



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 AM GMT

PDB ID : 2FME  
Title : Crystal structure of the mitotic kinesin eg5 (ksp) in complex with mg-adp and (r)-4-(3-hydroxyphenyl)-n,n,7,8-tetramethyl-3,4-dihydroisoquinoline-2(1h)-carboxamide  
Authors : Sheriff, S.  
Deposited on : 2006-01-09  
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

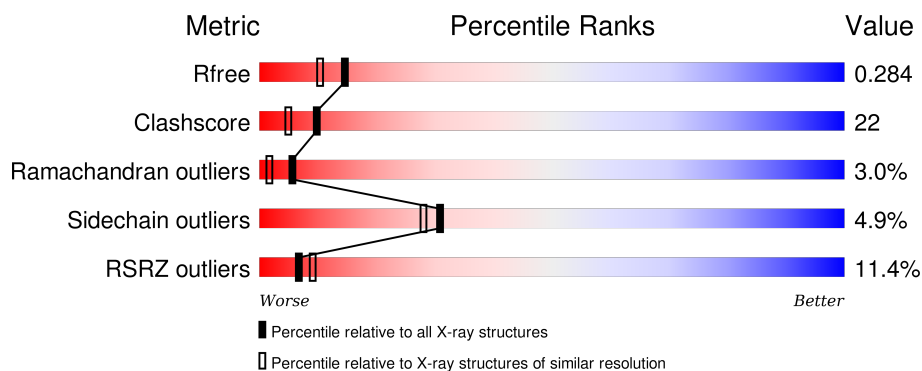
# 1 Overall quality at a glance

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	<div> <div>11%</div> <div>58%</div> <div>26%</div> <div>•</div> <div>13%</div> </div>
1	B	368	<div> <div>10%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5282 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.

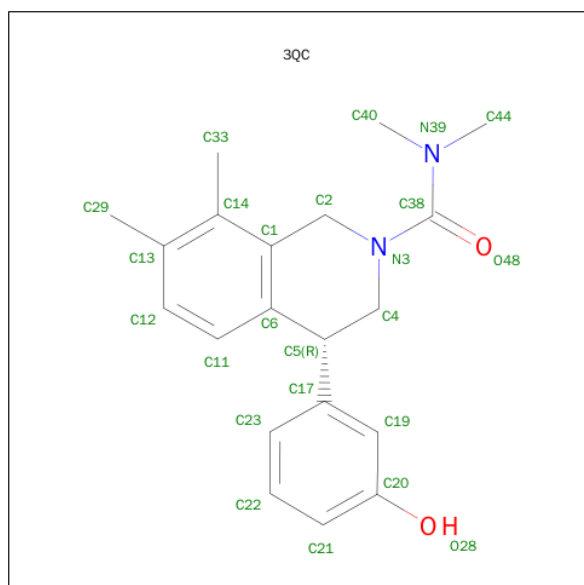
- Molecule 1 is a protein called Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	1
			2473	1549	430	484	10			
1	B	329	Total	C	N	O	S	0	0	1
			2527	1582	435	500	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

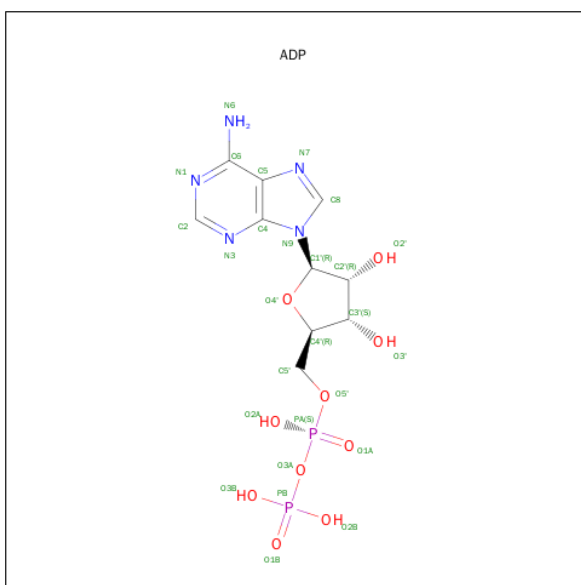
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (4R)-4-(3-HYDROXYPHENYL)-N,N,7,8-TETRAMETHYL-3,4-DIHYDROIS OQUINOLINE-2(1H)-CARBOXAMIDE (three-letter code: 3QC) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 24	C 20	N 2	O 2	0	0
3	B	1	Total 24	C 20	N 2	O 2	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 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

