



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:00 PM GMT

PDB ID : 1W0K  
Title : ADP inhibited bovine F1-ATPase  
Authors : Kagawa, R.; Montgomery, M.G.; Braig, K.; Walker, J.E.; Leslie, A.G.W.  
Deposited on : 2004-06-08  
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

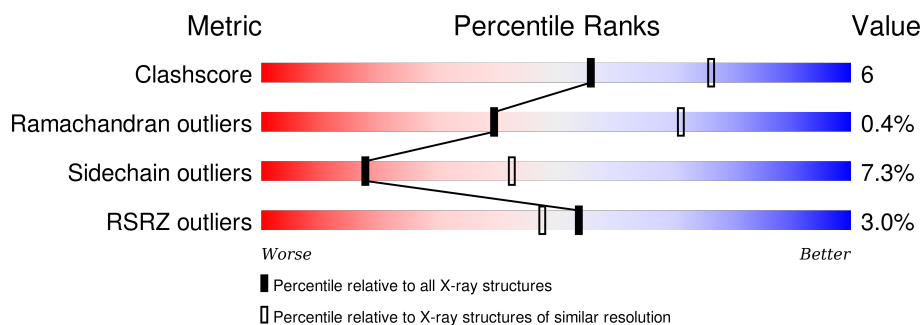
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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></div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	B	510	<div> <div></div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	C	510	<div> <div></div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
2	D	482	<div> <div></div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
2	E	482	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
2	F	482	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>
3	G	272	<div> <div>6%</div> <div> <div></div> <div>38%</div> <div>7%</div> <div>55%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	D	1477	-	-	-	X
6	GOL	D	1478	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23092 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 ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRECURSOR.

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
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

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

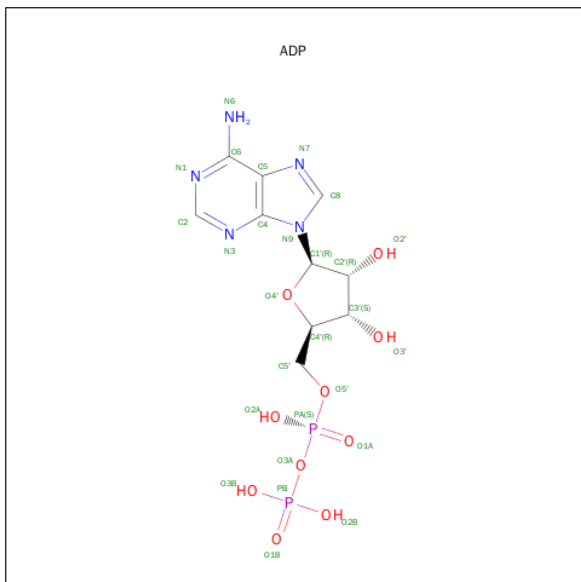
- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR.

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

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

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

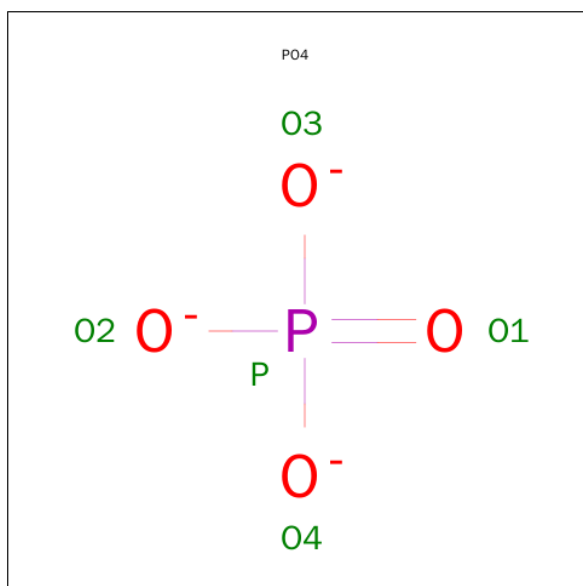
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

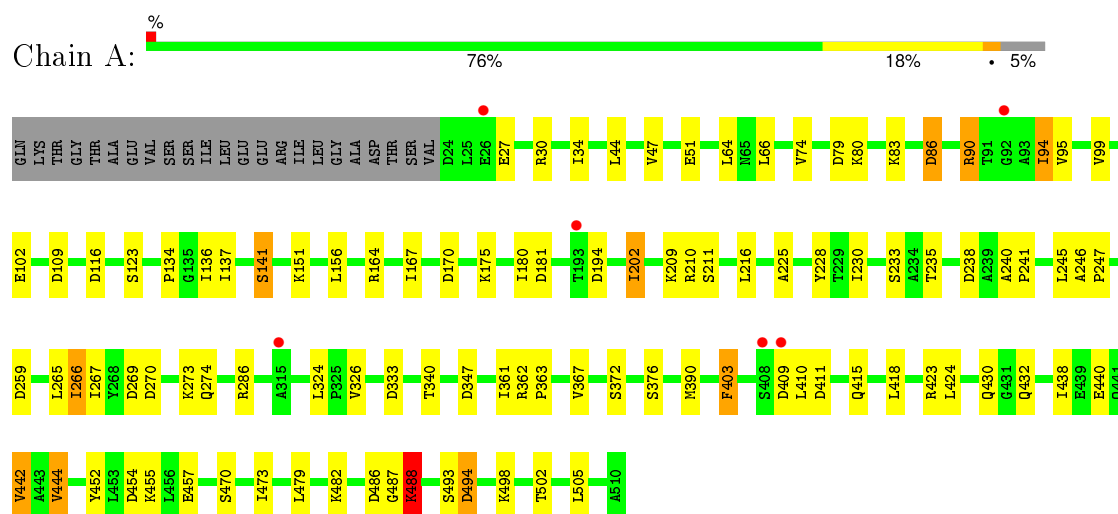
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	48	Total	O	0	0
			48	48		
8	B	40	Total	O	0	0
			40	40		
8	C	54	Total	O	0	0
			54	54		
8	D	51	Total	O	0	0
			51	51		
8	E	20	Total	O	0	0
			20	20		
8	F	48	Total	O	0	0
			48	48		
8	G	5	Total	O	0	0
			5	5		

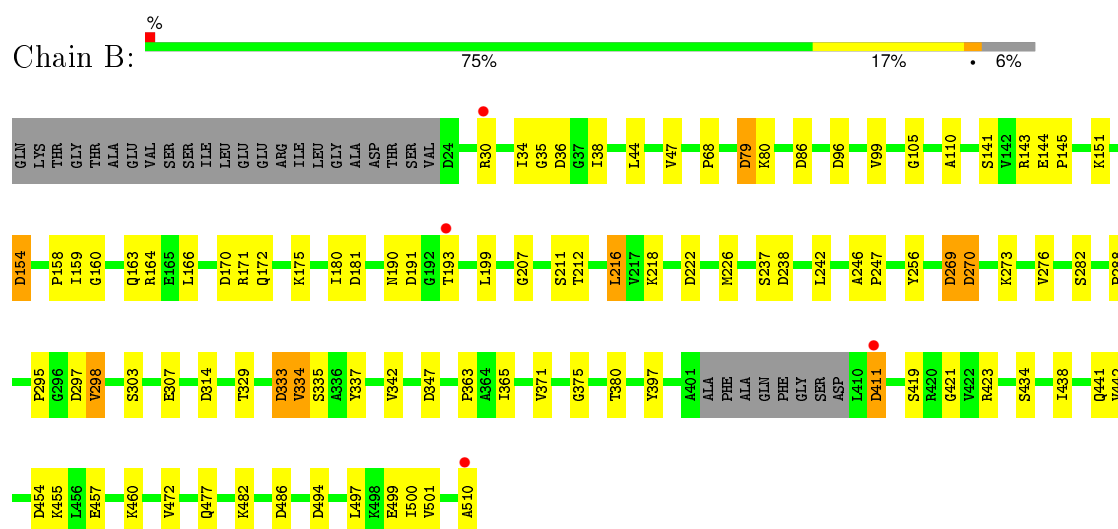
### 3 Residue-property plots [i](#)

