



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:35 PM GMT

PDB ID : 3U8X
Title : Crystal Structure of a chimera containing the N-terminal domain (residues 8-29) of drosophila Ciboulot and the C-terminal domain (residues 18-44) of bovine Thymosin-beta4, bound to G-actin-ATP
Authors : Renault, L.; Husson, C.; Carlier, M.F.; Didry, D.
Deposited on : 2011-10-17
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

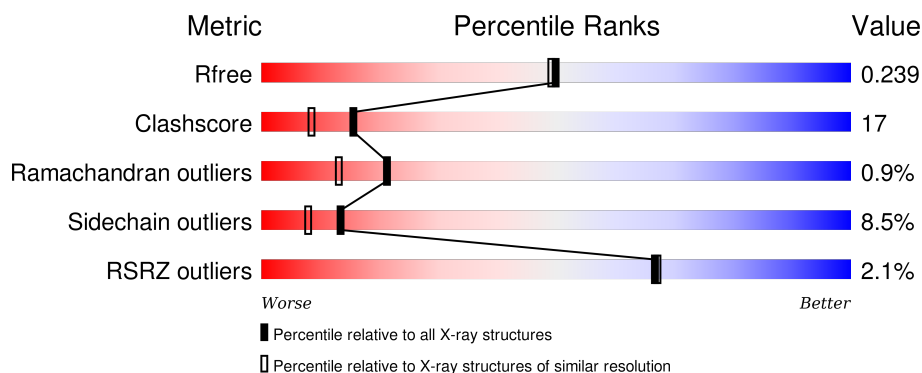
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	375	<div> <div>2%</div> <div>67%</div> <div>24%</div> <div>5%</div> </div>
1	C	375	<div> <div>%</div> <div>63%</div> <div>28%</div> <div>5%</div> </div>
2	B	54	<div> <div>7%</div> <div>17%</div> <div>17%</div> <div>6%</div> <div>61%</div> </div>
2	D	54	<div> <div>4%</div> <div>22%</div> <div>9%</div> <div>6%</div> <div>61%</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
4	MG	A	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5990 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2794	1771	469	536	18			
1	C	357	Total	C	N	O	S	0	0	0
			2794	1771	469	536	18			

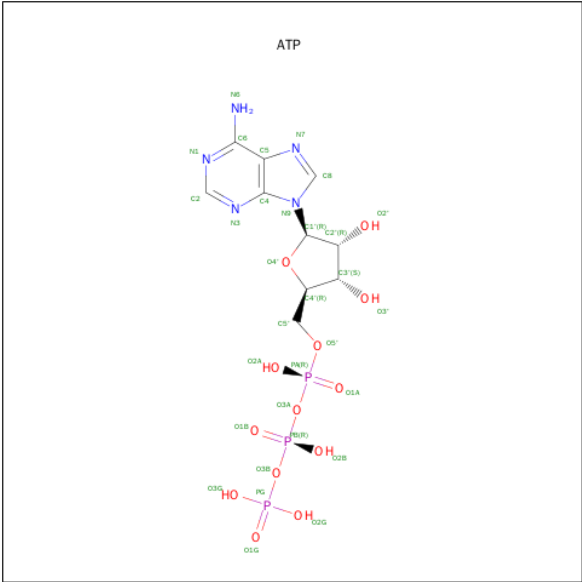
- Molecule 2 is a protein called Thymosin beta-4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	0	0	0
			169	107	30	32			
2	D	21	Total	C	N	O	0	0	0
			169	107	30	32			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	EXPRESSION TAG	UNP O97428
B	4	PRO	-	EXPRESSION TAG	UNP O97428
B	5	LEU	-	EXPRESSION TAG	UNP O97428
B	6	GLY	-	EXPRESSION TAG	UNP O97428
B	7	SER	-	EXPRESSION TAG	UNP O97428
D	3	GLY	-	EXPRESSION TAG	UNP O97428
D	4	PRO	-	EXPRESSION TAG	UNP O97428
D	5	LEU	-	EXPRESSION TAG	UNP O97428
D	6	GLY	-	EXPRESSION TAG	UNP O97428
D	7	SER	-	EXPRESSION TAG	UNP O97428

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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		