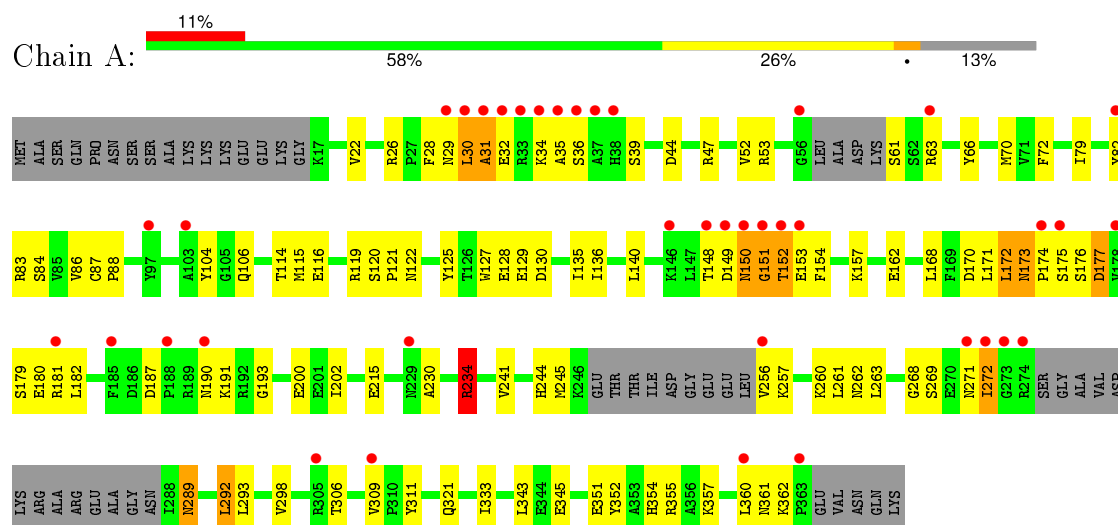
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 97 97	0	0
5	B	81	Total O 81 81	0	0

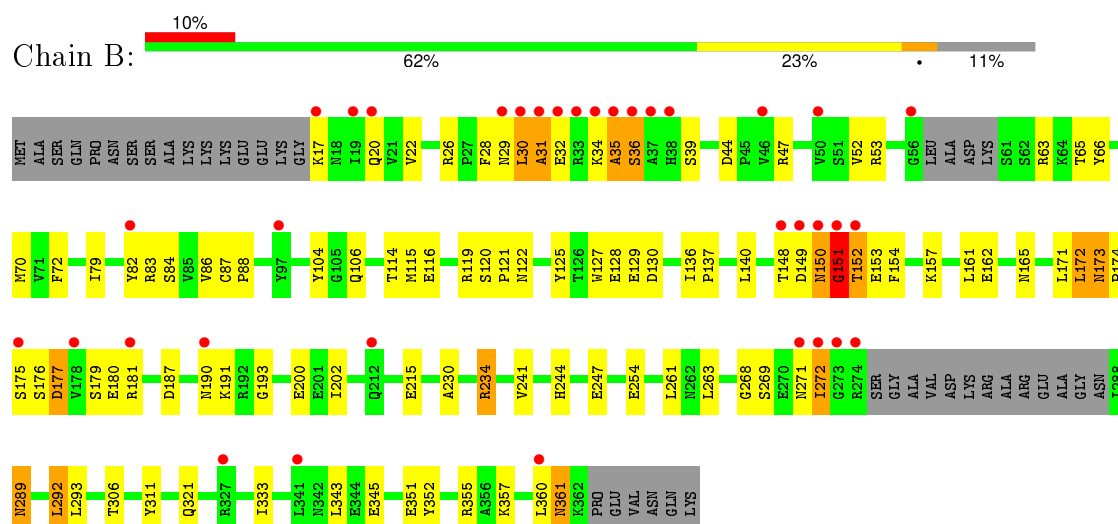
### 3 Residue-property plots

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-like protein KIF11



#### • Molecule 1: Kinesin-like protein KIF11



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.80 Å   80.00 Å   69.20 Å 90.00°   96.50°   90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.00-2.10) 93.4 (40.00-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 2.10 Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.280   ,   0.305 0.258   ,   0.284	Depositor DCC
$R_{free}$ test set	944 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 47350 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3QC, 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	0.37	0/2509	0.73	3/3398 (0.1%)
1	B	0.35	0/2564	0.72	4/3476 (0.1%)
All	All	0.36	0/5073	0.72	7/6874 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	234	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	B	234	ARG	NE-CZ-NH1	-12.73	113.93	120.30
1	B	234	ARG	NE-CZ-NH2	11.42	126.01	120.30
1	A	234	ARG	CD-NE-CZ	6.23	132.33	123.60
1	B	234	ARG	CD-NE-CZ	5.77	131.68	123.60
1	B	151	GLY	N-CA-C	-5.27	99.92	113.10

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	2473	0	2445	112	0
1	B	2527	0	2490	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	23	4	0
3	B	24	0	23	4	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	97	0	0	2	0
5	B	81	0	0	7	0
All	All	5282	0	5005	224	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.

