



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:11 AM GMT

PDB ID : 2W6E
Title : LOW RESOLUTION STRUCTURES OF BOVINE MITOCHONDRIAL F1-ATPASE DURING CONTROLLED DEHYDRATION: HYDRATION STATE 1.
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 : 6.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

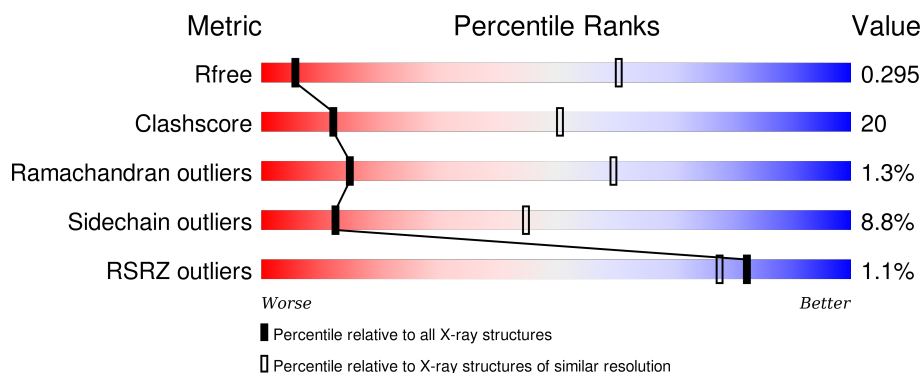
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	<div> <div>47%</div> <div>33%</div> <div>7%</div> <div>•</div> <div>12%</div> </div>
1	B	553	<div> <div>48%</div> <div>31%</div> <div>6%</div> <div>•</div> <div>13%</div> </div>
1	C	553	<div> <div>53%</div> <div>31%</div> <div>•</div> <div>•</div> <div>11%</div> </div>
2	D	528	<div> <div>54%</div> <div>29%</div> <div>5%</div> <div>•</div> <div>12%</div> </div>
2	E	528	<div> <div>45%</div> <div>37%</div> <div>5%</div> <div>•</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	528	
3	G	298	

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
4	ADP	D	1476	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22690 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			

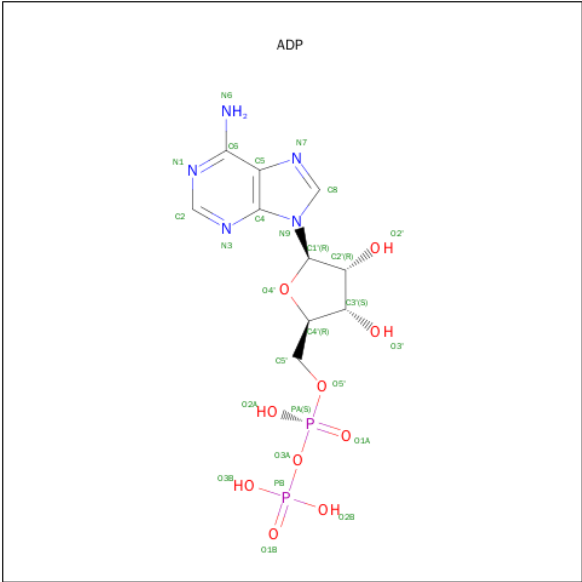
- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

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			

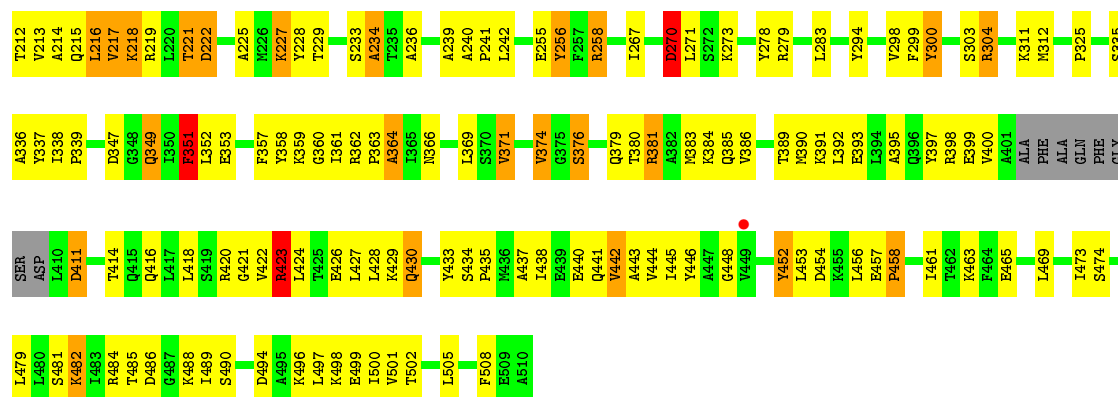
- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

