



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:00 am BST

PDB ID : 2W6I  
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 4B.  
Authors : Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.  
Deposited on : 2008-12-18  
Resolution : 4.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

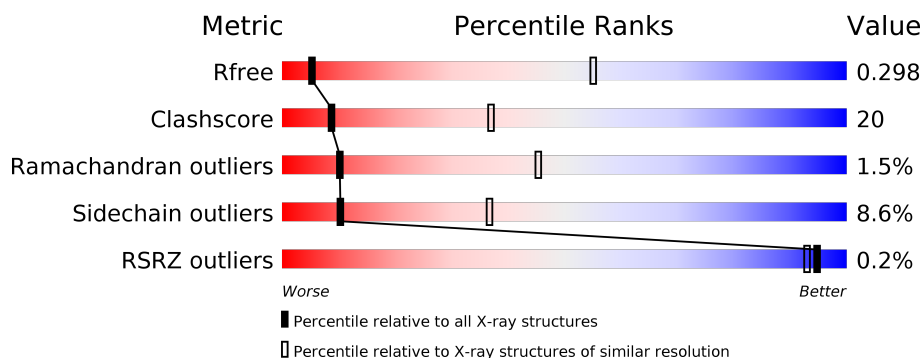
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	553	
1	B	553	
1	C	553	
2	D	528	
2	E	528	
2	F	528	

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Mol	Chain	Length	Quality of chain
3	G	298	<div><div></div><div>54%30%5%12%</div></div>
4	H	168	<div><div></div><div>9%9%82%</div></div>
5	I	51	<div><div></div><div>33%20%45%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24216 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, MITOCHONDRIAL.

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			

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

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 SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

- Molecule 4 is a protein called F1-ATPASE DELTA SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	31	Total	C	N	O	0	0	0
			235	147	39	49			

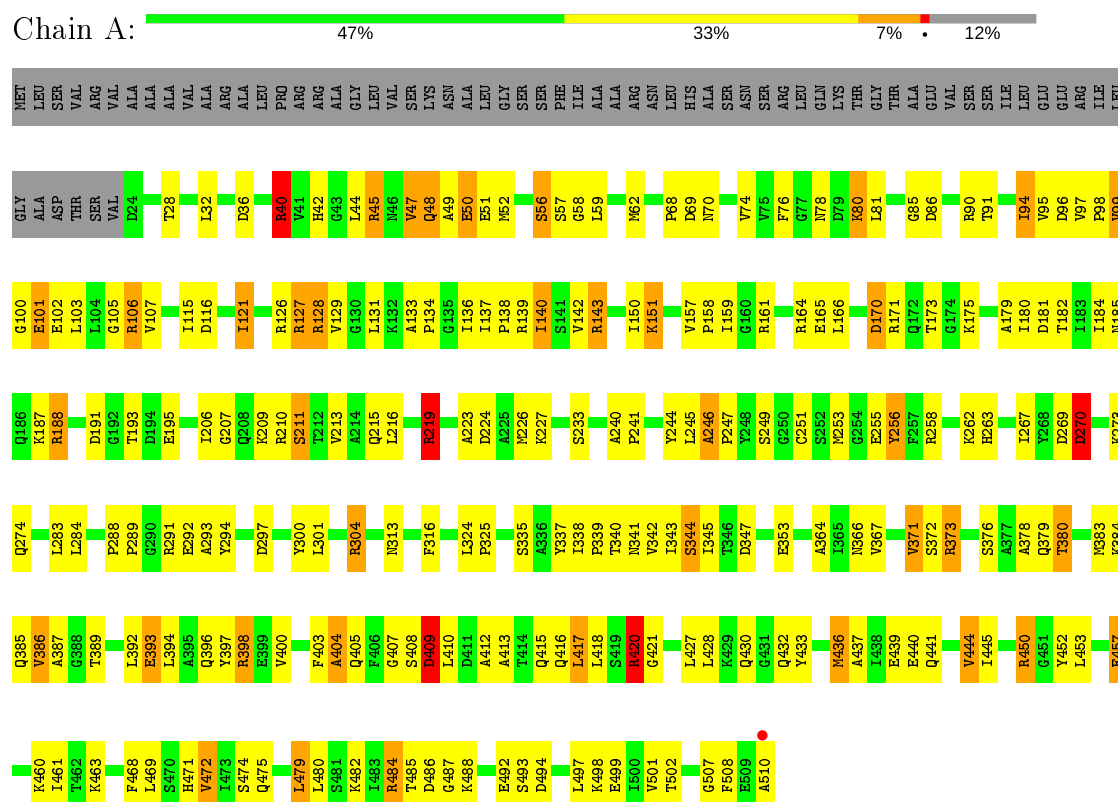
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	28	Total	C	N	O	S	0	0	0
			212	135	39	37	1			

