



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 11, 2018 – 02:15 PM EST

PDB ID : 5DN6  
Title : ATP synthase from *Paracoccus denitrificans*  
Authors : Morales-Rios, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2015-09-09  
Resolution : 3.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

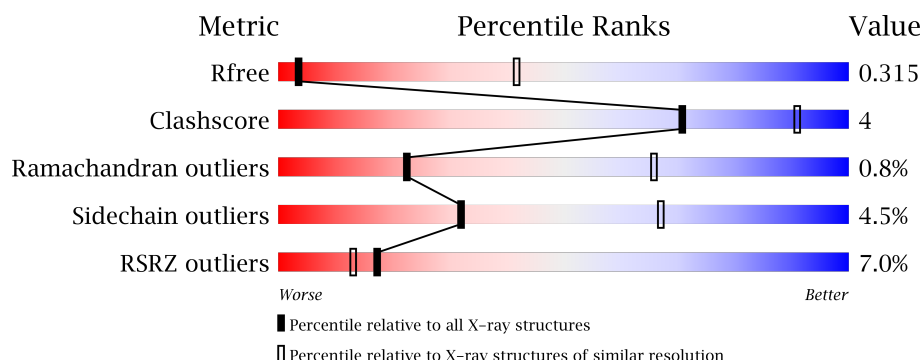
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 3.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1066 (4.36-3.60)
Clashscore	112137	1163 (4.36-3.60)
Ramachandran outliers	110173	1119 (4.36-3.60)
Sidechain outliers	110143	1108 (4.36-3.60)
RSRZ outliers	101464	1078 (4.36-3.60)

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	1	20	 100%
2	2	15	 100%
3	3	19	 100%
4	A	511	 3% 85% 14% ..
4	B	511	 1% 81% 14% ..

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	511	
5	D	474	
5	E	474	
5	F	474	
6	G	290	
7	H	188	
8	I	148	
9	J	77	
9	K	77	
9	L	77	
9	M	77	
9	N	77	
9	O	77	
9	P	77	
9	Q	77	
9	R	77	
9	S	77	
9	T	77	
9	U	77	
10	V	78	
11	W	124	
12	X	283	
13	Y	54	
14	Z	104	

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31527 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 Chain A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	1	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 2 is a protein called Chain B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	2	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 3 is a protein called Chain C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	3	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 4 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	505	Total	C	N	O	S	0	0	0
			3811	2395	665	735	16			
4	B	496	Total	C	N	O	S	0	0	0
			3754	2359	657	723	15			
4	C	484	Total	C	N	O	S	0	0	0
			3652	2293	640	703	16			

- Molecule 5 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	470	Total	C	N	O	S	0	0	0
			3508	2211	600	687	10			
5	E	466	Total	C	N	O	S	0	0	0
			3490	2198	596	686	10			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	466	Total	C	N	O	S	0	0	0
			3489	2199	596	684	10			

- Molecule 6 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	260	Total	C	N	O	S	0	0	0
			1978	1227	367	375	9			

- Molecule 7 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	110	Total	C	N	O	0	0	0
			544	324	110	110			

- Molecule 8 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	75	Total	C	N	O	0	0	0
			366	216	75	75			

- Molecule 9 is a protein called ATP synthase F0 subcomplex C subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	K	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	L	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	M	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	N	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	O	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	P	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	Q	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	R	74	Total	C	N	O	0	0	0
			358	210	74	74			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	T	74	Total	C	N	O	0	0	0
			358	210	74	74			
9	U	74	Total	C	N	O	0	0	0
			358	210	74	74			

- Molecule 10 is a protein called Chain V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	78	Total	C	N	O	0	0	0
			390	234	78	78			

- Molecule 11 is a protein called Chain W.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	W	124	Total	C	N	O	0	0	0
			620	372	124	124			

- Molecule 12 is a protein called ATP synthase subunit a,ATP synthase subunit a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	98	Total	C	N	O	0	0	0
			486	291	98	97			

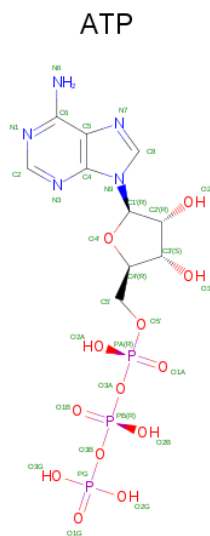
- Molecule 13 is a protein called Chain Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	Y	54	Total	C	N	O	0	0	0
			270	162	54	54			

- Molecule 14 is a protein called Zeta inhibitor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Z	54	Total	C	N	O	S	0	0	0
			447	274	88	84	1			

- Molecule 15 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>).

