



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y4I  
Title : KSR2-MEK1 HETERODIMER  
Authors : Brennan, D.F.; Barford, D.  
Deposited on : 2011-01-06  
Resolution : 3.46 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

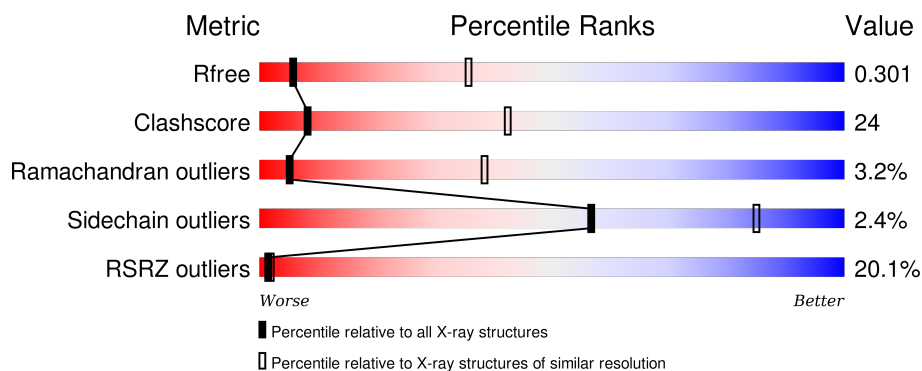
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.46 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	B	319	<div> <div>9%</div> <div>34%</div> <div>43%</div> <div>6%</div> <div>17%</div> </div>
2	C	395	<div> <div>22%</div> <div>49%</div> <div>29%</div> <div>•</div> <div>21%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4661 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 KINASE SUPPRESSOR OF RAS 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	265	2143	1385	367	379	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	632	GLY	-	EXPRESSION TAG	UNP Q6VAB6
B	633	PRO	-	EXPRESSION TAG	UNP Q6VAB6

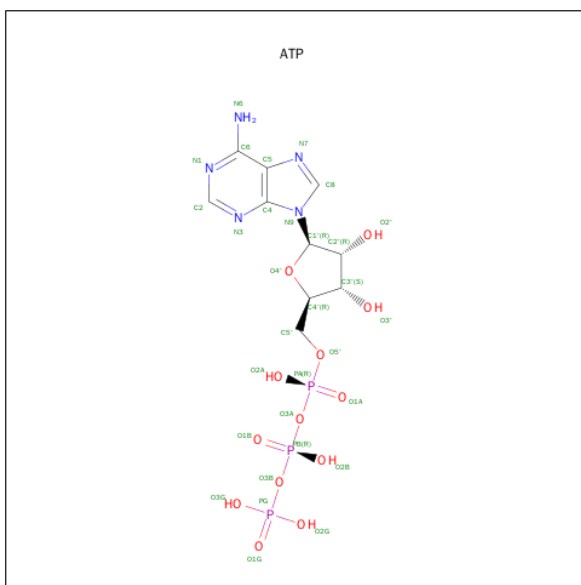
- Molecule 2 is a protein called DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	313	2453	1567	417	452	17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P29678
C	0	PRO	-	EXPRESSION TAG	UNP P29678
C	38	LEU	GLU	CONFLICT	UNP P29678

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

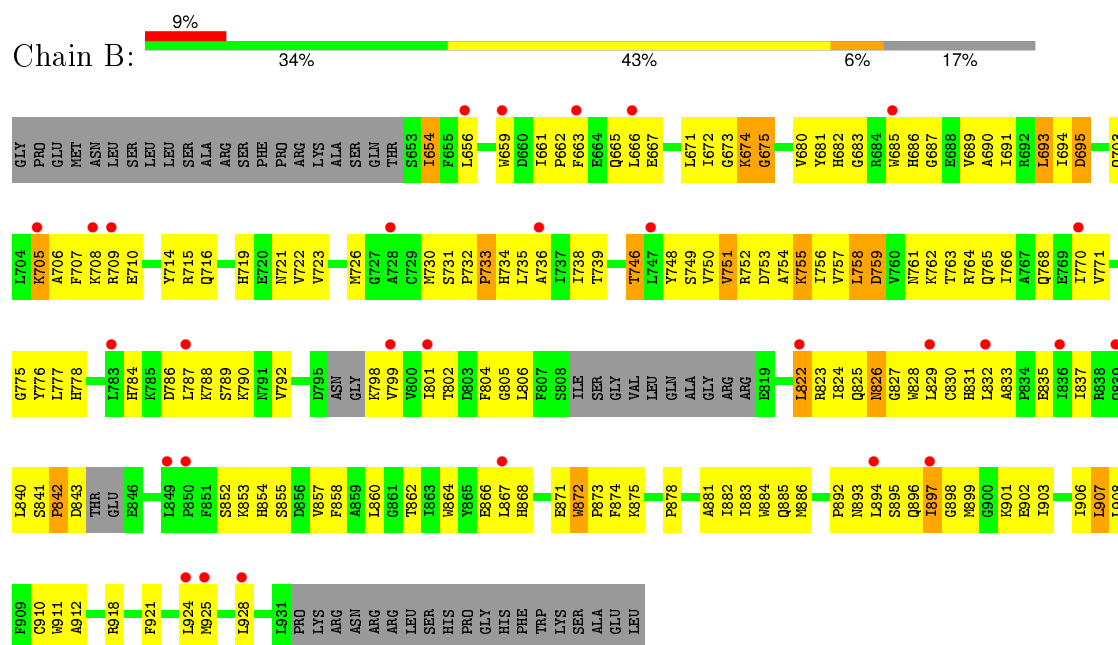
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

