



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:34 PM GMT

PDB ID : 3ZRY
Title : Rotor architecture in the F(1)-c(10)-ring complex of the yeast F-ATP synthase
Authors : Giraud, M.-F.; Dautant, A.
Deposited on : 2011-06-21
Resolution : 6.50 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 (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

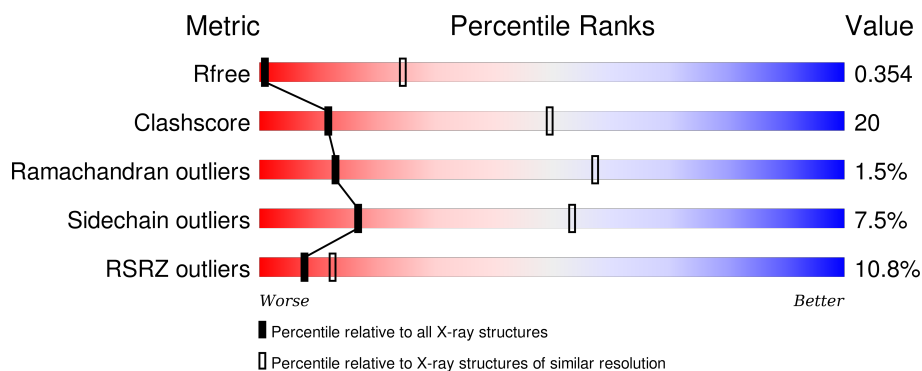
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

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>2%</div> <div>63%</div> <div>30%</div> <div>5%</div> </div>
1	B	510	<div> <div>3%</div> <div>57%</div> <div>33%</div> <div>5%</div> <div>5%</div> </div>
1	C	510	<div> <div>7%</div> <div>64%</div> <div>30%</div> <div>5%</div> </div>
2	D	478	<div> <div>8%</div> <div>69%</div> <div>27%</div> <div>•</div> </div>
2	E	478	<div> <div>11%</div> <div>64%</div> <div>33%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	478	
3	G	278	
4	H	138	
5	I	61	
6	J	76	
6	K	76	
6	L	76	
6	M	76	
6	N	76	
6	O	76	
6	P	76	
6	Q	76	
6	R	76	
6	S	76	

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
7	ANP	A	600	X	-	-	X
7	ANP	B	600	X	-	-	X
7	ANP	C	600	X	-	-	X
7	ANP	D	600	X	-	-	-
7	ANP	F	600	X	-	X	X
8	MG	F	700	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30100 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	1
			3665	2314	649	699	3			
1	B	484	Total	C	N	O	S	0	0	1
			3670	2317	650	700	3			
1	C	485	Total	C	N	O	S	0	0	1
			3674	2319	651	701	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	SER	PRO	VARIANT	UNP P07251
B	305	SER	PRO	VARIANT	UNP P07251
C	305	SER	PRO	VARIANT	UNP P07251

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	471	Total	C	N	O	S	0	0	1
			3550	2250	605	689	6			
2	E	469	Total	C	N	O	S	0	0	1
			3537	2243	603	685	6			
2	F	470	Total	C	N	O	S	0	0	1
			3544	2247	604	687	6			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	266	Total	C	N	O	S	0	0	1
			2022	1270	355	387	10			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	119	Total	C	N	O	S	0	0	0
			747	468	132	145	2			

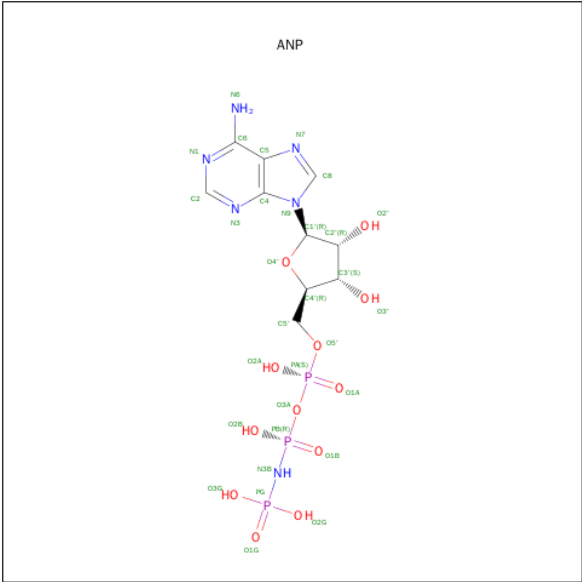
- Molecule 5 is a protein called ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O	S	0	0	1
			325	201	57	67				

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	73	Total	C	N	O	S	0	0	1
			515	343	81	88	3			
6	K	73	Total	C	N	O	S	0	0	1
			517	347	80	87	3			
6	L	72	Total	C	N	O	S	0	0	1
			507	337	80	87	3			
6	M	73	Total	C	N	O	S	0	0	1
			515	342	81	88	4			
6	N	73	Total	C	N	O	S	0	0	1
			515	342	81	88	4			
6	O	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	P	75	Total	C	N	O	S	0	0	1
			534	357	83	90	4			
6	Q	75	Total	C	N	O	S	0	0	1
			534	357	83	90	4			
6	R	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	S	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