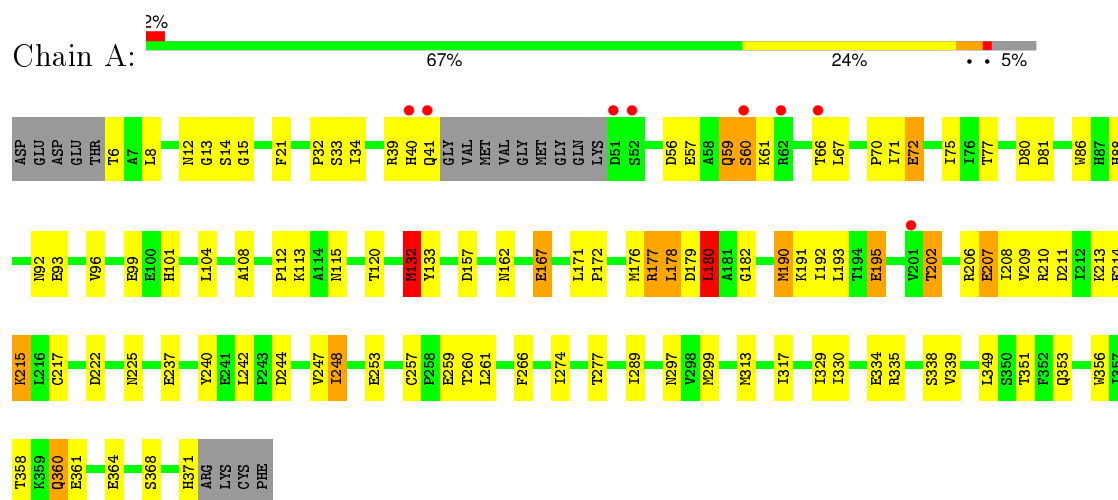
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

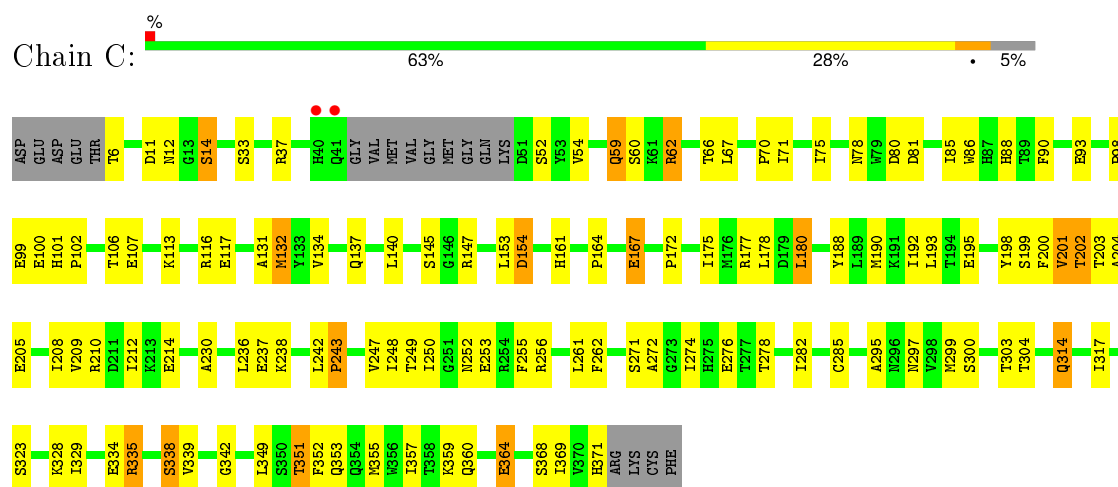
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

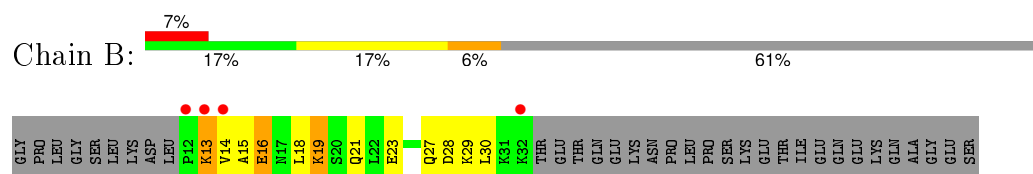
- Molecule 1: Actin, alpha skeletal muscle



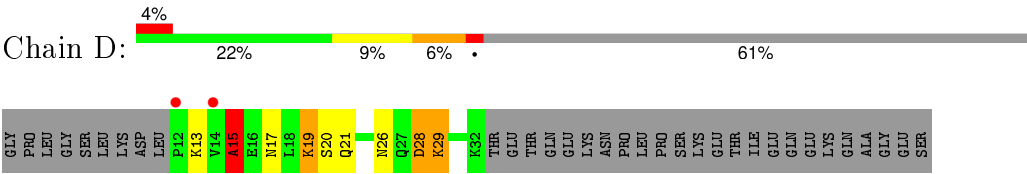
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Thymosin beta-4