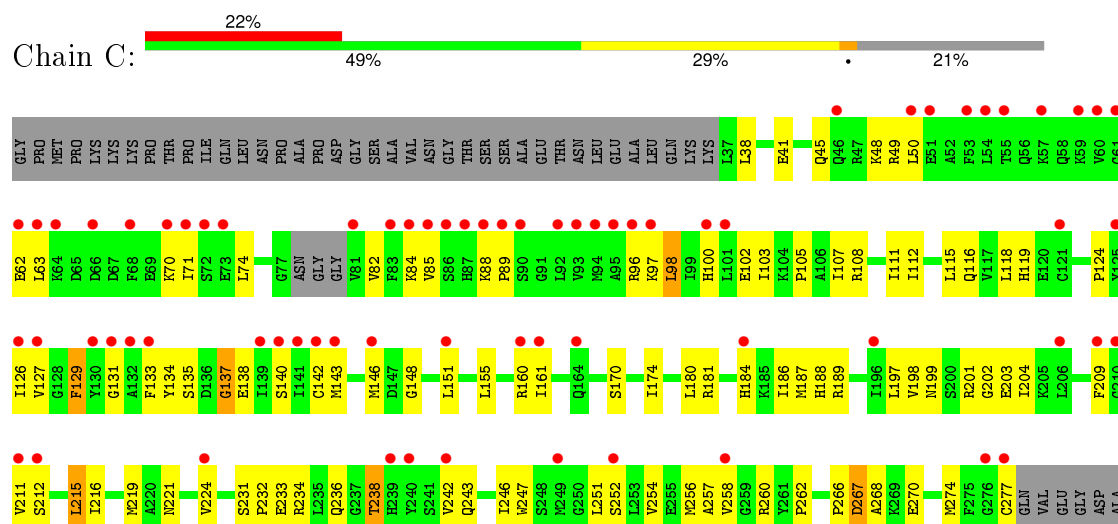
### 3 Residue-property plots

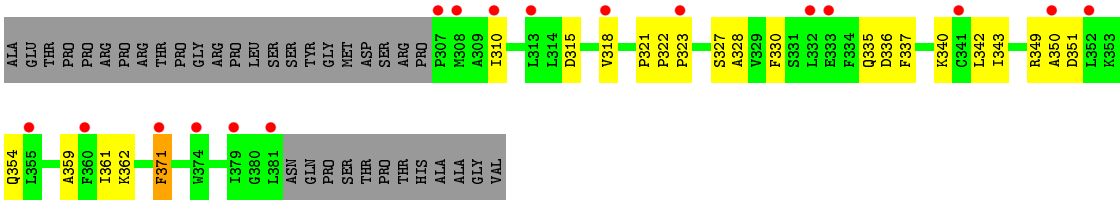
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: KINASE SUPPRESSOR OF RAS 2



#### • Molecule 2: DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.56 Å   130.56 Å   221.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	39.86 – 3.46 100.66 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.86-3.46) 99.5 (100.66-3.46)	Depositor EDS
$R_{merge}$	0.93	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.49 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.230   ,   0.293 0.237   ,   0.301	Depositor DCC
$R_{free}$ test set	762 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	133.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 134.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 15152 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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, ATP, CL

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	B	0.26	0/2192	0.43	0/2955
2	C	0.22	0/2499	0.38	0/3364
All	All	0.24	0/4691	0.41	0/6319

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	B	2143	0	2136	148	0
2	C	2453	0	2483	84	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	1	0	0	0	0
All	All	4661	0	4643	227	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 24.



