



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:02 PM GMT

PDB ID : 1II6  
Title : Crystal Structure of the Mitotic Kinesin Eg5 in Complex with Mg-ADP.  
Authors : Turner, J.; Anderson, R.; Guo, J.; Beraud, C.; Sakowicz, R.; Fletterick, R.  
Deposited on : 2001-04-20  
Resolution : 2.10 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](mailto: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.

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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

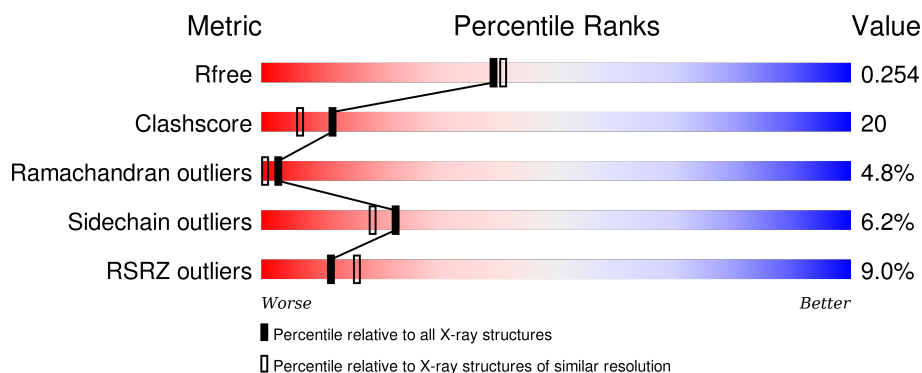
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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	368	
1	B	368	

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
4	ADP	A	2601	-	-	-	X
4	ADP	B	2600	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5704 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-RELATED MOTOR PROTEIN Eg5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2663	1665	467	521	10			
1	B	335	Total	C	N	O	S	0	0	0
			2626	1645	457	514	10			

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).

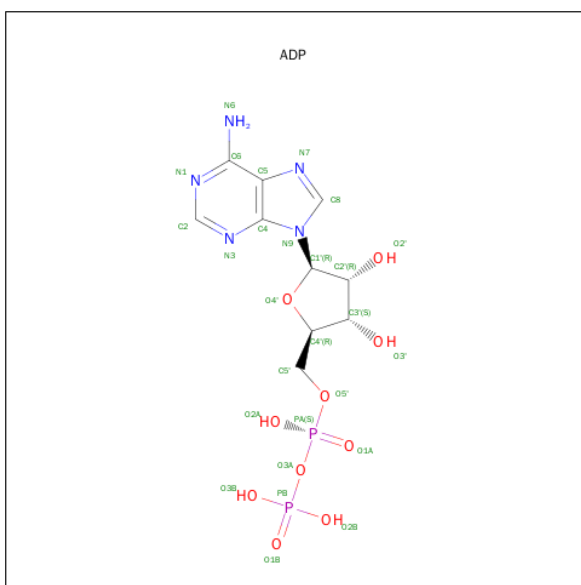


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		

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

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

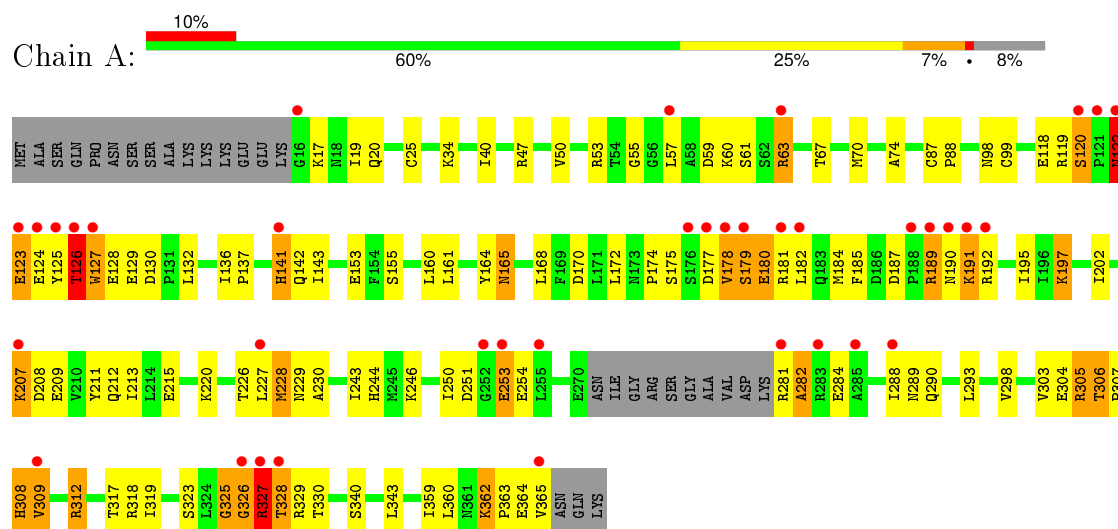
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	157	Total O 157 157	0	0
5	B	194	Total O 194 194	0	0