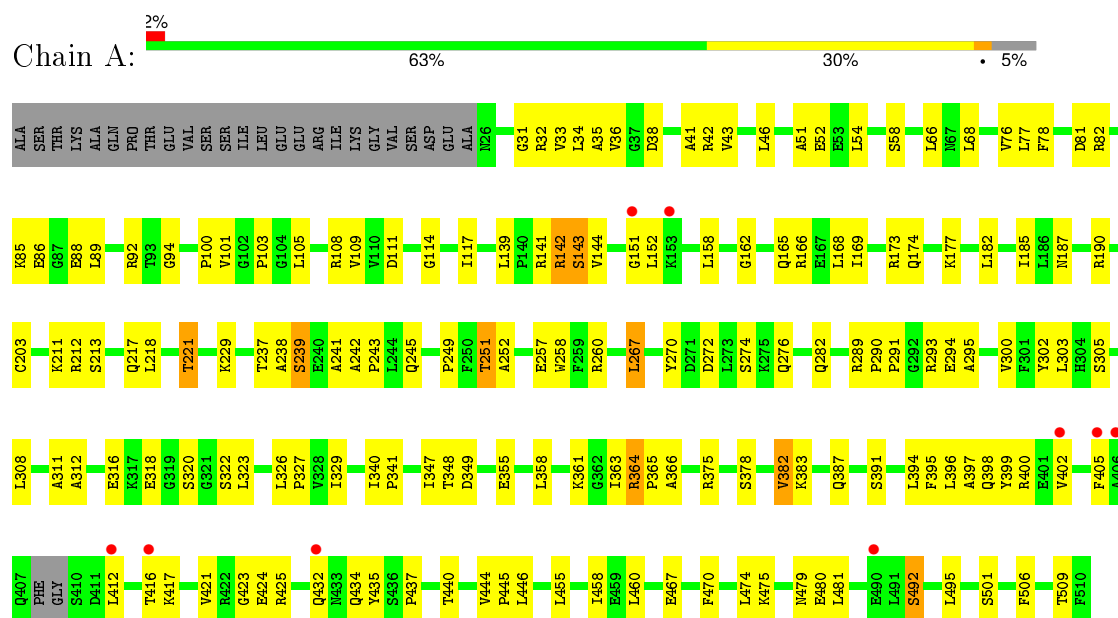
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

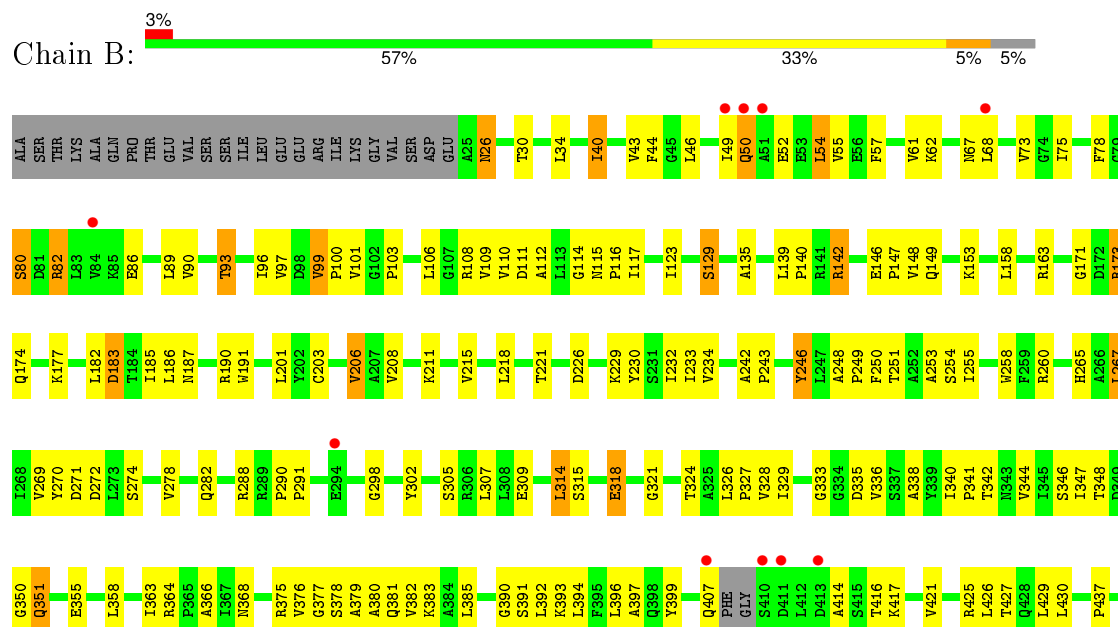
3 Residue-property plots

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 ($RSRZ > 2$). 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, MITOCHONDRIAL

