



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:59 am GMT

PDB ID : 1BMF
Title : BOVINE MITOCHONDRIAL F1-ATPASE
Authors : Abrahams, J.P.; Leslie, A.G.W.; Lutter, R.; Walker, J.E.
Deposited on : 1996-03-13
Resolution : 2.85 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

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 : trunk28620
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) : recalc28949

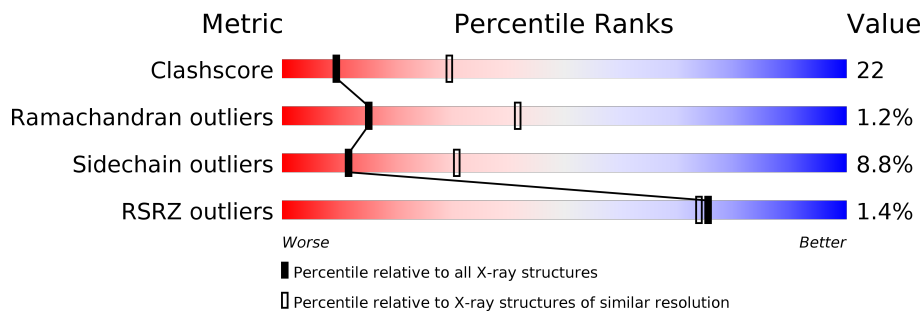
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	510	<div> <div>50%</div> <div>37%</div> <div>8%</div> <div>5%</div> </div>
1	B	510	<div> <div>52%</div> <div>36%</div> <div>6%</div> <div>5%</div> </div>
1	C	510	<div> <div>55%</div> <div>36%</div> <div>5%</div> <div>5%</div> </div>
2	D	482	<div> <div>58%</div> <div>33%</div> <div>5%</div> <div>5%</div> </div>
2	E	482	<div> <div>47%</div> <div>43%</div> <div>6%</div> <div>5%</div> </div>
2	F	482	<div> <div>60%</div> <div>33%</div> <div>5%</div> <div>5%</div> </div>
3	G	272	<div> <div>24%</div> <div>17%</div> <div>55%</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	D	601	-	-	-	X
4	MG	F	601	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23481 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	487	Total	C	N	O	S	59	0	0
			3715	2341	656	706	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	ENGINEERED	UNP P19483
B	481	GLY	SER	ENGINEERED	UNP P19483
C	481	GLY	SER	ENGINEERED	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

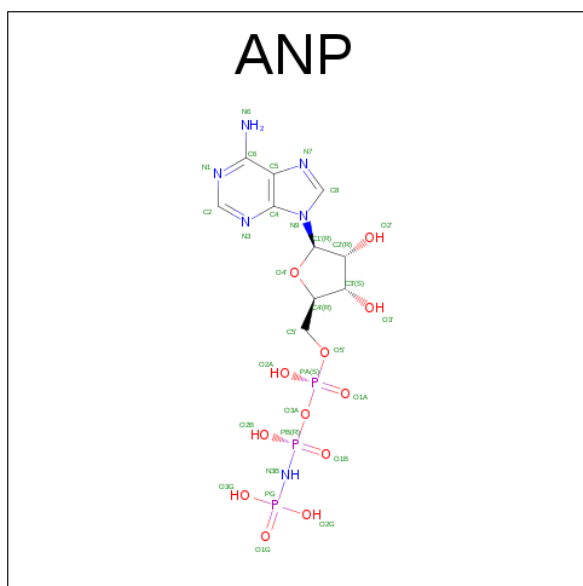
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

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

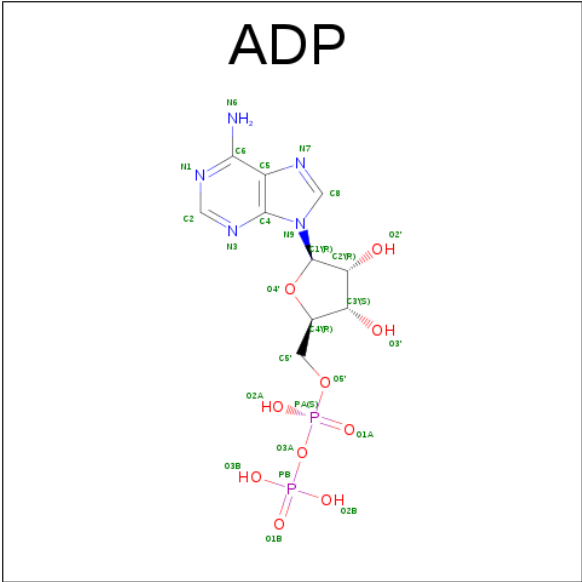
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0
5	C	1	Total C N O P 31 10 6 12 3	0	0
5	F	1	Total C N O P 31 10 6 12 3	0	0