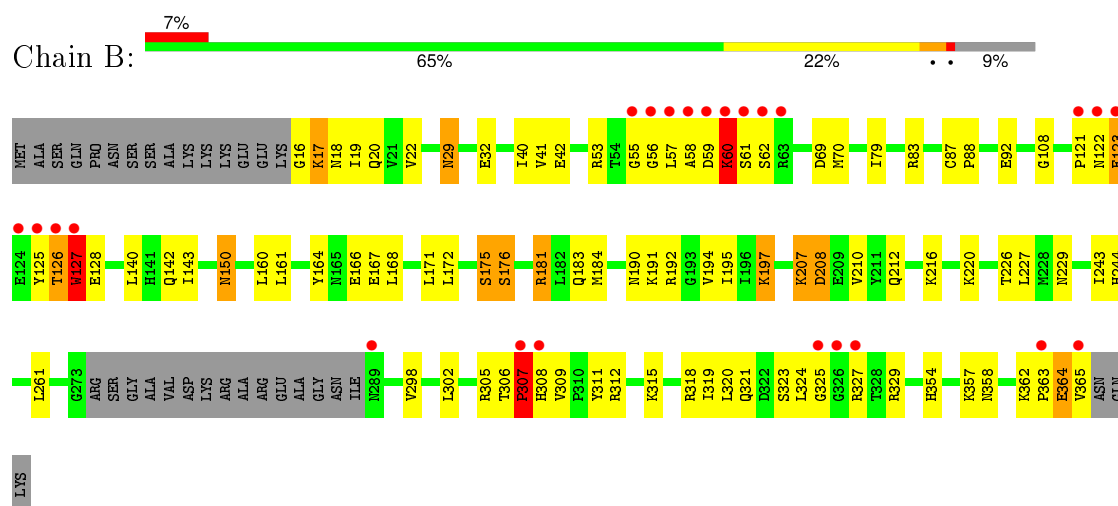
### 3 Residue-property plots [i](#)

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: KINESIN-RELATED MOTOR PROTEIN Eg5



#### • Molecule 1: KINESIN-RELATED MOTOR PROTEIN Eg5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.08Å 78.59Å 94.15Å 90.00° 93.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 47.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 94.8 (47.52-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.36 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.218 , 0.255 0.218 , 0.254	Depositor DCC
$R_{free}$ test set	4314 reflections (10.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 42888 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, NO3

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	0.32	0/2702	0.60	0/3653
1	B	0.34	0/2665	0.63	0/3603
All	All	0.33	0/5367	0.62	0/7256

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	2663	0	2684	125	0
1	B	2626	0	2653	97	0
2	A	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	1	0
5	A	157	0	0	8	0
5	B	194	0	0	10	0
All	All	5704	0	5361	213	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 20.