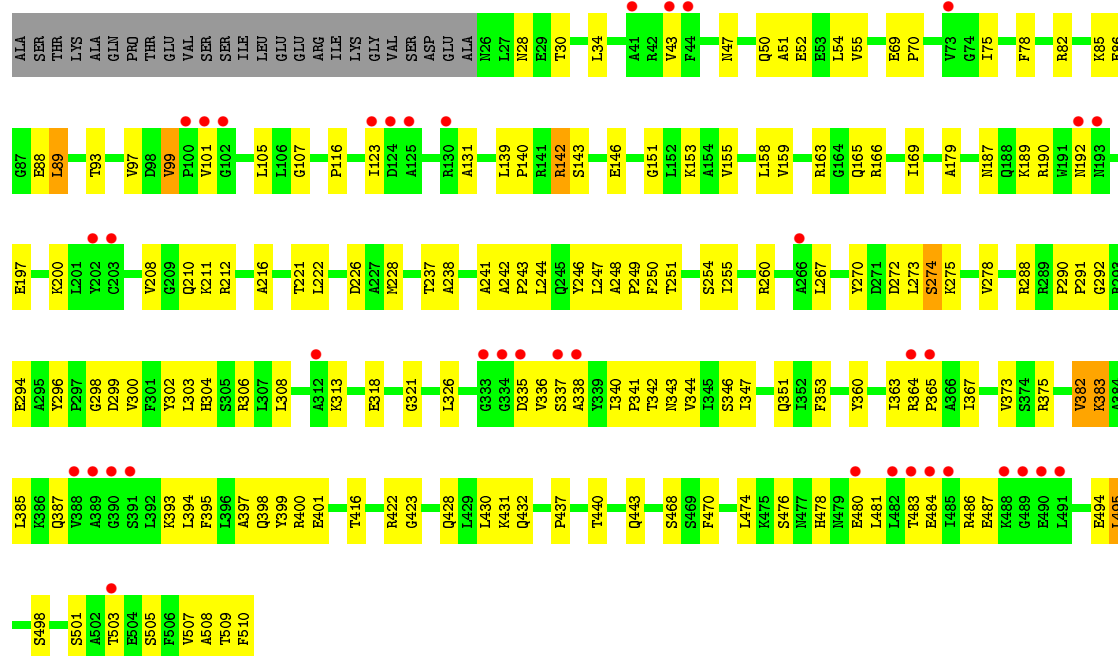


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

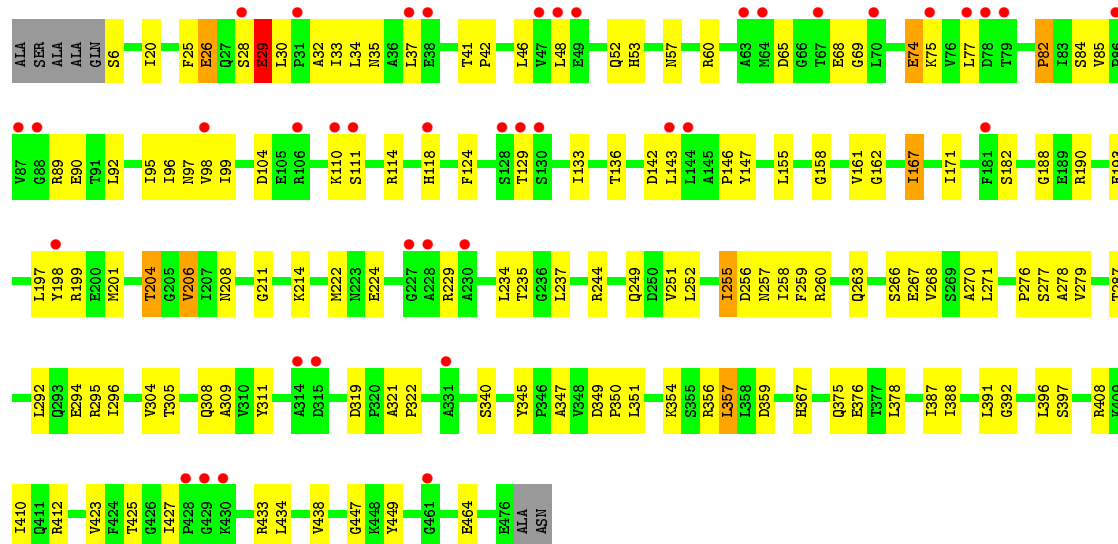




• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

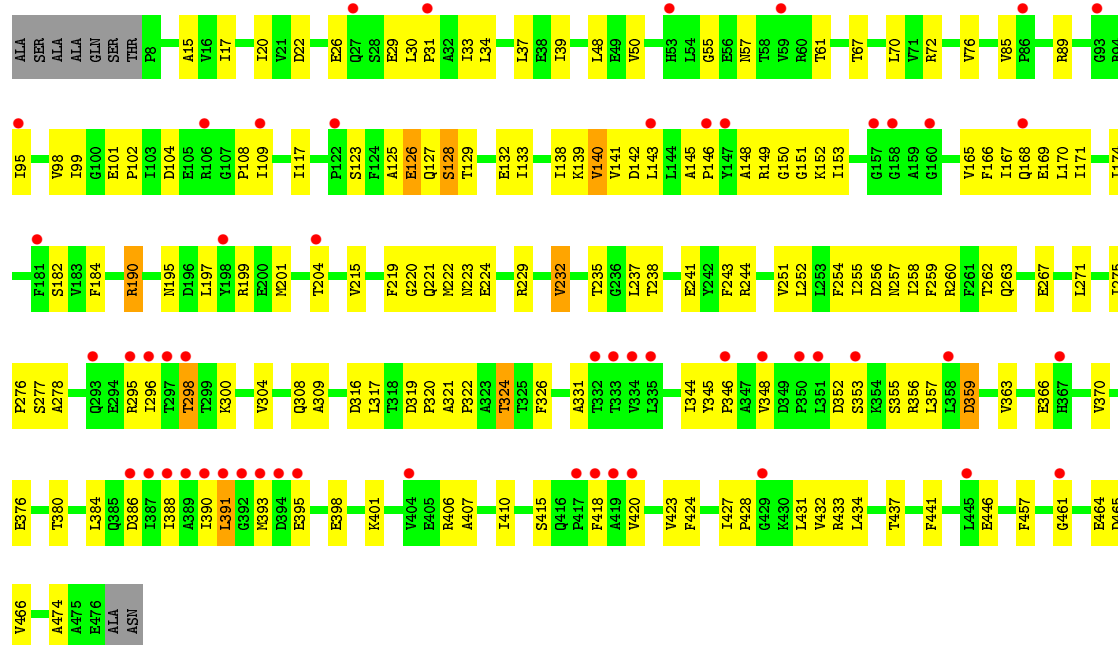


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

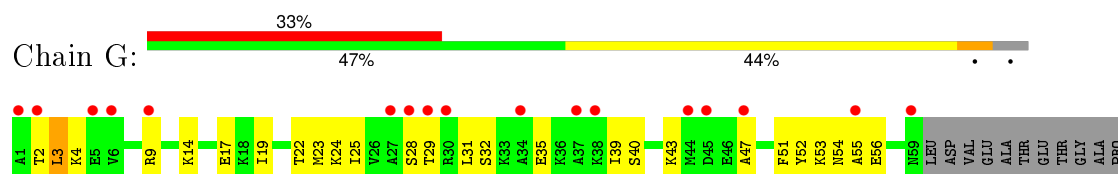


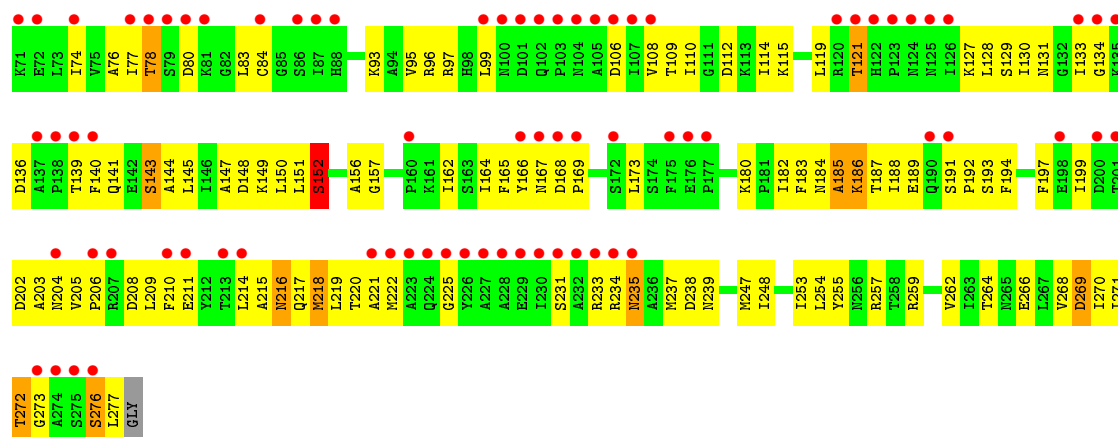