All (227) 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:B:719:HIS:HD2	1:B:721:ASN:H	1.27	0.82
1:B:654:ILE:HG23	1:B:730:MET:H	1.45	0.78
1:B:661:ILE:HD12	1:B:726:MET:HA	1.66	0.78
2:C:252:SER:O	2:C:256:MET:HG2	1.86	0.75
2:C:343:ILE:HD12	2:C:349:ARG:HA	1.67	0.75
1:B:854:HIS:HA	1:B:857:VAL:HG12	1.68	0.74
1:B:735:LEU:HD22	1:B:736:ALA:H	1.52	0.73
1:B:771:VAL:HG23	1:B:921:PHE:HD1	1.53	0.72
1:B:826:ASN:HA	2:C:221:ASN:CG	2.10	0.72
2:C:127:VAL:HG21	2:C:197:LEU:HD12	1.71	0.71
1:B:894:LEU:HD11	1:B:908:LEU:HD21	1.73	0.71
1:B:894:LEU:HD22	1:B:907:LEU:HD13	1.73	0.70
1:B:665:GLN:H	1:B:686:HIS:CE1	2.10	0.69
1:B:735:LEU:HD22	1:B:736:ALA:N	2.08	0.68
1:B:685:TRP:HE3	1:B:738:ILE:HG21	1.57	0.68
2:C:359:ALA:HA	2:C:362:LYS:HE2	1.76	0.67
1:B:878:PRO:O	1:B:882:ILE:HG12	1.95	0.67
1:B:903:ILE:H	1:B:903:ILE:HD12	1.59	0.66
1:B:784:HIS:CD2	1:B:804:PHE:HB3	2.31	0.66
1:B:864:TRP:CH2	1:B:906:ILE:HB	2.30	0.65
3:B:1932:ATP:H5'2	3:B:1932:ATP:PB	2.38	0.64
1:B:719:HIS:CD2	1:B:721:ASN:H	2.14	0.64
1:B:871:GLU:OE1	1:B:875:LYS:HD3	1.98	0.64
2:C:126:ILE:HD11	2:C:180:LEU:CD1	2.27	0.63
1:B:685:TRP:HB3	1:B:689:VAL:HG11	1.81	0.63
1:B:852:SER:O	1:B:855:SER:HB3	1.98	0.63
1:B:730:MET:HG2	1:B:735:LEU:HD23	1.80	0.62
2:C:199:ASN:OD1	2:C:203:GLU:HB2	2.00	0.62
1:B:833:ALA:HB1	1:B:918:ARG:NH2	2.14	0.62
1:B:764:ARG:O	1:B:768:GLN:HG2	2.00	0.62
1:B:829:LEU:HD21	1:B:883:ILE:HG13	1.81	0.62
2:C:70:LYS:HA	2:C:85:VAL:HG12	1.82	0.61
2:C:216:ILE:HA	2:C:219:MET:HB2	1.82	0.61
2:C:262:PRO:HB3	2:C:323:PRO:HB3	1.83	0.61
2:C:181:ARG:HH11	2:C:242:VAL:HG11	1.66	0.61
1:B:673:GLY:HA3	1:B:680:VAL:H	1.67	0.60
1:B:840:LEU:HB2	1:B:843:ASP:HB2	1.84	0.60
1:B:685:TRP:CD1	1:B:685:TRP:O	2.55	0.60
1:B:776:TYR:HD1	1:B:777:LEU:HD23	1.67	0.59
1:B:761:ASN:O	1:B:765:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:LYS:O	1:B:708:LYS:HD3	2.03	0.59
2:C:105:PRO:HA	2:C:108:ARG:NE	2.18	0.58
1:B:862:THR:HA	1:B:911:TRP:HZ2	1.67	0.58
2:C:112:ILE:O	2:C:116:GLN:HG2	2.04	0.58
1:B:827:GLY:O	1:B:831:HIS:HD2	1.85	0.58
1:B:732:PRO:HB2	1:B:733:PRO:HD3	1.85	0.58
1:B:752:ARG:NH2	1:B:866:GLU:OE2	2.36	0.57
1:B:841:SER:HB3	1:B:842:PRO:HD3	1.86	0.57
1:B:757:VAL:O	1:B:758:LEU:HD23	2.05	0.57
2:C:270:GLU:O	2:C:274:MET:HG3	2.03	0.57
1:B:674:LYS:HG3	1:B:675:GLY:H	1.70	0.56
1:B:685:TRP:HD1	1:B:685:TRP:O	1.88	0.56
1:B:824:ILE:HD13	1:B:829:LEU:HD13	1.87	0.56
1:B:719:HIS:HD2	1:B:721:ASN:N	1.99	0.56
1:B:759:ASP:H	1:B:762:LYS:HD2	1.71	0.56
2:C:184:HIS:O	2:C:186:ILE:HG13	2.06	0.56
1:B:778:HIS:HB2	1:B:853:LYS:HE2	1.88	0.55