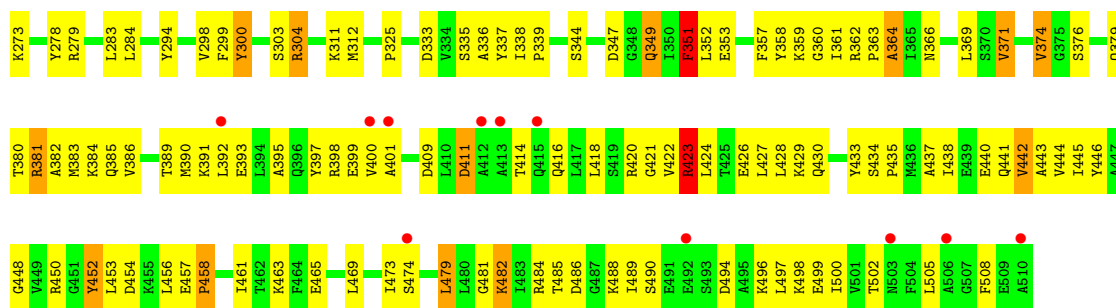
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is water.

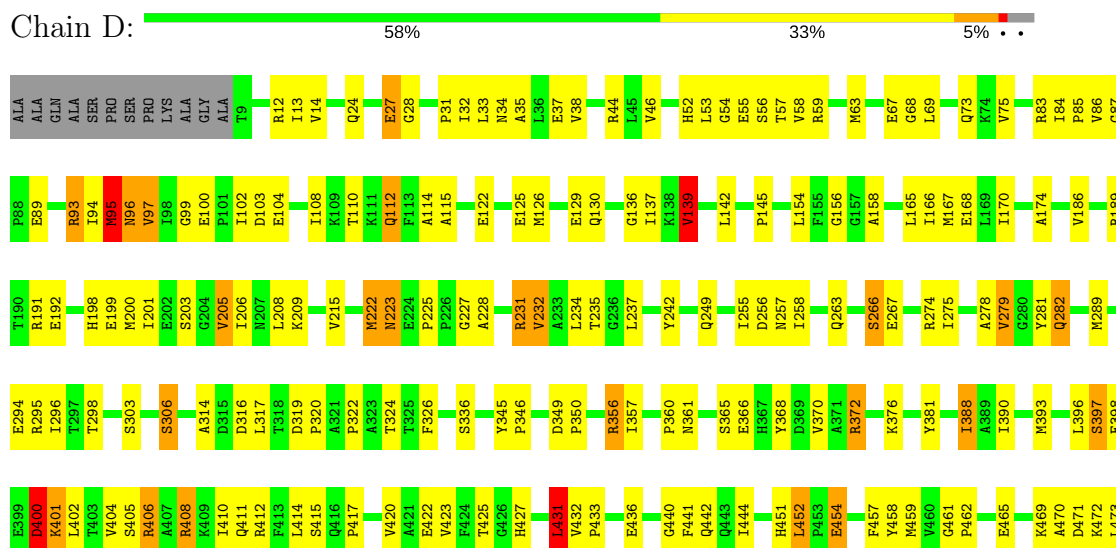
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	92	Total	O	0	0
			92	92		
7	B	96	Total	O	0	0
			96	96		
7	C	123	Total	O	0	0
			123	123		
7	D	105	Total	O	0	0
			105	105		
7	E	49	Total	O	0	0
			49	49		
7	F	104	Total	O	0	0
			104	104		
7	G	34	Total	O	0	0
			34	34		



• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

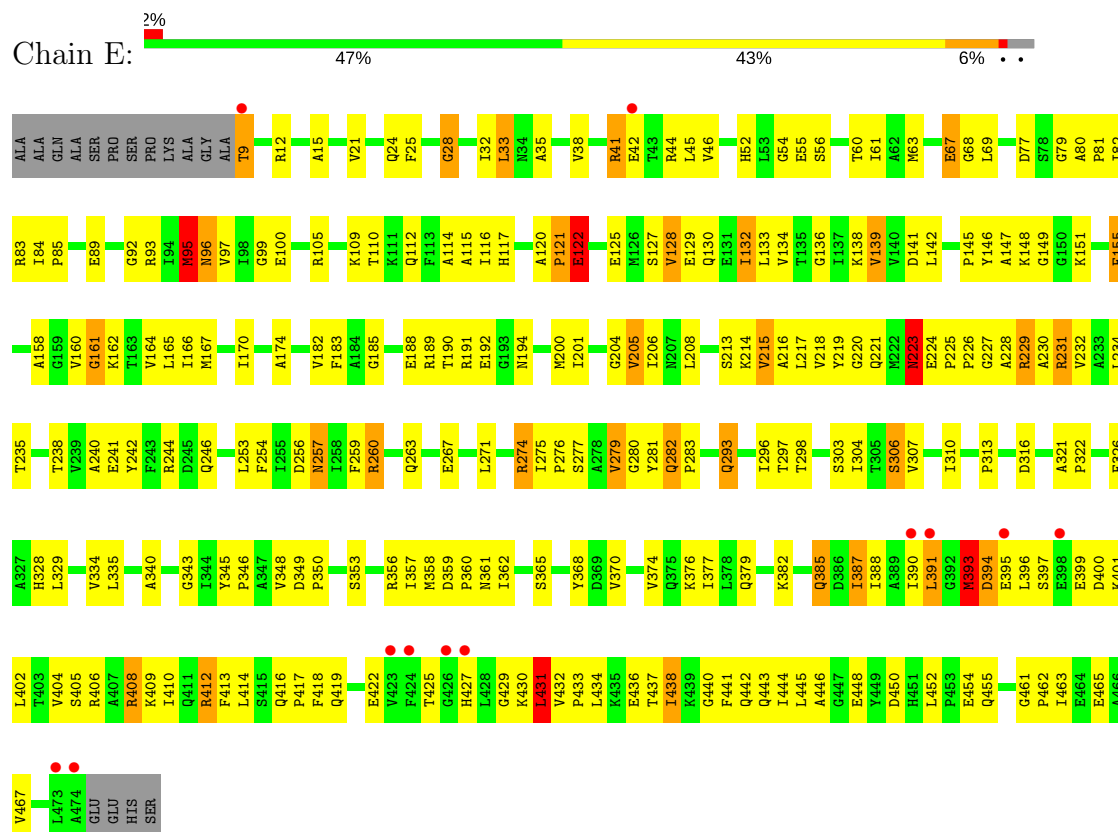


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

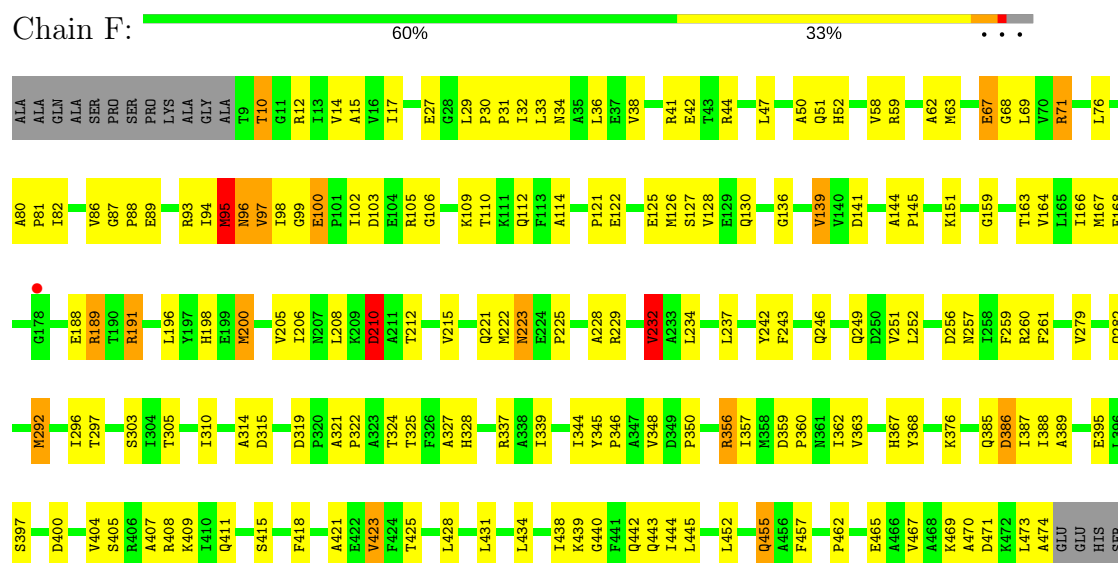




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

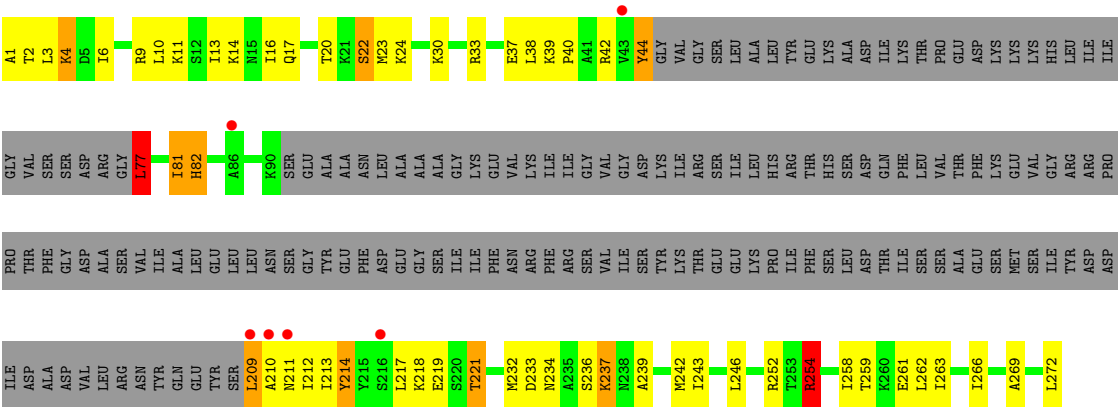


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	284.22Å 107.76Å 139.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.85 15.25 – 2.87	Depositor EDS
% Data completeness (in resolution range)	95.0 (6.00-2.85) 97.9 (15.25-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.86Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23481	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, 0.333 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, ANP, 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	0.60	0/3766	1.31	27/5080 (0.5%)
1	B	0.63	2/3766 (0.1%)	1.37	35/5080 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	27/4867 (0.6%)
3	G	0.52	0/949	1.15	5/1266 (0.4%)
All	All	0.61	2/23050 (0.0%)	1.34	159/31165 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	ALA	C-N	-7.54	1.16	1.34
1	B	409	ASP	C-N	-6.84	1.18	1.34

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	408	ARG	CD-NE-CZ	23.37	156.31	123.60
2	E	408	ARG	CD-NE-CZ	14.00	143.20	123.60