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 ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

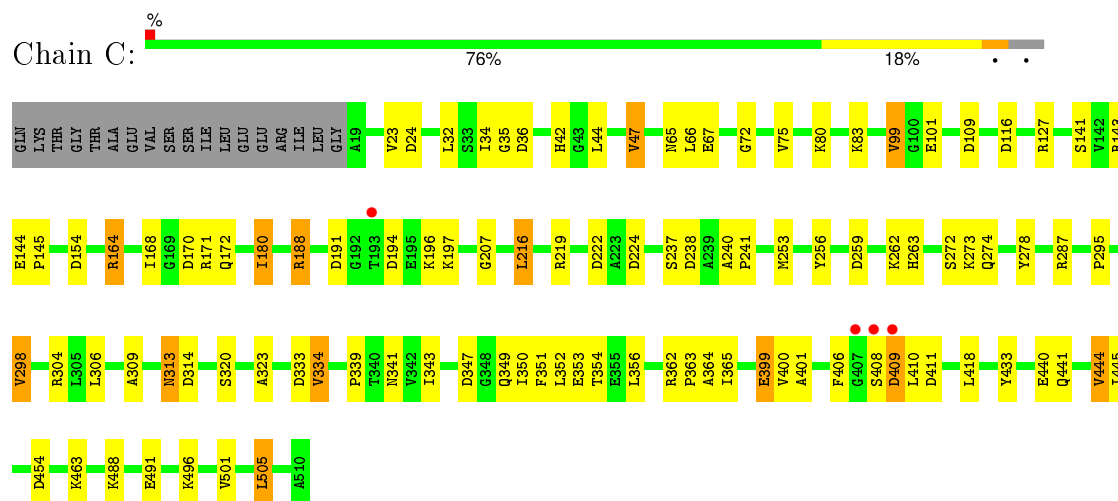


- Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

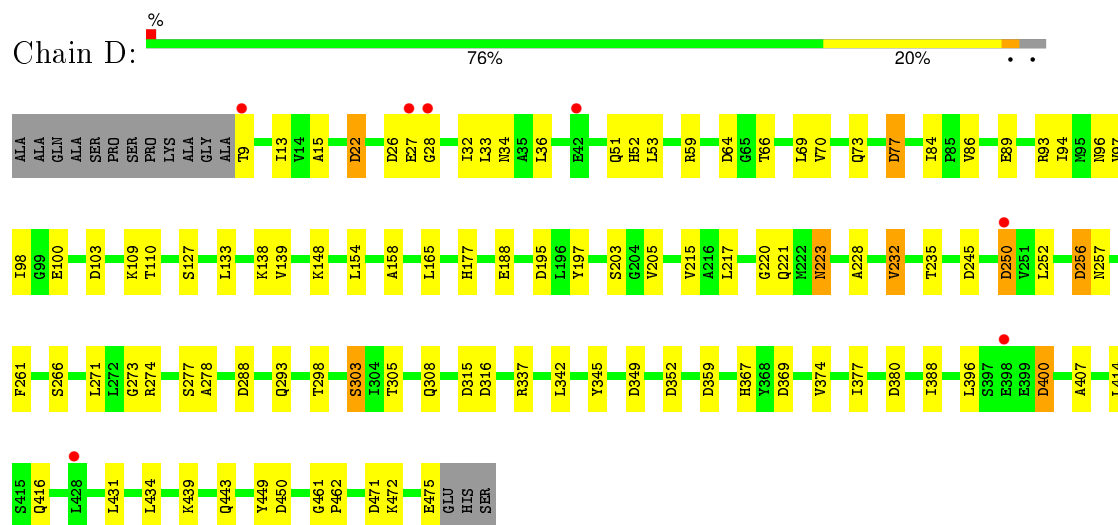


- Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

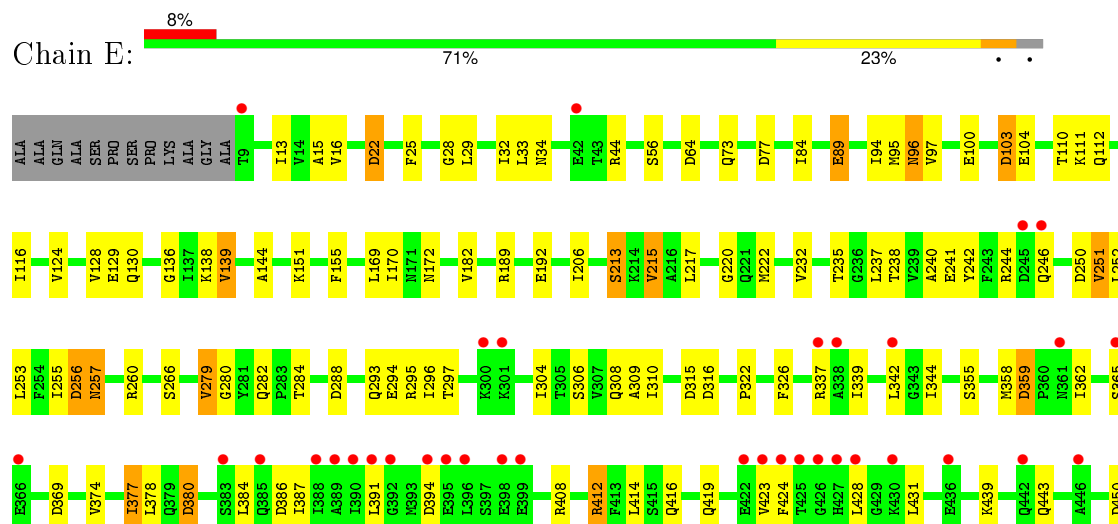


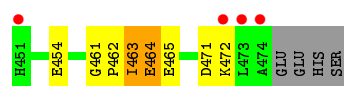


- Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR

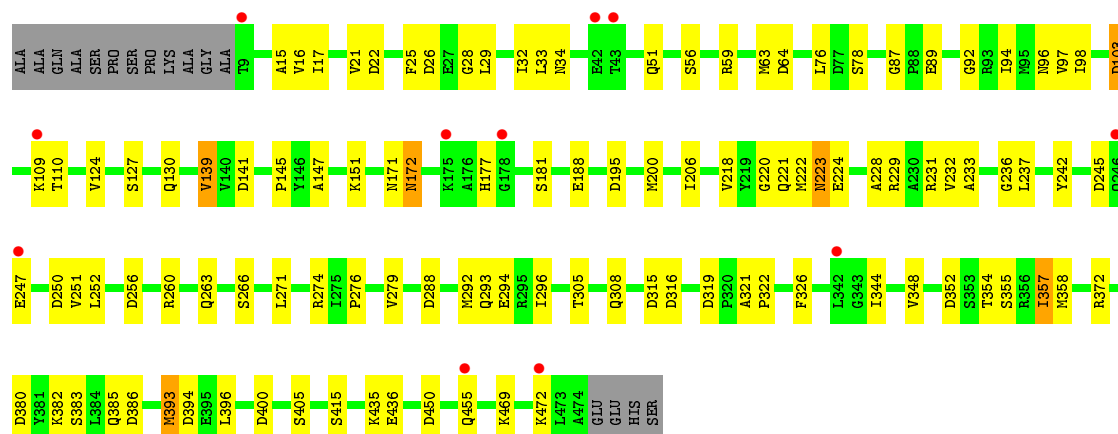
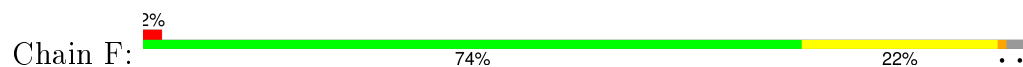


- Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR

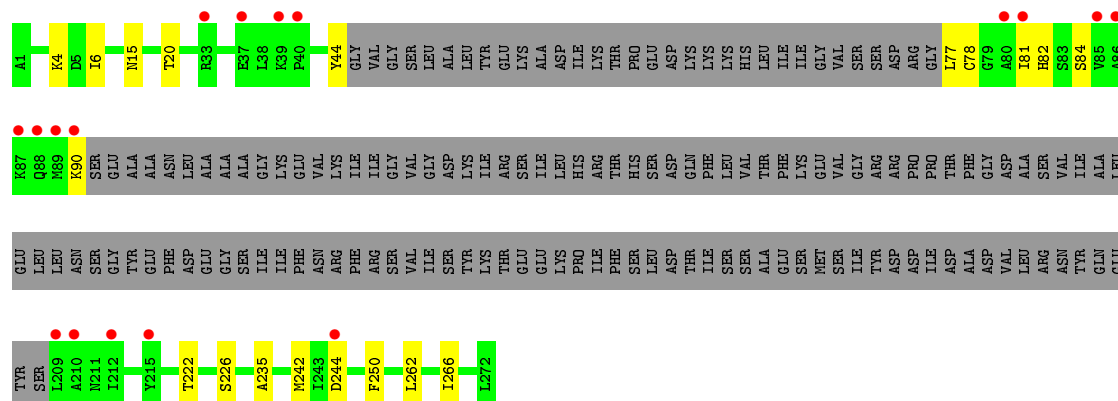
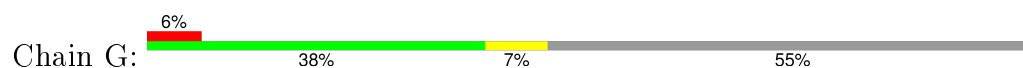




- Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR



- Molecule 3: ATP SYNTHASE GAMMA CHAIN, MITOCHONDRIAL PRECURSOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	283.04Å 107.61Å 139.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 19.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-2.85) 92.8 (19.99-2.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.51 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.222 , 0.278 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 92728 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: GOL, PO4, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/3766	0.71	14/5080 (0.3%)
1	B	0.35	0/3704	0.72	20/4995 (0.4%)
1	C	0.36	0/3799	0.73	18/5126 (0.4%)
2	D	0.34	0/3596	0.74	19/4879 (0.4%)
2	E	0.34	0/3587	0.70	15/4867 (0.3%)
2	F	0.35	0/3587	0.72	17/4867 (0.3%)
3	G	0.34	0/949	0.60	1/1266 (0.1%)
All	All	0.35	0/22988	0.71	104/31080 (0.3%)

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	103	ASP	CB-CG-OD2	7.44	125.00	118.30
2	E	316	ASP	CB-CG-OD2	7.17	124.76	118.30
2	D	77	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	109	ASP	CB-CG-OD2	7.02	124.62	118.30
2	D	256	ASP	CB-CG-OD2	6.86	124.47	118.30
2	D	22	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	36	ASP	CB-CG-OD2	6.75	124.38	118.30
2	D	195	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	96	ASP	CB-CG-OD2	6.66	124.30	118.30
1	C	191	ASP	CB-CG-OD2	6.59	124.23	118.30
2	E	77	ASP	CB-CG-OD2	6.58	124.22	118.30
2	D	359	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	333	ASP	CB-CG-OD2	6.48	124.13	118.30
1	C	109	ASP	CB-CG-OD2	6.46	124.11	118.30
2	D	349	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	194	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	486	ASP	CB-CG-OD2	6.30	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	369	ASP	CB-CG-OD2	6.29	123.96	118.30
2	E	103	ASP	CB-CG-OD2	6.28	123.95	118.30
2	F	195	ASP	CB-CG-OD2	6.25	123.92	118.30
2	D	380	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	238	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	454	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	454	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	194	ASP	CB-CG-OD2	6.21	123.89	118.30
2	E	22	ASP	CB-CG-OD2	6.19	123.87	118.30
2	F	103	ASP	CB-CG-OD2	6.18	123.86	118.30
2	D	315	ASP	CB-CG-OD2	6.17	123.85	118.30
2	D	64	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	36	ASP	CB-CG-OD2	6.09	123.78	118.30
2	F	450	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	259	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	454	ASP	CB-CG-OD2	6.08	123.78	118.30
2	D	400	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	333	ASP	CB-CG-OD2	6.06	123.76	118.30
2	F	141	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	181	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	191	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	170	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	154	ASP	CB-CG-OD2	5.96	123.67	118.30
2	F	319	ASP	CB-CG-OD2	5.96	123.67	118.30
2	F	22	ASP	CB-CG-OD2	5.95	123.66	118.30
2	E	256	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	222	ASP	CB-CG-OD2	5.93	123.64	118.30
2	E	394	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	259	ASP	CB-CG-OD2	5.88	123.60	118.30
2	F	394	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	116	ASP	CB-CG-OD2	5.83	123.55	118.30
2	D	471	ASP	CB-CG-OD2	5.79	123.51	118.30
2	F	245	ASP	CB-CG-OD2	5.79	123.51	118.30
2	F	400	ASP	CB-CG-OD2	5.76	123.48	118.30
2	D	26	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	314	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	238	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	170	ASP	CB-CG-OD2	5.69	123.42	118.30
2	E	471	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	116	ASP	CB-CG-OD2	5.68	123.42	118.30
2	D	245	ASP	CB-CG-OD2	5.67	123.40	118.30
2	D	288	ASP	CB-CG-OD2	5.65	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	380	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	154	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	297	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	79	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	79	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	314	ASP	CB-CG-OD2	5.56	123.31	118.30
2	E	380	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	181	ASP	CB-CG-OD2	5.51	123.26	118.30
2	F	316	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	270	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	269	ASP	CB-CG-OD2	5.46	123.21	118.30
2	F	386	ASP	CB-CG-OD2	5.44	123.20	118.30
2	F	64	ASP	CB-CG-OD2	5.44	123.19	118.30
2	F	352	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	409	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	86	ASP	CB-CG-OD2	5.42	123.17	118.30
2	F	256	ASP	CB-CG-OD2	5.37	123.14	118.30
2	F	26	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	409	ASP	CB-CG-OD2	5.35	123.12	118.30
2	F	288	ASP	CB-CG-OD2	5.35	123.12	118.30
1	C	170	ASP	CB-CG-OD2	5.33	123.09	118.30
2	E	386	ASP	CB-CG-OD2	5.27	123.05	118.30
2	E	315	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	224	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	24	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	347	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	222	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	494	ASP	CB-CG-OD2	5.22	123.00	118.30
2	D	316	ASP	CB-CG-OD2	5.21	122.99	118.30
2	E	288	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	333	ASP	CB-CG-OD2	5.20	122.98	118.30
3	G	244	ASP	CB-CG-OD2	5.16	122.94	118.30
2	E	64	ASP	CB-CG-OD2	5.13	122.92	118.30
2	E	250	ASP	CB-CG-OD2	5.12	122.90	118.30
2	E	359	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	494	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	411	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	450	ASP	CB-CG-OD2	5.05	122.85	118.30
2	E	369	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	238	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	411	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	411	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	352	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	347	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	347	ASP	CB-CG-OD2	5.00	122.80	118.30

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	3814	44	0
1	B	3656	0	3766	45	0
1	C	3748	0	3845	47	0
2	D	3539	0	3592	53	0
2	E	3530	0	3587	61	0
2	F	3530	0	3587	48	0
3	G	945	0	1019	6	0
4	A	27	0	12	0	0
4	B	27	0	12	1	0
4	C	27	0	12	0	0
4	D	27	0	12	1	0
4	F	27	0	12	0	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
6	B	6	0	8	0	0
6	C	6	0	8	1	0
6	D	6	0	8	1	0
7	E	5	0	0	0	0
8	A	48	0	0	1	0
8	B	40	0	0	2	0
8	C	54	0	0	3	0
8	D	51	0	0	1	0
8	E	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	48	0	0	0	0
8	G	5	0	0	0	0
All	All	23092	0	23294	286	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 6.

