



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:00 AM GMT

PDB ID : 2JIZ
Title : THE STRUCTURE OF F1-ATPASE INHIBITED BY RESVERATROL.
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2007-07-03
Resolution : 2.30 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

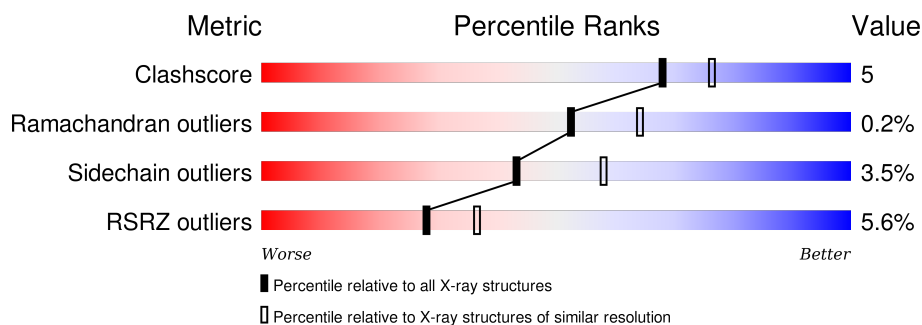
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	
1	B	510	
1	C	510	
1	H	510	
1	I	510	
1	J	510	
2	D	482	

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Mol	Chain	Length	Quality of chain
2	E	482	
2	F	482	
2	K	482	
2	L	482	
2	M	482	
3	G	272	
3	N	272	

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
10	STL	G	1273[A]	-	-	-	X
10	STL	G	1273[B]	-	-	-	X
10	STL	N	1273[A]	-	-	-	X
10	STL	N	1273[B]	-	-	-	X
6	GOL	A	1514	-	-	-	X
6	GOL	B	1512	-	-	-	X
6	GOL	C	1513	-	-	-	X
6	GOL	D	1479	-	-	-	X
6	GOL	H	1513	-	-	-	X
6	GOL	H	1514	-	-	-	X
6	GOL	I	1512	-	-	-	X
6	GOL	K	1479	-	-	-	X
8	AZI	D	1478	-	-	-	X
9	PO4	E	1475	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 50811 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 HEART ISOFORM.

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	479	Total	C	N	O	S	0	0	0
			3658	2305	647	694	12			
1	C	495	Total	C	N	O	S	0	0	0
			3768	2374	664	718	12			
1	H	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	I	479	Total	C	N	O	S	0	0	0
			3658	2305	647	694	12			
1	J	495	Total	C	N	O	S	0	0	0
			3768	2374	664	718	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	SEE REMARK 999	UNP P19483
B	1	GLU	GLN	SEE REMARK 999	UNP P19483
C	1	GLU	GLN	SEE REMARK 999	UNP P19483
H	1	GLU	GLN	SEE REMARK 999	UNP P19483
I	1	GLU	GLN	SEE REMARK 999	UNP P19483
J	1	GLU	GLN	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	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			

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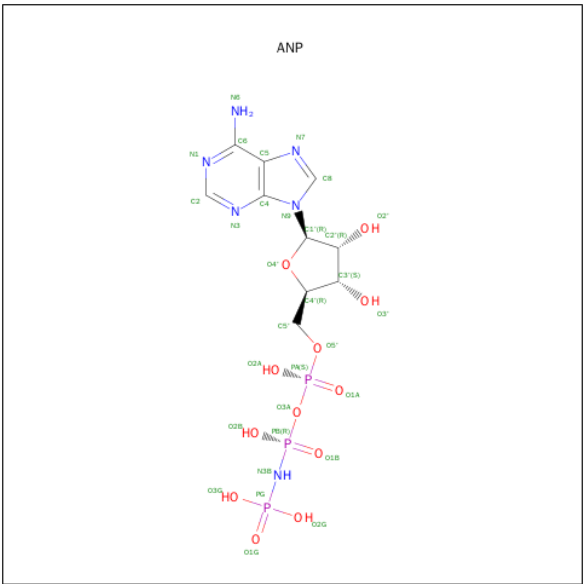
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	L	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	M	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	192	Total	C	N	O	S	0	0	0
			1492	942	268	275	7			
3	N	192	Total	C	N	O	S	0	0	0
			1492	942	268	275	7			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

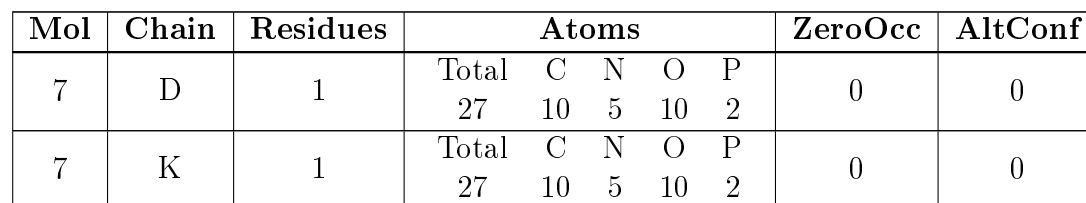
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		

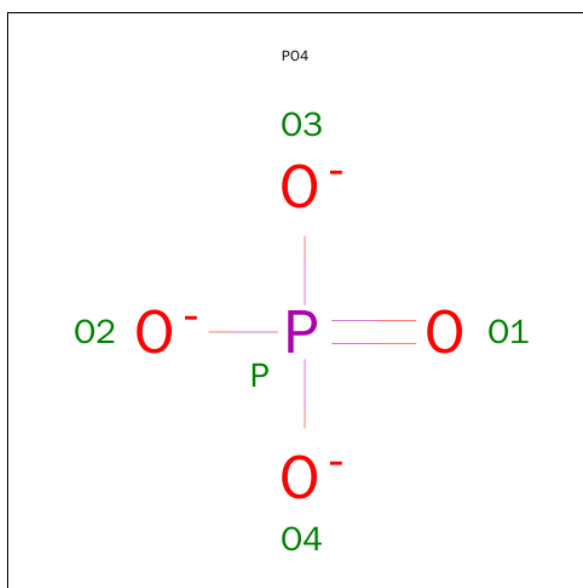
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- AZI
- N1 N⁻ N⁺ N⁻ N3

