



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 26, 2017 – 04:41 PM EDT

PDB ID : 4RH7
Title : Crystal structure of human cytoplasmic dynein 2 motor domain in complex with ADP.Vi
Authors : Schmidt, H.; Zalyte, R.; Urnavicius, L.; Carter, A.P.
Deposited on : unknown
Resolution : 3.41 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

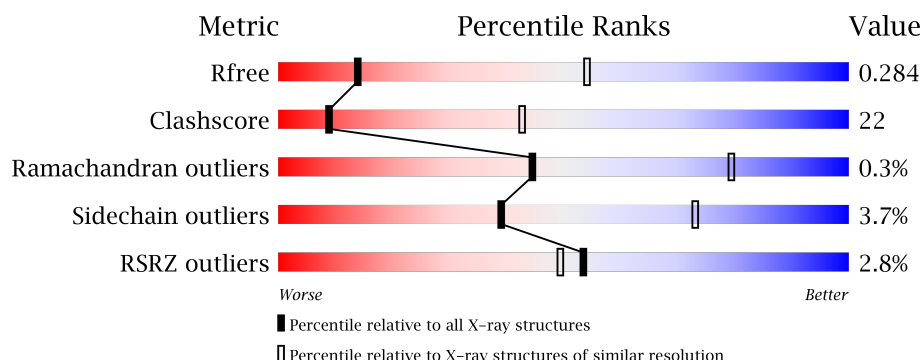
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	100719	1074 (3.50-3.34)
Clashscore	112137	1179 (3.50-3.34)
Ramachandran outliers	110173	1147 (3.50-3.34)
Sidechain outliers	110143	1148 (3.50-3.34)
RSRZ outliers	101464	1100 (3.50-3.34)

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	3450	<div> <div>2%</div> <div>59%</div> <div>27%</div> <div>13%</div> </div>

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	AOV	A	4401	-	-	X	-
3	MG	A	4404	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22816 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.

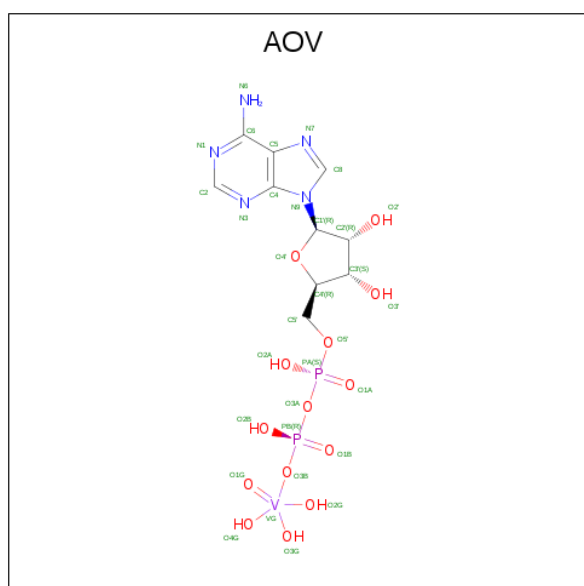
- Molecule 1 is a protein called Green fluorescent protein/Cytoplasmic dynein 2 heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	3005	22697	14414	3922	4263	98	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	GLY	-	LINKER	UNP Q8NCM8
A	1090	SER	-	LINKER	UNP Q8NCM8
A	1413	ARG	LYS	VARIANT	UNP Q8NCM8
A	2871	GLN	ARG	VARIANT	UNP Q8NCM8
A	3680	VAL	ALA	VARIANT	UNP Q8NCM8
A	4308	VAL	-	EXPRESSION TAG	UNP Q8NCM8

- Molecule 2 is ADP ORTHOVANADATE (three-letter code: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$).

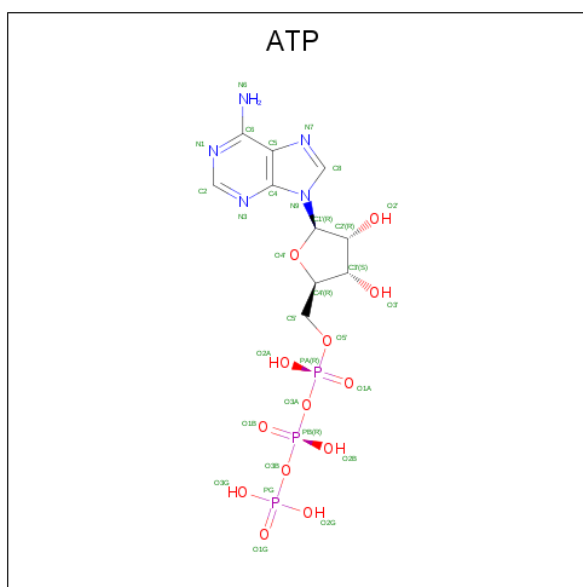


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	0	0
			32	10	5	14	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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