1:B:864:TRP:CZ3	1:B:906:ILE:HB	2.41	0.55
2:C:146:MET:HG3	2:C:197:LEU:CB	2.36	0.55
2:C:88:LYS:HB3	2:C:89:PRO:HD3	1.88	0.55
2:C:96:ARG:HE	2:C:140:SER:HB3	1.72	0.55
2:C:232:PRO:HD3	2:C:247:TRP:CE2	2.43	0.54
2:C:148:GLY:HA3	2:C:198:VAL:O	2.08	0.54
2:C:126:ILE:HD11	2:C:180:LEU:HD12	1.89	0.54
2:C:155:LEU:HD13	2:C:161:ILE:HG13	1.90	0.54
1:B:726:MET:HB2	1:B:738:ILE:HB	1.89	0.53
1:B:893:ASN:HD22	1:B:896:GLN:HE21	1.56	0.53
1:B:771:VAL:HG13	1:B:925:MET:HG2	1.90	0.53
2:C:232:PRO:O	2:C:236:GLN:HG3	2.08	0.53
1:B:901:LYS:O	1:B:902:GLU:HB2	2.08	0.53
1:B:862:THR:HG22	1:B:911:TRP:HE1	1.72	0.53
1:B:770:ILE:HD11	1:B:792:VAL:HG11	1.90	0.53
1:B:873:PRO:HB3	1:B:892:PRO:HG2	1.91	0.53
1:B:789:SER:HB2	1:B:866:GLU:OE1	2.10	0.52
1:B:674:LYS:CG	1:B:675:GLY:H	2.20	0.52
2:C:71:ILE:HB	2:C:84:LYS:O	2.09	0.52
2:C:146:MET:HG3	2:C:197:LEU:HB3	1.91	0.52
2:C:103:ILE:HB	2:C:107:ILE:HD12	1.91	0.52
1:B:722:VAL:HG21	1:B:777:LEU:HD21	1.92	0.51
2:C:126:ILE:HD11	2:C:180:LEU:HD11	1.90	0.51
1:B:862:THR:HG22	1:B:911:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:ILE:N	1:B:903:ILE:HD12	2.26	0.51
1:B:672:ILE:HD13	1:B:682:HIS:HB2	1.93	0.51
2:C:98:LEU:HD22	2:C:138:GLU:OE2	2.11	0.51
1:B:748:TYR:HB2	1:B:790:LYS:HG2	1.93	0.51
2:C:151:LEU:HD13	2:C:256:MET:HE2	1.93	0.50
1:B:654:ILE:HD11	1:B:659:TRP:HE1	1.76	0.50
1:B:694:ILE:O	1:B:695:ASP:C	2.50	0.50
2:C:327:SER:O	2:C:328:ALA:HB3	2.10	0.50
2:C:351:ASP:OD1	2:C:354:GLN:HG3	2.11	0.50
1:B:778:HIS:ND1	1:B:853:LYS:HE2	2.27	0.50
2:C:212:SER:O	2:C:216:ILE:HG13	2.11	0.50
1:B:732:PRO:CB	1:B:733:PRO:HD3	2.42	0.50
2:C:243:GLN:HA	2:C:246:ILE:HD12	1.92	0.50
1:B:860:LEU:HD23	1:B:860:LEU:C	2.32	0.50
1:B:895:SER:HA	1:B:899:MET:CB	2.42	0.49
1:B:893:ASN:ND2	1:B:896:GLN:HE21	2.09	0.49
2:C:74:LEU:HD12	2:C:82:VAL:HG12	1.94	0.49
2:C:233:GLU:HB2	2:C:238:THR:OG1	2.12	0.49
2:C:187:MET:O	2:C:189:ARG:HG3	2.13	0.49
1:B:825:GLN:C	2:C:221:ASN:HB3	2.33	0.49
2:C:180:LEU:HB3	2:C:186:ILE:O	2.12	0.49
2:C:202:GLY:HA2	2:C:371:PHE:CD1	2.48	0.49
1:B:862:THR:HA	1:B:911:TRP:CZ2	2.47	0.48
1:B:775:GLY:O	1:B:778:HIS:HB3	2.13	0.48
1:B:771:VAL:CG1	1:B:925:MET:HG2	2.43	0.48
1:B:756:ILE:O	1:B:756:ILE:HG13	2.12	0.48
1:B:801:ILE:HG22	1:B:802:THR:N	2.29	0.48
1:B:753:ASP:O	1:B:755:LYS:N	2.46	0.48
1:B:835:GLU:OE2	1:B:918:ARG:NH2	2.43	0.48
1:B:862:THR:CG2	1:B:911:TRP:HE1	2.27	0.48
1:B:756:ILE:HG13	1:B:758:LEU:HD22	1.94	0.48
1:B:833:ALA:HB1	1:B:918:ARG:HH22	1.76	0.48
1:B:746:THR:HG23	1:B:749:SER:OG	2.13	0.48
2:C:257:ALA:HB1	2:C:330:PHE:CZ	2.49	0.48
1:B:830:CYS:O	1:B:862:THR:HG21	2.14	0.47