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

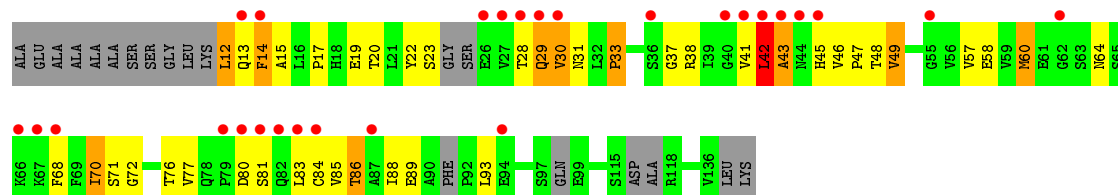


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

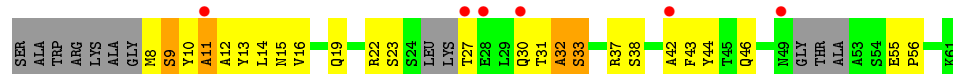




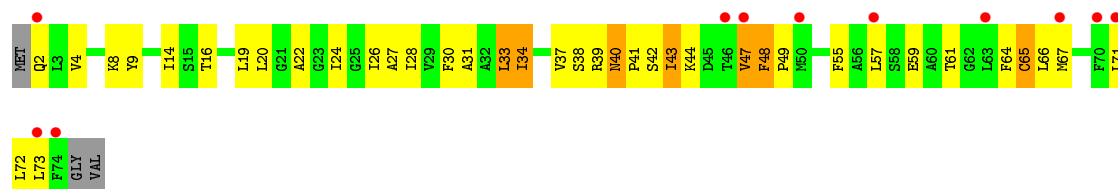
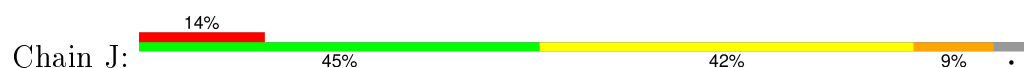
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



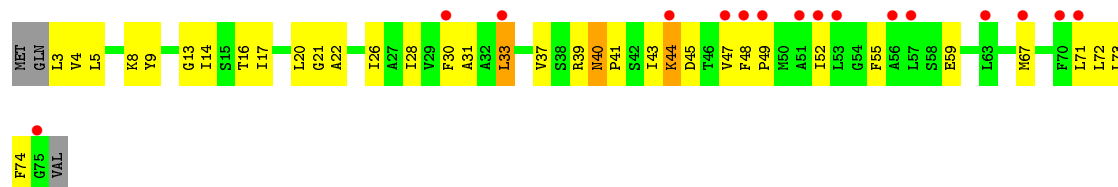