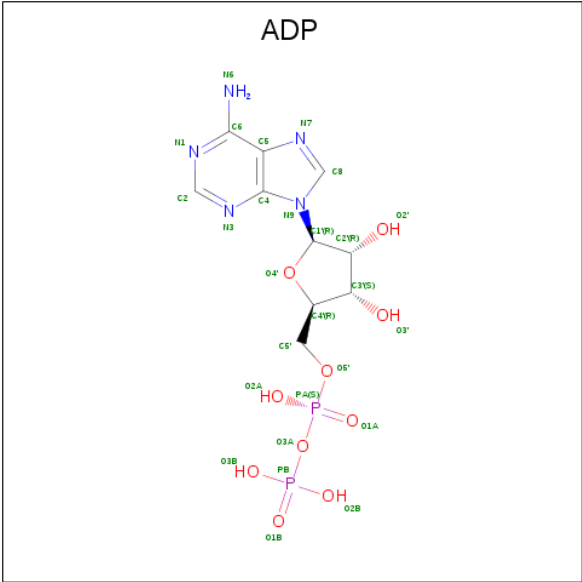


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
15	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
15	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
15	F	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total Mg 1 1	0	0
16	A	1	Total Mg 1 1	0	0
16	D	1	Total Mg 1 1	0	0
16	C	1	Total Mg 1 1	0	0
16	F	1	Total Mg 1 1	0	0

- Molecule 17 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
17	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



### 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 the various outlier classes 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: Chain A

Chain 1:  100%

There are no outlier residues recorded for this chain.

#### • Molecule 2: Chain B

Chain 2:  100%


There are no outlier residues recorded for this chain.

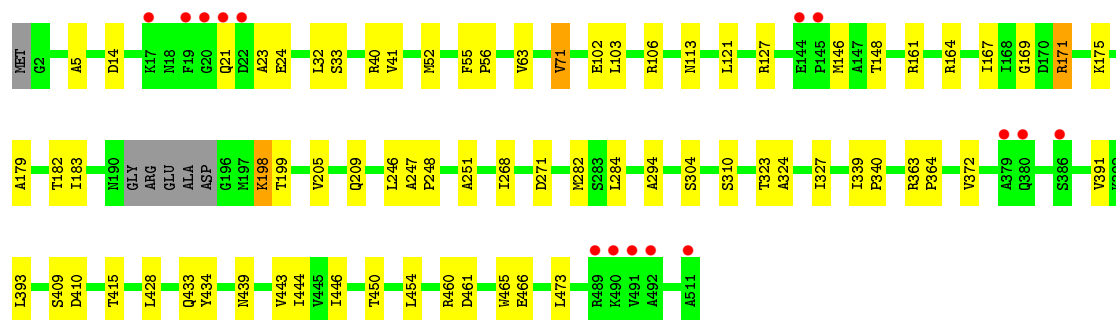
#### • Molecule 3: Chain C

Chain 3:  100%


There are no outlier residues recorded for this chain.

#### • Molecule 4: ATP synthase subunit alpha

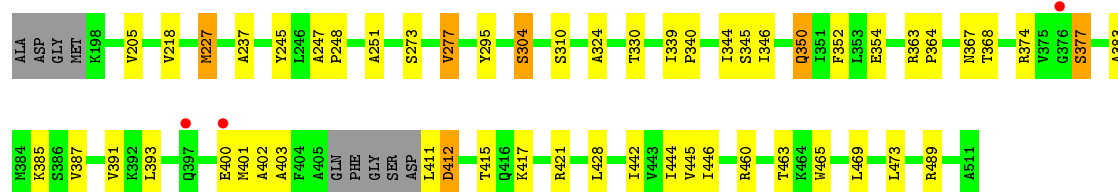
Chain A:  3% 85% 14% ..