All (213) 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:63:ARG:HH11	1:A:63:ARG:HB3	1.08	1.11
1:A:312:ARG:H	1:A:312:ARG:HD3	1.21	1.03
1:A:17:LYS:HE3	1:A:303:VAL:HA	1.42	1.00
1:A:160:LEU:HB3	1:A:172:LEU:HD13	1.52	0.89
1:A:63:ARG:NH1	1:A:63:ARG:HB3	1.87	0.88
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.57	0.84
1:A:63:ARG:CB	1:A:63:ARG:HH11	1.89	0.84
1:A:53:ARG:HG2	1:A:63:ARG:NH1	1.95	0.81
1:B:42:GLU:HG3	1:B:53:ARG:HH12	1.48	0.79
1:B:312:ARG:CZ	1:B:321:GLN:HE22	1.95	0.79
1:A:57:LEU:HB2	1:B:164:TYR:HE2	1.48	0.78
1:B:59:ASP:O	1:B:60:LYS:HG2	1.83	0.77
1:A:312:ARG:N	1:A:312:ARG:HD3	2.00	0.76
1:A:67:THR:HG22	1:A:359:ILE:HD11	1.67	0.75
1:A:177:ASP:O	1:A:178:VAL:HG23	1.87	0.74
1:B:29:ASN:HD22	1:B:29:ASN:C	1.91	0.74
1:B:40:ILE:HD12	1:B:41:VAL:HG13	1.71	0.73
1:B:29:ASN:HD21	1:B:32:GLU:HG3	1.54	0.71
1:B:123:GLU:HB3	1:B:125:TYR:CE1	2.27	0.70
1:A:362:LYS:NZ	1:A:362:LYS:H	1.89	0.70
1:B:29:ASN:ND2	1:B:32:GLU:H	1.89	0.70
1:A:362:LYS:H	1:A:362:LYS:HZ2	1.40	0.70
1:A:312:ARG:H	1:A:312:ARG:CD	1.94	0.69
1:A:67:THR:HG21	1:A:362:LYS:HE3	1.74	0.69
1:A:207:LYS:HD3	1:A:208:ASP:N	2.08	0.68
1:B:216:LYS:HE2	5:B:2740:HOH:O	1.93	0.68
1:A:17:LYS:HB3	1:A:17:LYS:HZ2	1.60	0.67
1:A:17:LYS:NZ	1:A:17:LYS:HB3	2.09	0.67
1:A:60:LYS:HZ1	1:B:229:ASN:ND2	1.92	0.67
1:B:298:VAL:O	1:B:302:LEU:HD23	1.95	0.66
1:B:29:ASN:ND2	1:B:32:GLU:HG3	2.12	0.65
1:A:136:ILE:HB	1:A:137:PRO:HD3	1.78	0.65
1:B:312:ARG:HH21	1:B:318:ARG:NH2	1.95	0.65
1:A:227:LEU:HA	1:B:56:GLY:O	1.98	0.64
1:A:226:THR:OG1	1:A:227:LEU:HD22	1.97	0.64
1:A:189:ARG:HG3	1:A:190:ASN:N	2.12	0.64
1:A:60:LYS:NZ	1:B:229:ASN:ND2	2.45	0.64
1:A:178:VAL:HG12	1:A:179:SER:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:HG2	5:A:2737:HOH:O	1.98	0.63
1:B:55:GLY:HA3	1:B:60:LYS:HB2	1.79	0.63
1:B:16:GLY:HA3	1:B:357:LYS:HE3	1.79	0.63
1:A:57:LEU:HD21	1:B:167:GLU:OE1	1.99	0.63
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.79	0.62
1:B:362:LYS:HB3	1:B:363:PRO:HD2	1.81	0.61
1:A:57:LEU:HB2	1:B:164:TYR:CE2	2.33	0.61
1:A:323:SER:O	1:A:328:THR:HG21	1.99	0.61
1:B:123:GLU:HB3	1:B:125:TYR:HE1	1.63	0.61
1:B:53:ARG:HH11	1:B:53:ARG:HG3	1.64	0.60
1:A:40:ILE:HD13	1:A:340:SER:HA	1.82	0.60
1:B:190:ASN:HB2	5:B:2729:HOH:O	2.00	0.60
1:A:120:SER:HB3	1:A:132:LEU:HD12	1.82	0.60
1:A:191:LYS:O	1:A:192:ARG:HB2	2.02	0.60
1:A:55:GLY:HA3	1:A:59:ASP:O	2.02	0.60
