



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:13 AM GMT

PDB ID : 2JJ2
Title : THE STRUCTURE OF F1-ATPASE INHIBITED BY QUERCETIN.
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2007-07-03
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

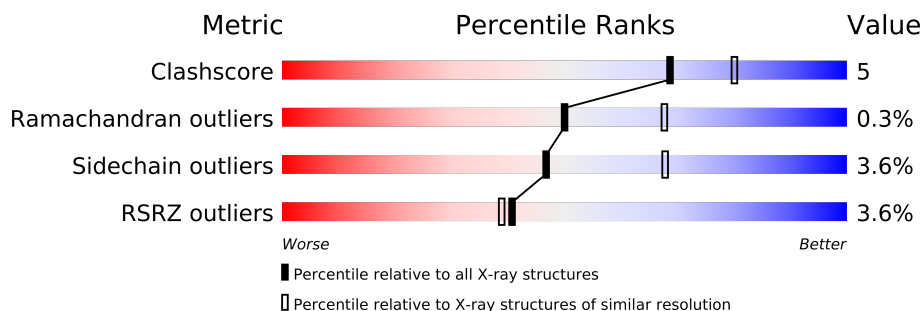
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. 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	
1	H	510	
1	I	510	
1	J	510	
2	D	482	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	A	1514	-	X
6	GOL	H	1514	-	X
6	GOL	K	1480	-	X
8	AZI	D	1478	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48794 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	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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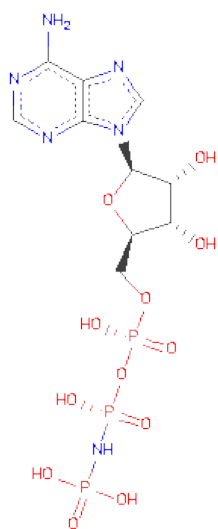
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	L	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	M	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	167	Total	C	N	O	S	0	0	0
			1296	810	237	242	7			
3	N	167	Total	C	N	O	S	0	0	0
			1296	810	237	242	7			

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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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).

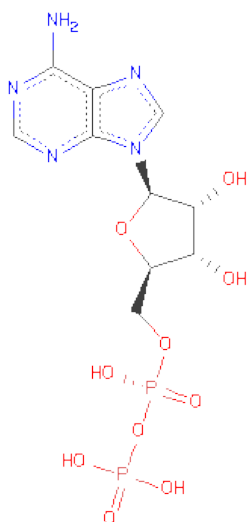
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	M	1	Total	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: $C_{10}H_{15}N_5O_{10}P_2$).



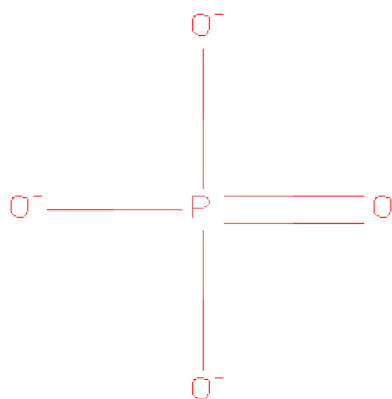
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is AZIDE ION (three-letter code: AZI) (formula: N_3).



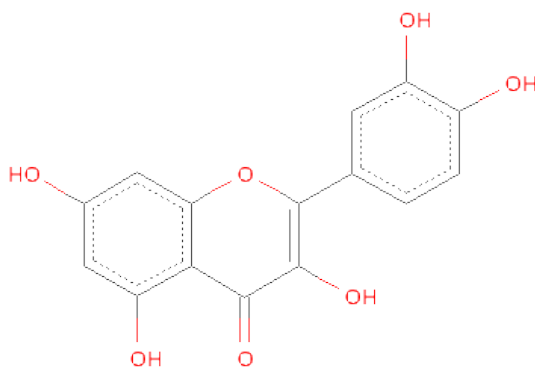
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	N	0	0
			3	3		
8	K	1	Total	N	0	0
			3	3		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: $\text{C}_{15}\text{H}_{10}\text{O}_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	1
			44	30	14		
10	N	1	Total	C	O	0	1
			44	30	14		

- Molecule 11 is water.