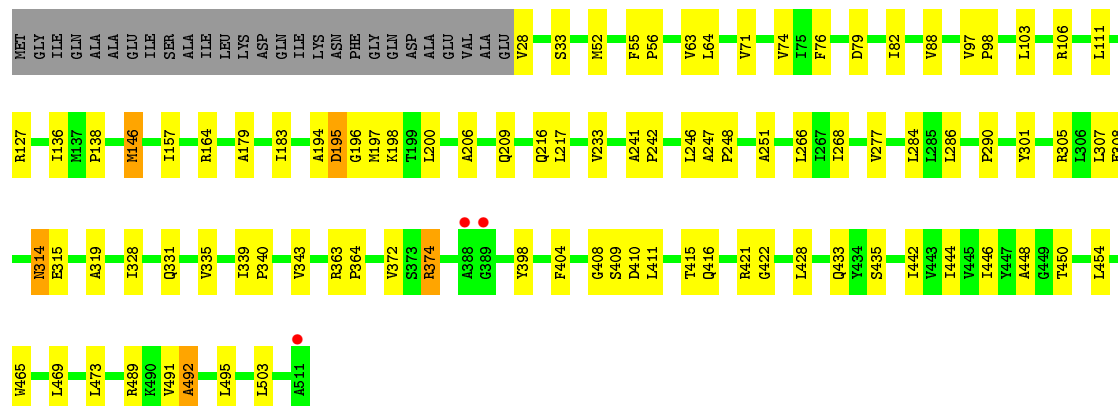
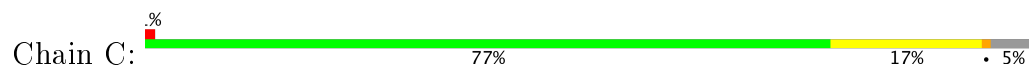
#### • Molecule 4: ATP synthase subunit alpha

Chain B:  3% 81% 14% ..

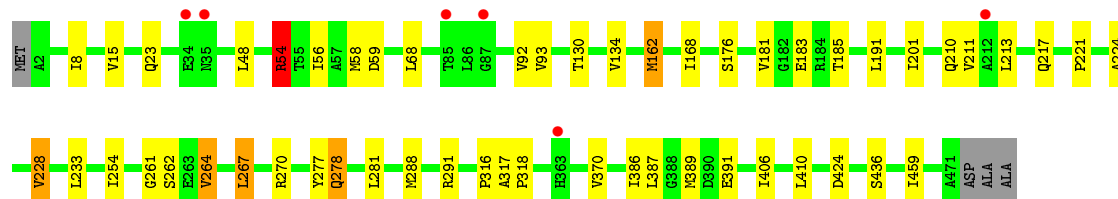
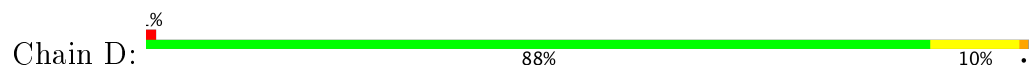




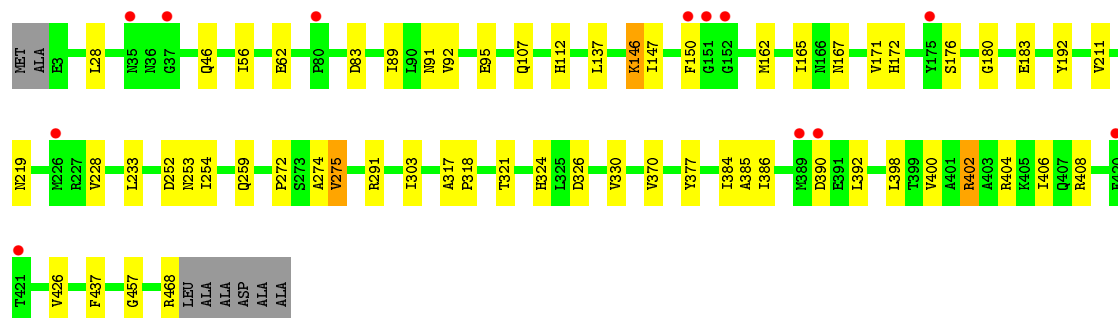
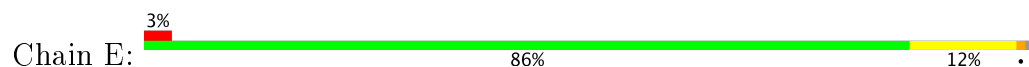
• Molecule 4: ATP synthase subunit alpha