1:A:122:ASN:O	1:A:123:GLU:HB2	2.02	0.60
1:A:17:LYS:HD2	1:A:303:VAL:HG13	1.84	0.59
1:B:184:MET:CE	1:B:194:VAL:HG11	2.32	0.59
1:B:363:PRO:C	1:B:365:VAL:H	2.04	0.59
1:B:323:SER:C	1:B:325:GLY:H	2.06	0.59
1:A:298:VAL:HG13	1:A:309:VAL:HG21	1.85	0.59
1:A:304:GLU:O	1:A:305:ARG:HB2	2.02	0.58
1:A:53:ARG:HH12	1:A:60:LYS:HE3	1.66	0.58
1:A:164:TYR:CE2	1:A:230:ALA:HA	2.38	0.58
1:A:197:LYS:HB2	1:A:197:LYS:NZ	2.19	0.58
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.34	0.57
1:B:87:CYS:HB2	1:B:88:PRO:HD3	1.86	0.57
1:B:244:HIS:HD2	5:B:2623:HOH:O	1.88	0.56
1:B:175:SER:O	1:B:176:SER:O	2.23	0.56
1:B:323:SER:O	1:B:324:LEU:HB2	2.06	0.56
1:B:181:ARG:HG2	5:B:2770:HOH:O	2.06	0.56
1:A:329:ARG:HH11	1:A:329:ARG:HG2	1.72	0.55
1:A:141:HIS:NE2	1:A:142:GLN:NE2	2.49	0.55
1:B:363:PRO:HG2	1:B:365:VAL:HG12	1.89	0.55
1:B:143:ILE:HD13	1:B:243:ILE:HD11	1.87	0.55
1:B:171:LEU:HA	1:B:220:LYS:HG2	1.89	0.55
1:A:160:LEU:HB3	1:A:172:LEU:CD1	2.32	0.54
1:A:57:LEU:HD13	1:B:164:TYR:CD2	2.42	0.54
1:A:184:MET:CE	1:A:318:ARG:HD3	2.37	0.54
1:B:53:ARG:NH1	1:B:53:ARG:HG3	2.22	0.54
1:A:281:ARG:HG2	1:A:282:ALA:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:HG2	5:B:2792:HOH:O	2.08	0.53
1:A:326:GLY:O	1:A:328:THR:HG22	2.08	0.53
1:B:57:LEU:HD13	1:B:60:LYS:HE3	1.91	0.53
1:B:92:GLU:OE1	1:B:329:ARG:HG3	2.08	0.53
1:B:321:GLN:O	1:B:323:SER:O	2.26	0.52
1:A:304:GLU:HB2	1:A:306:THR:HG22	1.91	0.52
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.74	0.52
1:B:184:MET:HE3	1:B:194:VAL:HG11	1.91	0.52
1:B:312:ARG:HH21	1:B:318:ARG:CZ	2.22	0.52
1:A:175:SER:C	1:A:177:ASP:H	2.12	0.52
1:A:305:ARG:HH11	1:A:305:ARG:HG3	1.75	0.51
1:B:212:GLN:O	1:B:216:LYS:HG3	2.09	0.51
1:A:181:ARG:HD3	1:A:182:LEU:H	1.75	0.51
1:A:61:SER:HA	5:A:2745:HOH:O	2.10	0.51
1:A:177:ASP:CG	1:A:220:LYS:HE3	2.31	0.50
1:B:17:LYS:HD3	5:B:2715:HOH:O	2.11	0.50
1:B:298:VAL:HG13	1:B:309:VAL:CG1	2.42	0.50
1:A:17:LYS:NZ	1:A:19:ILE:HG12	2.26	0.50
1:B:150:ASN:HD22	1:B:150:ASN:C	2.15	0.50
1:B:108:GLY:H	4:B:2600:ADP:PB	2.34	0.50
1:B:60:LYS:NZ	1:B:62:SER:HA	2.27	0.49
1:A:99:CYS:SG	1:A:328:THR:OG1	2.68	0.49
1:A:328:THR:OG1	1:A:329:ARG:N	2.45	0.49
1:A:325:GLY:O	1:A:326:GLY:C	2.51	0.49
1:A:120:SER:HB3	1:A:132:LEU:CD1	2.41	0.49
1:A:289:ASN:ND2	5:A:2758:HOH:O	2.46	0.49
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.95	0.48
1:A:253:GLU:HG2	1:A:254:GLU:N	2.28	0.48