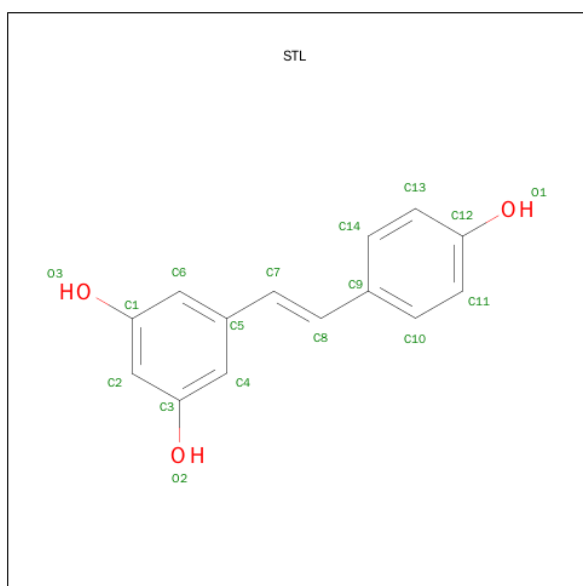
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total N 3 3	0	0
8	K	1	Total N 3 3	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	O	P	0	0
			5	4	1		
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is RESVERATROL (three-letter code: STL) (formula: C₁₄H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	1
			34	28	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	N	1	Total	C	O	0	1
			34	28	6		

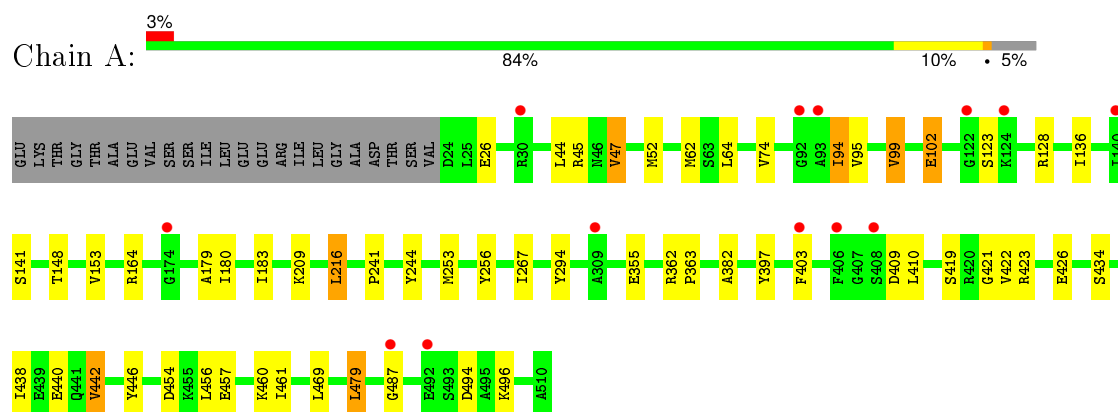
- Molecule 11 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	342	Total	O		0	0
			342	342			
11	B	284	Total	O		0	0
			284	284			
11	C	354	Total	O		0	0
			354	354			
11	D	299	Total	O		0	0
			299	299			
11	E	212	Total	O		0	0
			212	212			
11	F	328	Total	O		0	0
			328	328			
11	G	74	Total	O		0	0
			74	74			
11	H	336	Total	O		0	0
			336	336			
11	I	299	Total	O		0	0
			299	299			
11	J	363	Total	O		0	0
			363	363			
11	K	332	Total	O		0	0
			332	332			
11	L	250	Total	O		0	0
			250	250			
11	M	333	Total	O		0	0
			333	333			
11	N	73	Total	O		0	0
			73	73			

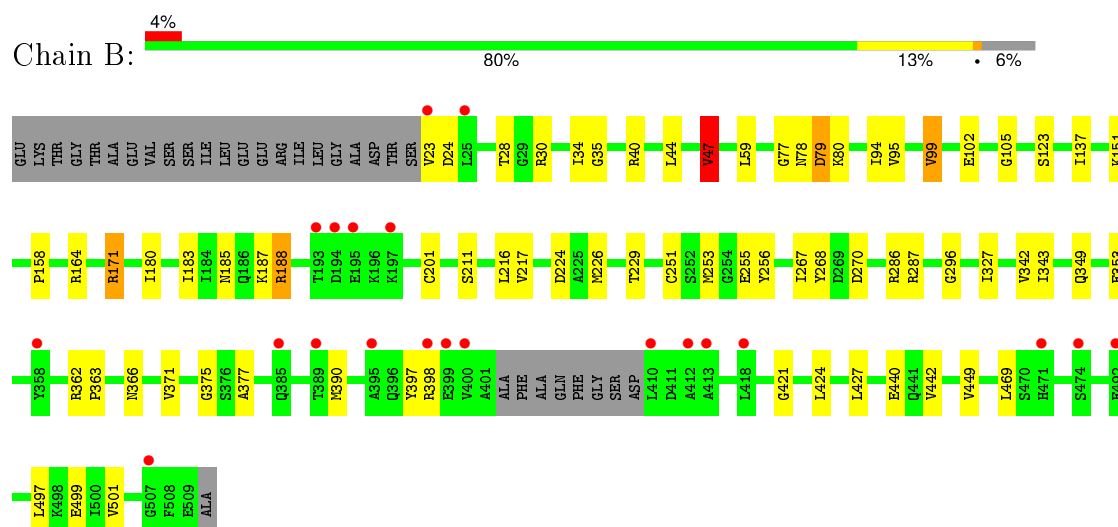
3 Residue-property plots

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.