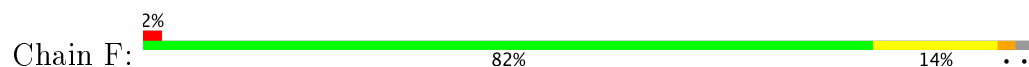
• Molecule 5: ATP synthase subunit beta



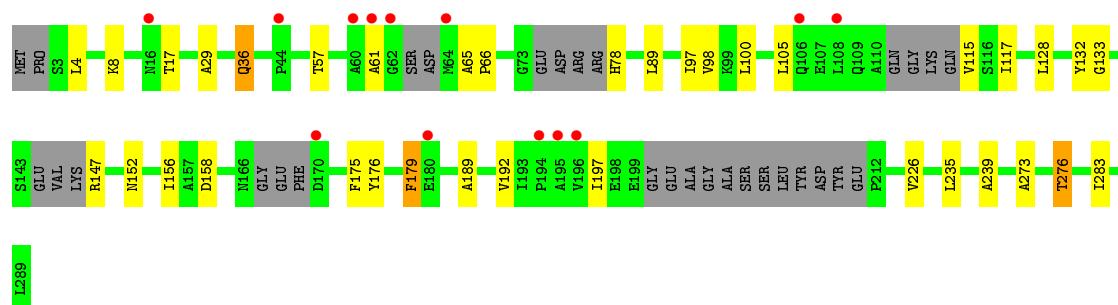
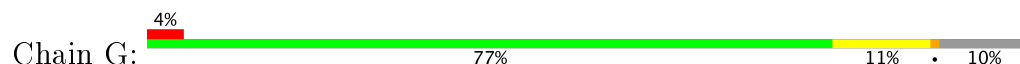
• Molecule 5: ATP synthase subunit beta



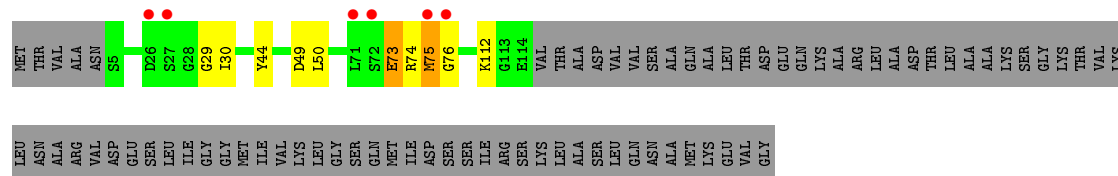
• Molecule 5: ATP synthase subunit beta



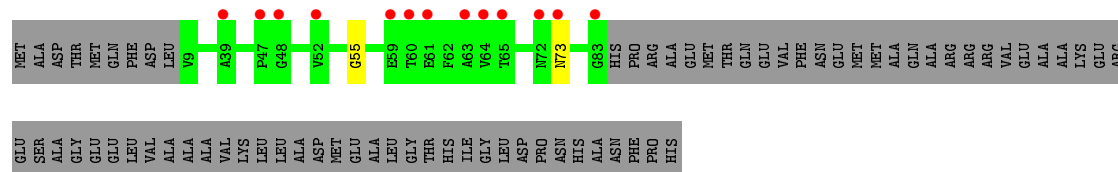
- Molecule 6: ATP synthase gamma chain



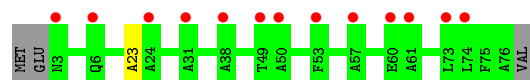
- Molecule 7: ATP synthase subunit delta



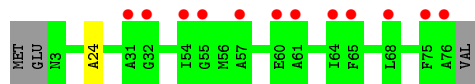
- Molecule 8: ATP synthase epsilon chain



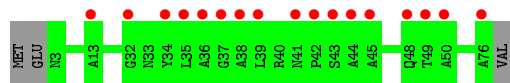
- Molecule 9: ATP synthase F0 subcomplex C subunit



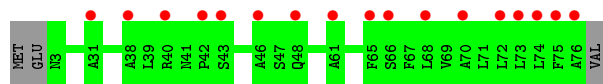
- Molecule 9: ATP synthase F0 subcomplex C subunit



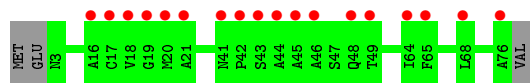
- Molecule 9: ATP synthase F0 subcomplex C subunit



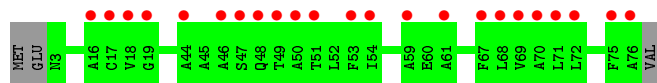
- Molecule 9: ATP synthase F0 subcomplex C subunit



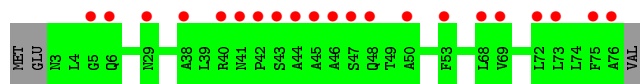
- Molecule 9: ATP synthase F0 subcomplex C subunit