1:B:363:PRO:C	1:B:365:VAL:N	2.67	0.48
1:B:363:PRO:O	1:B:365:VAL:N	2.46	0.48
1:B:61:SER:O	1:B:62:SER:HB2	2.12	0.48
1:B:122:ASN:O	1:B:123:GLU:C	2.51	0.48
1:B:56:GLY:O	1:B:57:LEU:HB2	2.13	0.48
1:B:184:MET:HE2	1:B:194:VAL:HG11	1.95	0.48
1:B:17:LYS:HE2	5:B:2713:HOH:O	2.14	0.48
1:A:192:ARG:NH1	1:A:325:GLY:HA3	2.29	0.48
1:A:197:LYS:HB2	1:A:197:LYS:HZ2	1.78	0.48
1:A:20:GLN:NE2	5:A:2742:HOH:O	2.42	0.48
1:B:60:LYS:HG3	1:B:62:SER:H	1.78	0.47
1:A:192:ARG:HG2	1:A:192:ARG:NH1	2.28	0.47
1:A:229:ASN:OD1	1:B:56:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:SER:O	1:A:180:GLU:C	2.53	0.47
1:A:126:THR:HB	1:A:127:TRP:H	1.45	0.47
1:B:55:GLY:HA3	1:B:60:LYS:CB	2.45	0.47
1:B:29:ASN:HD21	1:B:32:GLU:H	1.62	0.47
1:B:19:ILE:HD11	1:B:302:LEU:HB3	1.96	0.47
1:B:363:PRO:O	1:B:365:VAL:HG12	2.15	0.47
1:A:34:LYS:NZ	5:A:2699:HOH:O	2.47	0.47
1:B:20:GLN:HB2	5:B:2755:HOH:O	2.13	0.47
1:A:189:ARG:CG	1:A:190:ASN:N	2.77	0.47
1:A:184:MET:HE3	1:A:318:ARG:HH11	1.80	0.47
1:B:207:LYS:O	1:B:210:VAL:HG23	2.15	0.47
1:A:87:CYS:HB2	1:A:88:PRO:HD3	1.96	0.47
1:B:363:PRO:HG2	1:B:365:VAL:CG1	2.45	0.47
1:B:79:ILE:HG12	1:B:83:ARG:HD3	1.96	0.47
1:A:175:SER:O	1:A:177:ASP:N	2.44	0.46
1:A:153:GLU:OE1	1:A:246:LYS:HE2	2.14	0.46
1:A:212:GLN:HG3	1:A:213:ILE:N	2.30	0.46
1:B:327:ARG:HA	5:B:2707:HOH:O	2.15	0.46
1:A:126:THR:HB	1:A:128:GLU:OE1	2.16	0.46
1:B:69:ASP:O	1:B:70:MET:HG3	2.16	0.45
1:B:194:VAL:HG12	1:B:195:ILE:N	2.30	0.45
1:A:359:ILE:O	1:A:359:ILE:HG13	2.15	0.45
1:B:166:GLU:O	1:B:315:LYS:HD2	2.17	0.45
1:A:250:ILE:O	1:A:251:ASP:HB2	2.17	0.45
1:A:53:ARG:HG2	1:A:63:ARG:HH12	1.75	0.45
1:B:127:TRP:HD1	1:B:128:GLU:N	2.15	0.45
1:A:67:THR:CG2	1:A:362:LYS:HE3	2.46	0.45
1:A:53:ARG:NH1	1:A:60:LYS:HE3	2.32	0.45
1:A:129:GLU:HB2	5:A:2753:HOH:O	2.17	0.45
1:B:226:THR:HG22	1:B:227:LEU:HD23	1.99	0.44
1:A:284:GLU:O	1:A:288:ILE:HG13	2.17	0.44
1:A:325:GLY:O	1:A:327:ARG:N	2.50	0.44
1:B:197:LYS:HE2	1:B:197:LYS:HA	1.98	0.44
1:B:123:GLU:CB	1:B:125:TYR:HE1	2.30	0.44
1:A:17:LYS:CD	1:A:303:VAL:HG13	2.46	0.44
1:A:362:LYS:N	1:A:362:LYS:HZ2	2.12	0.44
1:A:122:ASN:HD22	1:A:122:ASN:HA	1.60	0.44
1:A:307:PRO:O	1:A:308:HIS:HB3	2.17	0.44
1:A:50:VAL:HG13	1:A:50:VAL:O	2.18	0.44
1:B:357:LYS:HA	5:B:2733:HOH:O	2.18	0.43
1:B:312:ARG:HE	1:B:318:ARG:NE	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ARG:HG3	1:B:318:ARG:HD3	2.00	0.43
