



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:47 AM GMT

PDB ID : 2JDI  
Title : GROUND STATE STRUCTURE OF F1-ATPASE FROM BOVINE HEART MITOCHONDRIA (BOVINE F1-ATPASE CRYSTALLISED IN THE ABSENCE OF AZIDE)  
Authors : Bowler, M.W.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2007-01-09  
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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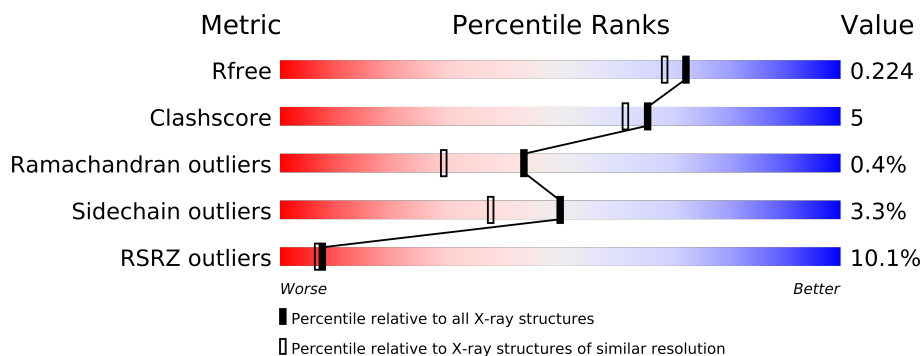
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	273	
4	H	146	
5	I	50	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	MG	A	1512	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26426 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	2	0
			3726	2348	659	707	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	SEE REMARK 999	UNP P19483
B	481	GLY	SER	SEE REMARK 999	UNP P19483
C	481	GLY	SER	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	3	1	0
			3544	2248	601	684	11			
2	E	458	Total	C	N	O	S	5	2	0
			3481	2207	593	671	10			
2	F	466	Total	C	N	O	S	1	2	0
			3538	2246	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	184	Total	C	N	O	S	0	0	0
			1417	894	252	265	6			

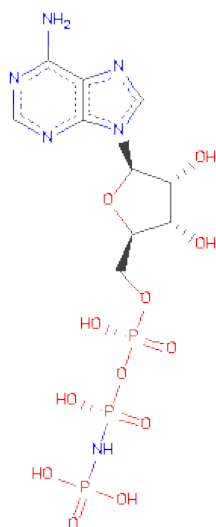
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	88	Total	C	N	O	S	0	0	0
			657	417	108	131	1			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	25	Total	C	N	O	S	0	0	0
			203	130	38	34	1			

- Molecule 6 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is water.

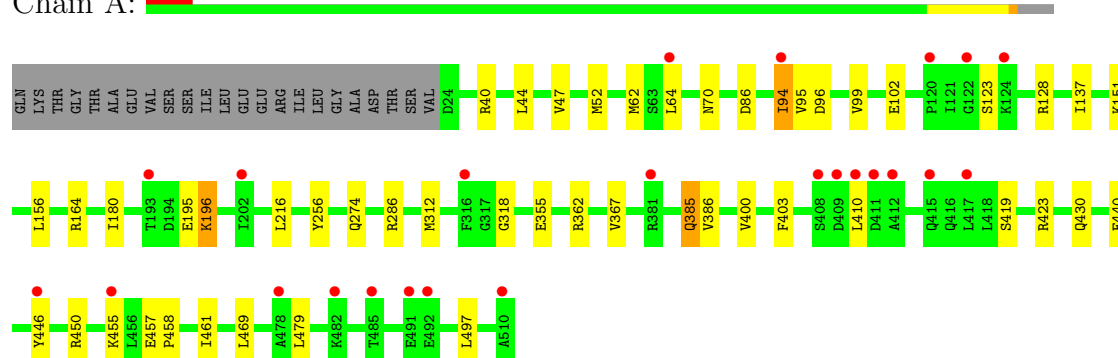
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	B	348	Total O 348 348	0	0
8	C	367	Total O 367 367	0	0
8	D	389	Total O 389 389	0	0
8	E	267	Total O 267 267	0	0
8	F	436	Total O 436 436	0	0
8	G	114	Total O 114 114	0	0
8	H	31	Total O 31 31	0	0
8	I	16	Total O 16 16	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