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

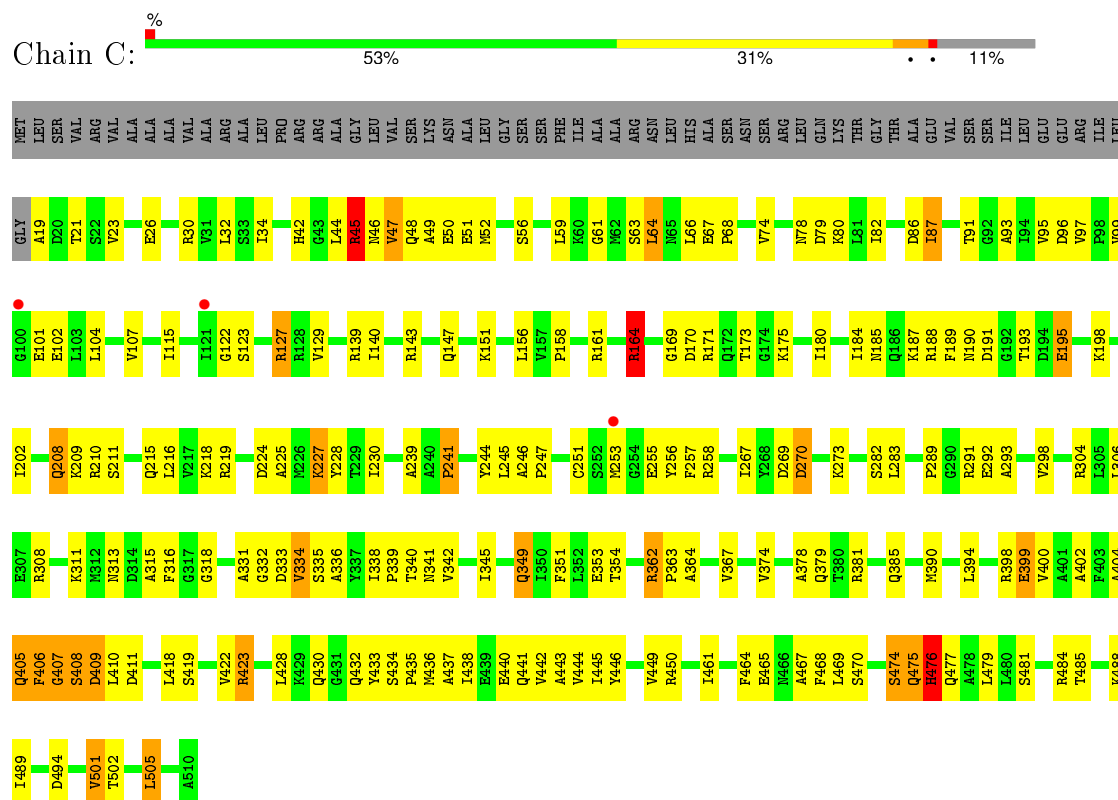
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



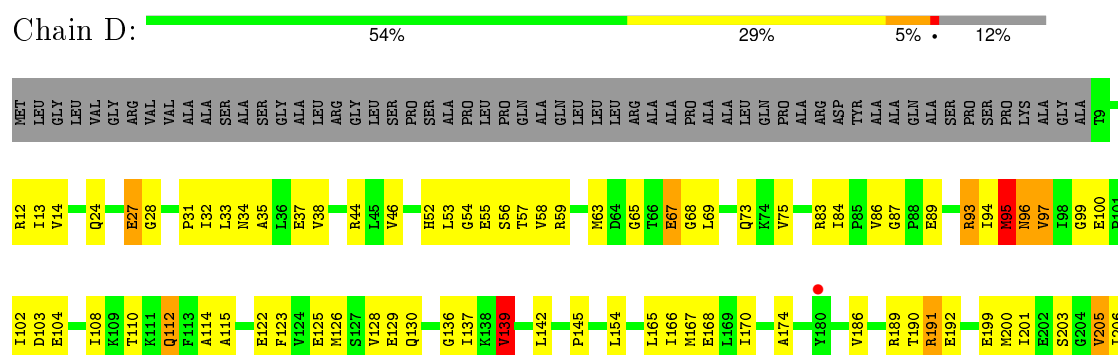
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