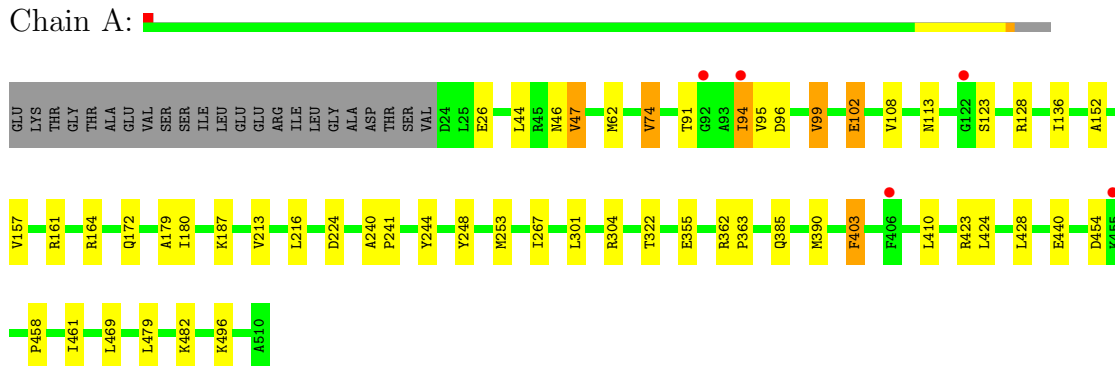
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	180	Total	O		0	0
			180	180			
11	B	153	Total	O		0	0
			153	153			
11	C	229	Total	O		0	0
			229	229			
11	D	179	Total	O		0	0
			179	179			
11	E	114	Total	O		0	0
			114	114			
11	F	205	Total	O		0	0
			205	205			
11	G	40	Total	O		0	0
			40	40			
11	H	207	Total	O		0	0
			207	207			
11	I	153	Total	O		0	0
			153	153			
11	J	236	Total	O		0	0
			236	236			
11	K	175	Total	O		0	0
			175	175			
11	L	122	Total	O		0	0
			122	122			
11	M	202	Total	O		0	0
			202	202			
11	N	39	Total	O		0	0
			39	39			

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.

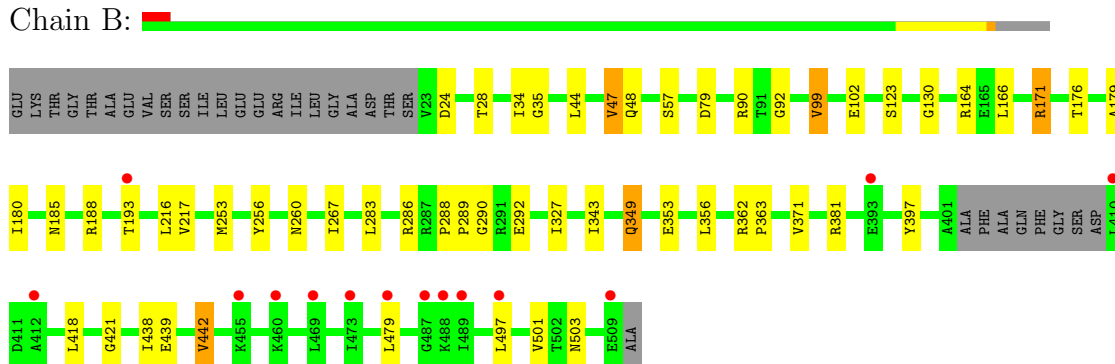
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain A:



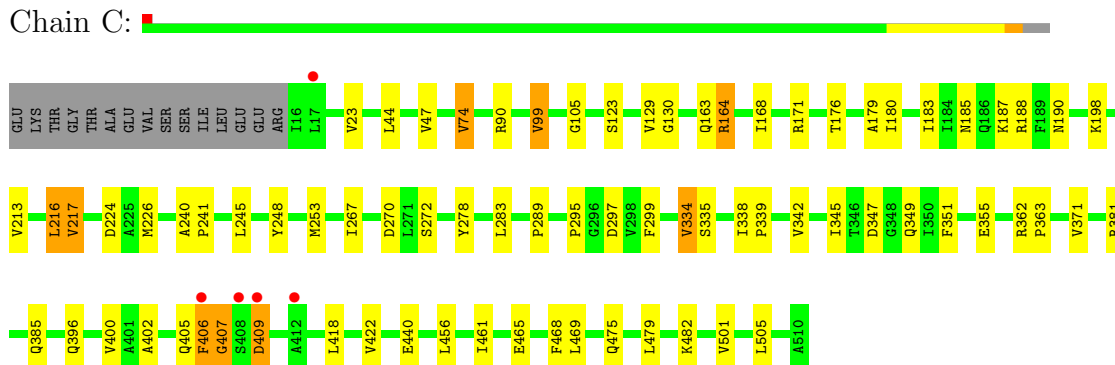
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain B:

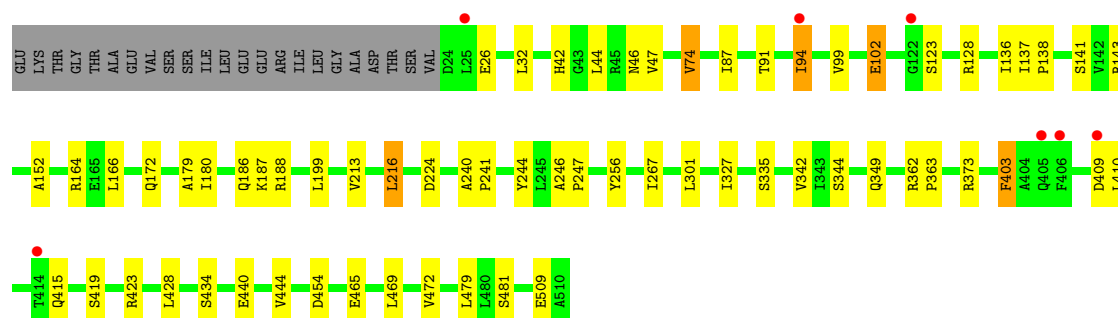


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

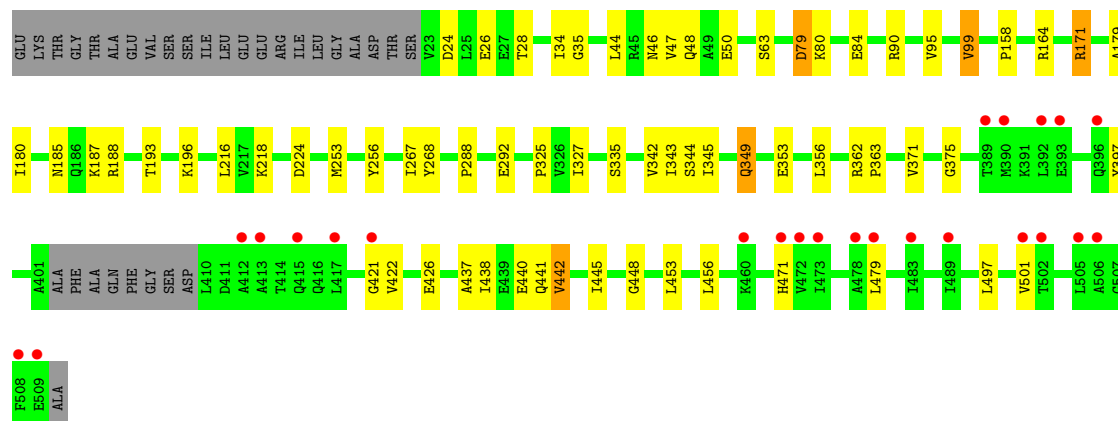
Chain C:



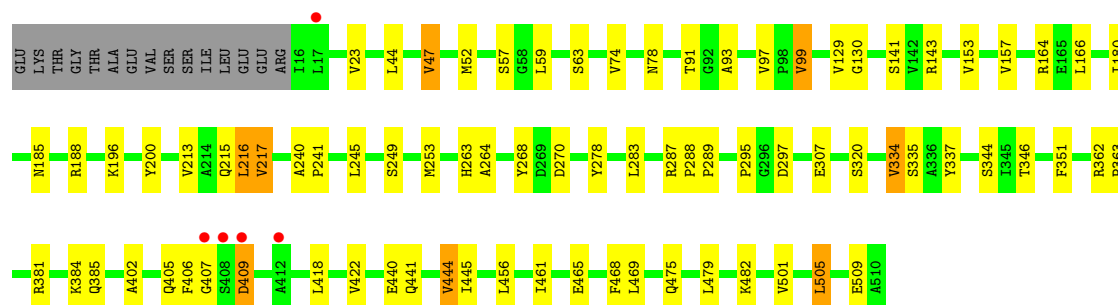
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain H: 

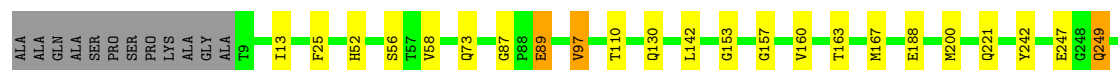
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

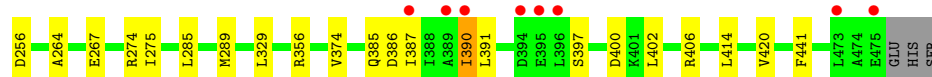
Chain I: 

- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain J: 

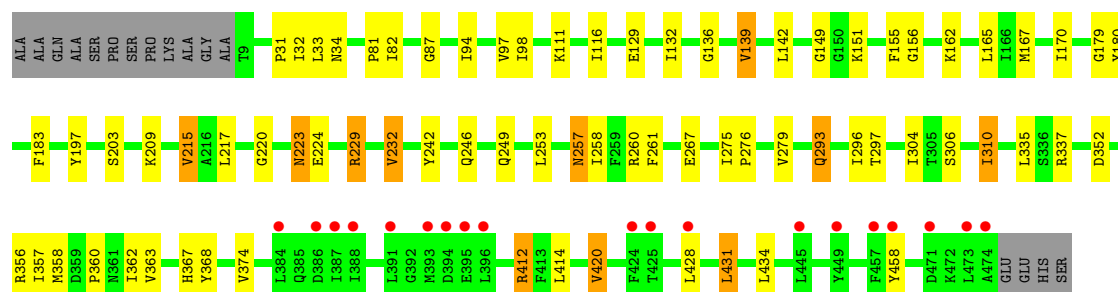
- Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain D: 