All (224) 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:31:ALA:HA	1:A:34:LYS:HD3	1.30	1.13
1:B:31:ALA:HA	1:B:34:LYS:HD3	1.34	1.08
1:B:119:ARG:HH12	1:B:130:ASP:HB2	1.36	0.90
1:A:119:ARG:HH12	1:A:130:ASP:HB2	1.35	0.90
1:B:20:GLN:HG2	5:B:443:HOH:O	1.75	0.87
1:A:115:MET:HE1	1:A:333:ILE:HD12	1.68	0.76
1:A:173:ASN:HD22	1:A:174:PRO:N	1.84	0.75
3:B:370:3QC:H402	3:B:370:3QC:H22A	1.68	0.75
1:A:187:ASP:HB3	1:A:190:ASN:HB2	1.69	0.75
1:A:28:PHE:HA	1:A:32:GLU:OE1	1.87	0.75
3:A:370:3QC:H402	3:A:370:3QC:H22A	1.69	0.74
1:B:272:ILE:HG23	1:B:292:LEU:HD13	1.70	0.73
1:B:187:ASP:HB3	1:B:190:ASN:HB2	1.69	0.73
1:B:28:PHE:HA	1:B:32:GLU:OE1	1.89	0.72
1:A:272:ILE:HG23	1:A:292:LEU:HD13	1.70	0.72
1:B:173:ASN:HD22	1:B:174:PRO:CD	2.03	0.71
1:A:173:ASN:HD22	1:A:174:PRO:CD	2.04	0.70
1:B:173:ASN:HD22	1:B:174:PRO:HD2	1.57	0.69
1:B:152:THR:HG22	1:B:153:GLU:N	2.07	0.69
1:B:115:MET:HE1	1:B:333:ILE:HD12	1.73	0.69
1:B:173:ASN:HD22	1:B:174:PRO:N	1.90	0.69
1:A:152:THR:HG22	1:A:153:GLU:N	2.06	0.69
1:A:53:ARG:NH1	1:A:63:ARG:HH22	1.90	0.69
1:B:152:THR:CG2	1:B:153:GLU:N	2.56	0.68
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:CG2	1:A:153:GLU:N	2.55	0.68
1:A:87:CYS:HB3	1:A:88:PRO:HD3	1.76	0.68
1:B:173:ASN:HA	1:B:200:GLU:HG3	1.74	0.68
1:B:53:ARG:NH1	1:B:63:ARG:HH22	1.91	0.67
1:A:31:ALA:CA	1:A:34:LYS:HD3	2.19	0.67
1:A:173:ASN:HA	1:A:200:GLU:HG3	1.76	0.67
1:B:119:ARG:HH12	1:B:130:ASP:CB	2.08	0.66
1:A:150:ASN:CG	1:A:151:GLY:N	2.48	0.66
1:B:29:ASN:OD1	1:B:29:ASN:O	2.14	0.65
1:A:150:ASN:CG	1:A:151:GLY:H	2.00	0.65
1:A:268:GLY:O	1:A:271:ASN:HB2	1.96	0.65
1:A:119:ARG:HH12	1:A:130:ASP:CB	2.10	0.65
1:B:152:THR:CG2	1:B:153:GLU:H	2.10	0.64
1:B:150:ASN:CG	1:B:151:GLY:N	2.51	0.64
1:A:245:MET:O	1:A:256:VAL:O	2.16	0.64
1:A:151:GLY:O	1:A:152:THR:CB	2.46	0.64
1:A:30:LEU:C	1:A:32:GLU:H	2.01	0.64
1:A:29:ASN:OD1	1:A:29:ASN:O	2.16	0.63
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.62	0.63
1:B:30:LEU:C	1:B:32:GLU:H	2.02	0.63
1:A:104:TYR:OH	1:A:272:ILE:HD11	1.98	0.62
1:B:268:GLY:O	1:B:271:ASN:HB2	1.99	0.62
1:B:104:TYR:OH	1:B:272:ILE:HD11	1.99	0.62
1:A:152:THR:CG2	1:A:153:GLU:H	2.13	0.62
1:B:176:SER:OG	1:B:180:GLU:HG3	2.00	0.61
1:A:176:SER:OG	1:A:180:GLU:HG3	2.00	0.61
1:A:173:ASN:ND2	1:A:175:SER:H	1.98	0.61
1:B:151:GLY:O	1:B:152:THR:CB	2.49	0.61
1:B:360:LEU:C	1:B:360:LEU:HD23	2.22	0.60
1:B:125:TYR:HB3	1:B:129:GLU:HG3	1.82	0.60
1:A:125:TYR:HB3	1:A:129:GLU:HG3	1.83	0.60
1:B:114:THR:HG22	1:B:115:MET:HE2	1.84	0.60
1:A:256:VAL:O	1:A:257:LYS:HB2	2.02	0.60
1:B:161:LEU:CD2	5:B:451:HOH:O	2.49	0.59