• Molecule 5: ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUBUNIT



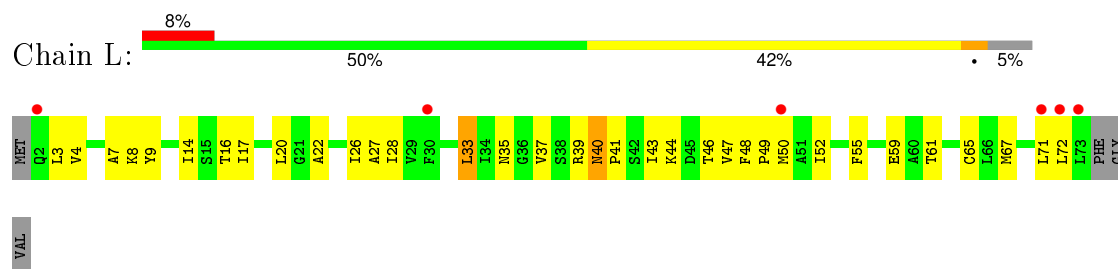
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



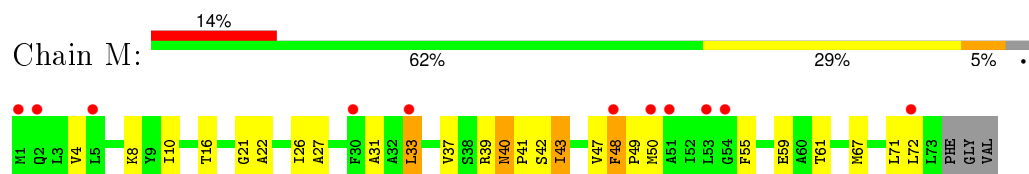
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



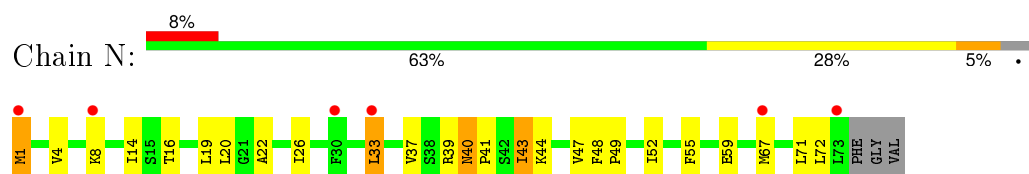
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