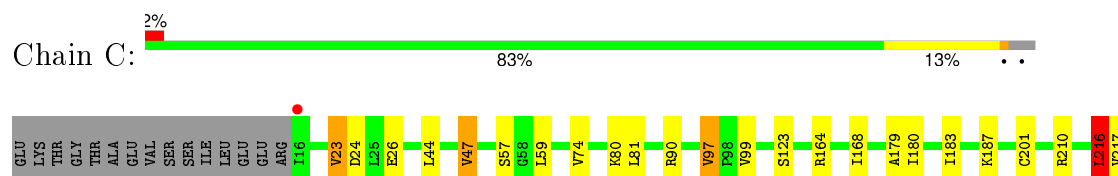
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

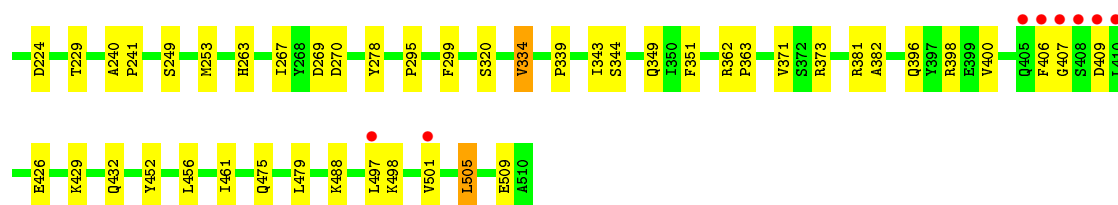


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

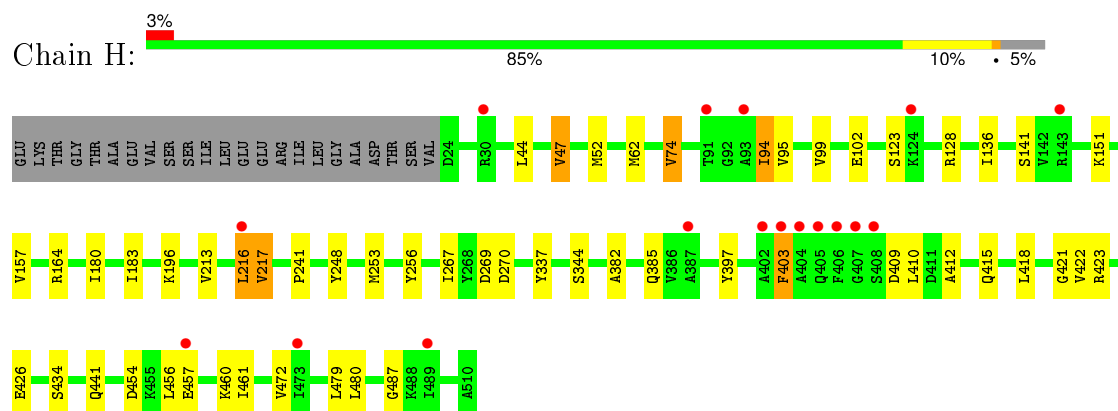


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

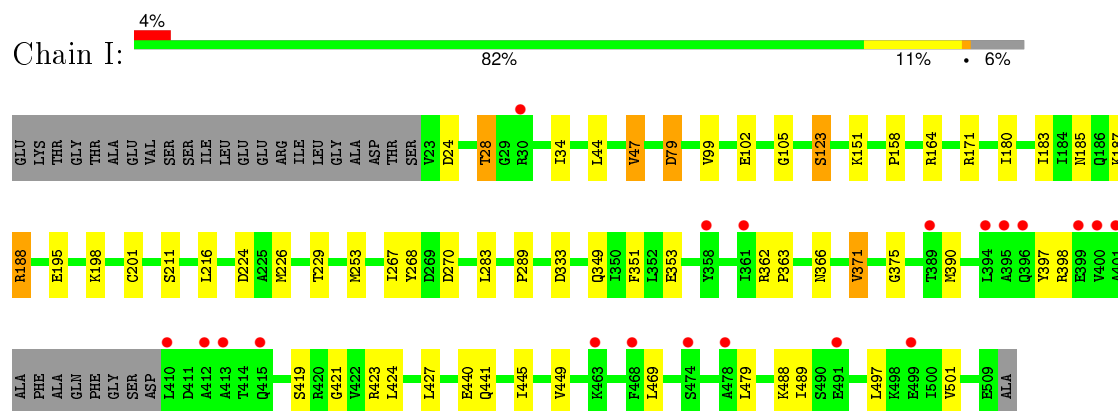




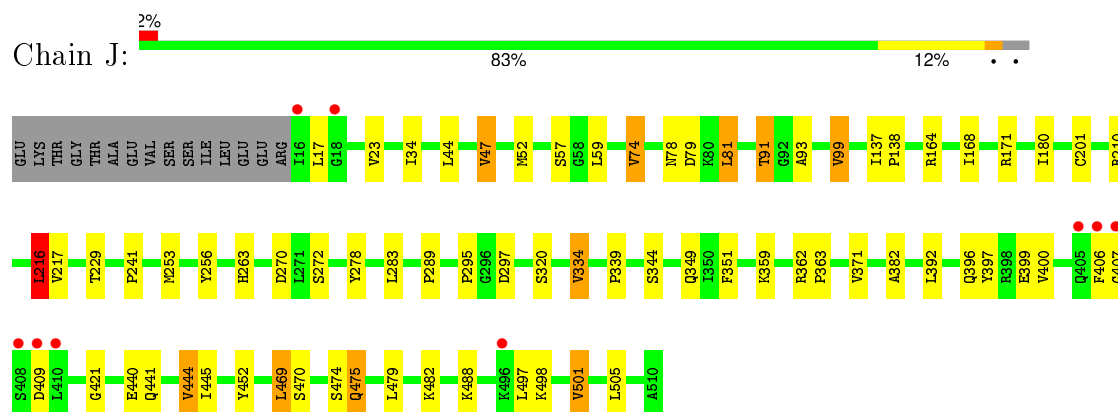
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