● Molecule 2: Thymosin beta-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.01Å 75.33Å 128.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.00 19.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.70-2.00) 97.9 (19.63-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.33 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.238 0.192 , 0.239	Depositor DCC
R_{free} test set	4171 reflections (7.75%)	DCC
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 12.1	EDS
Estimated twinning fraction	0.500 for H, K, L 0.500 for -H, -K, L 0.477 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -H, -K, L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 58182 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.05	2/2855 (0.1%)	1.07	11/3872 (0.3%)
1	C	1.17	2/2855 (0.1%)	1.09	6/3872 (0.2%)
2	B	1.06	0/170	0.97	1/223 (0.4%)
2	D	1.43	0/170	1.20	1/223 (0.4%)
All	All	1.12	4/6050 (0.1%)	1.08	19/8190 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	GLU	CG-CD	6.47	1.61	1.51
1	C	167	GLU	CB-CG	6.25	1.64	1.52
1	C	338	SER	CB-OG	-5.82	1.34	1.42
1	A	237	GLU	CB-CG	5.62	1.62	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	335	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	C	335	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	A	177	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	180	LEU	CA-CB-CG	6.76	130.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	132	MET	CG-SD-CE	6.33	110.33	100.20
1	A	335	ARG	CG-CD-NE	-6.26	98.65	111.80
1	A	72	GLU	N-CA-C	-6.23	94.17	111.00
1	C	154	ASP	CB-CG-OD1	-6.12	112.80	118.30
2	D	15	ALA	N-CA-C	5.95	127.06	111.00
1	A	178	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	351	THR	CA-CB-CG2	-5.58	104.59	112.40
1	A	335	ARG	CD-NE-CZ	5.52	131.33	123.60
1	A	180	LEU	CB-CG-CD1	-5.50	101.64	111.00
2	B	19	LYS	CD-CE-NZ	5.45	124.24	111.70
1	C	335	ARG	CG-CD-NE	-5.38	100.49	111.80
1	A	81	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	180	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	GLU	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	2794	0	2757	79	0
1	C	2794	0	2757	100	0
2	B	169	0	180	14	0
2	D	169	0	180	22	0
3	A	31	0	12	4	0
3	C	31	0	12	8	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	5990	0	5898	205	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 17.