1:B:323:SER:O	1:B:324:LEU:CB	2.65	0.43
1:B:298:VAL:O	1:B:302:LEU:CD2	2.64	0.43
1:A:298:VAL:HG13	1:A:309:VAL:CG2	2.47	0.43
1:A:161:LEU:HD12	1:A:161:LEU:C	2.38	0.43
1:A:141:HIS:CE1	5:A:2747:HOH:O	2.70	0.43
1:A:168:LEU:HD21	1:A:319:ILE:HD11	1.99	0.43
1:B:168:LEU:HD21	1:B:319:ILE:HD11	2.00	0.43
1:A:19:ILE:HA	1:A:330:THR:O	2.19	0.43
1:B:126:THR:O	1:B:127:TRP:CB	2.67	0.42
1:A:298:VAL:HG21	1:A:317:THR:HG21	2.01	0.42
1:A:182:LEU:HD21	5:A:2725:HOH:O	2.20	0.42
1:B:229:ASN:HD22	1:B:229:ASN:HA	1.69	0.42
1:A:364:GLU:O	1:A:365:VAL:O	2.38	0.42
1:A:181:ARG:CD	1:A:182:LEU:O	2.67	0.42
1:B:354:HIS:NE2	1:B:358:ASN:ND2	2.68	0.42
1:A:164:TYR:CD1	1:A:165:ASN:HB2	2.55	0.42
1:B:309:VAL:HG11	1:B:311:TYR:CZ	2.55	0.42
1:A:363:PRO:O	1:A:364:GLU:HB3	2.20	0.42
1:B:306:THR:HB	1:B:307:PRO:HD2	2.01	0.42
1:A:228:MET:CA	1:B:56:GLY:HA3	2.50	0.41
1:A:329:ARG:HG2	1:A:329:ARG:NH1	2.35	0.41
1:A:125:TYR:CE2	1:A:130:ASP:HA	2.55	0.41
1:B:140:LEU:CB	1:B:210:VAL:HG21	2.50	0.41
1:A:25:CYS:O	1:A:74:ALA:HA	2.20	0.41
1:A:187:ASP:HB3	1:A:195:ILE:HG13	2.02	0.41
1:B:192:ARG:HH11	1:B:325:GLY:HA3	1.84	0.41
1:B:181:ARG:H	1:B:181:ARG:HG2	1.77	0.41
1:A:184:MET:HE1	1:A:318:ARG:HD3	2.01	0.41
1:B:161:LEU:C	1:B:161:LEU:HD12	2.40	0.41
1:B:312:ARG:NE	1:B:321:GLN:HE22	2.15	0.41
1:B:29:ASN:HD22	1:B:32:GLU:H	1.67	0.41
1:A:122:ASN:O	1:A:123:GLU:CB	2.67	0.41
1:A:47:ARG:CZ	1:A:365:VAL:O	2.68	0.41
1:A:211:TYR:O	1:A:215:GLU:HG3	2.21	0.41
1:A:67:THR:HG22	1:A:359:ILE:CD1	2.45	0.41
1:A:184:MET:HE3	1:A:318:ARG:NH1	2.34	0.41
1:A:363:PRO:O	1:A:364:GLU:CB	2.68	0.41
1:A:155:SER:OG	1:A:244:HIS:HB2	2.21	0.41
1:A:281:ARG:HG2	1:A:282:ALA:H	1.85	0.41
1:A:172:LEU:HD23	1:A:202:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:SER:CB	1:A:132:LEU:HD12	2.50	0.41
1:A:125:TYR:O	1:A:126:THR:O	2.39	0.41
1:B:197:LYS:CE	1:B:197:LYS:HA	2.51	0.40
1:A:227:LEU:O	1:A:228:MET:HB2	2.22	0.40
1:B:16:GLY:O	1:B:18:ASN:N	2.54	0.40
1:A:98:ASN:OD1	1:A:323:SER:CB	2.70	0.40
1:A:119:ARG:O	1:A:120:SER:O	2.39	0.40
1:A:305:ARG:NH1	1:A:305:ARG:HG3	2.36	0.40
1:A:184:MET:HE3	1:A:318:ARG:HD3	2.03	0.40
1:A:306:THR:HA	1:A:307:PRO:HD2	1.95	0.40
1:B:160:LEU:HB3	1:B:172:LEU:HG	2.04	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	336/368 (91%)	303 (90%)	14 (4%)	19 (6%)	2	0
1	B	331/368 (90%)	310 (94%)	8 (2%)	13 (4%)	4	1
All	All	667/736 (91%)	613 (92%)	22 (3%)	32 (5%)	3	0