1:B:864:TRP:HZ3	1:B:907:LEU:N	2.12	0.47
1:B:833:ALA:HB2	1:B:858:PHE:CG	2.48	0.47
1:B:715:ARG:HG2	1:B:716:GLN:HG3	1.96	0.47
1:B:874:PHE:CE2	1:B:886:MET:HG2	2.49	0.47
1:B:685:TRP:O	1:B:686:HIS:HB2	2.13	0.47
1:B:685:TRP:O	1:B:687:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:PHE:HB2	1:B:685:TRP:CZ2	2.50	0.47
1:B:853:LYS:HE3	1:B:921:PHE:CD2	2.49	0.47
2:C:254:VAL:O	2:C:258:VAL:HG22	2.15	0.47
2:C:233:GLU:HG2	2:C:234:ARG:N	2.29	0.47
1:B:766:ILE:O	1:B:770:ILE:HG12	2.15	0.47
2:C:174:ILE:HD11	2:C:337:PHE:HZ	1.79	0.47
1:B:826:ASN:N	2:C:221:ASN:HB3	2.30	0.46
1:B:706:ALA:O	1:B:710:GLU:HB2	2.16	0.46
1:B:787:LEU:HG	1:B:787:LEU:O	2.14	0.46
1:B:666:LEU:HD11	1:B:691:ILE:HD11	1.98	0.46
2:C:50:LEU:HD11	2:C:124:PRO:HG3	1.97	0.46
2:C:260:ARG:HH12	2:C:266:PRO:HA	1.79	0.46
1:B:656:LEU:HD12	1:B:663:PHE:CZ	2.50	0.46
2:C:188:HIS:CD2	2:C:209:PHE:HB3	2.51	0.46
2:C:118:LEU:HD21	2:C:211:VAL:HG11	1.98	0.46
2:C:160:ARG:HH21	2:C:277:CYS:H	1.62	0.46
2:C:327:SER:HA	2:C:335:GLN:NE2	2.30	0.46
2:C:135:SER:C	2:C:137:GLY:H	2.18	0.46
1:B:874:PHE:HB3	1:B:882:ILE:CD1	2.46	0.46
2:C:111:ILE:O	2:C:115:LEU:HB2	2.14	0.46
2:C:49:ARG:HB3	2:C:201:ARG:NH1	2.31	0.46
1:B:666:LEU:HD12	1:B:667:GLU:N	2.31	0.45
1:B:837:ILE:HD12	1:B:886:MET:HB2	1.97	0.45
2:C:118:LEU:HB2	2:C:129:PHE:CZ	2.51	0.45
1:B:770:ILE:O	1:B:801:ILE:HD11	2.17	0.45
1:B:798:LYS:HB3	1:B:799:VAL:H	1.61	0.45
1:B:723:VAL:HG22	1:B:802:THR:HA	1.98	0.45
1:B:864:TRP:CH2	1:B:903:ILE:HA	2.52	0.45
1:B:714:TYR:CD1	1:B:714:TYR:N	2.84	0.45
1:B:674:LYS:HG3	1:B:675:GLY:N	2.32	0.45
1:B:910:CYS:SG	1:B:924:LEU:HD11	2.57	0.45
2:C:170:SER:O	2:C:174:ILE:HG13	2.16	0.45
1:B:690:ALA:O	1:B:739:THR:HG22	2.17	0.45
2:C:119:HIS:HA	2:C:129:PHE:HE1	1.82	0.44
1:B:703:GLN:HB3	1:B:706:ALA:HB3	1.99	0.44
1:B:763:THR:HG23	1:B:867:LEU:HB3	2.00	0.44
2:C:133:PHE:HD1	2:C:134:TYR:O	2.00	0.44
2:C:63:LEU:HD11	2:C:131:GLY:HA3	1.99	0.44
2:C:224:VAL:HG11	2:C:310:ILE:HD13	2.00	0.44
1:B:805:GLY:O	1:B:806:LEU:HD23	2.17	0.44
1:B:830:CYS:HA	1:B:886:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:ILE:H	1:B:903:ILE:CD1	2.28	0.44
2:C:215:LEU:O	2:C:219:MET:HG2	2.17	0.44
2:C:254:VAL:HG12	2:C:262:PRO:HG3	2.00	0.44
1:B:881:ALA:O	1:B:885:GLN:HG3	2.17	0.44
2:C:198:VAL:HG22	2:C:204:ILE:HG12	2.00	0.44
1:B:924:LEU:O	1:B:924:LEU:HD23	2.18	0.44
1:B:763:THR:HG21	1:B:868:HIS:CE1	2.53	0.44
1:B:666:LEU:HD13	1:B:685:TRP:HA	1.99	0.44
2:C:129:PHE:HA	2:C:143:MET:HA	1.99	0.44
1:B:735:LEU:C	1:B:735:LEU:HD13	2.39	0.43
1:B:771:VAL:HG23	1:B:921:PHE:CD1	2.42	0.43