All (205) 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:C:14:SER:HB2	3:C:501:ATP:O2G	1.34	1.21
1:C:14:SER:N	3:C:501:ATP:O1G	1.74	1.20
1:A:88:HIS:CD2	1:A:92:ASN:HD22	1.62	1.16
1:C:14:SER:CB	3:C:501:ATP:O2G	2.00	1.10
1:C:193:LEU:HD22	1:C:248:ILE:HD11	1.33	1.08
2:D:26:ASN:O	2:D:29:LYS:HG3	1.58	1.03
1:C:351:THR:O	1:C:351:THR:HG22	1.56	1.02
1:C:167:GLU:O	1:C:167:GLU:HG2	1.66	0.95
1:C:14:SER:HB2	3:C:501:ATP:PG	2.07	0.93
2:D:26:ASN:OD1	2:D:28:ASP:HB2	1.71	0.89
1:C:352:PHE:HA	1:C:355:MET:HG3	1.56	0.88
1:C:297:ASN:HD22	1:C:329:ILE:HD12	1.40	0.87
2:D:15:ALA:HB1	2:D:19:LYS:HZ3	1.41	0.85
2:D:15:ALA:HB1	2:D:19:LYS:NZ	1.91	0.85
1:A:88:HIS:CD2	1:A:92:ASN:ND2	2.44	0.84
1:A:13:GLY:HA2	3:A:501:ATP:O1G	1.78	0.84
1:C:359:LYS:HB3	1:C:360:GLN:NE2	1.95	0.82
1:A:162:ASN:HD22	1:A:176:MET:HB2	1.43	0.80
2:D:15:ALA:CB	2:D:19:LYS:NZ	2.45	0.79
1:A:99:GLU:OE2	1:C:99:GLU:HG3	1.82	0.79
1:C:278:THR:HG21	1:C:317:ILE:HD11	1.65	0.79
1:C:214:GLU:HG2	3:C:501:ATP:C5	2.17	0.79
1:C:359:LYS:HB3	1:C:360:GLN:HE22	1.49	0.78
1:C:335:ARG:HA	1:C:338:SER:OG	1.84	0.78
1:C:349:LEU:HB3	2:D:21:GLN:NE2	1.99	0.77
1:A:57:GLU:HA	1:A:60:SER:HB2	1.67	0.76
1:A:14:SER:H	3:A:501:ATP:PG	2.10	0.75
1:C:12:ASN:HD21	1:C:86:TRP:HE1	1.34	0.75
1:C:88:HIS:HE1	1:C:93:GLU:OE2	1.69	0.75
1:A:353:GLN:NE2	1:A:356:TRP:HE1	1.83	0.75
1:C:54:VAL:HB	1:C:88:HIS:CD2	2.22	0.75
1:C:209:VAL:HA	1:C:212:ILE:HD12	1.69	0.74
1:A:351:THR:HG21	2:B:18:LEU:N	2.02	0.74
1:A:162:ASN:ND2	1:A:277:THR:HB	2.03	0.73
1:C:364:GLU:OE1	1:C:364:GLU:HA	1.88	0.73
2:D:15:ALA:O	2:D:19:LYS:HD3	1.89	0.73
1:C:167:GLU:O	1:C:167:GLU:CG	2.37	0.72
1:A:162:ASN:HD21	1:A:277:THR:CB	2.01	0.72
1:A:192:ILE:HG21	1:A:253:GLU:HG2	1.73	0.71
1:C:154:ASP:OD1	1:C:300:SER:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:O	1:A:59:GLN:HB2	1.91	0.69
1:A:208:ILE:HG21	1:A:242:LEU:HD22	1.75	0.69
1:C:252:ASN:O	1:C:256:ARG:HG3	1.93	0.69
1:C:70:PRO:HB3	1:C:81:ASP:HB2	1.76	0.68
1:C:14:SER:HB3	3:C:501:ATP:O2G	1.93	0.68
2:D:15:ALA:CB	2:D:19:LYS:HZ2	2.08	0.66
1:C:238:LYS:O	1:C:249:THR:HG23	1.96	0.66
1:C:230:ALA:HB2	1:C:236:LEU:HD12	1.77	0.66
1:C:6:THR:O	1:C:101:HIS:HD2	1.79	0.66
2:D:15:ALA:CB	2:D:19:LYS:HZ3	2.07	0.66
2:D:15:ALA:HB2	2:D:19:LYS:HZ2	1.60	0.66
1:C:88:HIS:CE1	1:C:93:GLU:OE2	2.50	0.65
1:A:207:GLU:OE2	1:A:207:GLU:HA	1.97	0.65
1:C:107:GLU:OE1	1:C:116:ARG:HG3	1.97	0.65
1:C:352:PHE:CA	1:C:355:MET:HG3	2.26	0.64
2:D:26:ASN:CG	2:D:28:ASP:HB2	2.18	0.64
1:A:8:LEU:HD11	1:A:96:VAL:HG21	1.77	0.64
1:C:172:PRO:HA	1:C:175:ILE:HD12	1.80	0.63
1:C:33:SER:OG	1:C:71:ILE:HD12	1.99	0.63
1:A:162:ASN:HD21	1:A:277:THR:HB	1.62	0.63
1:C:201:VAL:O	1:C:202:THR:O	2.17	0.63
1:C:304:THR:O	1:C:335:ARG:NH1	2.34	0.61
1:C:188:TYR:CZ	1:C:192:ILE:HD11	2.35	0.61
1:A:104:LEU:HD12	1:A:133:TYR:HB3	1.83	0.61
1:C:59:GLN:O	1:C:62:ARG:HG3	2.01	0.60
1:C:117:GLU:OE2	1:C:371:HIS:HE1	1.85	0.60
1:C:78:ASN:CG	1:C:81:ASP:OD1	2.40	0.59
1:C:106:THR:HB	1:C:137:GLN:HG3	1.83	0.59
1:A:70:PRO:O	1:A:77:THR:HG22	2.02	0.59
1:A:297:ASN:HD22	1:A:329:ILE:CD1	2.16	0.59
2:B:14:VAL:O	2:B:14:VAL:HG12	2.03	0.59