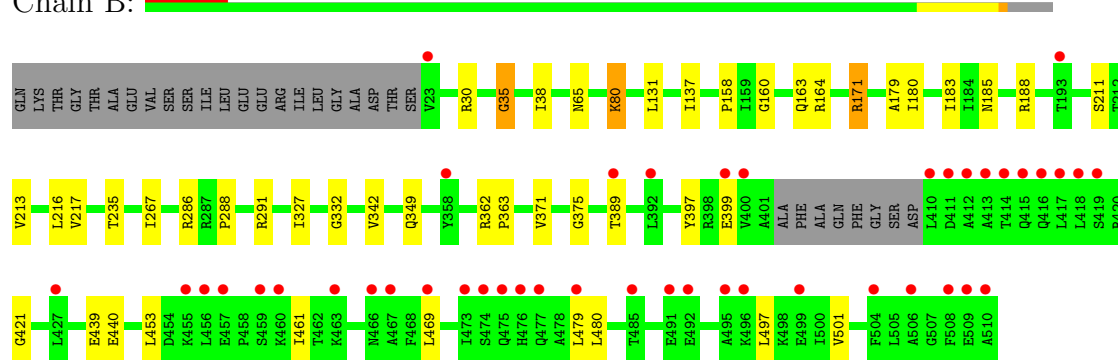
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain A:



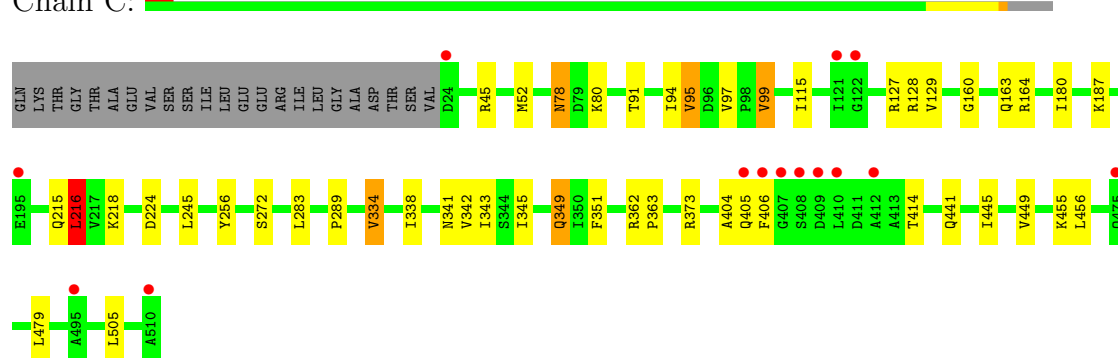
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain B:



#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

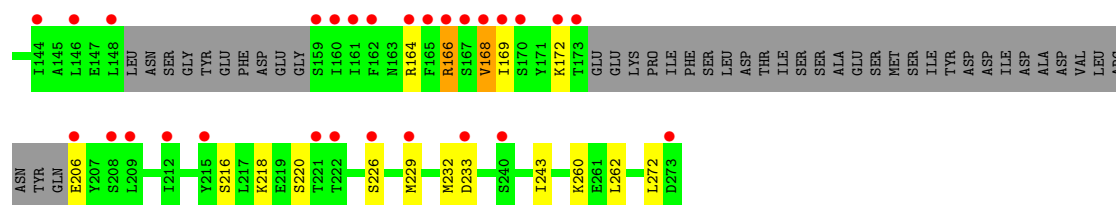
Chain C:



Chain D: 

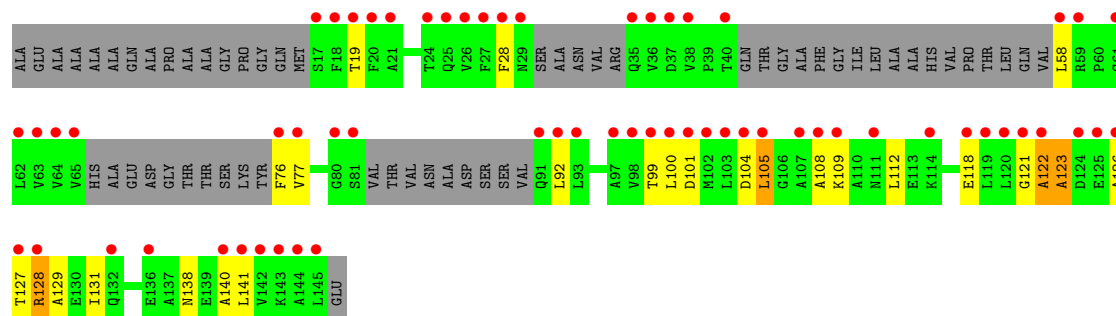






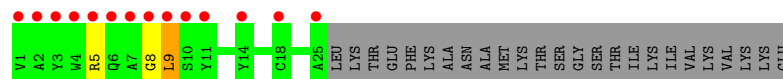
• Molecule 4: ATP SYNTHASE DELTA CHAIN

Chain H:



• Molecule 5: ATP SYNTHASE EPSILON CHAIN

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.61Å 123.13Å 261.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 23.15 – 1.85	Depositor EDS
% Data completeness (in resolution range)	72.7 (20.00-1.90) 67.6 (23.15-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.175 , 0.220 0.178 , 0.224	Depositor DCC
$R_{free}$ test set	9843 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 27.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 195694 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/3783	0.53	0/5102
1	B	0.39	0/3711	0.53	0/5005
1	C	0.39	0/3766	0.56	1/5080 (0.0%)
2	D	1.57	2/3604 (0.1%)	0.64	6/4891 (0.1%)
2	E	0.37	0/3543	0.54	1/4807 (0.0%)
2	F	0.41	0/3601	1.44	2/4887 (0.0%)
3	G	0.35	0/1426	0.49	0/1907
4	H	0.37	0/660	0.63	0/890
5	I	0.31	0/207	0.61	0/279
All	All	0.70	2/24301 (0.0%)	0.76	10/32848 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	275[A]	ILE	CB-CG2	64.47	3.52	1.52
2	D	275[B]	ILE	CB-CG2	64.47	3.52	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	97[A]	VAL	CG1-CB-CG2	-65.79	5.64	110.90
2	F	97[B]	VAL	CG1-CB-CG2	-65.79	5.64	110.90
2	D	275[A]	ILE	CA-CB-CG2	-13.16	84.58	110.90
2	D	275[B]	ILE	CA-CB-CG2	-13.16	84.58	110.90
2	D	275[A]	ILE	CG1-CB-CG2	6.93	126.64	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3726	0	3832	32	0
1	B	3663	0	3774	30	0
1	C	3715	0	3814	32	0
2	D	3544	0	3603	35	0
2	E	3481	0	3539	39	0
2	F	3538	0	3604	41	0
3	G	1417	0	1501	32	0
4	H	657	0	663	28	0
5	I	203	0	205	2	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	D	31	0	13	3	0
6	F	31	0	13	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	354	0	0	6	0
8	B	348	0	0	5	0
8	C	367	0	0	11	0
8	D	389	0	0	4	0
8	E	267	0	0	5	0
8	F	436	0	0	8	0
8	G	114	0	0	3	0
8	H	31	0	0	1	0
8	I	16	0	0	0	0
All	All	26426	0	24600	254	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 254 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:68:ILE:HB	3:G:69:ILE:HA	1.29	1.11
4:H:104:ASP:HA	4:H:105:LEU:CB	1.80	1.10
4:H:104:ASP:CA	4:H:105:LEU:HB2	1.82	1.08
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.31	1.07
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.09	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	487/510 (96%)	475 (98%)	11 (2%)	1 (0%)	56	44
1	B	476/510 (93%)	463 (97%)	12 (2%)	1 (0%)	56	44
1	C	485/510 (95%)	474 (98%)	10 (2%)	1 (0%)	56	44
2	D	466/482 (97%)	450 (97%)	16 (3%)	0	100	100
2	E	456/482 (95%)	442 (97%)	12 (3%)	2 (0%)	43	29
2	F	466/482 (97%)	453 (97%)	12 (3%)	1 (0%)	56	44
3	G	172/273 (63%)	163 (95%)	8 (5%)	1 (1%)	33	19
4	H	78/146 (53%)	65 (83%)	9 (12%)	4 (5%)	3	0
5	I	23/50 (46%)	22 (96%)	1 (4%)	0	100	100
All	All	3109/3445 (90%)	3007 (97%)	91 (3%)	11 (0%)	43	29

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	C	405	GLN
4	H	105	LEU
4	H	123	ALA
1	B	35	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	A	395/412 (96%)	388 (98%)	7 (2%)	71	66
1	B	389/412 (94%)	379 (97%)	10 (3%)	59	49
1	C	393/412 (95%)	379 (96%)	14 (4%)	47	33
2	D	378/386 (98%)	367 (97%)	11 (3%)	55	44
2	E	372/386 (96%)	357 (96%)	15 (4%)	42	29
2	F	378/386 (98%)	364 (96%)	14 (4%)	45	32
3	G	154/231 (67%)	144 (94%)	10 (6%)	24	11
4	H	70/109 (64%)	67 (96%)	3 (4%)	40	26
5	I	19/41 (46%)	18 (95%)	1 (5%)	32	18
All	All	2548/2775 (92%)	2463 (97%)	85 (3%)	50	37