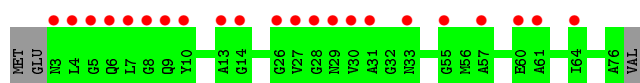
- Molecule 9: ATP synthase F0 subcomplex C subunit



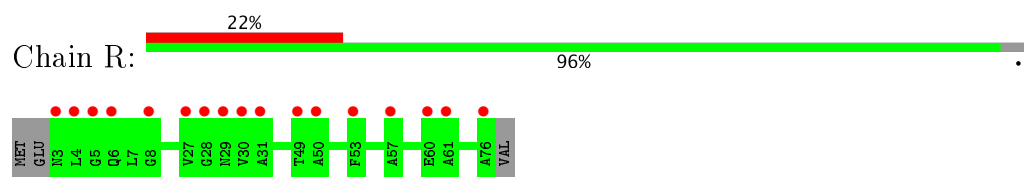
- Molecule 9: ATP synthase F0 subcomplex C subunit



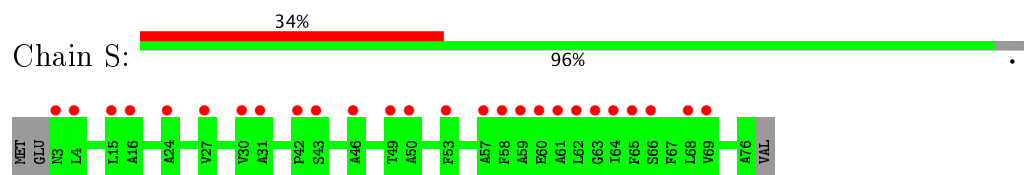
- Molecule 9: ATP synthase F0 subcomplex C subunit



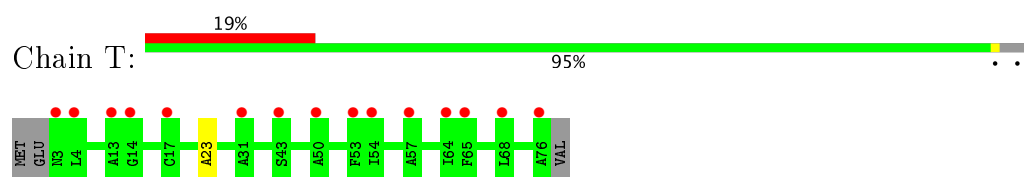
- Molecule 9: ATP synthase F0 subcomplex C subunit



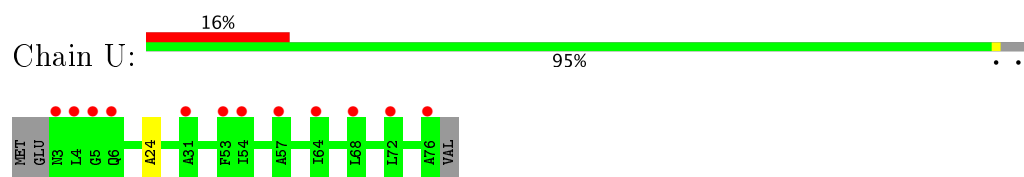
- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 9: ATP synthase F0 subcomplex C subunit



- Molecule 10: Chain V



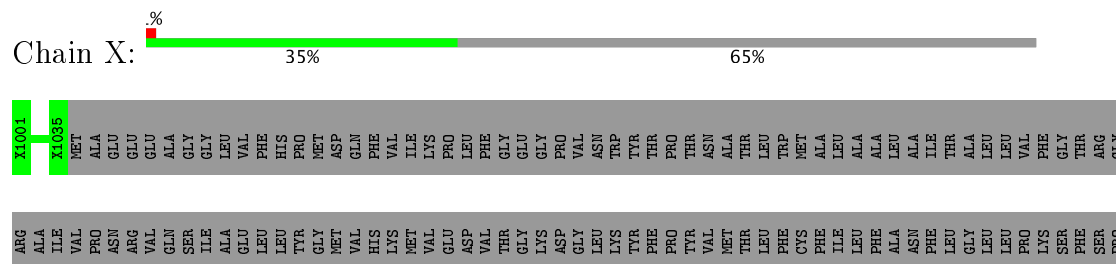
There are no outlier residues recorded for this chain.

- Molecule 11: Chain W



There are no outlier residues recorded for this chain.