1	C	291	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	B	40	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	B	279	ARG	NE-CZ-NH1	12.88	126.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3815	172	0
1	B	3715	0	3812	167	0
1	C	3748	0	3844	168	0
2	D	3539	0	3592	153	0
2	E	3530	0	3587	205	0
2	F	3530	0	3585	131	0
3	G	945	0	1019	55	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	13	2	0
5	B	31	0	13	5	0
5	C	31	0	13	4	0
5	F	31	0	13	4	0
6	D	27	0	12	2	0
7	A	92	0	0	9	0
7	B	96	0	0	14	0
7	C	123	0	0	11	0
7	D	105	0	0	6	0
7	E	49	0	0	6	0
7	F	104	0	0	3	0
7	G	34	0	0	1	0
All	All	23481	0	23318	994	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.

The worst 5 of 994 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:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.15
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.12	1.12
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.73	1.02
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.40	1.02

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	485/510 (95%)	442 (91%)	36 (7%)	7 (1%)	13	37
1	B	485/510 (95%)	435 (90%)	43 (9%)	7 (1%)	13	37
1	C	490/510 (96%)	444 (91%)	38 (8%)	8 (2%)	11	33
2	D	465/482 (96%)	419 (90%)	43 (9%)	3 (1%)	28	60
2	E	464/482 (96%)	408 (88%)	47 (10%)	9 (2%)	9	29
2	F	464/482 (96%)	432 (93%)	30 (6%)	2 (0%)	38	68
3	G	116/272 (43%)	97 (84%)	18 (16%)	1 (1%)	20	49
All	All	2969/3248 (91%)	2677 (90%)	255 (9%)	37 (1%)	15	42