All (286) 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)
2:D:138:LYS:H	2:D:416:GLN:HE22	1.22	0.86
2:F:293:GLN:HE22	2:F:308:GLN:HE22	1.24	0.82
1:B:190:ASN:HD21	1:B:199:LEU:H	1.30	0.79
2:D:96:ASN:HD22	2:D:98:ILE:HG13	1.48	0.79
1:C:313:ASN:HD22	1:C:313:ASN:C	1.84	0.78
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.69	0.75
1:A:94:ILE:HG13	1:A:95:VAL:N	2.03	0.74
1:A:94:ILE:HG13	1:A:95:VAL:H	1.53	0.73
1:B:44:LEU:O	1:B:47:VAL:HG23	1.87	0.73
1:A:151:LYS:H	1:A:430:GLN:HE22	1.37	0.73
1:B:160:GLY:H	1:B:163:GLN:HE21	1.38	0.71
1:B:175:LYS:HE3	4:B:1511:ADP:O1B	1.91	0.70
1:C:219:ARG:HD3	1:C:433:TYR:CE2	2.26	0.70
2:E:257:ASN:HD22	2:E:257:ASN:C	1.91	0.70
1:A:487:GLY:O	1:A:488:LYS:HB3	1.91	0.69
1:A:44:LEU:O	1:A:47:VAL:HG22	1.92	0.68
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.75	0.68
2:E:138:LYS:H	2:E:416:GLN:HE22	1.42	0.67
2:D:138:LYS:H	2:D:416:GLN:NE2	1.93	0.67
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.75	0.67
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.75	0.67
2:F:224:GLU:O	2:F:229:ARG:NH1	2.28	0.67
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.77	0.66
1:C:164:ARG:HD2	1:C:306:LEU:O	1.95	0.66
1:A:202:ILE:HD13	1:A:230:ILE:HD12	1.76	0.66
2:F:223:ASN:H	2:F:223:ASN:HD22	1.45	0.64
1:B:141:SER:HB3	1:B:143:ARG:HH21	1.62	0.64
2:F:252:LEU:HD23	2:F:305:THR:HB	1.79	0.63
2:E:206:ILE:HA	2:E:213:SER:HB3	1.80	0.63
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.81	0.62
1:C:141:SER:HB2	1:C:143:ARG:HE	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ARG:HB3	1:C:188:ARG:HH11	1.63	0.62
2:E:443:GLN:HE22	2:E:463:ILE:HG21	1.65	0.62
2:F:228:ALA:O	2:F:232:VAL:HG23	2.00	0.61
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.82	0.61
1:A:210:ARG:HG3	1:A:235:THR:HG21	1.83	0.61
1:B:151:LYS:HG2	1:B:441:GLN:HG2	1.84	0.59
2:E:89:GLU:CG	2:E:110:THR:HG22	2.33	0.58
2:F:32:ILE:O	2:F:33:LEU:HB2	2.03	0.58
2:E:462:PRO:HB2	2:E:464:GLU:HG2	1.85	0.58
1:B:460:LYS:HD3	1:B:510:ALA:HB1	1.85	0.58
2:F:94:ILE:HD12	2:F:103:ASP:HB3	1.84	0.58
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.39	0.57
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.87	0.57
2:F:200:MET:HB3	2:F:206:ILE:HG12	1.84	0.57
2:D:139:VAL:HG23	2:D:414:LEU:HD22	1.85	0.57
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.85	0.57
2:F:223:ASN:H	2:F:223:ASN:ND2	2.03	0.57
2:D:443:GLN:HE21	2:D:449:TYR:HE1	1.51	0.57
1:B:237:SER:HB3	2:E:294:GLU:HG3	1.86	0.57
2:D:96:ASN:HB2	2:D:100:GLU:O	2.05	0.56
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.88	0.55
1:C:313:ASN:ND2	1:C:313:ASN:C	2.58	0.55
1:B:303:SER:HB2	2:F:222:MET:HB3	1.86	0.55
2:D:298:THR:HG23	2:D:303:SER:HA	1.88	0.55
2:F:147:ALA:HB2	2:F:357:ILE:HD13	1.89	0.55
1:C:80:LYS:HE2	2:F:33:LEU:HD12	1.87	0.55
2:E:257:ASN:ND2	2:E:257:ASN:C	2.60	0.55
1:C:23:VAL:HG12	1:C:23:VAL:O	2.07	0.55
2:D:94:ILE:HG12	2:D:217:LEU:HD12	1.88	0.55
2:E:96:ASN:HB2	2:E:100:GLU:H	1.70	0.55
1:C:99:VAL:HG22	1:C:253:MET:HA	1.89	0.55
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.88	0.54
1:B:295:PRO:O	1:B:298:VAL:HG22	2.07	0.54
2:F:89:GLU:HG3	2:F:109:LYS:O	2.08	0.54
1:A:151:LYS:H	1:A:430:GLN:NE2	2.03	0.54
2:D:228:ALA:O	2:D:232:VAL:HG22	2.06	0.54
2:F:25:PHE:HB2	2:F:29:LEU:HD23	1.89	0.54
1:A:225:ALA:HA	1:A:228:TYR:CE2	2.42	0.54
1:B:44:LEU:HD13	1:B:47:VAL:HG21	1.90	0.53
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.90	0.53
1:B:158:PRO:O	1:B:375:GLY:HA3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:2038:HOH:O	2:F:383:SER:HB3	2.07	0.53
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.90	0.53
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.90	0.53
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.90	0.53
1:C:352:LEU:HA	1:C:364:ALA:O	2.08	0.53
1:B:333:ASP:HB3	8:B:2034:HOH:O	2.08	0.53
1:A:440:GLU:O	1:A:444:VAL:HG12	2.08	0.53
1:A:286:ARG:NH2	2:D:273:GLY:O	2.41	0.53
2:F:260:ARG:NH1	2:F:263:GLN:HE22	2.07	0.53
2:F:223:ASN:N	2:F:223:ASN:HD22	2.05	0.52
1:C:399:GLU:HB2	2:D:342:LEU:HD22	1.91	0.52
2:F:96:ASN:HD22	2:F:98:ILE:HG12	1.74	0.52
1:B:419:SER:O	1:B:423:ARG:HG2	2.08	0.52
2:D:158:ALA:O	2:D:337:ARG:NH2	2.41	0.52
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.91	0.52
2:D:223:ASN:HD22	2:D:223:ASN:H	1.57	0.52
1:A:240:ALA:N	1:A:241:PRO:HD2	2.25	0.52
2:E:322:PRO:O	2:E:326:PHE:HD1	1.92	0.52
2:D:96:ASN:ND2	2:D:98:ILE:HG13	2.21	0.51
2:E:138:LYS:H	2:E:416:GLN:NE2	2.08	0.51
2:E:25:PHE:HB2	2:E:29:LEU:HD23	1.91	0.51
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.41	0.51
1:A:64:LEU:HD12	1:A:74:VAL:HG21	1.93	0.51
2:D:36:LEU:HD22	2:D:77:ASP:HA	1.92	0.51
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.41	0.51