- Molecule 12: ATP synthase subunit a,ATP synthase subunit a



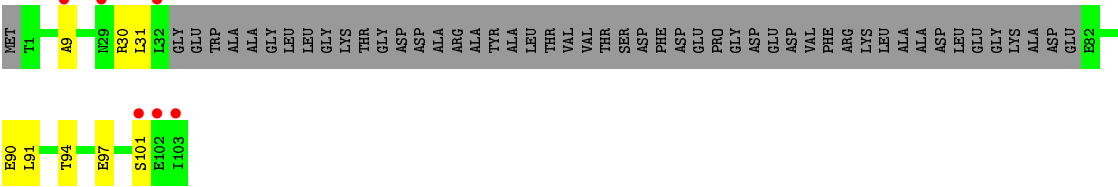


• Molecule 13: Chain Y



There are no outlier residues recorded for this chain.

• Molecule 14: Zeta inhibitor protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.00Å 187.94Å 164.72Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	36.84 – 3.98 36.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.84-3.98) 98.8 (36.84-3.98)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.295 , 0.324 0.292 , 0.315	Depositor DCC
$R_{free}$ test set	2789 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	119.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 63.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	31527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, 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
4	A	0.38	1/3864 (0.0%)	0.68	3/5227 (0.1%)
4	B	0.37	0/3805	0.66	2/5146 (0.0%)
4	C	0.36	0/3705	0.68	4/5015 (0.1%)
5	D	0.35	0/3562	0.65	2/4840 (0.0%)
5	E	0.36	1/3544 (0.0%)	0.62	2/4815 (0.0%)
5	F	0.35	0/3543	0.65	0/4814
6	G	0.40	0/1990	0.65	1/2674 (0.0%)
7	H	0.36	0/543	0.52	1/755 (0.1%)
8	I	0.29	0/365	0.55	0/504
9	J	0.43	0/357	0.51	0/491
9	K	0.43	0/357	0.51	0/491
9	L	0.43	0/357	0.52	0/491
9	M	0.43	0/357	0.51	0/491
9	N	0.43	0/357	0.51	0/491
9	O	0.43	0/357	0.51	0/491
9	P	0.43	0/357	0.51	0/491
9	Q	0.43	0/357	0.51	0/491
9	R	0.43	0/357	0.50	0/491
9	S	0.43	0/357	0.51	0/491
9	T	0.43	0/357	0.51	0/491
9	U	0.43	0/357	0.51	0/491
12	X	0.32	0/309	0.50	0/428
14	Z	0.49	0/450	0.69	0/599
All	All	0.38	2/29964 (0.0%)	0.63	15/40709 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	40	ARG	CZ-NH1	7.05	1.42	1.33
5	E	259	GLN	CD-OE1	5.44	1.35	1.24



The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	106	ARG	NE-CZ-NH2	9.18	124.89	120.30
4	B	139	ARG	NE-CZ-NH2	8.70	124.65	120.30
5	E	402	ARG	NE-CZ-NH2	8.17	124.39	120.30
4	A	40	ARG	NE-CZ-NH2	-7.87	116.37	120.30
4	A	40	ARG	NE-CZ-NH1	7.43	124.02	120.30

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	1	100	0	23	0	0
2	2	75	0	17	0	0
3	3	95	0	21	0	0
4	A	3811	0	3875	29	0
4	B	3754	0	3822	38	0
4	C	3652	0	3709	48	0
5	D	3508	0	3532	32	0
5	E	3490	0	3513	32	0
5	F	3489	0	3517	45	0
6	G	1978	0	2035	22	0
7	H	544	0	277	3	0
8	I	366	0	176	0	0
9	J	358	0	209	1	0
9	K	358	0	209	1	0
9	L	358	0	209	0	0
9	M	358	0	209	0	0
9	N	358	0	209	0	0
9	O	358	0	209	0	0
9	P	358	0	209	0	0
9	Q	358	0	209	0	0
9	R	358	0	209	0	0
9	S	358	0	209	0	0
9	T	358	0	209	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	358	0	209	1	0
10	V	390	0	80	0	0
11	W	620	0	127	0	0
12	X	486	0	181	0	0
13	Y	270	0	58	0	0
14	Z	447	0	449	4	0
15	A	31	0	12	0	0
15	C	31	0	12	0	0
15	D	31	0	12	0	0
15	F	31	0	12	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	F	1	0	0	0	0
17	B	27	0	12	0	0
All	All	31527	0	27980	242	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 4.