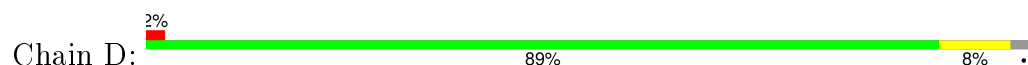
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

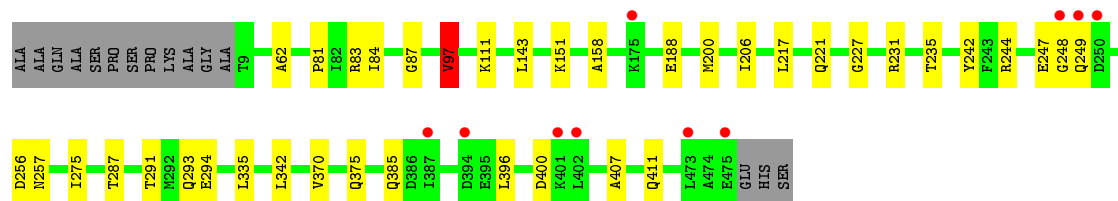


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

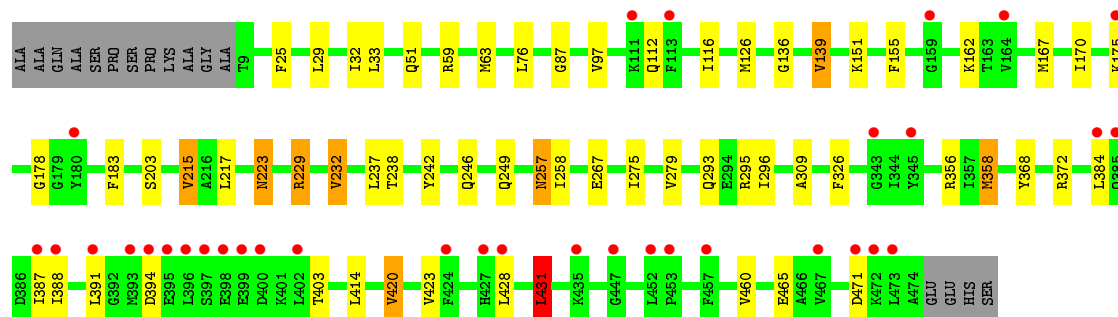
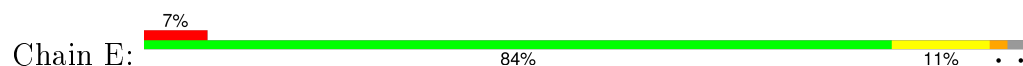


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

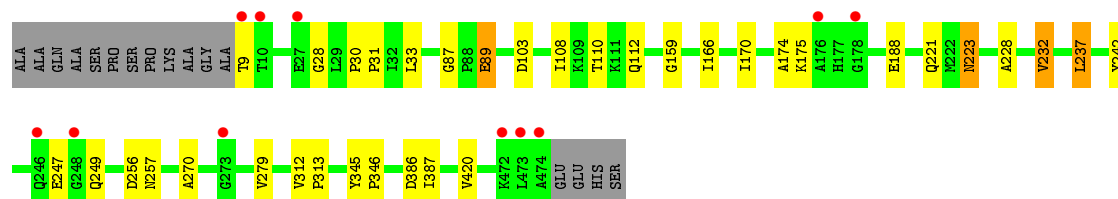
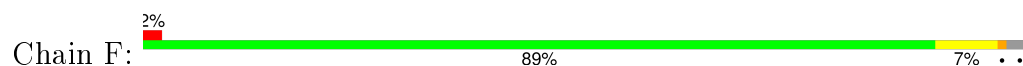




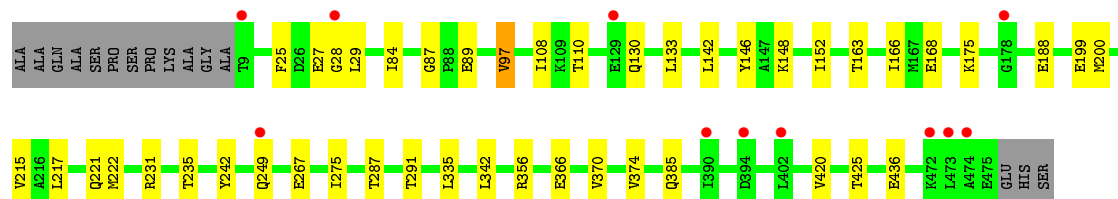
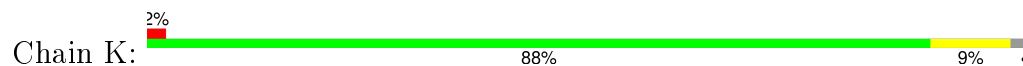
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