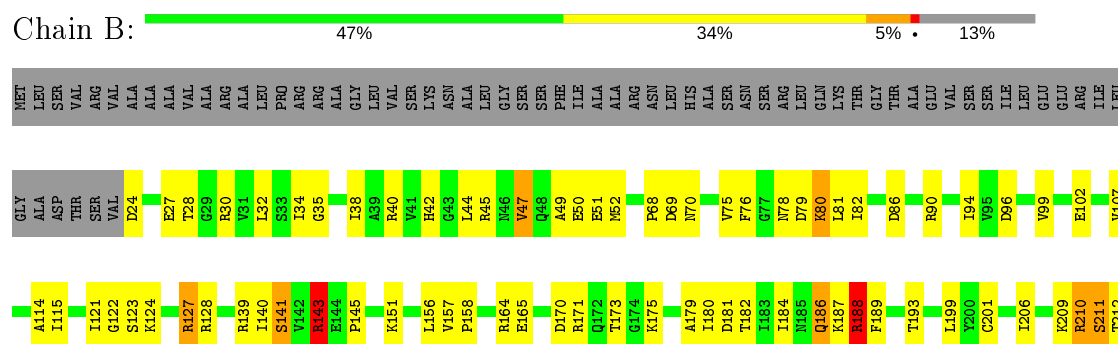
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

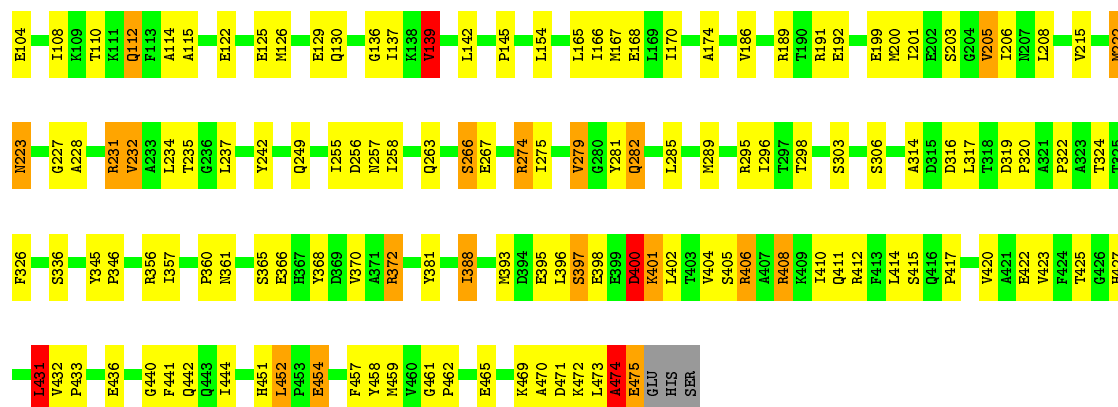
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL