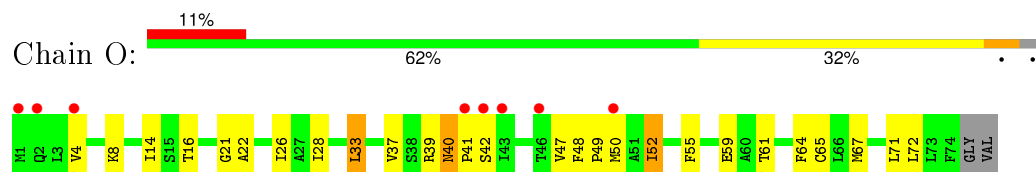
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



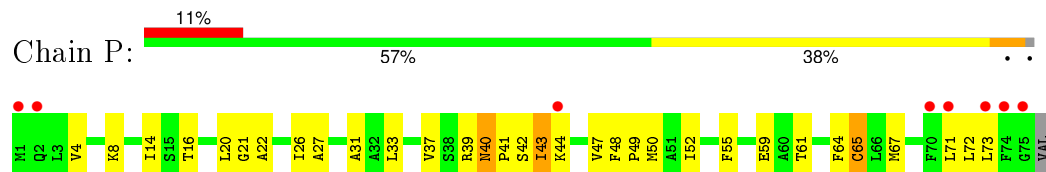
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



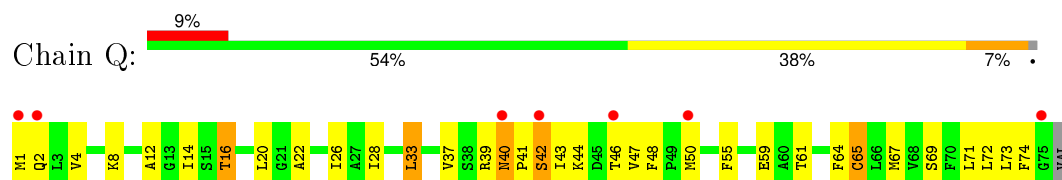
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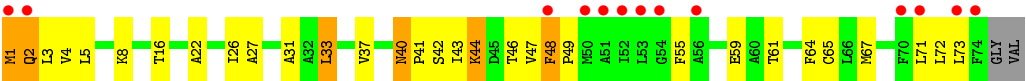


• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

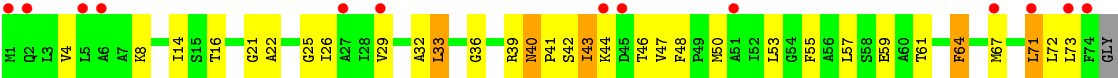


• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL





● Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.69Å 174.91Å 164.26Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	54.62 – 6.50 54.63 – 6.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (54.62-6.50) 96.6 (54.63-6.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 6.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.317 , 0.339 0.305 , 0.354	Depositor DCC
R_{free} test set	558 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	274.6	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 233.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 11677 reflections	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	30100	wwPDB-VP
Average B, all atoms (Å ²)	309.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.21	0/3719	0.46	0/5034
1	B	0.21	0/3724	0.46	0/5041
1	C	0.21	0/3729	0.47	0/5049
2	D	0.22	0/3606	0.47	0/4891
2	E	0.22	0/3593	0.46	1/4872 (0.0%)
2	F	0.21	0/3600	0.47	0/4883
3	G	0.24	0/2045	0.47	0/2752
4	H	0.22	0/755	0.47	0/1035
5	I	0.26	0/327	0.52	0/447
6	J	0.23	0/522	0.51	0/708
6	K	0.25	0/525	0.58	0/712
6	L	0.24	0/514	0.54	0/697
6	M	0.25	0/522	0.55	0/707
6	N	0.24	0/522	0.54	0/707
6	O	0.27	0/530	0.56	0/718
6	P	0.25	0/542	0.52	0/734
6	Q	0.25	0/542	0.51	0/734
6	R	0.25	0/530	0.54	0/718
6	S	0.27	0/530	0.61	0/718
All	All	0.22	0/30377	0.48	1/41157 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	391	LEU	CA-CB-CG	5.70	128.40	115.30

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	3665	0	3748	126	0
1	B	3670	0	3753	155	0
1	C	3674	0	3754	124	0
2	D	3550	0	3621	118	0
2	E	3537	0	3610	132	0
2	F	3544	0	3616	146	0
3	G	2022	0	2069	200	0
4	H	747	0	592	68	0
5	I	325	0	249	46	0
6	J	515	0	558	62	0
6	K	517	0	559	37	0
6	L	507	0	547	38	0
6	M	515	0	559	31	0
6	N	515	0	559	34	0
6	O	523	0	570	44	0
6	P	534	0	579	32	0
6	Q	534	0	579	37	0
6	R	523	0	570	35	0
6	S	523	0	570	51	0
7	A	31	0	10	0	0
7	B	31	0	10	1	0
7	C	31	0	10	4	0
7	D	31	0	10	5	0
7	F	31	0	10	9	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
All	All	30100	0	30712	1227	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 20.