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



S4239	A4150	R4033	D3932	V3830	K3711	ILE	R3525	D3857
P4240	I4151	E4034	M3953	E3831	L3718	ARG	R3533	N3363
S4241	Q4152		Y3934	L3836	E3719	D3612	D3536	F3366
V4245	N4153	S4037	V3939	K3837	I3720	E3621	R3543	F3367
L4246	N4154	N4038		L3840	E3721	R3622	I3544	L3368
P4247	K4157	E4039	Y3943	K3847	G3730	L3629	Q3545	L3370
C4248	L4040	S4041	L3944	N3841	A3731	A3632	L3548	T3372
F4249	P4042	V4043	V3952	R3842	D3732	L3632	L3551	N3374
W4252	S4166	E4166	I3953	V3844	P3733	L3633	Q3552	P3375
I4253	T4167	L4046	ASP	R3847	E3736	P3634	F3555	F3378
P4254	S4171	N4051	VAL	K3854	I3740	S3635	C3560	F3380
Q4255	E4172	Q4052	PHE	N3854		L3636	L3563	A3383
E4265		N4053	ASN	K3857	Y3750	T3639	D3567	A3384
C4266	D4177	S4054	GLN	T3857	I3760	L3640	V3575	S3385
I4267	N4055	N4055	ARG	T3858	C3641	C3641	G3578	T3386
S4268	L4180	L4056	ASN	R3859	R3755	F3642	F3571	V3387
L4269	I4057	I4057	LYS	R3860	G3756		F3575	T3388
P4270	R4184	I4072	LYS	L3864	Q3759	C3657	R3579	N3391
V4271	Q4186	L4073	SER	L3864	A3760	C3658	H3580	S3397
V4281	E4186	S4074	F3965	E3871	D3761	I3671	F3582	Q3448
T4282	A4188	F4075	P3966	Q3875	L3762		L3583	I3451
N4283	I4076	I4076	V3969	E3876	A3771	C3657	F3584	D3486
I4284	G4192	I4077	S3970	R3877	W3776	I3658	Q3585	D3490
D4285	R4193	L4078	C3975	I3881	K3780	P3662	E3586	A3491
V4286	E4079	Q4080	S3976	P3882	I3781		N3587	Y3492
P4287	Q4080	V4090	I3984	W3885	V3785	S3670	E3588	L3493
C4288	V4201	L4094	E3989	Y3900	K3788	I3671	V3589	P3494
G4288	A4201	L4097	D3991	I3903	L3789	F3672	D3590	L3495
G4290	A4202	L4097	F3996	D3904	P3790	Q3674	T3591	A3499
N4291	W4204	L4097		R3905	I3791	I3675	VAL	A3499
D4293	L4208	V4100	F3999	L3906	L3792	L3676	VAL	N3502
Q4296	Q4214	T4105	A4000	F3907	E3793	V3677	GLY	L3505
I4296	R4216	L4106	N4001	D3908	K3794		ASP	
C4298	I4217	V4111	I4002	G3909		V3680	NET	
L4302	L4220	L4118	Q4007	A3910	K3802	L3681	LEU	S3510
P4303	L4221	L4118	Q4017	K3911	F3805	R3682	ARG	K3511
L4304	L4222	P4124	Q4017	Q3914		R3685	LYS	T3512
K4305	E4223	P4124	Q4017	W3915	T3810	L3686	ALA	N3513
N4306	G4224	W4127	L4021	E3916	H3814	D3687	ASP	N3514
Q4307	C4225	W4127	G4022	F3917	P3815	S3688	SER	N3515
V4308	S4226	P4134	R4023	V3918		A3689	GLN	R3517
	F4227		S4024	V3919	P3819	R3690	LYS	F3518
	D4228		I4025	H3918	L3821		ALA	
	G4229		T4026	C3920	L3822		ASP	
	N4230		A4027	L3921			SER	
	Q4231		G4028	L3922			GLN	
	L4232		S4029	A3925			LYS	
	Q4236		F4030	C3929				
	L4237		F4031					
	D4238		D4032					

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	136.03Å 487.15Å 276.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.60 – 3.41 56.54 – 3.41	Depositor EDS
% Data completeness (in resolution range)	62.2 (56.60-3.41) 62.2 (56.54-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.285 0.239 , 0.284	Depositor DCC
R_{free} test set	3914 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 110.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: AOV, MG, ATP, 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	0.61	2/23147 (0.0%)	0.78	5/31474 (0.0%)