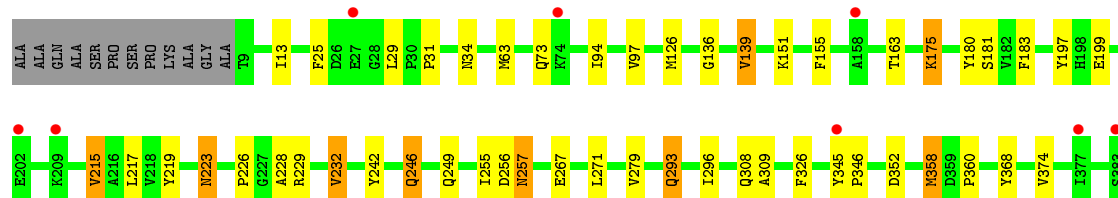
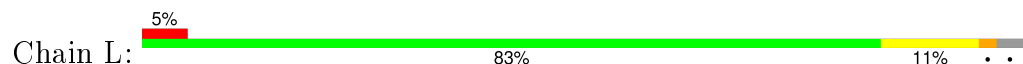
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

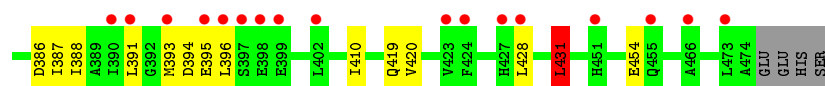


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

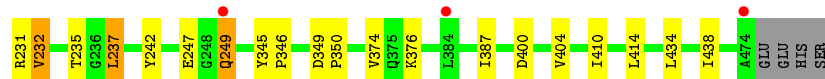
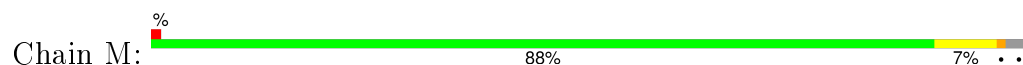


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

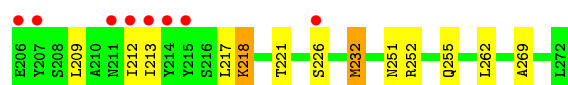
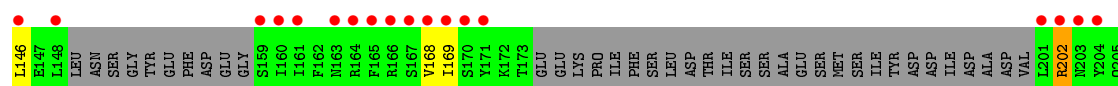
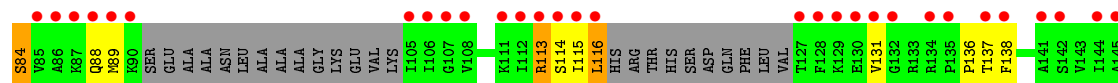
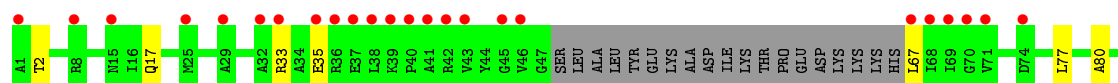




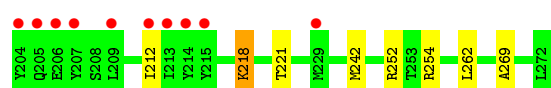
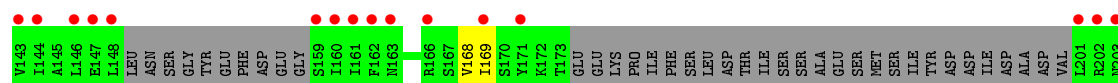
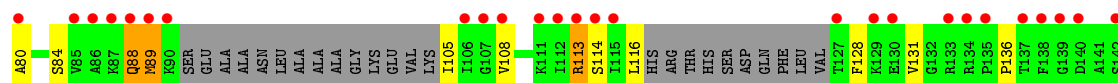
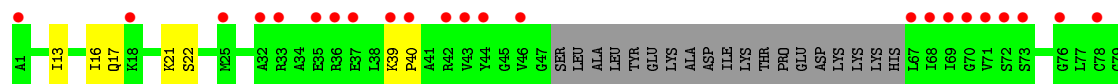
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• Molecule 3: ATP SYNTHASE GAMMA CHAIN