2:C:45:GLN:O	2:C:48:LYS:HB3	2.18	0.43
1:B:842:PRO:HB2	1:B:843:ASP:H	1.53	0.43
1:B:750:VAL:HG22	1:B:756:ILE:HD13	1.99	0.43
2:C:82:VAL:HG22	2:C:97:LYS:HB2	2.00	0.43
1:B:751:VAL:HG12	1:B:752:ARG:HG3	2.00	0.43
1:B:661:ILE:HA	1:B:662:PRO:HD3	1.91	0.43
1:B:842:PRO:O	1:B:843:ASP:C	2.56	0.43
1:B:751:VAL:CG1	1:B:752:ARG:HG3	2.48	0.43
2:C:349:ARG:HG2	2:C:350:ALA:N	2.34	0.43
2:C:327:SER:HA	2:C:335:GLN:HE22	1.83	0.43
1:B:758:LEU:HA	1:B:762:LYS:HD2	2.01	0.43
1:B:654:ILE:CG2	1:B:730:MET:H	2.23	0.43
1:B:683:GLY:HA3	1:B:691:ILE:CD1	2.48	0.43
2:C:251:LEU:N	2:C:342:LEU:HD21	2.34	0.43
2:C:231:SER:OG	2:C:234:ARG:HG3	2.19	0.42
1:B:714:TYR:HD1	1:B:714:TYR:N	2.17	0.42
1:B:681:TYR:CE1	1:B:693:LEU:HD22	2.54	0.42
1:B:750:VAL:CG2	1:B:756:ILE:HD13	2.48	0.42
1:B:874:PHE:CB	1:B:882:ILE:HD12	2.50	0.42
1:B:671:LEU:HB2	1:B:681:TYR:CE2	2.54	0.42
1:B:685:TRP:C	1:B:685:TRP:CD1	2.93	0.42
1:B:884:TRP:HE1	2:C:315:ASP:HA	1.85	0.42
2:C:63:LEU:HD13	2:C:133:PHE:HD2	1.85	0.42
2:C:321:PRO:HA	2:C:322:PRO:HD3	1.78	0.42
2:C:45:GLN:CD	2:C:49:ARG:HH21	2.24	0.41
1:B:707:PHE:C	1:B:709:ARG:N	2.72	0.41
2:C:105:PRO:O	2:C:108:ARG:HG2	2.20	0.41
2:C:361:ILE:HA	2:C:361:ILE:HD13	1.96	0.41
1:B:884:TRP:NE1	2:C:315:ASP:HA	2.36	0.41
1:B:822:LEU:HD12	1:B:823:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:ILE:HD13	2:C:211:VAL:HG23	2.02	0.41
1:B:853:LYS:HE3	1:B:921:PHE:CE2	2.55	0.41
1:B:748:TYR:CB	1:B:790:LYS:HG2	2.49	0.41
1:B:723:VAL:HG13	1:B:801:ILE:O	2.20	0.41
2:C:45:GLN:O	2:C:49:ARG:HG3	2.20	0.41
1:B:705:LYS:HG3	1:B:709:ARG:HD2	2.02	0.41
1:B:786:ASP:OD1	1:B:788:LYS:HG3	2.20	0.41
1:B:897:ILE:HA	1:B:898:GLY:HA2	1.63	0.41
1:B:731:SER:OG	1:B:734:HIS:CE1	2.74	0.41
1:B:893:ASN:O	1:B:894:LEU:HD23	2.21	0.41
1:B:864:TRP:HH2	1:B:903:ILE:HA	1.85	0.41
1:B:723:VAL:CG1	1:B:802:THR:HB	2.51	0.41
1:B:872:TRP:HB2	1:B:873:PRO:HD2	2.03	0.41
2:C:267:ASP:CG	2:C:268:ALA:H	2.24	0.41
2:C:336:ASP:O	2:C:340:LYS:HG2	2.21	0.41
2:C:215:LEU:HG	2:C:219:MET:HG2	2.03	0.41
1:B:911:TRP:O	1:B:912:ALA:C	2.58	0.40
2:C:133:PHE:HE2	2:C:142:CYS:SG	2.44	0.40
1:B:884:TRP:CZ2	2:C:318:VAL:HG11	2.57	0.40
1:B:663:PHE:HB2	1:B:685:TRP:CE2	2.57	0.40
1:B:837:ILE:HD12	1:B:886:MET:CB	2.51	0.40
2:C:100:HIS:CE1	2:C:102:GLU:HG2	2.56	0.40
1:B:828:TRP:CZ2	1:B:832:LEU:HD11	2.56	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	B	257/319 (81%)	203 (79%)	42 (16%)	12 (5%)	3	28
2	C	307/395 (78%)	261 (85%)	40 (13%)	6 (2%)	9	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	564/714 (79%)	464 (82%)	82 (14%)	18 (3%)	5	38