1:B:173:ASN:ND2	1:B:175:SER:H	2.00	0.59
1:B:150:ASN:CG	1:B:151:GLY:H	2.04	0.59
1:B:272:ILE:HG22	1:B:293:LEU:HD23	1.84	0.59
1:A:177:ASP:OD2	1:A:179:SER:HB3	2.03	0.58
1:B:151:GLY:O	1:B:152:THR:OG1	2.20	0.58
1:A:272:ILE:HG22	1:A:293:LEU:HD23	1.84	0.58
1:B:190:ASN:ND2	1:B:193:GLY:HA3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:ND2	1:B:174:PRO:HD2	2.18	0.57
1:B:360:LEU:C	1:B:361:ASN:HD22	2.08	0.57
1:A:360:LEU:HD23	1:A:360:LEU:C	2.25	0.57
1:A:119:ARG:NH1	1:A:130:ASP:HB2	2.14	0.56
1:B:150:ASN:O	1:B:151:GLY:O	2.23	0.56
1:A:151:GLY:O	1:A:152:THR:OG1	2.19	0.56
1:B:361:ASN:N	1:B:361:ASN:HD22	2.03	0.56
1:B:79:ILE:O	1:B:83:ARG:HG3	2.05	0.56
1:A:173:ASN:ND2	1:A:174:PRO:HD2	2.20	0.56
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.88	0.55
1:A:61:SER:HB3	1:B:65:THR:O	2.06	0.55
1:B:272:ILE:CG2	1:B:292:LEU:HD13	2.36	0.55
1:B:114:THR:HG22	1:B:115:MET:CE	2.37	0.55
1:A:79:ILE:O	1:A:83:ARG:HG3	2.06	0.55
1:A:190:ASN:ND2	1:A:193:GLY:HA3	2.21	0.55
1:A:311:TYR:CG	1:A:321:GLN:HG3	2.42	0.55
1:A:29:ASN:O	1:A:32:GLU:N	2.40	0.55
1:A:114:THR:HG22	1:A:115:MET:CE	2.37	0.54
1:B:29:ASN:O	1:B:32:GLU:N	2.41	0.54
1:A:272:ILE:CG2	1:A:292:LEU:HD13	2.38	0.54
1:B:177:ASP:OD2	1:B:179:SER:HB3	2.08	0.54
1:B:157:LYS:HA	1:B:202:ILE:O	2.08	0.54
1:A:187:ASP:OD1	1:A:190:ASN:ND2	2.41	0.54
1:B:311:TYR:CG	1:B:321:GLN:HG3	2.42	0.54
1:A:173:ASN:C	1:A:173:ASN:HD22	2.11	0.53
1:A:154:PHE:HA	1:A:244:HIS:O	2.07	0.53
1:B:172:LEU:HB2	5:B:385:HOH:O	2.09	0.53
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.91	0.53
1:A:114:THR:HG22	1:A:115:MET:HE2	1.91	0.53
1:A:269:SER:C	1:A:271:ASN:H	2.11	0.53
1:A:152:THR:O	1:A:153:GLU:HB2	2.09	0.53
1:B:119:ARG:NH1	1:B:130:ASP:CB	2.72	0.52
1:B:154:PHE:HA	1:B:244:HIS:O	2.09	0.52
1:A:61:SER:CB	1:B:65:THR:O	2.57	0.52
1:A:157:LYS:HA	1:A:202:ILE:O	2.09	0.52
1:A:82:TYR:CE1	1:A:86:VAL:HG11	2.45	0.52
1:B:31:ALA:CA	1:B:34:LYS:HD3	2.24	0.52
1:B:357:LYS:HB3	1:B:357:LYS:NZ	2.24	0.52
1:B:269:SER:C	1:B:271:ASN:H	2.14	0.52
1:A:357:LYS:NZ	1:A:357:LYS:HB3	2.25	0.52
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HG3	1:A:171:LEU:HD13	1.92	0.51
1:A:150:ASN:ND2	1:A:151:GLY:H	2.07	0.51
1:A:119:ARG:NH1	1:A:130:ASP:CB	2.73	0.51
1:A:52:VAL:O	1:A:63:ARG:HB2	2.11	0.51
1:A:245:MET:O	1:A:256:VAL:C	2.49	0.51
1:A:150:ASN:O	1:A:151:GLY:O	2.29	0.51
1:B:63:ARG:HB3	1:B:63:ARG:NH1	2.26	0.50
1:B:152:THR:HG23	1:B:153:GLU:H	1.76	0.50
1:B:82:TYR:CE1	1:B:86:VAL:HG11	2.46	0.50
1:A:30:LEU:C	1:A:32:GLU:N	2.65	0.50
1:B:52:VAL:O	1:B:63:ARG:HB2	2.12	0.50