1:C:247:VAL:HG12	1:C:247:VAL:O	2.01	0.58
1:A:6:THR:O	1:A:101:HIS:HD2	1.86	0.58
1:C:297:ASN:ND2	1:C:329:ILE:HD12	2.14	0.58
2:D:26:ASN:ND2	2:D:28:ASP:CB	2.67	0.58
1:C:304:THR:OG1	1:C:335:ARG:HD2	2.04	0.58
1:A:167:GLU:HG2	1:A:167:GLU:O	2.03	0.57
1:A:88:HIS:HD2	1:A:92:ASN:HD22	1.44	0.57
1:A:297:ASN:HD22	1:A:329:ILE:HD12	1.70	0.57
1:A:13:GLY:CA	3:A:501:ATP:O1G	2.49	0.57
1:C:252:ASN:HA	1:C:255:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ASN:ND2	2:D:28:ASP:HB3	2.19	0.57
1:C:90:PHE:HB3	1:C:98:PRO:HD3	1.86	0.56
1:A:178:LEU:HD11	1:A:180:LEU:HD12	1.88	0.56
1:C:180:LEU:HD22	1:C:261:LEU:HD23	1.88	0.56
2:B:15:ALA:HB1	2:B:19:LYS:HZ3	1.71	0.55
1:C:198:TYR:CE2	1:C:248:ILE:HD12	2.41	0.55
1:C:198:TYR:CD2	1:C:248:ILE:HD12	2.41	0.55
1:A:190:MET:HE1	1:A:206:ARG:HG3	1.89	0.55
2:D:26:ASN:HD21	2:D:28:ASP:CB	2.19	0.55
2:D:26:ASN:O	2:D:29:LYS:CG	2.47	0.55
1:C:11:ASP:HA	1:C:106:THR:OG1	2.06	0.54
1:A:167:GLU:HG3	2:B:19:LYS:HZ2	1.71	0.54
1:C:334:GLU:CD	1:C:334:GLU:H	2.10	0.54
1:A:351:THR:HG21	2:B:18:LEU:CA	2.38	0.54
2:B:28:ASP:O	2:B:30:LEU:N	2.40	0.54
1:A:190:MET:HG3	1:A:209:VAL:HG21	1.90	0.53
1:C:132:MET:CE	1:C:134:VAL:HG23	2.38	0.53
1:A:88:HIS:CE1	1:A:93:GLU:HG2	2.44	0.52
1:A:59:GLN:OE1	1:A:59:GLN:CA	2.58	0.52
1:A:313:MET:O	1:A:317:ILE:HD12	2.10	0.52
1:C:70:PRO:HB3	1:C:81:ASP:CB	2.40	0.52
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.57	0.52
1:A:12:ASN:ND2	1:A:86:TRP:HE1	2.09	0.51
1:C:303:THR:O	1:C:303:THR:HG22	2.09	0.51
1:C:278:THR:HG21	1:C:317:ILE:CD1	2.38	0.51
1:C:282:ILE:O	1:C:285:CYS:HB2	2.09	0.51
1:C:71:ILE:O	1:C:71:ILE:HG22	2.11	0.51
1:C:202:THR:HG22	1:C:203:THR:N	2.26	0.51
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.93	0.51
1:A:358:THR:OG1	1:A:361:GLU:HG2	2.11	0.51
1:A:192:ILE:CG2	1:A:253:GLU:HG2	2.42	0.50
1:C:172:PRO:HA	1:C:175:ILE:CD1	2.41	0.50
1:C:153:LEU:HB3	1:C:299:MET:CE	2.41	0.50
1:A:358:THR:OG1	1:A:361:GLU:CG	2.59	0.50
1:A:6:THR:O	1:A:101:HIS:CD2	2.65	0.50
1:C:12:ASN:ND2	1:C:86:TRP:HE1	2.07	0.50
1:C:262:PHE:N	1:C:262:PHE:CD2	2.80	0.49
2:D:26:ASN:HD21	2:D:28:ASP:HB3	1.76	0.49
1:C:272:ALA:HB1	1:C:276:GLU:HB2	1.94	0.49
1:A:60:SER:O	1:A:61:LYS:HG3	2.12	0.49
2:B:28:ASP:C	2:B:30:LEU:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:ALA:HB2	2:D:19:LYS:NZ	2.21	0.49
1:C:202:THR:HG22	1:C:203:THR:H	1.77	0.49
2:B:15:ALA:HB1	2:B:19:LYS:NZ	2.28	0.48
1:A:360:GLN:CD	1:A:360:GLN:H	2.16	0.48
1:A:261:LEU:HB3	1:A:274:ILE:HD13	1.95	0.48
1:A:191:LYS:HG2	1:A:195:GLU:OE1	2.14	0.48
2:D:26:ASN:ND2	2:D:28:ASP:HB2	2.29	0.48
1:C:352:PHE:C	1:C:355:MET:HG3	2.35	0.48
1:A:353:GLN:HE22	1:A:356:TRP:HE1	1.61	0.47
1:C:202:THR:HG22	1:C:204:ALA:H	1.79	0.47
1:A:313:MET:HG3	1:A:317:ILE:CD1	2.44	0.47
1:C:132:MET:HE1	1:C:134:VAL:HG23	1.96	0.47
1:A:222:ASP:HB3	1:A:225:ASN:HB2	1.97	0.47
1:A:34:ILE:HG13	1:A:34:ILE:O	2.15	0.47
1:C:6:THR:O	1:C:101:HIS:CD2	2.63	0.46
1:C:242:LEU:O	1:C:243:PRO:C	2.54	0.46
1:A:88:HIS:HD2	1:A:92:ASN:ND2	2.06	0.46
1:A:215:LYS:HA	1:A:215:LYS:HD3	1.80	0.46
1:A:358:THR:O	1:A:361:GLU:HB2	2.16	0.46
1:A:167:GLU:CG	2:B:19:LYS:HZ2	2.28	0.46
2:D:15:ALA:O	2:D:19:LYS:CD	2.62	0.46