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	351 (89%)	42 (11%)	8	21
1	B	393/412 (95%)	346 (88%)	47 (12%)	6	15
1	C	397/412 (96%)	369 (93%)	28 (7%)	17	41
2	D	377/386 (98%)	346 (92%)	31 (8%)	13	34
2	E	376/386 (97%)	343 (91%)	33 (9%)	12	31
2	F	376/386 (97%)	354 (94%)	22 (6%)	23	51
3	G	102/230 (44%)	92 (90%)	10 (10%)	9	25
All	All	2414/2624 (92%)	2201 (91%)	213 (9%)	12	31

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	164	ARG
2	D	56	SER
2	F	292	MET
1	C	208	GLN
1	C	406	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	442	GLN
2	E	130	GLN
2	F	282	GLN
2	E	51	GLN
2	E	194	ASN

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
5	ANP	A	600	4	29,33,33	1.23	4 (13%)	28,52,52	0.93	2 (7%)
5	ANP	B	600	4	29,33,33	1.32	4 (13%)	28,52,52	1.15	3 (10%)
5	ANP	C	600	4	29,33,33	1.49	4 (13%)	28,52,52	1.75	9 (32%)
6	ADP	D	600	4	25,29,29	0.86	0	24,45,45	1.23	4 (16%)
5	ANP	F	600	4	29,33,33	1.21	3 (10%)	28,52,52	1.45	4 (14%)

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
5	ANP	A	600	4	-	0/13/38/38	0/3/3/3
5	ANP	B	600	4	-	2/13/38/38	0/3/3/3
5	ANP	C	600	4	-	0/13/38/38	0/3/3/3
6	ADP	D	600	4	-	0/12/32/32	0/3/3/3
5	ANP	F	600	4	-	0/13/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	600	ANP	PG-O3G	-4.37	1.44	1.56
5	B	600	ANP	PG-O2G	-3.52	1.47	1.56
5	A	600	ANP	PG-O3G	-3.37	1.47	1.56
5	C	600	ANP	PB-O2B	-3.35	1.47	1.56
5	F	600	ANP	PG-O3G	-3.07	1.48	1.56

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	600	ANP	O1G-PG-N3B	-3.91	105.94	111.79
5	C	600	ANP	PA-O3A-PB	-3.42	120.30	132.38
5	C	600	ANP	O2G-PG-O1G	-3.31	105.00	113.41
5	C	600	ANP	O3A-PB-N3B	-3.11	97.97	106.59
5	C	600	ANP	O3'-C3'-C2'	-2.80	102.85	111.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	600	ANP	O1G-PG-N3B-PB
5	B	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ANP	2	0
5	B	600	ANP	5	0
5	C	600	ANP	4	0
6	D	600	ADP	2	0
5	F	600	ANP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	487/510 (95%)	-0.66	4 (0%) 86 85	16, 38, 67, 97	0
1	B	479/510 (93%)	-0.59	12 (2%) 58 54	15, 37, 75, 98	0
1	C	492/510 (96%)	-0.79	6 (1%) 79 77	13, 33, 63, 95	0
2	D	467/482 (96%)	-0.88	0 100 100	13, 34, 62, 83	0
2	E	466/482 (96%)	-0.44	12 (2%) 56 52	18, 45, 79, 98	0
2	F	466/482 (96%)	-0.83	1 (0%) 94 95	13, 34, 63, 87	0
3	G	122/272 (44%)	-0.01	6 (4%) 30 26	13, 60, 100, 100	0
All	All	2979/3248 (91%)	-0.67	41 (1%) 75 74	13, 37, 74, 100	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	473	LEU	4.3
1	C	407	GLY	4.3
1	C	408	SER	4.0
1	A	408	SER	3.7
2	E	395	GLU	3.6

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, 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(Å ²)	Q<0.9
4	MG	F	601	1/1	0.94	0.29	16.38	24,24,24,24	0
4	MG	D	601	1/1	0.93	0.36	11.22	22,22,22,22	0
5	ANP	B	600	31/31	0.97	0.12	-0.42	30,34,37,38	0
5	ANP	A	600	31/31	0.97	0.11	-0.51	25,27,32,32	0
5	ANP	F	600	31/31	0.98	0.10	-0.63	26,28,29,31	0
6	ADP	D	600	27/27	0.99	0.09	-0.68	20,23,24,25	0
5	ANP	C	600	31/31	0.98	0.09	-1.09	19,24,26,29	0
4	MG	B	601	1/1	0.94	0.22	-	36,36,36,36	0
4	MG	A	601	1/1	0.93	0.16	-	26,26,26,26	0
4	MG	C	601	1/1	0.96	0.23	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.