1:A:136:ILE:HG12	1:A:263:LEU:HD13	1.94	0.50
1:B:187:ASP:OD1	1:B:190:ASN:ND2	2.45	0.49
1:A:152:THR:HG23	1:A:153:GLU:H	1.77	0.49
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.42	0.49
3:A:370:3QC:H22A	3:A:370:3QC:C40	2.41	0.49
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.94	0.49
1:A:30:LEU:O	1:A:32:GLU:N	2.46	0.49
3:B:370:3QC:C40	3:B:370:3QC:H22A	2.40	0.49
1:B:149:ASP:O	1:B:150:ASN:O	2.31	0.48
1:B:150:ASN:ND2	1:B:151:GLY:H	2.11	0.48
1:A:149:ASP:O	1:A:150:ASN:O	2.31	0.48
1:A:119:ARG:NH1	1:A:130:ASP:OD1	2.46	0.48
1:B:17:LYS:HA	1:B:361:ASN:O	2.13	0.48
1:B:162:GLU:HG3	1:B:171:LEU:HD13	1.96	0.48
1:A:29:ASN:O	1:A:31:ALA:N	2.46	0.48
1:B:30:LEU:C	1:B:32:GLU:N	2.66	0.48
1:B:165:ASN:HB3	5:B:407:HOH:O	2.14	0.48
1:B:289:ASN:ND2	1:B:292:LEU:H	2.12	0.48
1:B:119:ARG:NH1	1:B:130:ASP:HB2	2.15	0.47
1:B:152:THR:O	1:B:153:GLU:HB2	2.13	0.47
1:A:360:LEU:HD23	1:A:361:ASN:O	2.14	0.47
1:B:241:VAL:CG1	1:B:261:LEU:HB3	2.44	0.47
1:A:63:ARG:NH1	1:A:63:ARG:HB3	2.28	0.47
1:B:360:LEU:HD23	1:B:361:ASN:N	2.29	0.47
1:B:30:LEU:O	1:B:32:GLU:N	2.48	0.47
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.76	0.47
1:B:44:ASP:OD2	1:B:47:ARG:HD2	2.14	0.47
1:B:119:ARG:NH1	1:B:130:ASP:OD1	2.47	0.47
1:A:152:THR:HG22	1:A:153:GLU:HG2	1.97	0.47
1:A:83:ARG:HD3	5:A:423:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.45	0.47
3:A:370:3QC:H331	3:A:370:3QC:H291	1.62	0.47
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.74	0.47
1:A:289:ASN:ND2	1:A:292:LEU:H	2.12	0.47
1:B:230:ALA:O	1:B:234:ARG:HG3	2.14	0.47
1:B:173:ASN:HD22	1:B:173:ASN:C	2.18	0.46
1:B:116:GLU:HG2	1:B:136:ILE:HD12	1.97	0.46
1:A:269:SER:C	1:A:271:ASN:N	2.68	0.46
1:A:241:VAL:CG1	1:A:261:LEU:HB3	2.46	0.46
1:A:116:GLU:HG2	1:A:136:ILE:HD12	1.98	0.46
1:B:106:GLN:NE2	1:B:345:GLU:HG3	2.31	0.46
1:B:35:ALA:O	1:B:36:SER:O	2.34	0.46
1:B:173:ASN:CA	1:B:200:GLU:HG3	2.45	0.46
1:B:70:MET:HE1	1:B:84:SER:HB3	1.97	0.46
1:B:269:SER:C	1:B:271:ASN:N	2.70	0.45
1:A:119:ARG:NH1	1:A:127:TRP:HA	2.31	0.45
1:B:29:ASN:O	1:B:31:ALA:N	2.49	0.45
1:A:66:TYR:CE2	1:A:351:GLU:OE2	2.70	0.45
1:A:106:GLN:NE2	1:A:345:GLU:HG3	2.32	0.45
1:B:119:ARG:NH1	1:B:127:TRP:HA	2.32	0.45
1:A:28:PHE:CE1	1:A:39:SER:HB2	2.52	0.44
1:A:79:ILE:HG13	1:A:83:ARG:HD2	2.00	0.44
1:B:66:TYR:CE2	1:B:351:GLU:OE2	2.70	0.44
1:B:152:THR:HG22	1:B:153:GLU:HG2	2.00	0.44
1:B:28:PHE:CE1	1:B:39:SER:HB2	2.52	0.44
1:A:215:GLU:HA	3:A:370:3QC:H401	2.00	0.44
1:A:352:TYR:O	1:A:355:ARG:HG2	2.17	0.44
1:A:29:ASN:O	1:A:30:LEU:C	2.56	0.43
1:A:173:ASN:CA	1:A:200:GLU:HG3	2.46	0.43