• Molecule 3: ATP SYNTHASE GAMMA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.78Å 277.37Å 137.83Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	138.68 – 2.30 66.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	84.6 (138.68-2.30) 83.8 (66.88-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.160 , 0.217 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.5	EDS
Estimated twinning fraction	0.387 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 299016 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50811	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, MG, ADP, GOL, STL, PO4, 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	0.47	0/3766	0.60	0/5080
1	B	0.46	0/3706	0.61	1/4998 (0.0%)
1	C	0.49	0/3819	0.62	1/5153 (0.0%)
1	H	0.46	0/3766	0.60	1/5080 (0.0%)
1	I	0.46	0/3706	0.60	1/4998 (0.0%)
1	J	0.50	0/3819	0.63	1/5153 (0.0%)
2	D	0.47	0/3596	0.59	1/4879 (0.0%)
2	E	0.43	0/3587	0.59	3/4867 (0.1%)
2	F	0.47	0/3587	0.61	1/4867 (0.0%)
2	K	0.48	0/3596	0.60	1/4879 (0.0%)
2	L	0.43	0/3587	0.59	2/4867 (0.0%)
2	M	0.47	0/3587	0.63	3/4867 (0.1%)
3	G	0.41	0/1502	0.52	0/2006
3	N	0.39	0/1502	0.51	0/2006
All	All	0.46	0/47126	0.60	16/63700 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	237	LEU	CA-CB-CG	8.32	134.44	115.30
2	F	237	LEU	CA-CB-CG	7.94	133.56	115.30
1	I	371	VAL	CB-CA-C	-6.28	99.47	111.40
2	K	97	VAL	CB-CA-C	-6.17	99.68	111.40
1	J	216	LEU	CA-CB-CG	6.02	129.15	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	3715	0	3812	40	0
1	B	3658	0	3767	45	0
1	C	3768	0	3867	35	0
1	H	3715	0	3812	33	0
1	I	3658	0	3767	39	0
1	J	3768	0	3867	42	0
2	D	3539	0	3592	23	0
2	E	3530	0	3587	49	0
2	F	3530	0	3586	21	0
2	K	3539	0	3592	31	0
2	L	3530	0	3587	45	0
2	M	3530	0	3586	30	0
3	G	1492	0	1587	15	0
3	N	1492	0	1587	16	0
4	A	31	0	13	0	0
4	B	31	0	13	0	0
4	C	31	0	13	0	0
4	F	31	0	13	1	0
4	H	31	0	13	0	0
4	I	31	0	13	0	0
4	J	31	0	13	0	0
4	M	31	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
6	A	12	0	16	1	0
6	B	12	0	16	1	0
6	C	6	0	8	0	0
6	D	6	0	8	1	0
6	H	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	6	0	8	0	0
6	J	6	0	8	0	0
6	K	12	0	16	2	0
7	D	27	0	12	1	0
7	K	27	0	12	0	0
8	D	3	0	0	1	0
8	K	3	0	0	1	0
9	E	5	0	0	0	0
9	L	5	0	0	0	0
10	G	34	0	20	0	0
10	N	34	0	19	1	0
11	A	342	0	0	1	0
11	B	284	0	0	5	0
11	C	354	0	0	4	0
11	D	299	0	0	3	0
11	E	212	0	0	5	0
11	F	328	0	0	3	0
11	G	74	0	0	4	0
11	H	336	0	0	3	0
11	I	299	0	0	2	0
11	J	363	0	0	2	0
11	K	332	0	0	7	0
11	L	250	0	0	2	0
11	M	333	0	0	3	0
11	N	73	0	0	1	0
All	All	50811	0	47859	443	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 5.

The worst 5 of 443 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:A:94:ILE:HD11	1:A:128:ARG:HG2	1.42	1.00
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.43	0.98
2:E:203:SER:HB2	2:E:420:VAL:HG22	1.46	0.95
2:L:223:ASN:HD22	2:L:223:ASN:H	1.14	0.89
2:M:223:ASN:HD22	2:M:223:ASN:H	1.22	0.86

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	485/510 (95%)	474 (98%)	11 (2%)	0	100	100
1	B	475/510 (93%)	466 (98%)	8 (2%)	1 (0%)	52	64
1	C	493/510 (97%)	480 (97%)	11 (2%)	2 (0%)	39	48
1	H	485/510 (95%)	475 (98%)	9 (2%)	1 (0%)	52	64
1	I	475/510 (93%)	464 (98%)	11 (2%)	0	100	100
1	J	493/510 (97%)	482 (98%)	9 (2%)	2 (0%)	39	48
2	D	465/482 (96%)	448 (96%)	16 (3%)	1 (0%)	52	64
2	E	464/482 (96%)	445 (96%)	18 (4%)	1 (0%)	52	64
2	F	464/482 (96%)	449 (97%)	14 (3%)	1 (0%)	52	64
2	K	465/482 (96%)	447 (96%)	17 (4%)	1 (0%)	52	64
2	L	464/482 (96%)	448 (97%)	15 (3%)	1 (0%)	52	64
2	M	464/482 (96%)	452 (97%)	11 (2%)	1 (0%)	52	64
3	G	180/272 (66%)	176 (98%)	4 (2%)	0	100	100
3	N	180/272 (66%)	176 (98%)	4 (2%)	0	100	100
All	All	6052/6496 (93%)	5882 (97%)	158 (3%)	12 (0%)	52	64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	409	ASP
1	C	407	GLY
2	D	385	GLN
1	J	407	GLY
1	J	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	393/413 (95%)	378 (96%)	15 (4%)	40	54
1	B	389/413 (94%)	377 (97%)	12 (3%)	47	64
1	C	399/413 (97%)	380 (95%)	19 (5%)	31	42
1	H	393/413 (95%)	380 (97%)	13 (3%)	45	61
1	I	389/413 (94%)	380 (98%)	9 (2%)	58	75
1	J	399/413 (97%)	377 (94%)	22 (6%)	27	36
2	D	377/386 (98%)	373 (99%)	4 (1%)	80	90
2	E	376/386 (97%)	361 (96%)	15 (4%)	38	52
2	F	376/386 (97%)	364 (97%)	12 (3%)	46	62
2	K	377/386 (98%)	375 (100%)	2 (0%)	92	97
2	L	376/386 (97%)	360 (96%)	16 (4%)	35	47
2	M	376/386 (97%)	366 (97%)	10 (3%)	52	70
3	G	162/230 (70%)	145 (90%)	17 (10%)	8	9
3	N	162/230 (70%)	154 (95%)	8 (5%)	31	41
All	All	4944/5254 (94%)	4770 (96%)	174 (4%)	43	58

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	35	GLU
1	H	141	SER
2	M	166	ILE
3	G	88	GLN
3	G	212	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	88	GLN