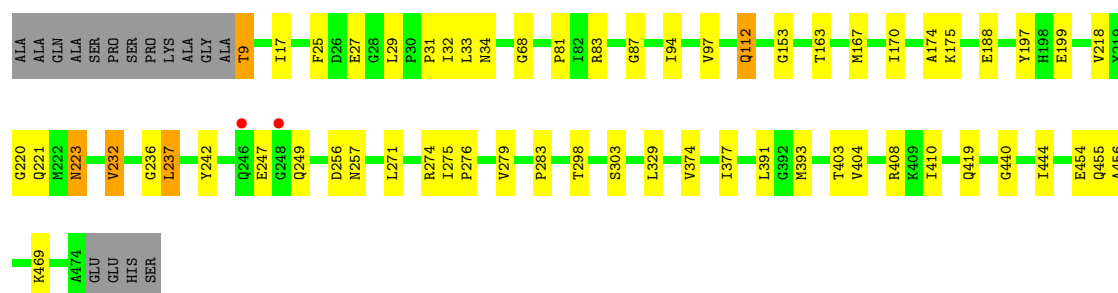
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain E:



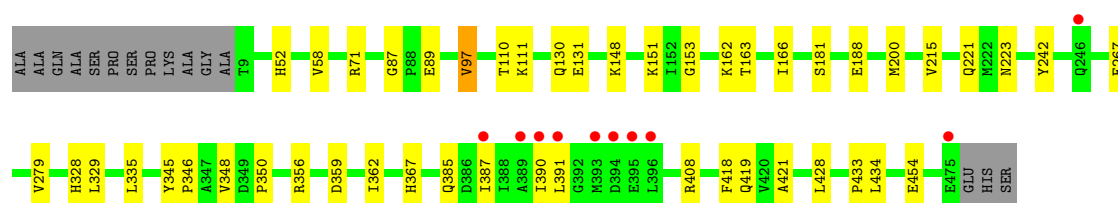
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain F:



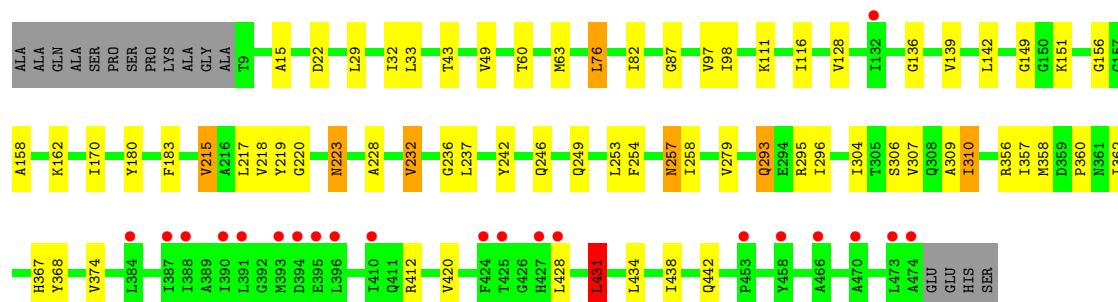
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain K:



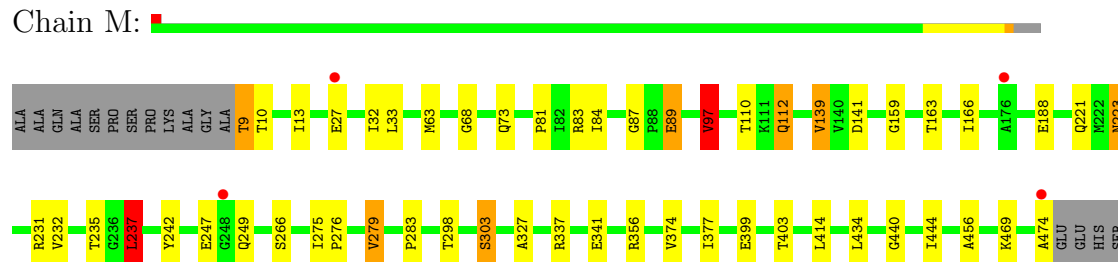
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain L:



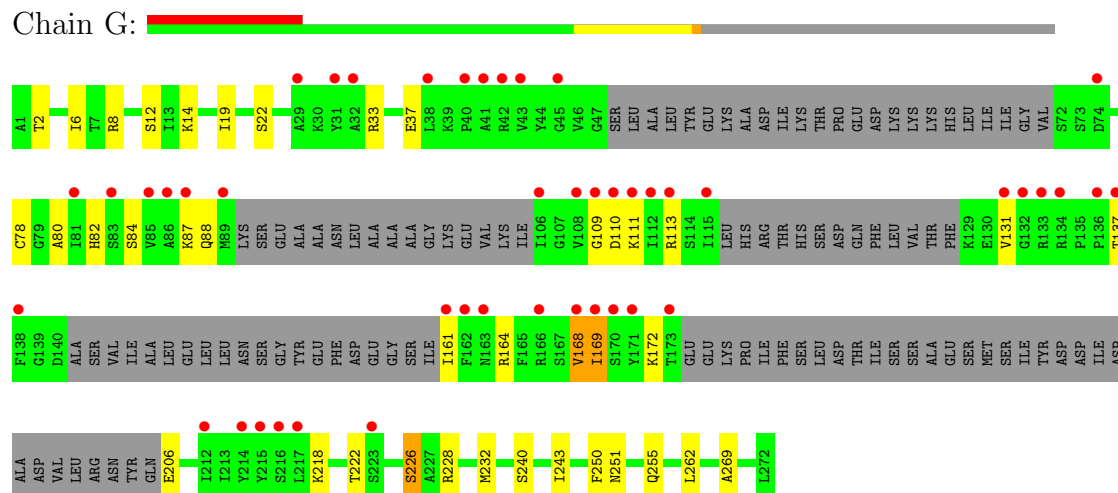
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain M:



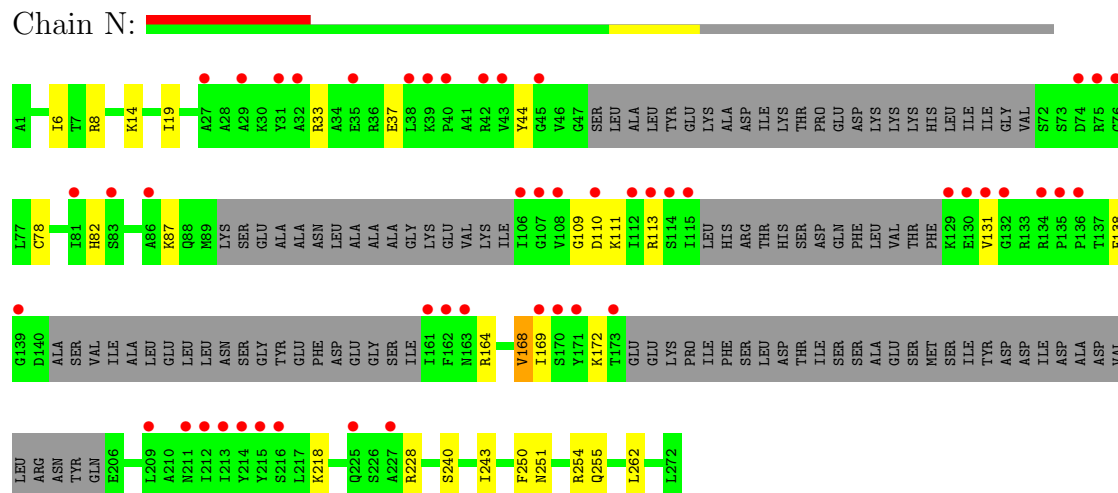
• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain G:



• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.40Å 282.02Å 138.09Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 80.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.1 (80.58-2.40) 92.1 (80.48-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.238 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.8	EDS
Estimated twinning fraction	0.328 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 297351 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	48794	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 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: AZI, MG, ADP, GOL, PO4, QUE, 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	0.41	0/3766	0.56	0/5080
1	B	0.40	0/3706	0.57	0/4998
1	C	0.43	0/3819	0.59	0/5153
1	H	0.40	0/3766	0.56	0/5080
1	I	0.41	0/3706	0.56	0/4998
1	J	0.43	0/3819	0.60	1/5153 (0.0%)
2	D	0.42	0/3596	0.57	1/4879 (0.0%)
2	E	0.39	0/3587	0.56	1/4867 (0.0%)
2	F	0.41	0/3587	0.58	1/4867 (0.0%)
2	K	0.42	0/3596	0.57	1/4879 (0.0%)
2	L	0.38	0/3587	0.57	2/4867 (0.0%)
2	M	0.42	0/3587	0.59	2/4867 (0.0%)
3	G	0.36	0/1304	0.48	0/1737
3	N	0.36	0/1304	0.49	0/1737
All	All	0.41	0/46730	0.57	9/63162 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	237	LEU	CA-CB-CG	7.28	132.04	115.30
2	M	237	LEU	CA-CB-CG	6.81	130.96	115.30
2	L	431	LEU	CA-CB-CG	6.09	129.30	115.30
2	D	97	VAL	CB-CA-C	-5.67	100.62	111.40
1	J	216	LEU	CA-CB-CG	5.67	128.35	115.30