1:B:79:ILE:HG13	1:B:83:ARG:HD2	1.99	0.43
1:B:357:LYS:HB3	5:B:419:HOH:O	2.18	0.43
1:A:70:MET:HE1	1:A:84:SER:HB3	2.01	0.43
1:B:352:TYR:O	1:B:355:ARG:HG2	2.18	0.43
1:A:172:LEU:HB2	5:A:382:HOH:O	2.19	0.43
1:B:120:SER:HA	1:B:121:PRO:HD3	1.86	0.43
1:A:187:ASP:HB3	1:A:190:ASN:HD22	1.84	0.43
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.48	0.43
1:B:28:PHE:HE1	1:B:39:SER:HB2	1.84	0.43
1:B:190:ASN:HD22	1:B:193:GLY:HA3	1.83	0.43
1:A:309:VAL:CG1	1:A:311:TYR:CE2	3.02	0.42
1:A:241:VAL:HG13	1:A:261:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:HIS:O	1:A:357:LYS:HG3	2.18	0.42
1:A:115:MET:HE2	1:A:135:ILE:HD12	2.01	0.42
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.49	0.42
1:B:247:GLU:O	1:B:254:GLU:HA	2.19	0.42
1:A:170:ASP:HB2	1:A:182:LEU:HD11	2.01	0.42
1:B:215:GLU:HA	3:B:370:3QC:H401	2.02	0.42
1:A:187:ASP:HB3	1:A:190:ASN:ND2	2.34	0.42
1:B:66:TYR:HE2	1:B:351:GLU:OE2	2.03	0.42
1:B:26:ARG:HH22	1:B:32:GLU:CD	2.23	0.42
1:B:187:ASP:HB3	1:B:190:ASN:ND2	2.34	0.42
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.85	0.42
1:A:26:ARG:HH22	1:A:32:GLU:CD	2.23	0.42
1:A:190:ASN:HD22	1:A:193:GLY:HA3	1.85	0.42
1:B:29:ASN:O	1:B:30:LEU:C	2.58	0.41
1:A:70:MET:HE1	1:A:72:PHE:CZ	2.55	0.41
1:A:28:PHE:HE1	1:A:39:SER:HB2	1.84	0.41
1:A:298:VAL:HG13	1:A:309:VAL:CG2	2.49	0.41
1:A:230:ALA:O	1:A:234:ARG:HG3	2.20	0.41
1:A:66:TYR:HE2	1:A:351:GLU:OE2	2.03	0.41
1:B:187:ASP:HB3	1:B:190:ASN:HD22	1.84	0.41
1:B:161:LEU:HD23	5:B:451:HOH:O	2.14	0.41
1:A:357:LYS:NZ	1:A:357:LYS:CB	2.84	0.41
1:A:29:ASN:O	1:A:32:GLU:HB2	2.21	0.41
1:A:63:ARG:HG3	1:B:63:ARG:HG2	2.01	0.41
1:A:120:SER:HA	1:A:121:PRO:HD3	1.86	0.41
3:B:370:3QC:H291	3:B:370:3QC:H331	1.63	0.41
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.86	0.41
1:B:177:ASP:O	1:B:180:GLU:HG2	2.20	0.41
1:B:357:LYS:CB	1:B:357:LYS:NZ	2.84	0.41
1:A:245:MET:O	1:A:256:VAL:HA	2.21	0.40
1:B:161:LEU:HD22	5:B:451:HOH:O	2.20	0.40
1:A:309:VAL:HG13	1:A:311:TYR:CE2	2.57	0.40
1:A:257:LYS:HB2	1:A:257:LYS:HE3	1.86	0.40
1:B:70:MET:HE1	1:B:72:PHE:HZ	1.86	0.40
1:B:136:ILE:N	1:B:137:PRO:HD2	2.37	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	313/368 (85%)	291 (93%)	12 (4%)	10 (3%)	5	1
1	B	323/368 (88%)	304 (94%)	10 (3%)	9 (3%)	6	2
All	All	636/736 (86%)	595 (94%)	22 (4%)	19 (3%)	5	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	150	ASN
1	A	152	THR
1	A	191	LYS
1	A	362	LYS
1	B	30	LEU
1	B	150	ASN
1	B	152	THR
1	B	191	LYS
1	A	31	ALA
1	A	36	SER
1	A	151	GLY
1	B	31	ALA
1	B	35	ALA
1	B	36	SER
1	B	151	GLY
1	A	35	ALA
1	A	272	ILE
1	B	272	ILE