1:C:113:LYS:O	1:C:117:GLU:HG3	2.16	0.46
1:C:117:GLU:OE2	1:C:371:HIS:CE1	2.67	0.45
1:C:131:ALA:HA	1:C:357:ILE:O	2.16	0.45
1:C:214:GLU:HG2	3:C:501:ATP:C4	2.51	0.45
2:B:19:LYS:HG2	2:B:23:GLU:OE2	2.17	0.45
1:A:57:GLU:O	1:A:60:SER:N	2.49	0.45
1:C:178:LEU:HD21	1:C:180:LEU:HD13	1.98	0.45
1:A:259:GLU:O	1:A:259:GLU:HG3	2.17	0.45
1:A:213:LYS:HA	1:A:217:CYS:SG	2.57	0.45
1:A:71:ILE:C	1:A:72:GLU:O	2.49	0.45
1:C:214:GLU:HG2	3:C:501:ATP:C6	2.51	0.44
1:C:314:GLN:HE21	1:C:329:ILE:HG12	1.82	0.44
1:A:353:GLN:NE2	1:A:356:TRP:NE1	2.60	0.44
2:B:16:GLU:H	2:B:16:GLU:HG2	1.66	0.44
1:A:330:ILE:HD12	1:A:330:ILE:N	2.33	0.44
1:A:353:GLN:HE21	1:A:356:TRP:HE1	1.61	0.44
1:A:15:GLY:O	1:A:32:PRO:HA	2.17	0.44
1:C:351:THR:O	1:C:351:THR:CG2	2.36	0.44
1:C:237:GLU:O	1:C:238:LYS:HD3	2.17	0.44
1:C:200:PHE:HD1	1:C:205:GLU:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HB3	1:A:371:HIS:NE2	2.31	0.44
1:C:317:ILE:HD13	1:C:317:ILE:HG21	1.65	0.44
1:C:102:PRO:HA	1:C:131:ALA:O	2.18	0.44
1:C:295:ALA:O	1:C:328:LYS:HB3	2.19	0.43
1:A:59:GLN:OE1	1:A:59:GLN:N	2.51	0.43
1:C:357:ILE:HG23	1:C:369:ILE:HD13	2.01	0.43
1:A:120:THR:HG23	1:A:132:MET:SD	2.59	0.43
1:C:161:HIS:CE1	1:C:177:ARG:HG3	2.54	0.43
1:C:210:ARG:NH1	1:C:214:GLU:OE2	2.52	0.43
1:A:349:LEU:HD13	2:B:21:GLN:HB2	2.01	0.43
1:C:140:LEU:O	1:C:342:GLY:HA3	2.19	0.43
1:C:297:ASN:HD22	1:C:329:ILE:CD1	2.21	0.43
1:A:182:GLY:O	1:A:213:LYS:NZ	2.51	0.43
1:A:162:ASN:ND2	1:A:277:THR:CB	2.67	0.42
1:C:349:LEU:HB3	2:D:21:GLN:HE22	1.80	0.42
1:A:40:HIS:O	1:A:41:GLN:HB3	2.19	0.42
1:C:85:ILE:O	1:C:88:HIS:HB3	2.20	0.42
1:A:177:ARG:NH2	1:A:179:ASP:OD2	2.49	0.42
1:C:360:GLN:H	1:C:360:GLN:CD	2.23	0.42
1:A:360:GLN:O	1:A:364:GLU:HG2	2.20	0.42
1:A:21:PHE:N	1:A:21:PHE:CD2	2.87	0.42
1:A:338:SER:O	1:A:339:VAL:C	2.54	0.42
2:D:15:ALA:HB1	2:D:19:LYS:HD3	2.02	0.41
1:A:351:THR:HB	2:B:21:GLN:OE1	2.20	0.41
2:B:14:VAL:O	2:B:14:VAL:CG1	2.68	0.41
1:C:153:LEU:HD21	1:C:274:ILE:HD12	2.01	0.41
1:C:303:THR:O	1:C:303:THR:CG2	2.68	0.41
1:A:157:ASP:OD1	3:A:501:ATP:O3'	2.26	0.41
1:C:351:THR:H	2:D:21:GLN:HE22	1.68	0.41
1:C:352:PHE:HA	1:C:355:MET:CG	2.41	0.41
1:A:210:ARG:O	1:A:214:GLU:HG3	2.21	0.41
1:C:250:ILE:HB	1:C:253:GLU:HB2	2.03	0.41
1:A:75:ILE:HD13	1:A:108:ALA:HB3	2.02	0.41
1:C:352:PHE:O	1:C:355:MET:HG3	2.20	0.41
1:C:137:GLN:HG2	1:C:339:VAL:HG11	2.02	0.41
1:A:171:LEU:O	1:A:172:PRO:C	2.58	0.41
1:C:145:SER:HB2	1:C:147:ARG:NH1	2.36	0.41
1:C:75:ILE:HD12	1:C:75:ILE:HG23	1.81	0.41
1:A:193:LEU:HD13	1:A:248:ILE:CD1	2.51	0.40
1:A:192:ILE:HG21	1:A:253:GLU:CG	2.49	0.40
1:C:153:LEU:HB3	1:C:299:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:OD2	1:A:240:TYR:OH	2.27	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	353/375 (94%)	339 (96%)	13 (4%)	1 (0%)	46	41
1	C	353/375 (94%)	328 (93%)	22 (6%)	3 (1%)	24	15
2	B	19/54 (35%)	15 (79%)	2 (10%)	2 (10%)	1	0
2	D	19/54 (35%)	17 (90%)	1 (5%)	1 (5%)	2	0
All	All	744/858 (87%)	699 (94%)	38 (5%)	7 (1%)	21	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	LYS
1	C	202	THR
2	D	15	ALA
2	B	29	LYS
1	A	202	THR
1	C	201	VAL
1	C	60	SER