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	3715	0	3812	33	0
1	B	3658	0	3767	36	0
1	C	3768	0	3867	45	0
1	H	3715	0	3812	43	0
1	I	3658	0	3767	40	0
1	J	3768	0	3867	42	0
2	D	3539	0	3592	31	0
2	E	3530	0	3587	47	0
2	F	3530	0	3586	33	0
2	K	3539	0	3592	26	0
2	L	3530	0	3587	37	0
2	M	3530	0	3586	31	0
3	G	1296	0	1365	19	0
3	N	1296	0	1365	13	0
4	A	31	0	13	1	0
4	B	31	0	13	0	0
4	C	31	0	13	0	0
4	F	31	0	13	0	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	2	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	4	0
6	B	12	0	16	2	0
6	C	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	6	0	8	0	0
6	H	12	0	16	0	0
6	I	6	0	8	0	0
6	J	6	0	8	2	0
6	K	12	0	16	0	0
7	D	27	0	12	0	0
7	K	27	0	12	0	0
8	D	3	0	0	0	0
8	K	3	0	0	1	0
9	E	5	0	0	0	0
9	L	5	0	0	0	0
10	G	44	0	12	4	0
10	N	44	0	15	2	0
11	A	180	0	0	3	0
11	B	153	0	0	3	0
11	C	229	0	0	2	0
11	D	179	0	0	3	0
11	E	114	0	0	1	0
11	F	205	0	0	4	0
11	G	40	0	0	3	0
11	H	207	0	0	5	0
11	I	153	0	0	4	0
11	J	236	0	0	2	0
11	K	175	0	0	2	0
11	L	122	0	0	0	0
11	M	202	0	0	5	0
11	N	39	0	0	1	0
All	All	48794	0	47403	453	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 453 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:223:ASN:H	2:E:223:ASN:HD22	1.25	0.83
1:B:290:GLY:HA3	6:B:1513:GOL:H12	1.62	0.81
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.15	0.81
2:L:183:PHE:HB3	2:L:217:LEU:HD23	1.64	0.78
1:J:180:ILE:HD11	1:J:216:LEU:HD21	1.66	0.78

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%)	469 (97%)	15 (3%)	1 (0%)	56	74
1	B	475/510 (93%)	458 (96%)	16 (3%)	1 (0%)	56	74
1	C	493/510 (97%)	481 (98%)	10 (2%)	2 (0%)	43	61
1	H	485/510 (95%)	469 (97%)	16 (3%)	0	100	100
1	I	475/510 (93%)	462 (97%)	12 (2%)	1 (0%)	56	74
1	J	493/510 (97%)	480 (97%)	10 (2%)	3 (1%)	33	47
2	D	465/482 (96%)	441 (95%)	23 (5%)	1 (0%)	56	74
2	E	464/482 (96%)	444 (96%)	17 (4%)	3 (1%)	33	47
2	F	464/482 (96%)	446 (96%)	18 (4%)	0	100	100
2	K	465/482 (96%)	442 (95%)	21 (4%)	2 (0%)	43	61
2	L	464/482 (96%)	446 (96%)	16 (3%)	2 (0%)	43	61
2	M	464/482 (96%)	445 (96%)	18 (4%)	1 (0%)	56	74
3	G	155/272 (57%)	152 (98%)	3 (2%)	0	100	100
3	N	155/272 (57%)	151 (97%)	4 (3%)	0	100	100
All	All	6002/6496 (92%)	5786 (96%)	199 (3%)	17 (0%)	50	68

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
1	J	407	GLY
1	C	409	ASP
1	J	409	ASP
1	A	385	GLN

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%)	379 (96%)	14 (4%)	47	68
1	B	389/413 (94%)	377 (97%)	12 (3%)	52	74
1	C	399/413 (97%)	384 (96%)	15 (4%)	44	65
1	H	393/413 (95%)	379 (96%)	14 (4%)	47	68
1	I	389/413 (94%)	377 (97%)	12 (3%)	52	74
1	J	399/413 (97%)	383 (96%)	16 (4%)	42	63
2	D	377/386 (98%)	372 (99%)	5 (1%)	80	93
2	E	376/386 (97%)	358 (95%)	18 (5%)	35	53
2	F	376/386 (97%)	364 (97%)	12 (3%)	51	72
2	K	377/386 (98%)	371 (98%)	6 (2%)	75	89
2	L	376/386 (97%)	360 (96%)	16 (4%)	40	59
2	M	376/386 (97%)	360 (96%)	16 (4%)	40	59
3	G	140/230 (61%)	126 (90%)	14 (10%)	11	16
3	N	140/230 (61%)	132 (94%)	8 (6%)	29	44
All	All	4900/5254 (93%)	4722 (96%)	178 (4%)	47	68

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	110	ASP
1	H	403	PHE
2	M	249	GLN
3	G	137	THR
1	H	74	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	443	GLN
1	I	48	GLN
2	M	419	GLN
3	G	15	ASN
3	G	211	ASN