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.51
1:C:263:HIS:HD2	1:C:320:SER:OG	1.94	0.51
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.93	0.50
2:D:133:LEU:HD12	2:D:148:LYS:HG2	1.92	0.50
2:D:138:LYS:HE3	2:D:416:GLN:HB2	1.92	0.50
1:C:66:LEU:O	2:D:15:ALA:HA	2.12	0.50
1:A:482:LYS:O	1:A:486:ASP:HB2	2.11	0.50
1:C:401:ALA:HA	1:C:418:LEU:HD21	1.94	0.50
2:E:116:ILE:HA	2:E:238:THR:OG1	2.11	0.50
1:B:159:ILE:HA	1:B:163:GLN:NE2	2.27	0.50
1:B:497:LEU:O	1:B:501:VAL:HG23	2.11	0.50
2:F:145:PRO:HG2	2:F:357:ILE:HG22	1.94	0.49
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.93	0.49
1:C:362:ARG:HA	1:C:363:PRO:C	2.31	0.49
2:E:32:ILE:O	2:E:33:LEU:HB2	2.12	0.49
2:E:155:PHE:HZ	2:E:326:PHE:CZ	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:VAL:O	1:C:505:LEU:HB2	2.12	0.49
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.48	0.49
1:C:44:LEU:O	1:C:47:VAL:HG22	2.13	0.49
1:B:273:LYS:HA	1:B:276:VAL:HG13	1.94	0.49
1:B:44:LEU:HB3	1:B:47:VAL:HG21	1.94	0.49
2:F:260:ARG:HH11	2:F:263:GLN:HE22	1.59	0.48
3:G:222:THR:O	3:G:226:SER:HB2	2.12	0.48
2:E:257:ASN:HB2	2:E:309:ALA:O	2.12	0.48
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.93	0.48
1:B:160:GLY:H	1:B:163:GLN:NE2	2.09	0.48
2:E:257:ASN:HD21	2:E:260:ARG:HG3	1.78	0.48
1:A:47:VAL:HG12	1:A:90:ARG:HG3	1.95	0.48
3:G:6:ILE:HG21	3:G:250:PHE:HB2	1.96	0.48
1:C:505:LEU:HB3	8:C:2050:HOH:O	2.14	0.48
2:D:70:VAL:H	2:D:73:GLN:HE21	1.62	0.48
2:F:188:GLU:O	2:F:221:GLN:HB3	2.14	0.48
2:D:377:ILE:HG12	2:D:407:ALA:HB2	1.94	0.48
2:D:223:ASN:N	2:D:223:ASN:HD22	2.12	0.48
2:F:382:LYS:HA	2:F:385:GLN:HE21	1.78	0.48
1:A:273:LYS:HE3	8:D:2034:HOH:O	2.13	0.48
2:D:32:ILE:O	2:D:33:LEU:HB2	2.13	0.48
1:B:105:GLY:HA2	1:B:226:MET:O	2.14	0.48
2:D:89:GLU:HB2	2:D:110:THR:HG22	1.96	0.47
2:D:293:GLN:HE22	2:D:308:GLN:HE22	1.61	0.47
1:B:438:ILE:O	1:B:442:VAL:HG13	2.14	0.47
2:E:182:VAL:HB	2:E:253:LEU:HD12	1.96	0.47
2:E:189:ARG:HB2	2:E:192:GLU:HG3	1.96	0.47
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.96	0.47
1:A:487:GLY:O	1:A:488:LYS:CB	2.59	0.47
2:E:359:ASP:HB3	2:E:362:ILE:HD12	1.96	0.47
2:D:96:ASN:HD22	2:D:98:ILE:CG1	2.23	0.47
1:C:350:ILE:HG23	1:C:365:ILE:HG12	1.96	0.47
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.96	0.47
1:A:202:ILE:HG23	1:A:230:ILE:HB	1.95	0.47
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.95	0.47
2:D:138:LYS:N	2:D:416:GLN:HE22	2.03	0.47
2:E:89:GLU:HG3	2:E:110:THR:HG22	1.97	0.47
2:F:228:ALA:O	2:F:232:VAL:CG2	2.63	0.47
2:F:233:ALA:HB1	2:F:292:MET:HE3	1.97	0.47
1:C:295:PRO:HD2	1:C:298:VAL:HG13	1.97	0.46
2:D:274:ARG:HH22	6:D:1478:GOL:H11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.96	0.46
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.98	0.46
2:E:339:ILE:HG23	2:E:344:ILE:HB	1.97	0.46
2:E:94:ILE:HB	2:E:103:ASP:HB3	1.96	0.46
1:A:403:PHE:N	1:A:403:PHE:CD2	2.83	0.46
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.96	0.46
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.97	0.46
2:E:255:ILE:HB	2:E:308:GLN:HG2	1.96	0.46
3:G:20:THR:HG21	3:G:235:ALA:HB3	1.97	0.46
2:F:16:VAL:HG22	2:F:21:VAL:HG13	1.97	0.46
2:F:17:ILE:HG13	2:F:271:LEU:HD22	1.97	0.46
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.45	0.46
1:B:166:LEU:HD13	1:B:342:VAL:HG11	1.98	0.46
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.16	0.46
2:D:177:HIS:CE1	2:D:250:ASP:HB3	2.51	0.46
2:E:256:ASP:HA	2:E:257:ASN:HA	1.69	0.45
1:B:171:ARG:O	1:B:172:GLN:HB2	2.16	0.45
1:B:180:ILE:HD11	1:B:216:LEU:HD11	1.97	0.45
8:A:2036:HOH:O	2:E:222:MET:HE2	2.16	0.45
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.97	0.45
2:D:252:LEU:HD23	2:D:305:THR:HB	1.98	0.45
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.97	0.45
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.47	0.45
1:C:171:ARG:HD2	2:F:326:PHE:HB3	1.99	0.45
1:B:154:ASP:HB2	1:B:441:GLN:HE22	1.82	0.45
1:B:207:GLY:HA3	1:B:273:LYS:HD3	1.98	0.45
1:C:75:VAL:O	1:C:241:PRO:HG2	2.16	0.45
2:E:240:ALA:O	2:E:251:VAL:HG21	2.17	0.45
1:C:180:ILE:HD11	1:C:216:LEU:HD11	1.98	0.45
2:F:220:GLY:HA3	2:F:232:VAL:HG21	1.99	0.45
1:C:263:HIS:CD2	1:C:320:SER:OG	2.70	0.45
1:C:287:ARG:HD3	2:D:271:LEU:HD21	1.98	0.45
2:D:96:ASN:ND2	2:D:98:ILE:CG1	2.79	0.45
2:E:89:GLU:HG2	2:E:89:GLU:H	1.54	0.45
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.98	0.45
1:A:269:ASP:HA	1:A:270:ASP:HA	1.76	0.44
1:C:237:SER:HB3	2:F:294:GLU:HG3	1.98	0.44
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.18	0.44
1:A:202:ILE:HB	1:A:266:ILE:HD12	1.98	0.44
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.52	0.44