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	754	ALA
1	B	758	LEU
1	B	822	LEU
1	B	826	ASN
2	C	267	ASP
1	B	675	GLY
1	B	755	LYS
1	B	759	ASP
1	B	842	PRO
2	C	41	GLU
2	C	371	PHE
1	B	674	LYS
1	B	695	ASP
1	B	733	PRO
1	B	897	ILE
2	C	38	LEU
2	C	62	GLU
2	C	137	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	B	228/278 (82%)	220 (96%)	8 (4%)	43	78
2	C	270/339 (80%)	266 (98%)	4 (2%)	72	90
All	All	498/617 (81%)	486 (98%)	12 (2%)	57	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	654	ILE
1	B	693	LEU
1	B	705	LYS
1	B	746	THR
1	B	751	VAL
1	B	872	TRP
1	B	907	LEU
1	B	928	LEU
2	C	98	LEU
2	C	129	PHE
2	C	215	LEU
2	C	238	THR

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

Mol	Chain	Res	Type
1	B	734	HIS
1	B	765	GLN
1	B	831	HIS
1	B	896	GLN
1	B	915	GLN
2	C	116	GLN
2	C	335	GLN

### 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 5 ligands modelled in this entry, 3 are 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
3	ATP	B	1932	4	24,33,33	0.95	1 (4%)	31,52,52	1.91	5 (16%)
3	ATP	C	1382	4	24,33,33	0.97	1 (4%)	31,52,52	1.93	5 (16%)

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	ATP	B	1932	4	-	0/18/38/38	0/3/3/3
3	ATP	C	1382	4	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1932	ATP	C5-C4	3.01	1.47	1.40
3	C	1382	ATP	C5-C4	3.15	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1382	ATP	N3-C2-N1	-6.76	123.72	128.89
3	B	1932	ATP	N3-C2-N1	-6.69	123.77	128.89
3	B	1932	ATP	PB-O3B-PG	-3.90	119.60	132.67
3	C	1382	ATP	C2'-C1'-N9	-3.85	108.41	114.29
3	B	1932	ATP	C2'-C1'-N9	-3.81	108.47	114.29
3	C	1382	ATP	PB-O3B-PG	-3.66	120.38	132.67
3	B	1932	ATP	C4-C5-N7	-3.19	106.55	109.48
3	C	1382	ATP	PA-O3A-PB	-3.16	123.85	132.73
3	C	1382	ATP	C4-C5-N7	-2.94	106.77	109.48
3	B	1932	ATP	PA-O3A-PB	-2.46	125.81	132.73