### 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	273/322 (85%)	259 (95%)	14 (5%)	29	26
1	B	279/322 (87%)	266 (95%)	13 (5%)	32	30
All	All	552/644 (86%)	525 (95%)	27 (5%)	31	28

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	128	GLU
1	A	140	LEU
1	A	148	THR
1	A	168	LEU
1	A	172	LEU
1	A	173	ASN
1	A	177	ASP
1	A	181	ARG
1	A	234	ARG
1	A	289	ASN
1	A	292	LEU
1	A	306	THR
1	A	343	LEU
1	B	122	ASN
1	B	128	GLU
1	B	140	LEU
1	B	148	THR
1	B	172	LEU
1	B	173	ASN
1	B	177	ASP
1	B	181	ARG
1	B	289	ASN
1	B	292	LEU
1	B	306	THR
1	B	343	LEU
1	B	361	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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Mol	Chain	Res	Type
1	A	98	ASN
1	A	122	ASN
1	A	141	HIS
1	A	142	GLN
1	A	173	ASN
1	A	190	ASN
1	A	205	HIS
1	A	262	ASN
1	A	289	ASN
1	B	18	ASN
1	B	98	ASN
1	B	122	ASN
1	B	141	HIS
1	B	142	GLN
1	B	173	ASN
1	B	190	ASN
1	B	205	HIS
1	B	262	ASN
1	B	289	ASN
1	B	361	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 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
3	3QC	A	370	-	26,26,26	2.12	9 (34%)	31,38,38	2.02	3 (9%)
4	ADP	A	371	2	22,29,29	1.45	6 (27%)	27,45,45	3.42	7 (25%)
3	3QC	B	370	-	26,26,26	2.08	9 (34%)	31,38,38	2.01	7 (22%)
4	ADP	B	371	2	22,29,29	1.50	4 (18%)	27,45,45	3.29	8 (29%)