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	282	GLN
2	E	257[A]	ASN
3	G	206	GLU
2	D	341	GLU
2	E	139	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	194	ASN
2	E	223	ASN
3	G	15	ASN
2	D	282	GLN
2	E	249	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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$
6	ANP	A	1511	7	33,33,33	3.12	6 (18%)	51,52,52	2.16	10 (19%)
6	ANP	B	1511	7	33,33,33	3.23	6 (18%)	51,52,52	1.95	10 (19%)
6	ANP	C	1511	7	33,33,33	3.36	6 (18%)	51,52,52	2.04	9 (17%)
6	ANP	D	1480	7	33,33,33	2.99	6 (18%)	51,52,52	2.12	10 (19%)
6	ANP	F	1479	7	33,33,33	2.87	6 (18%)	51,52,52	2.08	11 (21%)

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
6	ANP	A	1511	7	-	0/18/38/38	0/1/3/3
6	ANP	B	1511	7	-	0/18/38/38	0/1/3/3
6	ANP	C	1511	7	-	0/18/38/38	0/1/3/3
6	ANP	D	1480	7	-	0/18/38/38	0/1/3/3
6	ANP	F	1479	7	-	1/18/38/38	0/1/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1511	ANP	PB-N3B	12.11	1.74	1.64
6	B	1511	ANP	PB-N3B	12.09	1.74	1.64
6	C	1511	ANP	PG-N3B	12.05	1.74	1.64
6	B	1511	ANP	PG-N3B	11.22	1.74	1.64
6	A	1511	ANP	PB-N3B	11.21	1.74	1.64

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1480	ANP	O1G-PG-N3B	-8.88	98.41	111.83
6	C	1511	ANP	O1G-PG-N3B	-7.68	100.22	111.83
6	F	1479	ANP	O1G-PG-N3B	-7.47	100.54	111.83
6	A	1511	ANP	O1G-PG-N3B	-7.38	100.67	111.83
6	A	1511	ANP	N3-C2-N1	-6.86	122.97	128.71

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1479	ANP	O1B-PB-N3B-PG

There are no ring outliers.

## 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	A	487/510 (95%)	0.32	24 (4%) 28 28	5, 15, 36, 66	3 (0%)
1	B	480/510 (94%)	0.55	44 (9%) 9 8	5, 14, 48, 78	1 (0%)
1	C	487/510 (95%)	0.31	14 (2%) 49 50	8, 15, 32, 70	0
2	D	467/482 (96%)	0.21	13 (2%) 50 51	6, 14, 34, 71	1 (0%)
2	E	458/482 (95%)	0.73	63 (13%) 4 3	7, 18, 60, 81	2 (0%)
2	F	466/482 (96%)	0.38	16 (3%) 43 44	8, 14, 38, 59	1 (0%)
3	G	184/273 (67%)	1.79	67 (36%) 1 1	5, 32, 48, 54	1 (0%)
4	H	88/146 (60%)	3.33	62 (70%) 0 0	2, 20, 42, 50	0
5	I	25/50 (50%)	2.81	14 (56%) 0 0	2, 7, 32, 34	0
All	All	3142/3445 (91%)	0.60	317 (10%) 7 7	2, 15, 45, 81	9 (0%)

The worst 5 of 317 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	273	ASP	13.1
4	H	27	PHE	9.2
4	H	18	PHE	8.7
1	C	407	GLY	8.5
4	H	64	VAL	8.4

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	A	1512	1/1	0.12	7.40	16,16,16,16	0
7	MG	F	1480	1/1	0.16	0.62	13,13,13,13	0
7	MG	D	1481	1/1	0.14	0.32	14,14,14,14	0
7	MG	C	1512	1/1	0.10	-0.23	13,13,13,13	0
6	ANP	F	1479	31/31	0.11	-0.49	8,12,18,21	0
6	ANP	D	1480	31/31	0.11	-0.50	6,10,14,16	0
7	MG	B	1512	1/1	0.09	-0.50	15,15,15,15	0
6	ANP	C	1511	31/31	0.10	-0.69	8,12,17,25	0
6	ANP	B	1511	31/31	0.09	-0.71	8,15,24,33	0
6	ANP	A	1511	31/31	0.09	-0.78	8,12,19,21	0

## 6.5 Other polymers

There are no such residues in this entry.