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 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	33,33,33	3.13	8 (24%)	51,52,52	2.10	12 (23%)
6	GOL	A	1513	-	5,5,5	0.31	0	5,5,5	0.55	0
6	GOL	A	1514	-	5,5,5	0.32	0	5,5,5	0.72	0
4	ANP	B	1510	5	33,33,33	3.31	6 (18%)	51,52,52	2.01	12 (23%)
6	GOL	B	1512	-	5,5,5	0.39	0	5,5,5	0.30	0
6	GOL	B	1513	-	5,5,5	0.31	0	5,5,5	0.48	0
4	ANP	C	1511	5	33,33,33	3.09	7 (21%)	51,52,52	2.13	13 (25%)
6	GOL	C	1513	-	5,5,5	0.36	0	5,5,5	0.22	0
7	ADP	D	1476	5	29,29,29	1.20	2 (6%)	45,45,45	1.71	7 (15%)
8	AZI	D	1478	-	2,2,2	1.19	0	0,1,1	0.00	-
6	GOL	D	1479	-	5,5,5	0.36	0	5,5,5	0.38	0
9	PO4	E	1475	-	4,4,4	0.25	0	6,6,6	0.31	0
4	ANP	F	1475	5	33,33,33	3.33	6 (18%)	51,52,52	2.13	12 (23%)
10	QUE	G	1273[A]	-	23,24,24	2.46	6 (26%)	33,36,36	1.68	6 (18%)
10	QUE	G	1273[B]	-	23,24,24	2.40	6 (26%)	33,36,36	1.61	5 (15%)
4	ANP	H	1511	5	33,33,33	3.29	6 (18%)	51,52,52	2.00	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	H	1513	-	5,5,5	0.39	0	5,5,5	0.33	0
6	GOL	H	1514	-	5,5,5	0.37	0	5,5,5	0.43	0
4	ANP	I	1510	5	33,33,33	3.19	6 (18%)	51,52,52	2.16	11 (21%)
6	GOL	I	1512	-	5,5,5	0.37	0	5,5,5	0.41	0
4	ANP	J	1511	5	33,33,33	3.18	7 (21%)	51,52,52	1.94	12 (23%)
6	GOL	J	1513	-	5,5,5	0.37	0	5,5,5	0.49	0
7	ADP	K	1476	5	29,29,29	1.20	2 (6%)	45,45,45	1.67	7 (15%)
8	AZI	K	1478	-	2,2,2	1.30	0	0,1,1	0.00	-
6	GOL	K	1479	-	5,5,5	0.41	0	5,5,5	0.24	0
6	GOL	K	1480	-	5,5,5	0.29	0	5,5,5	0.45	0
9	PO4	L	1475	-	4,4,4	0.28	0	6,6,6	0.31	0
4	ANP	M	1475	5	33,33,33	3.23	6 (18%)	51,52,52	2.11	13 (25%)
10	QUE	N	1273[A]	-	23,24,24	2.53	6 (26%)	33,36,36	1.73	5 (15%)
10	QUE	N	1273[B]	-	23,24,24	2.43	6 (26%)	33,36,36	1.64	5 (15%)

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	-	0/18/38/38	0/1/3/3
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	-	0/18/38/38	0/1/3/3
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	-	0/18/38/38	0/1/3/3
6	GOL	C	1513	-	-	0/4/4/4	0/0/0/0
7	ADP	D	1476	5	-	0/16/32/32	0/1/3/3
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	-	0/18/38/38	0/1/3/3
10	QUE	G	1273[A]	-	-	0/4/4/4	0/1/3/3
10	QUE	G	1273[B]	-	-	0/4/4/4	0/1/3/3
4	ANP	H	1511	5	-	0/18/38/38	0/1/3/3
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	-	0/18/38/38	0/1/3/3
6	GOL	I	1512	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	J	1511	5	-	0/18/38/38	0/1/3/3
6	GOL	J	1513	-	-	0/4/4/4	0/0/0/0
7	ADP	K	1476	5	-	0/16/32/32	0/1/3/3
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	-	0/18/38/38	0/1/3/3
10	QUE	N	1273[A]	-	-	0/4/4/4	0/1/3/3
10	QUE	N	1273[B]	-	-	0/4/4/4	0/1/3/3

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1511	ANP	PB-N3B	12.45	1.75	1.64
4	F	1475	ANP	PG-N3B	12.16	1.74	1.64
4	B	1510	ANP	PB-N3B	12.13	1.74	1.64
4	J	1511	ANP	PB-N3B	11.99	1.74	1.64
4	I	1510	ANP	PB-N3B	11.69	1.74	1.64

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1511	ANP	N3-C2-N1	-7.48	122.46	128.71
4	F	1475	ANP	O1G-PG-N3B	-7.38	100.67	111.83
4	I	1510	ANP	O1G-PG-N3B	-7.17	101.00	111.83
4	M	1475	ANP	O1G-PG-N3B	-6.98	101.28	111.83
4	A	1511	ANP	N3-C2-N1	-6.74	123.07	128.71

There are no chirality outliers.

There are no torsion outliers.