2:D:70:VAL:H	2:D:73:GLN:NE2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:GLU:HG3	1:C:400:VAL:N	2.31	0.44
2:E:144:ALA:HA	2:E:355:SER:HB2	1.99	0.44
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.98	0.44
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.53	0.44
1:B:212:THR:O	1:B:216:LEU:HB2	2.16	0.44
2:E:384:LEU:HA	2:E:387:ILE:HD12	1.98	0.44
1:C:164:ARG:HG3	1:C:323:ALA:HB3	1.97	0.44
1:B:329:THR:HG21	1:B:334:VAL:HG12	2.00	0.44
1:A:51:GLU:OE2	1:A:90:ARG:HG2	2.18	0.44
1:C:164:ARG:CD	1:C:309:ALA:HB3	2.48	0.44
1:C:343:ILE:HG22	2:D:158:ALA:HB1	2.00	0.43
2:E:279:VAL:O	2:E:279:VAL:HG12	2.18	0.43
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.99	0.43
2:D:84:ILE:HG21	2:D:235:THR:HG23	2.00	0.43
2:E:266:SER:HA	2:E:282:GLN:HB3	2.00	0.43
1:B:30:ARG:HD2	8:B:2001:HOH:O	2.18	0.43
1:B:110:ALA:HB3	1:B:242:LEU:HD23	2.01	0.43
2:E:244:ARG:HD3	2:E:304:ILE:HG13	2.00	0.43
1:A:34:ILE:HG22	2:D:52:HIS:HB2	2.01	0.43
1:C:353:GLU:HB2	1:C:356:LEU:HD12	2.00	0.43
1:A:180:ILE:HA	1:A:180:ILE:HD13	1.85	0.43
2:D:188:GLU:O	2:D:221:GLN:HB3	2.18	0.43
2:F:151:LYS:NZ	2:F:293:GLN:HE21	2.17	0.43
2:D:277:SER:OG	2:D:278:ALA:N	2.52	0.43
2:D:345:TYR:HB3	4:D:1476:ADP:C6	2.53	0.43
1:C:67:GLU:HG2	8:C:2004:HOH:O	2.18	0.43
1:A:95:VAL:HG11	1:A:245:LEU:HD13	2.01	0.42
2:F:218:VAL:HG21	2:F:236:GLY:HA2	2.00	0.42
1:C:34:ILE:HG13	1:C:35:GLY:N	2.33	0.42
2:E:257:ASN:ND2	2:E:260:ARG:H	2.16	0.42
2:F:63:MET:CE	2:F:97:VAL:HG11	2.49	0.42
1:C:207:GLY:HA3	1:C:273:LYS:HD3	2.01	0.42
2:F:139:VAL:HG11	2:F:348:VAL:HB	2.01	0.42
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.45	0.42
2:F:393:MET:HG2	2:F:396:LEU:HD12	2.00	0.42
1:B:363:PRO:HB2	1:B:365:ILE:HD12	2.01	0.42
1:A:438:ILE:O	1:A:442:VAL:HG12	2.19	0.42
1:C:32:LEU:HG	1:C:42:HIS:HB2	2.01	0.42
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.54	0.42
2:F:171:ASN:HD22	2:F:172:ASN:ND2	2.18	0.42
1:C:440:GLU:O	1:C:444:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ARG:HA	1:A:363:PRO:C	2.39	0.42
1:A:175:LYS:HE2	1:A:175:LYS:HB2	1.92	0.42
1:C:44:LEU:HB3	1:C:47:VAL:HG22	2.01	0.42
2:D:66:THR:HB	2:D:69:LEU:HD12	2.02	0.42
2:E:253:LEU:O	2:E:306:SER:HA	2.20	0.42
1:A:83:LYS:O	1:A:86:ASP:HB2	2.19	0.42
1:B:246:ALA:HB3	1:B:247:PRO:HD3	2.02	0.42
3:G:266:ILE:HA	3:G:266:ILE:HD13	1.93	0.42
2:F:51:GLN:HG2	2:F:59:ARG:HB3	2.01	0.41
1:C:99:VAL:HG13	1:C:256:TYR:HB2	2.02	0.41
1:A:137:ILE:HG13	2:E:104:GLU:HG3	2.03	0.41
2:E:241:GLU:OE1	2:E:295:ARG:HB3	2.20	0.41
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.94	0.41
2:F:25:PHE:O	2:F:56:SER:HB3	2.20	0.41
1:C:172:GLN:HG3	2:F:354:THR:HG21	2.01	0.41
1:A:66:LEU:HD12	2:E:16:VAL:HB	2.01	0.41
1:B:34:ILE:HG13	1:B:35:GLY:N	2.35	0.41
1:A:209:LYS:HZ3	1:A:211:SER:HB2	1.85	0.41
1:A:102:GLU:CD	1:A:102:GLU:H	2.24	0.41
1:A:390:MET:HG3	1:A:424:LEU:HD22	2.02	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.86	0.41
2:E:242:TYR:CD1	2:E:246:GLN:HG3	2.56	0.41
1:A:167:ILE:HB	1:A:326:VAL:HG22	2.02	0.41
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.89	0.41
2:E:95:MET:HA	2:E:100:GLU:O	2.21	0.41
1:B:282:SER:OG	1:B:295:PRO:HG3	2.21	0.41
2:D:53:LEU:HD11	2:D:59:ARG:HB2	2.03	0.41
1:C:240:ALA:HB3	1:C:241:PRO:HD3	2.03	0.40
1:A:27:GLU:O	1:A:90:ARG:HB2	2.21	0.40
1:B:218:LYS:HG3	2:E:128:VAL:HB	2.01	0.40
1:A:415:GLN:HA	1:A:418:LEU:HD12	2.03	0.40
1:C:65:ASN:HB2	1:C:72:GLY:HA3	2.03	0.40
1:C:304:ARG:HH21	6:C:1513:GOL:H32	1.86	0.40
2:E:387:ILE:HG23	2:E:391:LEU:HD12	2.02	0.40
2:D:51:GLN:HB2	2:D:59:ARG:HB3	2.04	0.40
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.51	0.40
1:A:156:LEU:HD13	1:A:367:VAL:HG11	2.03	0.40
2:D:374:VAL:O	2:D:377:ILE:HG22	2.22	0.40
1:C:144:GLU:HA	1:C:145:PRO:HD3	1.87	0.40
1:B:269:ASP:HA	1:B:270:ASP:HA	1.73	0.40
2:E:408:ARG:O	2:E:412:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:LEU:HB3	2:E:252:LEU:HD21	2.03	0.40
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.57	0.40
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.40
2:E:355:SER:HB3	2:E:358:MET:HB2	2.03	0.40
1:C:441:GLN:O	1:C:445:ILE:HG12	2.22	0.40
1:B:472:VAL:HG12	1:B:500:ILE:HG21	2.04	0.40
3:G:242:MET:HE3	3:G:242:MET:HB2	1.97	0.40
2:E:374:VAL:O	2:E:377:ILE:HG22	2.22	0.40
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	459 (95%)	22 (4%)	4 (1%)	24	56
1	B	475/510 (93%)	451 (95%)	22 (5%)	2 (0%)	39	71
1	C	490/510 (96%)	469 (96%)	20 (4%)	1 (0%)	52	82
2	D	465/482 (96%)	437 (94%)	27 (6%)	1 (0%)	52	82
2	E	464/482 (96%)	433 (93%)	28 (6%)	3 (1%)	30	63
2	F	464/482 (96%)	436 (94%)	26 (6%)	2 (0%)	39	71
3	G	116/272 (43%)	116 (100%)	0	0	100	100
All	All	2959/3248 (91%)	2801 (95%)	145 (5%)	13 (0%)	39	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	LYS
1	A	141	SER