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

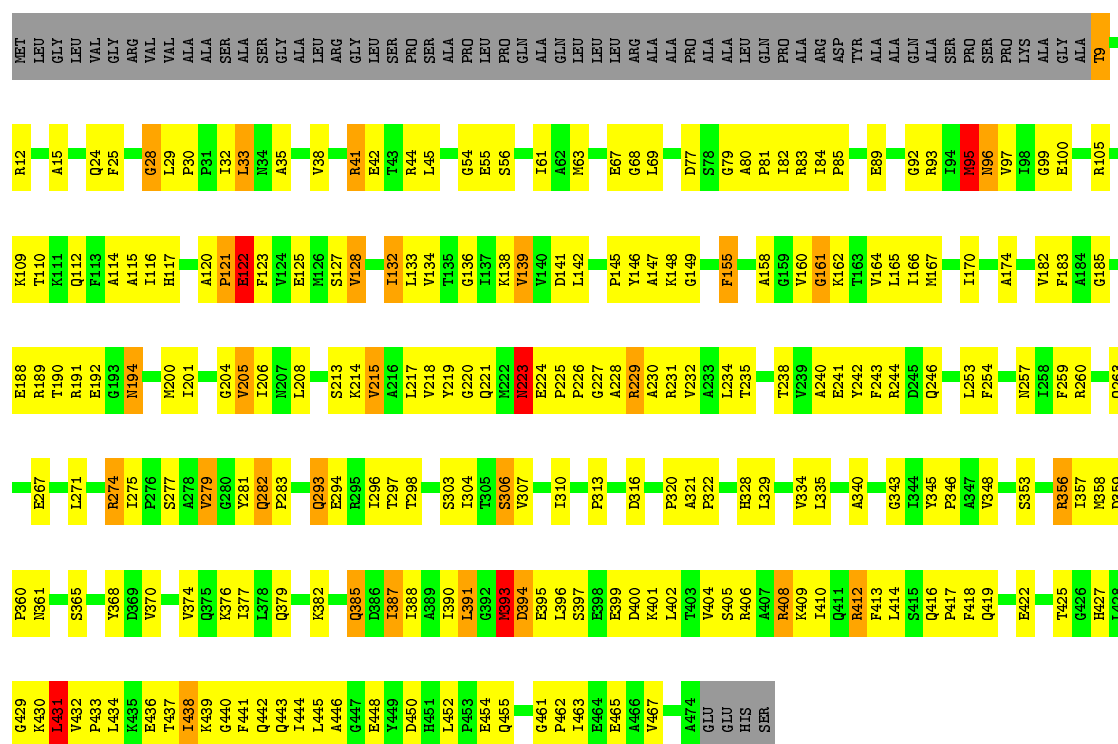






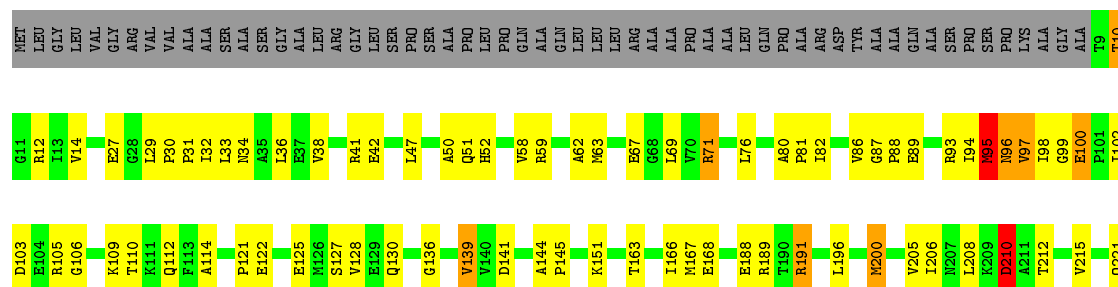
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 44% 38% 5% • 12%



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F: 57% 28% • 12%







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.92Å 131.33Å 267.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 100.87 – 4.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-4.00) 92.7 (100.87-4.00)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, $R_{free}$	0.299 , 0.300 0.303 , 0.298	Depositor DCC
$R_{free}$ test set	1557 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 9.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	24216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.60	0/3766	1.31	26/5080 (0.5%)
1	B	0.61	0/3704	1.36	30/4995 (0.6%)
1	C	0.62	0/3799	1.38	25/5126 (0.5%)
2	D	0.62	0/3596	1.36	22/4879 (0.5%)
2	E	0.60	0/3587	1.32	17/4867 (0.3%)
2	F	0.62	0/3587	1.36	28/4867 (0.6%)
3	G	0.35	0/2074	0.72	3/2785 (0.1%)
4	H	0.31	0/232	0.61	0/308
5	I	0.34	0/212	0.75	0/281
All	All	0.59	0/24557	1.30	151/33188 (0.5%)

There are no bond length outliers.