The worst 5 of 1227 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)
6:M:40:ASN:HB3	6:M:41:PRO:HA	1.20	1.15
1:C:291:PRO:HD2	3:G:273:GLY:CA	1.76	1.15
2:E:390:ILE:HG21	3:G:28:SER:CB	1.76	1.14
1:C:509:THR:HG23	1:C:510:PHE:N	1.54	1.14
3:G:191:SER:HB2	3:G:194:PHE:CB	1.77	1.12

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	479/510 (94%)	430 (90%)	46 (10%)	3 (1%)	30	74
1	B	480/510 (94%)	433 (90%)	45 (9%)	2 (0%)	39	80
1	C	483/510 (95%)	445 (92%)	36 (8%)	2 (0%)	39	80
2	D	469/478 (98%)	429 (92%)	37 (8%)	3 (1%)	30	74
2	E	467/478 (98%)	425 (91%)	36 (8%)	6 (1%)	15	60
2	F	468/478 (98%)	419 (90%)	41 (9%)	8 (2%)	11	55
3	G	260/278 (94%)	225 (86%)	28 (11%)	7 (3%)	6	44
4	H	109/138 (79%)	88 (81%)	16 (15%)	5 (5%)	3	32
5	I	43/61 (70%)	27 (63%)	8 (19%)	8 (19%)	0	3
6	J	71/76 (93%)	64 (90%)	6 (8%)	1 (1%)	14	58
6	K	71/76 (93%)	65 (92%)	5 (7%)	1 (1%)	14	58
6	L	70/76 (92%)	65 (93%)	4 (6%)	1 (1%)	14	58
6	M	71/76 (93%)	66 (93%)	3 (4%)	2 (3%)	6	44
6	N	71/76 (93%)	66 (93%)	3 (4%)	2 (3%)	6	44
6	O	72/76 (95%)	67 (93%)	4 (6%)	1 (1%)	14	58
6	P	73/76 (96%)	67 (92%)	4 (6%)	2 (3%)	6	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	73/76 (96%)	63 (86%)	9 (12%)	1 (1%)	14	58
6	R	72/76 (95%)	66 (92%)	5 (7%)	1 (1%)	14	58
6	S	72/76 (95%)	66 (92%)	4 (6%)	2 (3%)	6	44
All	All	3974/4201 (95%)	3576 (90%)	340 (9%)	58 (2%)	13	57

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	29	GLU
2	F	28	SER
3	G	152	SER
3	G	185	ALA
3	G	186	LYS

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	388/412 (94%)	370 (95%)	18 (5%)	33	68
1	B	388/412 (94%)	351 (90%)	37 (10%)	11	41
1	C	388/412 (94%)	363 (94%)	25 (6%)	22	58
2	D	380/384 (99%)	361 (95%)	19 (5%)	30	66
2	E	378/384 (98%)	359 (95%)	19 (5%)	30	66
2	F	379/384 (99%)	360 (95%)	19 (5%)	30	66
3	G	216/236 (92%)	190 (88%)	26 (12%)	6	31
4	H	53/112 (47%)	43 (81%)	10 (19%)	2	13
5	I	23/48 (48%)	20 (87%)	3 (13%)	5	28
6	J	53/56 (95%)	42 (79%)	11 (21%)	1	10
6	K	53/56 (95%)	48 (91%)	5 (9%)	11	42
6	L	52/56 (93%)	49 (94%)	3 (6%)	25	61
6	M	53/56 (95%)	48 (91%)	5 (9%)	11	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	N	53/56 (95%)	49 (92%)	4 (8%)	17	53
6	O	54/56 (96%)	49 (91%)	5 (9%)	11	42
6	P	55/56 (98%)	51 (93%)	4 (7%)	17	54
6	Q	55/56 (98%)	48 (87%)	7 (13%)	5	29
6	R	54/56 (96%)	46 (85%)	8 (15%)	4	24
6	S	54/56 (96%)	48 (89%)	6 (11%)	8	34
All	All	3129/3344 (94%)	2895 (92%)	234 (8%)	17	53

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	232	VAL
2	F	324	THR
6	Q	48	PHE
2	E	352	ASP
2	F	58	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	210	GLN
1	C	452	ASN
6	J	2	GLN
1	C	225	HIS
1	C	407	GLN

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$
7	ANP	A	600	8	27,33,33	14.49	8 (29%)	30,52,52	9.24	18 (60%)
7	ANP	B	600	8	27,33,33	14.69	8 (29%)	30,52,52	9.14	18 (60%)
7	ANP	C	600	8	27,33,33	14.06	8 (29%)	30,52,52	9.29	18 (60%)
7	ANP	D	600	8	27,33,33	14.43	9 (33%)	30,52,52	9.23	17 (56%)
7	ANP	F	600	8	27,33,33	14.40	8 (29%)	30,52,52	9.23	18 (60%)