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Mol	Chain	Res	Type
1	I	466	ASN
2	M	419	GLN
3	G	211	ASN
1	H	432	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 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	$\# Z > 2$
4	ANP	A	1511	5	27,33,33	2.06	6 (22%)	30,52,52	2.18	6 (20%)
6	GOL	A	1513	-	5,5,5	0.32	0	5,5,5	0.51	0
6	GOL	A	1514	-	5,5,5	0.35	0	5,5,5	0.80	0
4	ANP	B	1510	5	27,33,33	1.98	7 (25%)	30,52,52	2.09	6 (20%)
6	GOL	B	1512	-	5,5,5	0.34	0	5,5,5	0.35	0
6	GOL	B	1513	-	5,5,5	0.30	0	5,5,5	1.11	1 (20%)
4	ANP	C	1511	5	27,33,33	2.20	9 (33%)	30,52,52	2.40	7 (23%)
6	GOL	C	1513	-	5,5,5	0.40	0	5,5,5	0.58	0
7	ADP	D	1476	5	22,29,29	1.02	1 (4%)	27,45,45	1.76	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	AZI	D	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	D	1479	-	5,5,5	0.39	0	5,5,5	0.26	0
9	PO4	E	1475	-	4,4,4	0.47	0	6,6,6	0.27	0
4	ANP	F	1475	5	27,33,33	2.17	8 (29%)	30,52,52	2.41	8 (26%)
10	STL	G	1273[A]	-	18,18,18	0.49	0	24,24,24	0.76	1 (4%)
10	STL	G	1273[B]	-	18,18,18	0.49	0	24,24,24	0.72	0
4	ANP	H	1511	5	27,33,33	2.11	7 (25%)	30,52,52	2.39	8 (26%)
6	GOL	H	1513	-	5,5,5	0.33	0	5,5,5	0.57	0
6	GOL	H	1514	-	5,5,5	0.30	0	5,5,5	0.80	0
4	ANP	I	1510	5	27,33,33	1.99	6 (22%)	30,52,52	2.35	5 (16%)
6	GOL	I	1512	-	5,5,5	0.29	0	5,5,5	0.36	0
4	ANP	J	1511	5	27,33,33	2.00	8 (29%)	30,52,52	2.52	6 (20%)
6	GOL	J	1513	-	5,5,5	0.39	0	5,5,5	0.49	0
7	ADP	K	1476	5	22,29,29	1.00	1 (4%)	27,45,45	1.87	3 (11%)
8	AZI	K	1478	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	K	1479	-	5,5,5	0.35	0	5,5,5	0.26	0
6	GOL	K	1480	-	5,5,5	0.40	0	5,5,5	0.32	0
9	PO4	L	1475	-	4,4,4	0.42	0	6,6,6	0.27	0
4	ANP	M	1475	5	27,33,33	2.22	10 (37%)	30,52,52	2.38	6 (20%)
10	STL	N	1273[A]	-	18,18,18	0.46	0	24,24,24	0.79	0
10	STL	N	1273[B]	-	18,18,18	0.42	0	24,24,24	0.65	0

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
4	ANP	A	1511	5	-	0/12/38/38	0/3/3/3
6	GOL	A	1513	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1514	-	-	0/4/4/4	0/0/0/0
4	ANP	B	1510	5	-	0/12/38/38	0/3/3/3
6	GOL	B	1512	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1513	-	-	0/4/4/4	0/0/0/0
4	ANP	C	1511	5	-	1/12/38/38	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	0/0/0/0
7	ADP	D	1476	5	-	0/12/32/32	0/3/3/3
8	AZI	D	1478	-	-	0/0/0/0	0/0/0/0
6	GOL	D	1479	-	-	0/4/4/4	0/0/0/0
9	PO4	E	1475	-	-	0/0/0/0	0/0/0/0
4	ANP	F	1475	5	-	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	STL	G	1273[A]	-	-	0/5/5/5	0/2/2/2
10	STL	G	1273[B]	-	-	0/5/5/5	0/2/2/2
4	ANP	H	1511	5	-	1/12/38/38	0/3/3/3
6	GOL	H	1513	-	-	0/4/4/4	0/0/0/0
6	GOL	H	1514	-	-	0/4/4/4	0/0/0/0
4	ANP	I	1510	5	-	0/12/38/38	0/3/3/3
6	GOL	I	1512	-	-	0/4/4/4	0/0/0/0
4	ANP	J	1511	5	-	0/12/38/38	0/3/3/3
6	GOL	J	1513	-	-	0/4/4/4	0/0/0/0
7	ADP	K	1476	5	-	0/12/32/32	0/3/3/3
8	AZI	K	1478	-	-	0/0/0/0	0/0/0/0
6	GOL	K	1479	-	-	0/4/4/4	0/0/0/0
6	GOL	K	1480	-	-	0/4/4/4	0/0/0/0
9	PO4	L	1475	-	-	0/0/0/0	0/0/0/0
4	ANP	M	1475	5	-	1/12/38/38	0/3/3/3
10	STL	N	1273[A]	-	-	0/5/5/5	0/2/2/2
10	STL	N	1273[B]	-	-	0/5/5/5	0/2/2/2

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1511	ANP	PG-O2G	-3.30	1.47	1.56
4	M	1475	ANP	PG-O2G	-2.65	1.49	1.56
4	C	1511	ANP	PB-O2B	-2.49	1.49	1.56
4	M	1475	ANP	PB-O2B	-2.45	1.49	1.56
4	F	1475	ANP	PG-O3G	-2.44	1.49	1.56

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1511	ANP	O1G-PG-N3B	-9.33	97.59	111.90
4	I	1510	ANP	O1G-PG-N3B	-8.06	99.53	111.90
4	C	1511	ANP	O1G-PG-N3B	-7.45	100.47	111.90
4	C	1511	ANP	N3-C2-N1	-7.44	123.19	128.89
4	H	1511	ANP	N3-C2-N1	-7.37	123.25	128.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1511	ANP	O1B-PB-N3B-PG

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Mol	Chain	Res	Type	Atoms
4	H	1511	ANP	O1B-PB-N3B-PG
4	M	1475	ANP	O1B-PB-N3B-PG