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	23.38	156.33	123.60
2	E	408	ARG	CD-NE-CZ	13.90	143.07	123.60
1	C	291	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	B	40	ARG	NE-CZ-NH1	13.11	126.85	120.30
1	B	279	ARG	NE-CZ-NH1	12.83	126.71	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3813	165	3
1	B	3656	0	3764	149	52
1	C	3748	0	3843	152	53
2	D	3539	0	3593	146	0
2	E	3530	0	3587	198	0
2	F	3530	0	3586	123	2
3	G	2051	0	2115	114	0
4	H	235	0	230	18	0
5	I	212	0	232	13	0
All	All	24216	0	24763	1003	55

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1003 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:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.16
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.25	1.11
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.11	1.07
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.04
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.73	1.03

The worst 5 of 55 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLY:O	1:C:20:ASP:OD2[4_555]	0.43	1.77
1:B:314:ASP:N	1:C:21:THR:C[4_555]	0.83	1.37
1:B:318:GLY:N	1:C:22:SER:OG[4_555]	0.92	1.28
1:B:313:ASN:O	1:C:22:SER:CA[4_555]	0.99	1.21
1:B:314:ASP:O	1:C:22:SER:O[4_555]	1.06	1.14

## 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	485/553 (88%)	443 (91%)	35 (7%)	7 (1%)	11	46
1	B	475/553 (86%)	427 (90%)	41 (9%)	7 (2%)	10	45
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	9	44
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	25	63
2	E	464/528 (88%)	407 (88%)	47 (10%)	10 (2%)	6	37
2	F	464/528 (88%)	433 (93%)	29 (6%)	2 (0%)	34	71
3	G	257/298 (86%)	223 (87%)	26 (10%)	8 (3%)	4	31
4	H	21/168 (12%)	21 (100%)	0	0	100	100
5	I	24/51 (47%)	20 (83%)	2 (8%)	2 (8%)	1	13
All	All	3145/3760 (84%)	2837 (90%)	261 (8%)	47 (2%)	10	45

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	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	393/444 (88%)	351 (89%)	42 (11%)	6	27
1	B	388/444 (87%)	341 (88%)	47 (12%)	5	23
1	C	397/444 (89%)	369 (93%)	28 (7%)	14	42
2	D	377/417 (90%)	346 (92%)	31 (8%)	11	38
2	E	376/417 (90%)	343 (91%)	33 (9%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	376/417 (90%)	354 (94%)	22 (6%)	19	48
3	G	225/251 (90%)	210 (93%)	15 (7%)	16	44
4	H	27/128 (21%)	26 (96%)	1 (4%)	34	60
5	I	23/42 (55%)	21 (91%)	2 (9%)	10	35
All	All	2582/3004 (86%)	2361 (91%)	221 (9%)	10	37

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	208	GLN
2	D	112	GLN
3	G	67	LEU
1	C	282	SER
1	C	477	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	328	HIS
2	E	130	GLN
3	G	234	ASN
2	D	442	GLN
2	E	39	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 [i](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	487/553 (88%)	-0.04	1 (0%) 95 93	20, 20, 20, 20	0
1	B	479/553 (86%)	-0.11	1 (0%) 95 93	20, 20, 20, 20	0
1	C	492/553 (88%)	-0.17	1 (0%) 95 93	20, 20, 20, 20	0
2	D	467/528 (88%)	-0.15	0 100 100	20, 20, 20, 20	0
2	E	466/528 (88%)	-0.12	0 100 100	20, 20, 20, 20	0
2	F	466/528 (88%)	-0.16	2 (0%) 92 87	20, 20, 20, 20	0
3	G	263/298 (88%)	0.31	1 (0%) 92 87	20, 20, 20, 20	0
4	H	31/168 (18%)	0.32	0 100 100	20, 20, 20, 20	0
5	I	28/51 (54%)	0.43	0 100 100	20, 20, 20, 20	0
All	All	3179/3760 (84%)	-0.08	6 (0%) 95 93	20, 20, 20, 20	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	ALA	3.6
1	C	19	ALA	3.1
3	G	175	GLU	2.4
2	F	469	LYS	2.4
1	B	448	GLY	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.