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	THR
1	A	178	VAL
1	A	191	LYS
1	A	282	ALA
1	B	123	GLU
1	B	127	TRP
1	B	176	SER

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Mol	Chain	Res	Type
1	B	207	LYS
1	B	208	ASP
1	A	120	SER
1	A	124	GLU
1	A	180	GLU
1	A	189	ARG
1	A	228	MET
1	A	253	GLU
1	A	326	GLY
1	A	327	ARG
1	B	126	THR
1	B	364	GLU
1	A	122	ASN
1	A	174	PRO
1	A	209	GLU
1	B	58	ALA
1	B	175	SER
1	B	307	PRO
1	A	123	GLU
1	A	308	HIS
1	B	17	LYS
1	B	60	LYS
1	B	121	PRO
1	A	179	SER
1	A	325	GLY

### 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	298/322 (92%)	277 (93%)	21 (7%)	19	15
1	B	296/322 (92%)	280 (95%)	16 (5%)	27	24
All	All	594/644 (92%)	557 (94%)	37 (6%)	23	19

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

Mol	Chain	Res	Type
1	A	63	ARG
1	A	118	GLU
1	A	122	ASN
1	A	126	THR
1	A	127	TRP
1	A	141	HIS
1	A	165	ASN
1	A	185	PHE
1	A	197	LYS
1	A	207	LYS
1	A	290	GLN
1	A	293	LEU
1	A	305	ARG
1	A	306	THR
1	A	309	VAL
1	A	312	ARG
1	A	327	ARG
1	A	328	THR
1	A	343	LEU
1	A	360	LEU
1	A	362	LYS
1	B	29	ASN
1	B	60	LYS
1	B	127	TRP
1	B	142	GLN
1	B	150	ASN
1	B	181	ARG
1	B	183	GLN
1	B	191	LYS
1	B	197	LYS
1	B	208	ASP
1	B	261	LEU
1	B	305	ARG
1	B	307	PRO
1	B	308	HIS
1	B	320	LEU
1	B	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	38	HIS

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	183	GLN
1	A	262	ASN
1	A	290	GLN
1	A	321	GLN
1	B	20	GLN
1	B	29	ASN
1	B	150	ASN
1	B	212	GLN
1	B	229	ASN
1	B	244	HIS
1	B	262	ASN
1	B	321	GLN
1	B	342	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
2	NO3	A	2000	-	3,3,3	0.69	0	3,3,3	0.67	0
2	NO3	A	2001	-	3,3,3	0.68	0	3,3,3	0.67	0
4	ADP	A	2601	3	22,29,29	1.25	3 (13%)	27,45,45	2.24	7 (25%)
4	ADP	B	2600	3	22,29,29	1.28	2 (9%)	27,45,45	2.88	6 (22%)