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
3	3QC	A	370	-	-	0/12/24/24	0/3/3/3
4	ADP	A	371	2	-	0/12/32/32	0/3/3/3
3	3QC	B	370	-	-	0/12/24/24	0/3/3/3
4	ADP	B	371	2	-	0/12/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	371	ADP	PA-O2A	-2.68	1.43	1.54
3	A	370	3QC	C33-C14	-2.52	1.46	1.51
4	A	371	ADP	PB-O3B	-2.39	1.46	1.54
4	B	371	ADP	PB-O3B	-2.28	1.46	1.54
3	B	370	3QC	C33-C14	-2.02	1.47	1.51
4	A	371	ADP	C5-C4	2.01	1.45	1.40
3	A	370	3QC	C22-C21	2.19	1.43	1.38
4	A	371	ADP	C2-N1	2.20	1.38	1.33
4	A	371	ADP	C4-N3	2.43	1.39	1.35
4	B	371	ADP	C4-N3	2.44	1.39	1.35
3	B	370	3QC	C12-C11	2.51	1.43	1.38
4	B	371	ADP	C2-N1	2.56	1.38	1.33
3	A	370	3QC	C12-C11	2.57	1.43	1.38
3	B	370	3QC	C21-C20	2.58	1.44	1.38
3	A	370	3QC	C22-C23	2.77	1.44	1.38
4	A	371	ADP	C2-N3	3.04	1.37	1.32
3	B	370	3QC	C22-C23	3.11	1.45	1.38
3	B	370	3QC	C22-C21	3.20	1.45	1.38
3	B	370	3QC	C19-C17	3.36	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	370	3QC	C11-C6	3.43	1.44	1.39
3	A	370	3QC	C21-C20	3.51	1.46	1.38
3	A	370	3QC	C11-C6	3.56	1.44	1.39
3	A	370	3QC	C19-C17	3.56	1.45	1.39
4	B	371	ADP	C2-N3	3.71	1.38	1.32
3	B	370	3QC	C23-C17	4.14	1.45	1.39
3	A	370	3QC	C19-C20	4.39	1.46	1.39
3	A	370	3QC	C23-C17	4.47	1.46	1.39
3	B	370	3QC	C19-C20	4.75	1.46	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	371	ADP	N3-C2-N1	-15.74	116.84	128.89
4	B	371	ADP	N3-C2-N1	-15.13	117.31	128.89
3	A	370	3QC	C20-C19-C17	-3.62	116.85	120.14
4	A	371	ADP	C2'-C3'-C4'	-3.60	95.21	102.61
4	B	371	ADP	C2'-C3'-C4'	-3.33	95.77	102.61
4	A	371	ADP	C2'-C1'-N9	-3.31	109.23	114.29
3	B	370	3QC	C20-C19-C17	-3.31	117.14	120.14
3	B	370	3QC	C23-C22-C21	-3.15	115.74	120.24
4	B	371	ADP	C2'-C1'-N9	-2.95	109.78	114.29
4	B	371	ADP	C4'-O4'-C1'	-2.73	106.72	109.72
3	A	370	3QC	C23-C22-C21	-2.72	116.35	120.24
3	B	370	3QC	O48-C38-N3	-2.37	118.45	123.72
3	B	370	3QC	C29-C13-C14	-2.13	117.49	121.17
4	B	371	ADP	C4-C5-N7	-2.07	107.58	109.48
3	B	370	3QC	C11-C12-C13	-2.07	119.13	122.00
4	A	371	ADP	C4-C5-N7	-2.05	107.59	109.48
3	B	370	3QC	C22-C21-C20	2.21	122.70	119.37
4	A	371	ADP	O5'-C5'-C4'	2.27	117.50	109.12
4	B	371	ADP	O5'-C5'-C4'	2.28	117.54	109.12
4	B	371	ADP	C2-N1-C6	2.38	123.02	118.77
4	A	371	ADP	C2-N1-C6	2.82	123.80	118.77
4	B	371	ADP	O4'-C1'-N9	2.90	114.16	108.10
4	A	371	ADP	O4'-C1'-N9	3.13	114.66	108.10
3	B	370	3QC	C17-C5-C6	7.35	123.14	113.25
3	A	370	3QC	C17-C5-C6	7.74	123.67	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	370	3QC	4	0
3	B	370	3QC	4	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	321/368 (87%)	1.15	39 (12%) 6 7	11, 25, 44, 53	0
1	B	329/368 (89%)	0.95	35 (10%) 8 11	13, 26, 46, 53	0
All	All	650/736 (88%)	1.05	74 (11%) 7 9	11, 26, 46, 53	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	20.2
1	B	36	SER	13.8
1	B	35	ALA	13.4
1	A	273	GLY	11.0
1	B	272	ILE	10.7
1	B	37	ALA	9.9
1	A	272	ILE	9.8
1	A	274	ARG	9.5
1	A	150	ASN	8.8
1	B	34	LYS	8.3
1	A	149	ASP	8.3
1	A	31	ALA	8.0
1	A	151	GLY	7.9
1	A	36	SER	7.9
1	B	273	GLY	7.6
1	B	31	ALA	7.4
1	A	34	LYS	7.1
1	B	274	ARG	6.9
1	A	30	LEU	6.2
1	A	38	HIS	6.1
1	B	38	HIS	6.0
1	A	56	GLY	5.9
1	A	148	THR	5.5
1	A	152	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	360	LEU	5.4
1	A	190	ASN	5.1
1	A	97	TYR	5.0
1	B	33	ARG	5.0
1	A	33	ARG	5.0
1	A	32	GLU	4.8
1	B	152	THR	4.6
1	A	256	VAL	4.5
1	B	56	GLY	4.4
1	A	271	ASN	4.4
1	B	149	ASP	4.4
1	A	37	ALA	4.3
1	A	153	GLU	4.2
1	A	305	ARG	4.2
1	B	30	LEU	4.1
1	B	190	ASN	4.0
1	A	175	SER	3.8
1	B	151	GLY	3.5
1	A	174	PRO	3.4
1	B	271	ASN	3.4
1	B	32	GLU	3.3
1	B	97	TYR	3.3
1	A	188	PRO	3.2
1	A	82	TYR	3.2
1	B	178	VAL	3.2
1	A	29	ASN	3.1
1	B	20	GLN	3.0
1	A	178	VAL	2.9
1	B	17	LYS	2.9
1	B	29	ASN	2.9
1	B	150	ASN	2.9
1	B	46	VAL	2.9
1	B	341	LEU	2.7
1	B	148	THR	2.7
1	A	181	ARG	2.6
1	A	185	PHE	2.6
1	B	181	ARG	2.5
1	A	363	PRO	2.4
1	B	175	SER	2.4
1	B	212	GLN	2.2
1	A	63	ARG	2.1
1	A	229	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	ALA	2.1
1	A	146	LYS	2.1
1	B	327	ARG	2.1
1	B	19	ILE	2.1
1	B	50	VAL	2.0
1	A	360	LEU	2.0
1	A	309	VAL	2.0
1	B	82	TYR	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<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(Å <sup>2</sup> )	Q<0.9
3	3QC	A	370	24/24	0.93	0.19	0.83	14,20,21,22	0
3	3QC	B	370	24/24	0.93	0.16	0.46	14,19,20,21	0
4	ADP	B	371	27/27	0.96	0.14	0.07	13,23,25,29	0
4	ADP	A	371	27/27	0.97	0.14	-0.51	14,19,21,23	0
2	MG	A	369	1/1	0.97	0.29	-	21,21,21,21	0
2	MG	B	369	1/1	0.97	0.23	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.