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
7	ANP	A	600	8	3/3/7/8	0/12/38/38	0/3/3/3
7	ANP	B	600	8	3/3/7/8	0/12/38/38	0/3/3/3
7	ANP	C	600	8	3/3/7/8	0/12/38/38	0/3/3/3
7	ANP	D	600	8	3/3/7/8	1/12/38/38	0/3/3/3
7	ANP	F	600	8	3/3/7/8	0/12/38/38	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	600	ANP	PB-O3A	-10.70	1.45	1.59
7	C	600	ANP	PB-O3A	-10.48	1.46	1.59
7	B	600	ANP	PB-O3A	-10.36	1.46	1.59
7	A	600	ANP	PB-O3A	-10.31	1.46	1.59
7	D	600	ANP	PB-O3A	-10.29	1.46	1.59

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	600	ANP	O4'-C1'-N9	-37.79	28.99	108.10
7	C	600	ANP	O4'-C1'-N9	-37.64	29.30	108.10
7	B	600	ANP	O4'-C1'-N9	-37.50	29.60	108.10
7	F	600	ANP	O4'-C1'-N9	-36.98	30.69	108.10
7	D	600	ANP	O4'-C1'-N9	-36.97	30.71	108.10

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	F	600	ANP	C4'
7	F	600	ANP	C3'
7	F	600	ANP	C1'
7	B	600	ANP	C4'
7	B	600	ANP	C3'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	600	ANP	1	0
7	C	600	ANP	4	0
7	D	600	ANP	5	0
7	F	600	ANP	9	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	483/510 (94%)	0.23	9 (1%) 70 65	190, 219, 279, 304	0
1	B	484/510 (94%)	0.33	16 (3%) 50 46	184, 237, 325, 351	0
1	C	485/510 (95%)	0.61	38 (7%) 16 19	255, 279, 425, 448	0
2	D	471/478 (98%)	0.55	40 (8%) 13 17	217, 250, 325, 361	0
2	E	469/478 (98%)	0.63	54 (11%) 6 11	215, 255, 301, 336	0
2	F	470/478 (98%)	0.70	53 (11%) 7 12	242, 287, 363, 404	0
3	G	266/278 (95%)	1.56	93 (34%) 0 4	315, 367, 397, 413	0
4	H	119/138 (86%)	1.29	27 (22%) 1 6	339, 382, 438, 476	0
5	I	49/61 (80%)	0.92	6 (12%) 5 11	298, 368, 423, 442	0
6	J	73/76 (96%)	0.94	11 (15%) 3 9	407, 446, 474, 482	0
6	K	73/76 (96%)	0.59	16 (21%) 1 6	414, 437, 478, 491	0
6	L	72/76 (94%)	0.40	6 (8%) 14 18	399, 482, 524, 524	0
6	M	73/76 (96%)	0.82	11 (15%) 3 9	424, 488, 520, 520	0
6	N	73/76 (96%)	0.58	6 (8%) 14 18	430, 526, 526, 526	0
6	O	74/76 (97%)	0.60	8 (10%) 8 12	420, 455, 487, 493	0
6	P	75/76 (98%)	0.65	8 (10%) 8 13	419, 452, 487, 506	0
6	Q	75/76 (98%)	0.84	7 (9%) 11 15	445, 458, 488, 517	0
6	R	74/76 (97%)	0.83	13 (17%) 2 7	414, 436, 466, 485	0
6	S	74/76 (97%)	0.98	13 (17%) 2 7	378, 432, 464, 480	0
All	All	4032/4201 (95%)	0.65	435 (10%) 8 12	184, 280, 466, 526	0

The worst 5 of 435 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	J	74	PHE	10.7

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Mol	Chain	Res	Type	RSRZ
6	P	75	GLY	8.4
2	F	461	GLY	8.1
3	G	134	GLY	7.7
3	G	122	HIS	7.5

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
8	MG	F	700	1/1	0.84	0.65	5.14	376,376,376,376	0
7	ANP	B	600	31/31	0.81	0.41	0.50	190,214,226,227	0
7	ANP	A	600	31/31	0.80	0.53	0.47	199,210,219,227	0
7	ANP	D	600	31/31	0.89	0.40	0.22	231,238,281,287	0
7	ANP	F	600	31/31	0.78	0.42	-0.05	216,249,272,272	0
7	ANP	C	600	31/31	0.73	0.41	-0.21	309,327,335,341	0
8	MG	D	700	1/1	0.90	0.45	-	395,395,395,395	0
8	MG	A	700	1/1	0.95	0.74	-	394,394,394,394	0
8	MG	C	700	1/1	0.89	0.74	-	405,405,405,405	0
8	MG	B	700	1/1	0.80	0.90	-	410,410,410,410	0

6.5 Other polymers [i](#)

There are no such residues in this entry.