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Mol	Chain	Res	Type
1	A	361	ILE
2	D	28	GLY
2	E	28	GLY
1	A	123	SER
1	B	411	ASP
1	C	409	ASP
1	B	334	VAL
2	F	279	VAL
2	E	279	VAL
2	E	423	VAL
2	F	28	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	358 (91%)	35 (9%)	12	32
1	B	388/412 (94%)	370 (95%)	18 (5%)	33	66
1	C	397/412 (96%)	367 (92%)	30 (8%)	16	40
2	D	377/386 (98%)	358 (95%)	19 (5%)	30	62
2	E	376/386 (97%)	338 (90%)	38 (10%)	9	25
2	F	376/386 (97%)	348 (93%)	28 (7%)	17	42
3	G	102/230 (44%)	93 (91%)	9 (9%)	12	33
All	All	2409/2624 (92%)	2232 (93%)	177 (7%)	17	42

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	80	LYS
1	A	86	ASP
1	A	90	ARG
1	A	94	ILE
1	A	99	VAL

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Mol	Chain	Res	Type
1	A	134	PRO
1	A	136	ILE
1	A	141	SER
1	A	164	ARG
1	A	202	ILE
1	A	216	LEU
1	A	233	SER
1	A	265	LEU
1	A	266	ILE
1	A	274	GLN
1	A	340	THR
1	A	372	SER
1	A	376	SER
1	A	403	PHE
1	A	410	LEU
1	A	423	ARG
1	A	432	GLN
1	A	442	VAL
1	A	444	VAL
1	A	455	LYS
1	A	457	GLU
1	A	470	SER
1	A	473	ILE
1	A	479	LEU
1	A	488	LYS
1	A	493	SER
1	A	494	ASP
1	A	502	THR
1	A	505	LEU
1	B	38	ILE
1	B	80	LYS
1	B	164	ARG
1	B	193	THR
1	B	211	SER
1	B	216	LEU
1	B	298	VAL
1	B	307	GLU
1	B	335	SER
1	B	337	TYR
1	B	371	VAL
1	B	380	THR
1	B	434	SER

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Mol	Chain	Res	Type
1	B	455	LYS
1	B	457	GLU
1	B	477	GLN
1	B	482	LYS
1	B	499	GLU
1	C	47	VAL
1	C	83	LYS
1	C	99	VAL
1	C	101	GLU
1	C	127	ARG
1	C	164	ARG
1	C	180	ILE
1	C	188	ARG
1	C	196	LYS
1	C	197	LYS
1	C	216	LEU
1	C	262	LYS
1	C	272	SER
1	C	274	GLN
1	C	298	VAL
1	C	313	ASN
1	C	334	VAL
1	C	341	ASN
1	C	349	GLN
1	C	354	THR
1	C	399	GLU
1	C	406	PHE
1	C	408	SER
1	C	410	LEU
1	C	444	VAL
1	C	463	LYS
1	C	488	LYS
1	C	491	GLU
1	C	496	LYS
1	C	505	LEU
2	D	9	THR
2	D	27	GLU
2	D	34	ASN
2	D	86	VAL
2	D	93	ARG
2	D	97	VAL
2	D	109	LYS

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Mol	Chain	Res	Type
2	D	127	SER
2	D	223	ASN
2	D	232	VAL
2	D	250	ASP
2	D	261	PHE
2	D	266	SER
2	D	303	SER
2	D	388	ILE
2	D	431	LEU
2	D	439	LYS
2	D	472	LYS
2	D	475	GLU
2	E	34	ASN
2	E	44	ARG
2	E	89	GLU
2	E	96	ASN
2	E	97	VAL
2	E	111	LYS
2	E	112	GLN
2	E	124	VAL
2	E	129	GLU
2	E	130	GLN
2	E	139	VAL
2	E	172	ASN
2	E	213	SER
2	E	215	VAL
2	E	237	LEU
2	E	251	VAL
2	E	257	ASN
2	E	284	THR
2	E	293	GLN
2	E	297	THR
2	E	310	ILE
2	E	337	ARG
2	E	342	LEU
2	E	365	SER
2	E	377	ILE
2	E	378	LEU
2	E	380	ASP
2	E	412	ARG
2	E	419	GLN
2	E	424	PHE

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Mol	Chain	Res	Type
2	E	428	LEU
2	E	439	LYS
2	E	450	ASP
2	E	454	GLU
2	E	463	ILE
2	E	464	GLU
2	E	465	GLU
2	E	472	LYS
2	F	34	ASN
2	F	76	LEU
2	F	78	SER
2	F	110	THR
2	F	124	VAL
2	F	127	SER
2	F	139	VAL
2	F	172	ASN
2	F	177	HIS
2	F	181	SER
2	F	223	ASN
2	F	247	GLU
2	F	250	ASP
2	F	251	VAL
2	F	266	SER
2	F	274	ARG
2	F	315	ASP
2	F	355	SER
2	F	357	ILE
2	F	358	MET
2	F	372	ARG
2	F	393	MET
2	F	405	SER
2	F	435	LYS
2	F	436	GLU
2	F	455	GLN
2	F	469	LYS
2	F	472	LYS
3	G	4	LYS
3	G	15	ASN
3	G	44	TYR
3	G	77	LEU
3	G	78	CYS
3	G	81	ILE

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Mol	Chain	Res	Type
3	G	82	HIS
3	G	84	SER
3	G	90	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	172	GLN
1	A	263	HIS
1	A	274	GLN
1	A	415	GLN
1	A	430	GLN
1	A	471	HIS
1	A	475	GLN
1	A	476	HIS
1	A	477	GLN
1	B	147	GLN
1	B	163	GLN
1	B	190	ASN
1	B	260	ASN
1	B	341	ASN
1	B	379	GLN
1	B	396	GLN
1	B	415	GLN
1	B	430	GLN
1	B	441	GLN
1	B	466	ASN
1	B	503	ASN
1	C	147	GLN
1	C	263	HIS
1	C	274	GLN
1	C	280	GLN
1	C	313	ASN
1	C	341	ASN
1	C	349	GLN
1	C	471	HIS
1	C	475	GLN
2	D	34	ASN
2	D	51	GLN
2	D	73	GLN
2	D	96	ASN

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Mol	Chain	Res	Type
2	D	130	GLN
2	D	172	ASN
2	D	177	HIS
2	D	223	ASN
2	D	293	GLN
2	D	416	GLN
2	E	34	ASN
2	E	172	ASN
2	E	249	GLN
2	E	257	ASN
2	E	293	GLN
2	E	308	GLN
2	E	367	HIS
2	E	385	GLN
2	E	416	GLN
2	E	443	GLN
2	F	73	GLN
2	F	96	ASN
2	F	172	ASN
2	F	194	ASN
2	F	223	ASN
2	F	263	GLN
2	F	293	GLN
2	F	361	ASN
2	F	385	GLN
2	F	455	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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	ADP	A	1511	5	22,29,29	1.23	2 (9%)	27,45,45	2.43	2 (7%)
4	ADP	B	1511	5	22,29,29	1.20	2 (9%)	27,45,45	2.49	2 (7%)
6	GOL	B	1513	-	5,5,5	0.37	0	5,5,5	0.22	0
4	ADP	C	1511	5	22,29,29	1.17	2 (9%)	27,45,45	2.50	3 (11%)
6	GOL	C	1513	-	5,5,5	0.30	0	5,5,5	0.38	0
4	ADP	D	1476	5	22,29,29	1.17	2 (9%)	27,45,45	2.48	4 (14%)
6	GOL	D	1478	-	5,5,5	0.38	0	5,5,5	0.28	0
7	PO4	E	1475	-	4,4,4	0.47	0	6,6,6	0.28	0
4	ADP	F	1475	5	22,29,29	1.29	2 (9%)	27,45,45	2.33	3 (11%)