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, 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%)	0.11	5 (1%) 79 79	19, 38, 62, 98	0
1	B	479/510 (93%)	0.14	14 (2%) 49 47	16, 37, 90, 105	0
1	C	495/510 (97%)	-0.03	5 (1%) 79 79	14, 32, 54, 94	0
1	H	487/510 (95%)	0.10	7 (1%) 72 71	17, 38, 61, 100	0
1	I	479/510 (93%)	0.25	24 (5%) 28 25	16, 37, 90, 104	0
1	J	495/510 (97%)	-0.06	5 (1%) 79 79	17, 32, 53, 94	0
2	D	467/482 (96%)	0.09	8 (1%) 67 65	16, 33, 65, 92	0
2	E	466/482 (96%)	0.38	19 (4%) 35 33	19, 46, 90, 117	0
2	F	466/482 (96%)	-0.07	2 (0%) 90 90	13, 31, 57, 73	0
2	K	467/482 (96%)	0.10	10 (2%) 60 58	17, 33, 65, 92	0
2	L	466/482 (96%)	0.39	21 (4%) 32 30	20, 46, 89, 117	0
2	M	466/482 (96%)	-0.09	4 (0%) 81 81	15, 30, 57, 74	0
3	G	167/272 (61%)	1.31	46 (27%) 1 1	16, 78, 123, 128	0
3	N	167/272 (61%)	1.33	49 (29%) 1 1	18, 76, 124, 129	0
All	All	6054/6496 (93%)	0.18	219 (3%) 41 39	13, 37, 87, 129	0

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	40	PRO	6.8
3	N	169	ILE	6.6
1	H	406	PHE	6.5
2	K	390	ILE	6.3
3	N	161	ILE	6.2

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	A	1514	6/6	0.37	12.27	32,38,46,54	0
6	GOL	H	1514	6/6	0.26	4.16	36,45,46,53	0
8	AZI	D	1478	3/3	0.19	4.02	10,10,12,22	0
6	GOL	K	1480	6/6	0.24	2.29	38,45,47,50	0
6	GOL	B	1513	6/6	0.16	1.74	28,38,39,42	0
10	QUE	N	1273[B]	22/22	0.17	1.32	49,51,51,51	22
10	QUE	N	1273[A]	22/22	0.17	1.28	34,42,44,45	22
6	GOL	H	1513	6/6	0.19	1.19	44,46,49,53	0
6	GOL	C	1513	6/6	0.16	0.87	36,38,41,47	0
6	GOL	J	1513	6/6	0.15	0.26	31,33,37,37	0
6	GOL	A	1513	6/6	0.16	0.23	39,41,46,48	0
9	PO4	L	1475	5/5	0.17	0.08	84,84,85,86	0
4	ANP	M	1475	31/31	0.14	0.00	18,25,30,33	0
7	ADP	D	1476	27/27	0.15	-0.04	13,25,29,29	0
4	ANP	I	1510	31/31	0.15	-0.13	20,37,44,52	0
10	QUE	G	1273[B]	22/22	0.14	-0.22	65,65,66,66	22
10	QUE	G	1273[A]	22/22	0.14	-0.25	37,41,43,43	22
7	ADP	K	1476	27/27	0.14	-0.29	20,26,29,30	0
4	ANP	J	1511	31/31	0.14	-0.36	14,26,28,30	0
4	ANP	C	1511	31/31	0.13	-0.49	18,24,32,34	0
5	MG	J	1512	1/1	0.13	-0.50	18,18,18,18	0
4	ANP	B	1510	31/31	0.14	-0.51	22,36,42,48	0
6	GOL	B	1512	6/6	0.14	-0.51	20,23,24,31	0
4	ANP	A	1511	31/31	0.14	-0.60	18,25,32,33	0
4	ANP	H	1511	31/31	0.14	-0.65	20,29,34,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ANP	F	1475	31/31	0.13	-0.81	13,22,35,36	0
6	GOL	K	1479	6/6	0.14	-0.92	38,41,44,49	0
9	PO4	E	1475	5/5	0.10	-1.51	70,70,71,71	0
6	GOL	D	1479	6/6	0.12	-1.83	29,37,40,43	0
6	GOL	I	1512	6/6	0.13	-2.02	19,27,28,37	0
5	MG	H	1512	1/1	0.11	-2.12	25,25,25,25	0
5	MG	C	1512	1/1	0.10	-2.20	14,14,14,14	0
5	MG	M	1476	1/1	0.10	-2.36	16,16,16,16	0
5	MG	A	1512	1/1	0.12	-2.62	28,28,28,28	0
5	MG	B	1511	1/1	0.07	-2.79	29,29,29,29	0
8	AZI	K	1478	3/3	0.10	-2.79	6,6,12,18	0
5	MG	K	1477	1/1	0.09	-3.14	22,22,22,22	0
5	MG	D	1477	1/1	0.08	-5.68	18,18,18,18	0
5	MG	I	1511	1/1	0.06	-8.22	29,29,29,29	0
5	MG	F	1476	1/1	0.08	-9.68	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.