HD13	1:A:335:ASP:HA	1.99	0.45
1:A:36:THR:HB	1:A:47:PRO:HB2	1.99	0.44
1:A:260:ALA:C	1:A:263:THR:HG23	2.38	0.44
1:A:273:LYS:CD	1:A:308:ASP:O	2.59	0.44
1:A:201:LYS:O	1:A:205:VAL:HG13	2.18	0.44
1:A:12:VAL:CG2	1:A:333:PRO:HB3	2.48	0.44
1:A:235:ASN:OD1	1:A:235:ASN:C	2.55	0.43
1:A:157:LEU:HD11	1:A:203:ARG:HD3	1.99	0.43
1:A:156:ASP:HB2	1:A:166:LEU:HD21	2.00	0.43
1:A:260:ALA:HA	1:A:261:LYS:HA	1.47	0.42
1:A:168:VAL:HG22	1:A:178:VAL:HG22	2.01	0.42
1:A:303:PHE:CE1	1:A:303:PHE:O	2.73	0.42
1:A:146:TYR:CD2	1:A:199:GLY:HA3	2.55	0.42
1:A:169:ARG:HB3	1:A:169:ARG:HE	1.78	0.42
1:A:148:GLU:HG3	1:A:157:LEU:HD11	2.03	0.41
1:A:228:LYS:NZ	1:A:228:LYS:CB	2.83	0.41
1:A:243:LYS:HE3	5:A:627:HOH:O	2.21	0.41
1:A:11:ARG:HG3	1:A:56:TYR:CB	2.50	0.41
1:A:139:SER:O	1:A:228:LYS:NZ	2.54	0.41
1:A:111:GLN:NE2	1:A:193:GLN:HE22	2.18	0.41
1:A:8:VAL:HG21	1:A:352:LYS:HG2	2.03	0.41
1:A:161:LYS:HG3	1:A:161:LYS:O	2.21	0.41
1:A:13:ARG:HB2	1:A:14:PRO:CD	2.51	0.41
1:A:126:LEU:CD2	1:A:223:ILE:HD11	2.51	0.40
1:A:84:HIS:NE2	1:A:89:TYR:CB	2.81	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	332/366 (91%)	313 (94%)	17 (5%)	2 (1%)	30	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	LYS
1	A	162	ASN

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	294/322 (91%)	256 (87%)	38 (13%)	5	3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	63	GLU
1	A	66	ASN
1	A	92	CYS
1	A	98	GLN
1	A	108	MET
1	A	111	GLN
1	A	112	GLU
1	A	113	LYS

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Mol	Chain	Res	Type
1	A	132	ASP
1	A	136	ASP
1	A	139	SER
1	A	146	TYR
1	A	159	ASN
1	A	163	LYS
1	A	166	LEU
1	A	167	ARG
1	A	169	ARG
1	A	197	ASP
1	A	201	LYS
1	A	223	ILE
1	A	229	ARG
1	A	234	THR
1	A	236	ILE
1	A	237	THR
1	A	238	THR
1	A	254	ARG
1	A	261	LYS
1	A	263	THR
1	A	264	ARG
1	A	265	LEU
1	A	272	ASN
1	A	285	LEU
1	A	322	ASN
1	A	323	SER
1	A	324	ARG
1	A	342	LEU
1	A	352	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	70	GLN
1	A	111	GLN
1	A	116	GLN
1	A	159	ASN
1	A	171	HIS
1	A	211	ASN
1	A	218	HIS
1	A	227	GLN

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Mol	Chain	Res	Type
1	A	272	ASN
1	A	322	ASN

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 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	VO4	A	400	-	1,4,4	1.54	0	0,6,6	0.00	-
4	ADP	A	500	3	22,29,29	1.19	4 (18%)	27,45,45	2.44	9 (33%)

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	VO4	A	400	-	-	0/0/0/0	0/0/0/0
4	ADP	A	500	3	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	ADP	C8-N7	-2.56	1.29	1.34
4	A	500	ADP	PA-O2A	-2.05	1.46	1.54
4	A	500	ADP	O4'-C1'	2.08	1.43	1.41
4	A	500	ADP	C2'-C3'	2.09	1.59	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	ADP	O2A-PA-O3A	-6.21	76.91	105.09
4	A	500	ADP	O3A-PA-O5'	-4.82	90.16	102.94
4	A	500	ADP	N3-C2-N1	-3.49	126.22	128.89
4	A	500	ADP	C1'-N9-C4	-2.27	123.52	126.94
4	A	500	ADP	O4'-C1'-N9	2.10	112.50	108.10
4	A	500	ADP	PA-O3A-PB	2.17	139.94	132.67
4	A	500	ADP	O5'-C5'-C4'	2.81	119.48	109.12
4	A	500	ADP	O2A-PA-O1A	3.76	132.89	112.53
4	A	500	ADP	C4'-O4'-C1'	5.93	116.24	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	ADP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	338/366 (92%)	0.20	21 (6%) 24 25	12, 27, 64, 73	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	ILE	7.2
1	A	292	PRO	5.8
1	A	291	GLY	4.7
1	A	164	GLY	4.6
1	A	134	THR	4.5
1	A	163	LYS	4.4
1	A	230	HIS	3.7
1	A	303	PHE	3.4
1	A	133	THR	3.0
1	A	229	ARG	2.6
1	A	167	ARG	2.6
1	A	235	ASN	2.6
1	A	287	GLU	2.5
1	A	290	SER	2.4
1	A	162	ASN	2.4
1	A	238	THR	2.3
1	A	322	ASN	2.2
1	A	320	GLY	2.1
1	A	84	HIS	2.1
1	A	260	ALA	2.0
1	A	160	PRO	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, 95th 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(\AA^2)	Q<0.9
2	VO4	A	400	5/5	0.69	0.40	11.00	60,60,63,68	0
4	ADP	A	500	27/27	0.92	0.20	3.08	16,27,35,47	0
3	MG	A	501	1/1	0.90	0.25	-	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.