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	ADP	A	1511	5	-	0/12/32/32	0/3/3/3
4	ADP	B	1511	5	-	0/12/32/32	0/3/3/3
6	GOL	B	1513	-	-	0/4/4/4	0/0/0/0
4	ADP	C	1511	5	-	0/12/32/32	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	0/0/0/0
4	ADP	D	1476	5	-	0/12/32/32	0/3/3/3
6	GOL	D	1478	-	-	0/4/4/4	0/0/0/0
7	PO4	E	1475	-	-	0/0/0/0	0/0/0/0
4	ADP	F	1475	5	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1476	ADP	C2-N1	2.41	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1511	ADP	C2-N1	2.49	1.38	1.33
4	C	1511	ADP	C2-N1	2.58	1.38	1.33
4	A	1511	ADP	C2-N1	2.72	1.39	1.33
4	F	1475	ADP	C2-N1	2.82	1.39	1.33
4	C	1511	ADP	C2-N3	3.55	1.38	1.32
4	D	1476	ADP	C2-N3	3.63	1.38	1.32
4	A	1511	ADP	C2-N3	3.79	1.38	1.32
4	B	1511	ADP	C2-N3	3.81	1.38	1.32
4	F	1475	ADP	C2-N3	4.16	1.39	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1511	ADP	N3-C2-N1	-11.90	119.78	128.89
4	C	1511	ADP	N3-C2-N1	-11.83	119.83	128.89
4	A	1511	ADP	N3-C2-N1	-11.71	119.93	128.89
4	D	1476	ADP	N3-C2-N1	-11.27	120.27	128.89
4	F	1475	ADP	N3-C2-N1	-10.71	120.70	128.89
4	D	1476	ADP	C2'-C1'-N9	-3.75	108.56	114.29
4	F	1475	ADP	PA-O3A-PB	-3.64	120.45	132.67
4	C	1511	ADP	PA-O3A-PB	-3.16	122.09	132.67
4	B	1511	ADP	PA-O3A-PB	-2.94	122.81	132.67
4	F	1475	ADP	C2'-C1'-N9	-2.66	110.22	114.29
4	D	1476	ADP	PA-O3A-PB	-2.42	124.55	132.67
4	A	1511	ADP	O2B-PB-O3A	2.07	114.50	105.09
4	D	1476	ADP	C4'-O4'-C1'	2.23	112.17	109.72
4	C	1511	ADP	C4'-O4'-C1'	2.49	112.46	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1511	ADP	1	0
6	C	1513	GOL	1	0
4	D	1476	ADP	1	0
6	D	1478	GOL	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	487/510 (95%)	-0.19	6 (1%) 81 78	41, 62, 80, 109	0
1	B	479/510 (93%)	-0.23	4 (0%) 87 86	39, 58, 95, 110	0
1	C	492/510 (96%)	-0.33	4 (0%) 87 86	38, 50, 70, 101	0
2	D	467/482 (96%)	-0.33	7 (1%) 76 73	38, 56, 79, 94	0
2	E	466/482 (96%)	0.15	39 (8%) 14 9	43, 72, 118, 136	0
2	F	466/482 (96%)	-0.22	11 (2%) 62 57	39, 55, 78, 97	0
3	G	122/272 (44%)	0.61	17 (13%) 4 2	44, 85, 122, 127	0
All	All	2979/3248 (91%)	-0.16	88 (2%) 54 47	38, 59, 99, 136	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	474	ALA	6.7
3	G	39	LYS	6.0
1	C	407	GLY	5.6
2	E	398	GLU	5.6
2	E	390	ILE	5.2
2	F	178	GLY	5.0
3	G	209	LEU	4.9
3	G	88	GLN	4.4
2	E	395	GLU	4.4
2	E	388	ILE	4.2
2	E	446	ALA	4.2
2	E	473	LEU	4.2
3	G	210	ALA	4.0
3	G	87	LYS	3.9
3	G	89	MET	3.8
3	G	86	ALA	3.7
2	E	424	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
3	G	90	LYS	3.6
3	G	40	PRO	3.6
2	E	427	HIS	3.6
2	E	394	ASP	3.5
2	F	9	THR	3.5
2	E	423	VAL	3.3
1	B	193	THR	3.3
2	E	426	GLY	3.2
3	G	215	TYR	3.2
3	G	212	ILE	3.2
2	E	472	LYS	3.1
1	C	409	ASP	3.1
1	A	408	SER	3.0
2	E	361	ASN	3.0
3	G	80	ALA	3.0
2	E	389	ALA	2.9
3	G	33	ARG	2.9
1	A	193	THR	2.9
2	E	425	THR	2.9
2	F	246	GLN	2.9
1	C	193	THR	2.9
2	E	9	THR	2.8
2	E	391	LEU	2.8
2	E	301	LYS	2.8
2	E	385	GLN	2.8
3	G	37	GLU	2.7
1	B	510	ALA	2.7
2	E	42	GLU	2.7
3	G	244	ASP	2.7
2	E	396	LEU	2.7
2	D	27	GLU	2.7
2	F	455	GLN	2.6
2	D	9	THR	2.5
2	E	342	LEU	2.5
2	F	42	GLU	2.5
2	E	338	ALA	2.5
2	E	451	HIS	2.5
2	E	430	LYS	2.5
1	A	409	ASP	2.5
2	D	250	ASP	2.4
2	F	247	GLU	2.4
2	E	428	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLY	2.3
2	E	436	GLU	2.3
1	A	315	ALA	2.3
2	E	366	GLU	2.3
1	B	30	ARG	2.3
2	E	337	ARG	2.3
2	D	42	GLU	2.3
1	B	411	ASP	2.3
2	E	422	GLU	2.3
2	E	442	GLN	2.2
2	D	398	GLU	2.2
1	C	408	SER	2.2
2	F	175	LYS	2.2
2	E	392	GLY	2.2
2	E	246	GLN	2.2
2	E	399	GLU	2.2
3	G	81	ILE	2.2
2	E	383	SER	2.1
3	G	85	VAL	2.1
2	F	43	THR	2.1
2	F	472	LYS	2.1
2	E	365	SER	2.1
2	E	300	LYS	2.1
2	E	245	ASP	2.1
1	A	26	GLU	2.1
2	F	109	LYS	2.1
2	F	342	LEU	2.1
2	D	428	LEU	2.0
2	D	28	GLY	2.0

## 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 [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	D	1477	1/1	0.93	0.55	31.69	50,50,50,50	0
6	GOL	D	1478	6/6	0.92	0.23	2.19	67,67,68,68	0
6	GOL	C	1513	6/6	0.92	0.15	-0.33	49,52,53,53	0
6	GOL	B	1513	6/6	0.96	0.12	-0.95	46,46,47,47	0
7	PO4	E	1475	5/5	0.86	0.15	-0.95	101,101,101,101	0
4	ADP	F	1475	27/27	0.97	0.12	-1.01	35,46,47,48	0
4	ADP	C	1511	27/27	0.98	0.11	-1.08	37,42,43,45	0
4	ADP	B	1511	27/27	0.96	0.13	-1.21	51,56,59,59	0
4	ADP	A	1511	27/27	0.97	0.10	-1.27	47,48,52,52	0
4	ADP	D	1476	27/27	0.98	0.11	-1.40	41,48,54,55	0
5	MG	F	1476	1/1	0.81	0.39	-	47,47,47,47	0
5	MG	A	1512	1/1	0.94	0.30	-	48,48,48,48	0
5	MG	C	1512	1/1	0.95	0.24	-	29,29,29,29	0
5	MG	B	1512	1/1	0.92	0.26	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.