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
3	B	1932	ATP	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	B	265/319 (83%)	0.91	29 (10%) 7 8	97, 135, 226, 274	0
2	C	313/395 (79%)	1.31	87 (27%) 1 1	95, 168, 234, 302	0
All	All	578/714 (80%)	1.13	116 (20%) 1 2	95, 151, 232, 302	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	94	MET	7.8
2	C	63	LEU	5.9
1	B	685	TRP	5.6
2	C	93	VAL	5.3
2	C	139	ILE	5.3
2	C	85	VAL	5.2
2	C	141	ILE	5.2
2	C	60	VAL	5.1
2	C	132	ALA	4.7
2	C	68	PHE	4.4
2	C	90	SER	4.3
2	C	352	LEU	4.2
2	C	310	ILE	4.0
2	C	53	PHE	3.9
2	C	240	TYR	3.9
1	B	822	LEU	3.9
2	C	210	GLY	3.7
2	C	211	VAL	3.7
1	B	728	ALA	3.6
2	C	46	GLN	3.6
2	C	142	CYS	3.6
2	C	50	LEU	3.6
2	C	95	ALA	3.5
2	C	84	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	89	PRO	3.4
2	C	87	HIS	3.3
2	C	374	TRP	3.3
2	C	277	CYS	3.3
2	C	88	LYS	3.2
2	C	125	TYR	3.2
1	B	850	PRO	3.2
2	C	64	LYS	3.1
2	C	308	MET	3.1
1	B	656	LEU	3.1
2	C	151	LEU	3.0
2	C	55	THR	3.0
2	C	70	LYS	2.9
2	C	307	PRO	2.9
1	B	705	LYS	2.9
1	B	897	ILE	2.9
1	B	708	LYS	2.9
2	C	161	ILE	2.9
1	B	894	LEU	2.9
1	B	829	LEU	2.8
2	C	127	VAL	2.8
2	C	97	LYS	2.8
1	B	747	LEU	2.8
1	B	787	LEU	2.8
2	C	62	GLU	2.7
2	C	212	SER	2.7
2	C	73	GLU	2.7
2	C	57	LYS	2.7
2	C	184	HIS	2.7
2	C	96	ARG	2.7
2	C	92	LEU	2.6
2	C	131	GLY	2.6
2	C	242	VAL	2.6
2	C	276	GLY	2.6
2	C	224	VAL	2.6
1	B	783	LEU	2.6
1	B	709	ARG	2.6
2	C	59	LYS	2.6
2	C	341	CYS	2.5
2	C	379	ILE	2.5
2	C	83	PHE	2.5
2	C	66	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	239	HIS	2.5
2	C	209	PHE	2.5
1	B	659	TRP	2.4
2	C	130	TYR	2.4
2	C	164	GLN	2.4
1	B	928	LEU	2.4
2	C	332	LEU	2.4
2	C	206	LEU	2.4
2	C	249	MET	2.4
2	C	51	GLU	2.4
1	B	770	ILE	2.4
2	C	196	ILE	2.4
1	B	839	GLN	2.4
2	C	86	SER	2.3
2	C	160	ARG	2.3
2	C	61	GLY	2.3
2	C	252	SER	2.3
2	C	318	VAL	2.3
1	B	867	LEU	2.3
2	C	81	VAL	2.3
2	C	355	LEU	2.3
2	C	360	PHE	2.3
2	C	140	SER	2.3
2	C	101	LEU	2.2
2	C	72	SER	2.2
1	B	849	LEU	2.2
1	B	799	VAL	2.2
2	C	143	MET	2.2
2	C	146	MET	2.2
1	B	666	LEU	2.2
2	C	126	ILE	2.2
2	C	323	PRO	2.1
2	C	333	GLU	2.1
1	B	836	ILE	2.1
2	C	381	LEU	2.1
2	C	350	ALA	2.1
2	C	371	PHE	2.1
1	B	832	LEU	2.1
2	C	100	HIS	2.1
2	C	133	PHE	2.1
2	C	71	ILE	2.1
2	C	258	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	54	LEU	2.1
1	B	925	MET	2.1
1	B	801	ILE	2.0
2	C	121	CYS	2.0
1	B	663	PHE	2.0
1	B	736	ALA	2.0
1	B	924	LEU	2.0
2	C	313	LEU	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
5	CL	C	1384	1/1	0.59	0.31	0.81	143,143,143,143	0
3	ATP	C	1382	31/31	0.84	0.27	-0.40	110,136,174,305	0
3	ATP	B	1932	31/31	0.95	0.28	-0.41	86,105,134,268	0
4	MG	C	1383	1/1	0.97	0.20	-0.55	185,185,185,185	0
4	MG	B	1933	1/1	0.99	0.23	-	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.