The worst 5 of 242 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)
5:F:278:GLN:H	5:F:278:GLN:HE21	1.24	0.83
5:D:386:ILE:HD11	6:G:17:THR:HG22	1.59	0.82
5:E:176:SER:HB2	5:E:211:VAL:HG12	1.62	0.80
14:Z:31:LEU:HD23	14:Z:91:LEU:HD22	1.64	0.80
5:D:48:LEU:HD21	5:D:54:ARG:HG3	1.67	0.77

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	
4	A	501/511 (98%)	470 (94%)	24 (5%)	7 (1%)	13	55
4	B	490/511 (96%)	459 (94%)	26 (5%)	5 (1%)	18	61
4	C	482/511 (94%)	463 (96%)	15 (3%)	4 (1%)	22	66
5	D	468/474 (99%)	448 (96%)	19 (4%)	1 (0%)	51	84
5	E	464/474 (98%)	439 (95%)	22 (5%)	3 (1%)	28	70
5	F	464/474 (98%)	439 (95%)	23 (5%)	2 (0%)	38	77
6	G	246/290 (85%)	233 (95%)	8 (3%)	5 (2%)	9	50
7	H	108/188 (57%)	90 (83%)	12 (11%)	6 (6%)	2	27
8	I	73/148 (49%)	66 (90%)	5 (7%)	2 (3%)	6	43
9	J	72/77 (94%)	72 (100%)	0	0	100	100
9	K	72/77 (94%)	72 (100%)	0	0	100	100
9	L	72/77 (94%)	72 (100%)	0	0	100	100
9	M	72/77 (94%)	72 (100%)	0	0	100	100
9	N	72/77 (94%)	72 (100%)	0	0	100	100
9	O	72/77 (94%)	72 (100%)	0	0	100	100
9	P	72/77 (94%)	72 (100%)	0	0	100	100
9	Q	72/77 (94%)	72 (100%)	0	0	100	100
9	R	72/77 (94%)	72 (100%)	0	0	100	100
9	S	72/77 (94%)	72 (100%)	0	0	100	100
9	T	72/77 (94%)	72 (100%)	0	0	100	100
9	U	72/77 (94%)	72 (100%)	0	0	100	100
12	X	59/283 (21%)	58 (98%)	1 (2%)	0	100	100
14	Z	50/104 (48%)	47 (94%)	2 (4%)	1 (2%)	9	50
All	All	4269/4892 (87%)	4076 (96%)	157 (4%)	36 (1%)	22	66

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	23	ALA
4	A	199	THR
4	B	402	ALA
4	C	197	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	C	492	ALA

### 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	
4	A	396/401 (99%)	375 (95%)	21 (5%)	26	63
4	B	391/401 (98%)	369 (94%)	22 (6%)	25	61
4	C	379/401 (94%)	360 (95%)	19 (5%)	28	64
5	D	371/375 (99%)	358 (96%)	13 (4%)	41	73
5	E	372/375 (99%)	361 (97%)	11 (3%)	46	75
5	F	372/375 (99%)	352 (95%)	20 (5%)	26	62
6	G	203/227 (89%)	196 (97%)	7 (3%)	42	73
14	Z	45/81 (56%)	43 (96%)	2 (4%)	33	67
All	All	2529/2636 (96%)	2414 (96%)	115 (4%)	32	67

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	217	LEU
5	D	59	ASP
6	G	36	GLN
4	C	277	VAL
4	C	410	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	375	GLN
5	E	217	GLN
5	F	278	GLN
5	E	107	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	189	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z  > 2$
15	ATP	A	600	16	27,33,33	1.06	2 (7%)	25,52,52	1.74	3 (12%)
17	ADP	B	600	16	25,29,29	1.07	2 (8%)	24,45,45	1.81	2 (8%)
15	ATP	C	600	16	27,33,33	1.01	1 (3%)	25,52,52	1.74	3 (12%)
15	ATP	D	600	16	27,33,33	1.01	2 (7%)	25,52,52	1.79	2 (8%)
15	ATP	F	600	16	27,33,33	1.07	2 (7%)	25,52,52	1.69	3 (12%)