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	303/318 (95%)	279 (92%)	24 (8%)	15	9
1	C	303/318 (95%)	281 (93%)	22 (7%)	17	11
2	B	19/48 (40%)	16 (84%)	3 (16%)	3	1
2	D	19/48 (40%)	13 (68%)	6 (32%)	0	0
All	All	644/732 (88%)	589 (92%)	55 (8%)	13	8

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	39	ARG
1	A	59	GLN
1	A	60	SER
1	A	66	THR
1	A	67	LEU
1	A	80	ASP
1	A	112	PRO
1	A	115	ASN
1	A	132	MET
1	A	180	LEU
1	A	190	MET
1	A	195	GLU
1	A	202	THR
1	A	207	GLU
1	A	215	LYS
1	A	244	ASP
1	A	247	VAL
1	A	248	ILE
1	A	257	CYS
1	A	289	ILE
1	A	299	MET
1	A	360	GLN
1	A	368	SER
2	B	13	LYS
2	B	16	GLU
2	B	27	GLN
1	C	14	SER
1	C	37	ARG
1	C	52	SER

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Mol	Chain	Res	Type
1	C	59	GLN
1	C	62	ARG
1	C	66	THR
1	C	67	LEU
1	C	80	ASP
1	C	100	GLU
1	C	132	MET
1	C	164	PRO
1	C	190	MET
1	C	195	GLU
1	C	199	SER
1	C	208	ILE
1	C	243	PRO
1	C	271	SER
1	C	314	GLN
1	C	323	SER
1	C	353	GLN
1	C	364	GLU
1	C	368	SER
2	D	13	LYS
2	D	17	ASN
2	D	19	LYS
2	D	20	SER
2	D	28	ASP
2	D	29	LYS