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1514	GOL	1	0
6	B	1513	GOL	1	0
7	D	1476	ADP	1	0
8	D	1478	AZI	1	0
6	D	1479	GOL	1	0
4	F	1475	ANP	1	0
6	H	1513	GOL	2	0
6	H	1514	GOL	1	0
8	K	1478	AZI	1	0
6	K	1479	GOL	1	0
6	K	1480	GOL	1	0
4	M	1475	ANP	1	0
10	N	1273[B]	STL	1	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	487/510 (95%)	0.61	13 (2%) 58 67	28, 42, 61, 88	0
1	B	479/510 (93%)	0.47	21 (4%) 38 47	28, 40, 72, 90	0
1	C	495/510 (97%)	0.35	9 (1%) 71 78	24, 36, 54, 87	0
1	H	487/510 (95%)	0.61	17 (3%) 48 56	29, 42, 61, 90	0
1	I	479/510 (93%)	0.48	20 (4%) 40 49	26, 41, 72, 91	0
1	J	495/510 (97%)	0.33	9 (1%) 71 78	25, 37, 53, 87	0
2	D	467/482 (96%)	0.43	10 (2%) 67 74	26, 37, 61, 78	0
2	E	466/482 (96%)	0.72	34 (7%) 18 25	30, 49, 91, 106	0
2	F	466/482 (96%)	0.31	11 (2%) 62 71	25, 36, 59, 77	0
2	K	467/482 (96%)	0.45	11 (2%) 62 71	24, 36, 62, 80	0
2	L	466/482 (96%)	0.69	25 (5%) 29 38	30, 50, 89, 106	0
2	M	466/482 (96%)	0.30	7 (1%) 76 81	26, 36, 59, 78	0
3	G	192/272 (70%)	2.31	80 (41%) 0 0	24, 82, 107, 117	0
3	N	192/272 (70%)	1.81	75 (39%) 0 0	24, 78, 109, 118	0
All	All	6104/6496 (93%)	0.58	342 (5%) 28 36	24, 40, 80, 118	0

The worst 5 of 342 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	128	PHE	9.9
1	B	410	LEU	9.0
3	N	146	LEU	8.7
3	G	43	VAL	8.7
3	G	40	PRO	8.5

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, 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
6	GOL	C	1513	6/6	0.92	0.28	8.02	30,33,33,35	0
6	GOL	D	1479	6/6	0.81	0.32	7.05	55,62,64,65	0
9	PO4	E	1475	5/5	0.68	0.43	5.71	137,138,138,139	0
6	GOL	H	1514	6/6	0.82	0.26	4.35	37,41,46,50	0
6	GOL	I	1512	6/6	0.95	0.27	3.88	27,32,36,36	0
6	GOL	B	1512	6/6	0.98	0.21	3.81	28,32,34,36	0
10	STL	G	1273[A]	17/17	0.96	0.22	3.58	29,34,38,40	17
10	STL	G	1273[B]	17/17	0.96	0.22	3.41	6,10,14,15	17
10	STL	N	1273[A]	17/17	0.95	0.22	3.13	31,34,39,41	17
6	GOL	A	1514	6/6	0.92	0.24	3.12	37,41,45,54	0
10	STL	N	1273[B]	17/17	0.95	0.22	3.10	2,6,13,14	17
6	GOL	K	1479	6/6	0.88	0.22	2.79	49,50,55,59	0
8	AZI	D	1478	3/3	0.95	0.25	2.75	28,28,34,36	0
6	GOL	H	1513	6/6	0.91	0.24	2.40	38,41,42,44	0
9	PO4	L	1475	5/5	0.84	0.26	1.90	102,102,104,105	0
8	AZI	K	1478	3/3	0.97	0.20	1.89	30,30,30,32	0
6	GOL	B	1513	6/6	0.93	0.18	1.76	35,46,48,51	0
6	GOL	K	1480	6/6	0.89	0.26	1.42	54,56,60,61	0
6	GOL	A	1513	6/6	0.85	0.22	1.36	43,46,47,50	0
6	GOL	J	1513	6/6	0.93	0.17	1.19	31,37,38,38	0
4	ANP	B	1510	31/31	0.96	0.18	0.84	30,40,50,58	0
4	ANP	C	1511	31/31	0.97	0.17	0.76	25,30,34,36	0
4	ANP	I	1510	31/31	0.97	0.19	0.46	24,40,49,61	0
7	ADP	K	1476	27/27	0.96	0.17	0.34	25,28,31,32	0
4	ANP	F	1475	31/31	0.97	0.16	0.21	26,31,34,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ANP	M	1475	31/31	0.97	0.17	0.18	26,31,35,40	0
7	ADP	D	1476	27/27	0.96	0.16	-0.09	24,29,32,34	0
4	ANP	H	1511	31/31	0.95	0.16	-0.15	25,37,42,49	0
4	ANP	J	1511	31/31	0.97	0.14	-0.51	25,29,33,36	0
5	MG	K	1477	1/1	0.92	0.16	-0.53	28,28,28,28	0
4	ANP	A	1511	31/31	0.96	0.14	-1.13	26,34,41,43	0
5	MG	F	1476	1/1	0.92	0.12	-1.94	23,23,23,23	0
5	MG	M	1476	1/1	0.94	0.09	-3.41	29,29,29,29	0
5	MG	D	1477	1/1	0.94	0.08	-4.61	24,24,24,24	0
5	MG	B	1511	1/1	0.87	0.14	-	33,33,33,33	0
5	MG	C	1512	1/1	0.91	0.14	-	24,24,24,24	0
5	MG	I	1511	1/1	0.96	0.08	-	34,34,34,34	0
5	MG	J	1512	1/1	0.97	0.11	-	28,28,28,28	0
5	MG	A	1512	1/1	0.94	0.13	-	36,36,36,36	0
5	MG	H	1512	1/1	0.90	0.06	-	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.