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
15	ATP	A	600	16	-	0/18/38/38	0/3/3/3
17	ADP	B	600	16	-	0/12/32/32	0/3/3/3
15	ATP	C	600	16	-	0/18/38/38	0/3/3/3
15	ATP	D	600	16	-	0/18/38/38	0/3/3/3
15	ATP	F	600	16	-	0/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	600	ATP	C2-N3	2.00	1.35	1.32
15	D	600	ATP	C2-N3	2.01	1.35	1.32
15	A	600	ATP	C2-N3	2.13	1.35	1.32
17	B	600	ADP	C2-N3	2.14	1.35	1.32
15	D	600	ATP	C5-C4	3.12	1.47	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	600	ADP	N3-C2-N1	-7.16	122.63	128.86
15	D	600	ATP	N3-C2-N1	-7.07	122.70	128.86
15	C	600	ATP	N3-C2-N1	-6.77	122.96	128.86
15	A	600	ATP	N3-C2-N1	-6.53	123.17	128.86
15	F	600	ATP	N3-C2-N1	-6.37	123.31	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	1	0/20	-	-	-	-
2	2	0/15	-	-	-	-
3	3	0/19	-	-	-	-
4	A	505/511 (98%)	-0.20	15 (2%) 51 40	73, 123, 205, 249	0
4	B	496/511 (97%)	-0.26	4 (0%) 86 79	59, 112, 185, 216	0
4	C	484/511 (94%)	-0.30	3 (0%) 89 84	67, 107, 159, 206	0
5	D	470/474 (99%)	-0.23	6 (1%) 77 68	73, 107, 156, 186	0
5	E	466/474 (98%)	-0.08	12 (2%) 56 46	72, 131, 203, 247	0
5	F	466/474 (98%)	-0.23	9 (1%) 67 58	58, 100, 153, 189	0
6	G	260/290 (89%)	0.08	13 (5%) 30 23	80, 143, 203, 224	0
7	H	110/188 (58%)	-0.21	6 (5%) 26 20	110, 152, 185, 215	0
8	I	75/148 (50%)	0.71	13 (17%) 2 3	167, 207, 238, 241	0
9	J	74/77 (96%)	1.10	13 (17%) 2 3	217, 279, 383, 417	0
9	K	74/77 (96%)	0.87	12 (16%) 2 3	182, 295, 402, 415	0
9	L	74/77 (96%)	0.87	17 (22%) 1 2	224, 296, 463, 488	0
9	M	74/77 (96%)	0.89	17 (22%) 1 2	209, 279, 409, 418	0
9	N	74/77 (96%)	0.96	18 (24%) 1 1	214, 273, 401, 421	0
9	O	74/77 (96%)	0.92	23 (31%) 0 1	220, 287, 352, 363	0
9	P	74/77 (96%)	1.39	21 (28%) 1 1	222, 304, 397, 443	0
9	Q	74/77 (96%)	1.32	22 (29%) 1 1	266, 349, 427, 451	0
9	R	74/77 (96%)	0.92	17 (22%) 1 2	200, 315, 439, 449	0
9	S	74/77 (96%)	1.71	26 (35%) 0 1	239, 320, 445, 471	0
9	T	74/77 (96%)	0.91	15 (20%) 1 2	260, 317, 430, 437	0
9	U	74/77 (96%)	0.56	12 (16%) 2 3	231, 279, 431, 447	0
10	V	0/78	-	-	-	-

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
11	W	0/124	-	-	-	-
12	X	63/283 (22%)	-0.47	3 (4%) 31 24	147, 201, 252, 268	0
13	Y	0/54	-	-	-	-
14	Z	54/104 (51%)	0.47	6 (11%) 6 6	135, 172, 218, 248	0
All	All	4337/5202 (83%)	0.08	303 (6%) 17 13	58, 131, 361, 488	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	P	76	ALA	9.3
9	S	3	ASN	7.6
9	N	43	SER	7.5
9	K	61	ALA	7.3
9	P	68	LEU	7.0

## 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
15	ATP	A	600	31/31	0.92	0.29	0.31	96,98,105,106	0
15	ATP	D	600	31/31	0.93	0.26	0.25	90,96,152,153	0
15	ATP	F	600	31/31	0.92	0.25	-0.20	69,74,109,110	0
17	ADP	B	600	27/27	0.86	0.25	-0.40	155,165,171,173	0
15	ATP	C	600	31/31	0.93	0.19	-0.50	103,110,115,118	0
16	MG	F	601	1/1	0.96	0.29	-	35,35,35,35	0

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	B	601	1/1	0.93	0.20	-	72,72,72,72	0
16	MG	C	601	1/1	0.99	0.35	-	48,48,48,48	0
16	MG	A	601	1/1	0.97	0.41	-	78,78,78,78	0
16	MG	D	601	1/1	0.96	0.28	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.