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	12	ASN
1	A	88	HIS
1	A	92	ASN
1	A	101	HIS
1	A	128	ASN
1	A	162	ASN
1	A	246	GLN
1	A	297	ASN
1	A	314	GLN
1	A	353	GLN
1	C	12	ASN
1	C	88	HIS
1	C	101	HIS

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Mol	Chain	Res	Type
1	C	111	ASN
1	C	161	HIS
1	C	162	ASN
1	C	297	ASN
1	C	314	GLN
1	C	360	GLN
1	C	371	HIS
2	D	21	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 4 ligands modelled in this entry, 2 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	A	501	4	24,33,33	1.67	4 (16%)	31,52,52	2.64	12 (38%)
3	ATP	C	501	-	24,33,33	1.25	3 (12%)	31,52,52	2.50	9 (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	ATP	A	501	4	-	0/18/38/38	0/3/3/3
3	ATP	C	501	-	-	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ATP	PG-O3G	-2.21	1.46	1.54
3	C	501	ATP	C5-C4	2.03	1.45	1.40
3	C	501	ATP	O4'-C1'	2.36	1.44	1.41
3	C	501	ATP	PG-O3G	2.53	1.63	1.54
3	A	501	ATP	C4-N3	2.96	1.40	1.35
3	A	501	ATP	C5-C4	3.32	1.48	1.40
3	A	501	ATP	O4'-C1'	5.07	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ATP	N3-C2-N1	-8.49	122.39	128.89
3	A	501	ATP	PB-O3B-PG	-6.82	109.82	132.67
3	C	501	ATP	N3-C2-N1	-6.54	123.89	128.89
3	C	501	ATP	PB-O3B-PG	-6.06	112.36	132.67
3	A	501	ATP	C2'-C1'-N9	-4.45	107.49	114.29
3	C	501	ATP	O2G-PG-O3B	-3.26	90.30	105.09
3	A	501	ATP	C4'-O4'-C1'	-3.13	106.28	109.72
3	C	501	ATP	C4'-O4'-C1'	-2.79	106.65	109.72
3	A	501	ATP	PA-O3A-PB	-2.78	124.93	132.73
3	A	501	ATP	C5'-C4'-C3'	-2.61	104.87	115.21
3	C	501	ATP	C2'-C1'-N9	-2.50	110.47	114.29
3	A	501	ATP	C1'-N9-C4	-2.50	123.18	126.94
3	A	501	ATP	O3G-PG-O1G	-2.02	104.06	110.58
3	A	501	ATP	O4'-C1'-N9	2.09	112.47	108.10
3	C	501	ATP	O2B-PB-O1B	2.16	124.22	112.53
3	A	501	ATP	O2G-PG-O3B	2.26	115.36	105.09
3	C	501	ATP	C2-N1-C6	2.32	122.91	118.77
3	C	501	ATP	N6-C6-N1	2.67	124.93	119.20
3	A	501	ATP	C2-N1-C6	2.90	123.94	118.77
3	A	501	ATP	O2A-PA-O3A	3.00	118.71	105.09
3	C	501	ATP	O3G-PG-O2G	6.93	133.76	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ATP	4	0
3	C	501	ATP	8	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, 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	357/375 (95%)	0.04	8 (2%) 65 66	9, 26, 63, 94	0
1	C	357/375 (95%)	-0.36	2 (0%) 90 90	2, 14, 35, 48	0
2	B	21/54 (38%)	1.05	4 (19%) 2 2	26, 44, 66, 89	0
2	D	21/54 (38%)	0.22	2 (9%) 10 11	11, 19, 29, 36	0
All	All	756/858 (88%)	-0.12	16 (2%) 67 67	2, 20, 56, 94	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	14	VAL	5.4
1	A	201	VAL	4.5
1	A	40	HIS	4.3
1	A	60	SER	3.5
2	D	14	VAL	3.5
1	A	66	THR	2.9
2	B	12	PRO	2.6
2	D	12	PRO	2.6
1	A	62	ARG	2.5
1	C	41	GLN	2.4
1	C	40	HIS	2.2
2	B	32	LYS	2.2
1	A	41	GLN	2.2
1	A	52	SER	2.2
2	B	13	LYS	2.1
1	A	51	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	A	502	1/1	0.96	0.17	2.22	10,10,10,10	0
3	ATP	C	501	31/31	0.95	0.11	0.96	3,12,23,32	0
3	ATP	A	501	31/31	0.95	0.10	-0.03	10,19,33,39	0
4	MG	C	502	1/1	0.99	0.08	-	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.