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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2275	PHE	CB-CG	-5.18	1.42	1.51
1	A	2826	GLU	CD-OE2	5.06	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2426	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	2275	PHE	CB-CA-C	-5.82	98.76	110.40
1	A	1915	CYS	CA-CB-SG	5.68	124.22	114.00
1	A	4253	ILE	CB-CA-C	-5.50	100.59	111.60
1	A	2426	ARG	NE-CZ-NH2	5.42	123.01	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	2247	GLU	Peptide
1	A	2275	PHE	Peptide
1	A	2310	SER	Peptide
1	A	2416	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	22697	0	21503	995	0
2	A	32	0	12	12	0
3	A	2	0	0	0	0
4	A	31	0	12	4	0
5	A	54	0	24	10	0
All	All	22816	0	21551	996	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 22.

The worst 5 of 996 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:3581:PRO:HA	1:A:3584:PHE:CE1	1.16	1.63
1:A:2284:LYS:CE	1:A:2401:GLN:HG3	1.33	1.55
1:A:2284:LYS:HE3	1:A:2401:GLN:CG	1.49	1.40
1:A:3291:LEU:O	1:A:3294:HIS:CE1	1.75	1.39
1:A:3581:PRO:CA	1:A:3584:PHE:CE1	2.04	1.38

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	2995/3450 (87%)	2834 (95%)	153 (5%)	8 (0%)	44 79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1820	PRO
1	A	3965	PHE
1	A	1589	SER
1	A	1645	VAL
1	A	3375	PRO

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	2286/3065 (75%)	2201 (96%)	85 (4%)	39 73

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3336	LEU
1	A	3584	PHE
1	A	4215	ILE
1	A	3343	ASP
1	A	3495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2362	ASN
1	A	2391	ASN

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Mol	Chain	Res	Type
1	A	3738	GLN
1	A	2269	GLN
1	A	2777	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](#)

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	$\# Z > 2$
2	AOV	A	4401	3	26,34,34	1.03	2 (7%)	23,56,56	1.82	3 (13%)
4	ATP	A	4403	3	27,33,33	0.88	1 (3%)	25,52,52	1.77	3 (12%)
5	ADP	A	4405	-	25,29,29	1.06	2 (8%)	24,45,45	1.63	3 (12%)
5	ADP	A	4406	-	25,29,29	1.07	2 (8%)	24,45,45	1.97	5 (20%)

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	AOV	A	4401	3	-	0/12/39/39	0/3/3/3
4	ATP	A	4403	3	-	0/18/38/38	0/3/3/3
5	ADP	A	4405	-	-	0/12/32/32	0/3/3/3
5	ADP	A	4406	-	-	0/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4405	ADP	C4-N3	-2.10	1.32	1.35
2	A	4401	AOV	C2-N3	2.23	1.35	1.32
4	A	4403	ATP	C5-C4	2.34	1.45	1.40
5	A	4405	ADP	C5-C4	2.36	1.45	1.40
5	A	4406	ADP	C5-C4	2.38	1.45	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4406	ADP	N3-C2-N1	-6.98	122.78	128.86
4	A	4403	ATP	N3-C2-N1	-6.92	122.83	128.86
2	A	4401	AOV	N3-C2-N1	-6.40	123.28	128.86
5	A	4405	ADP	C4-C5-N7	-4.50	105.06	109.41
5	A	4405	ADP	N3-C2-N1	-4.21	125.19	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4401	AOV	12	0
4	A	4403	ATP	4	0
5	A	4405	ADP	5	0
5	A	4406	ADP	5	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 [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	3005/3450 (87%)	-0.31	85 (2%)	53 49	39, 110, 274, 477	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3130	LEU	8.1
1	A	2975	ASP	5.9
1	A	3136	SER	5.5
1	A	2942	SER	4.7
1	A	2946	ALA	4.5

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(Å ²)	Q<0.9
3	MG	A	4404	1/1	1.00	0.22	3.95	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ATP	A	4403	31/31	0.97	0.18	0.37	49,80,97,108	0
5	ADP	A	4406	27/27	0.95	0.20	-0.10	66,85,103,111	0
5	ADP	A	4405	27/27	0.97	0.18	-0.29	42,46,57,61	0
2	AOV	A	4401	32/32	0.98	0.20	-0.40	41,69,88,93	0
3	MG	A	4402	1/1	0.99	0.21	-0.63	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.