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	NO3	A	2000	-	-	0/0/0/0	0/0/0/0
2	NO3	A	2001	-	-	0/0/0/0	0/0/0/0
4	ADP	A	2601	3	-	0/12/32/32	0/3/3/3
4	ADP	B	2600	3	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2600	ADP	C8-N7	-3.31	1.28	1.34
4	A	2601	ADP	C8-N7	-3.27	1.28	1.34
4	A	2601	ADP	C5-C4	-2.12	1.35	1.40
4	B	2600	ADP	O4'-C1'	2.16	1.43	1.41
4	A	2601	ADP	C2'-C3'	2.50	1.60	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2600	ADP	O3B-PB-O1B	-7.43	86.65	110.58
4	B	2600	ADP	O3B-PB-O2B	-6.74	81.72	107.38
4	A	2601	ADP	O2A-PA-O3A	-5.95	78.09	105.09
4	B	2600	ADP	O3B-PB-O3A	-5.34	80.85	105.09
4	A	2601	ADP	O3A-PA-O5'	-4.00	92.32	102.94
4	A	2601	ADP	N3-C2-N1	-3.82	125.97	128.89
4	B	2600	ADP	N3-C2-N1	-3.57	126.16	128.89
4	A	2601	ADP	O5'-C5'-C4'	2.02	116.57	109.12
4	A	2601	ADP	PA-O3A-PB	2.19	139.99	132.67
4	A	2601	ADP	O2A-PA-O1A	4.10	134.77	112.53
4	B	2600	ADP	C4'-O4'-C1'	4.48	114.64	109.72
4	A	2601	ADP	C4'-O4'-C1'	5.01	115.22	109.72
4	B	2600	ADP	O2B-PB-O1B	6.42	131.26	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2600	ADP	1	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	340/368 (92%)	0.67	37 (10%) 7 10	15, 36, 74, 82	0
1	B	335/368 (91%)	0.52	24 (7%) 18 25	13, 30, 63, 83	0
All	All	675/736 (91%)	0.60	61 (9%) 12 16	13, 32, 70, 83	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	SER	8.8
1	B	58	ALA	8.7
1	B	57	LEU	8.6
1	A	127	TRP	8.2
1	B	127	TRP	7.8
1	B	365	VAL	6.9
1	B	56	GLY	6.4
1	B	125	TYR	5.9
1	A	365	VAL	5.7
1	A	16	GLY	5.4
1	B	59	ASP	5.3
1	A	190	ASN	5.2
1	A	178	VAL	4.9
1	B	62	SER	4.5
1	A	120	SER	4.4
1	A	125	TYR	4.4
1	B	123	GLU	4.1
1	B	124	GLU	3.8
1	A	281	ARG	3.8
1	B	307	PRO	3.7
1	B	326	GLY	3.7
1	A	124	GLU	3.7
1	A	57	LEU	3.7
1	A	188	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	3.5
1	A	191	LYS	3.5
1	A	326	GLY	3.4
1	B	55	GLY	3.4
1	A	288	ILE	3.4
1	B	60	LYS	3.4
1	A	181	ARG	3.4
1	B	327	ARG	3.4
1	B	308	HIS	3.3
1	A	283	ARG	3.3
1	A	309	VAL	3.2
1	A	189	ARG	3.0
1	A	141	HIS	3.0
1	A	176	SER	2.9
1	B	289	ASN	2.8
1	B	126	THR	2.7
1	A	123	GLU	2.5
1	A	126	THR	2.5
1	B	325	GLY	2.5
1	A	63	ARG	2.5
1	B	121	PRO	2.5
1	A	182	LEU	2.4
1	A	179	SER	2.4
1	A	177	ASP	2.4
1	A	192	ARG	2.4
1	A	253	GLU	2.4
1	B	122	ASN	2.4
1	A	207	LYS	2.3
1	A	227	LEU	2.3
1	B	363	PRO	2.3
1	A	255	LEU	2.3
1	A	327	ARG	2.2
1	A	328	THR	2.2
1	A	252	GLY	2.2
1	A	122	ASN	2.2
1	B	63	ARG	2.1
1	A	285	ALA	2.1

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

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	ADP	B	2600	27/27	0.92	0.19	4.75	12,30,35,35	0
4	ADP	A	2601	27/27	0.93	0.19	2.15	22,29,36,43	0
2	NO3	A	2001	4/4	0.94	0.14	-0.64	48,48,50,51	0
2	NO3	A	2000	4/4	0.97	0.09	-2.46	23,24,27,28	0
3	MG	B	2602	1/1	0.96	0.20	-	25,25,25,25	0
3	MG	A	2603	1/1	0.95	0.20	-	29,29,29,29	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.