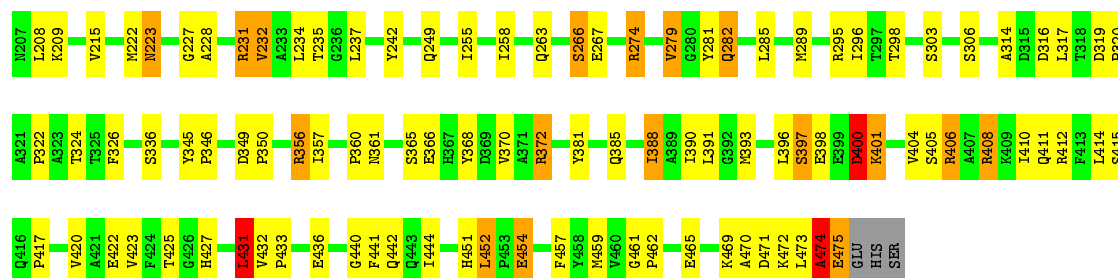


● Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

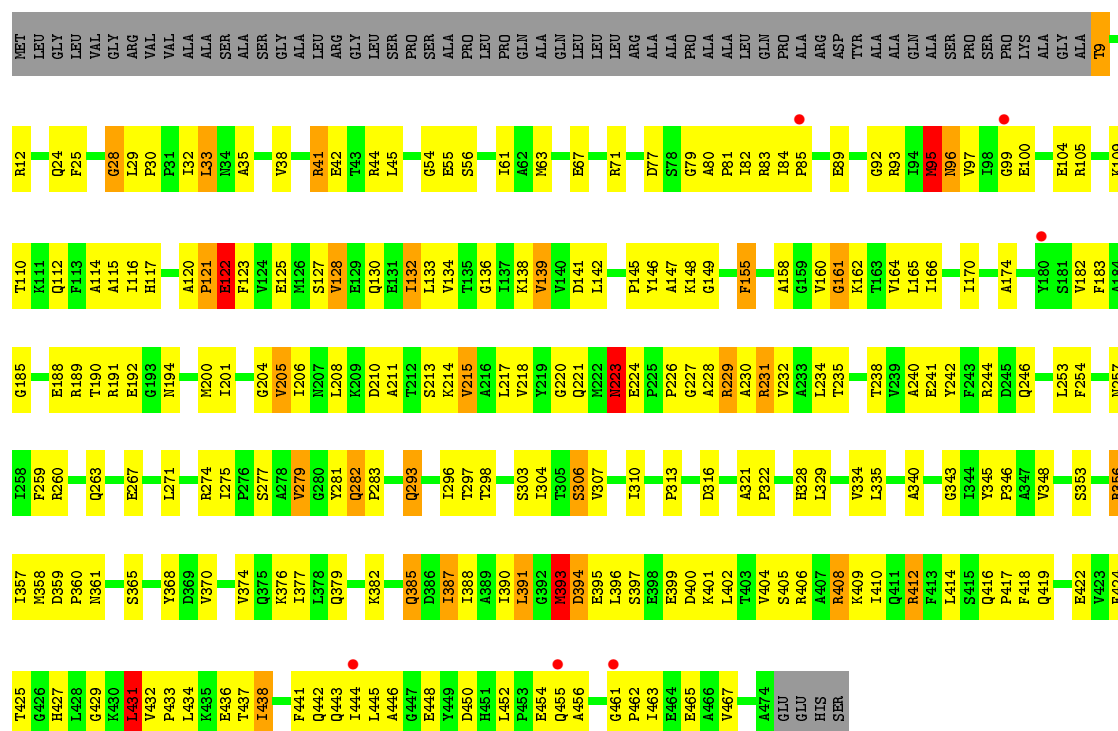


● Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

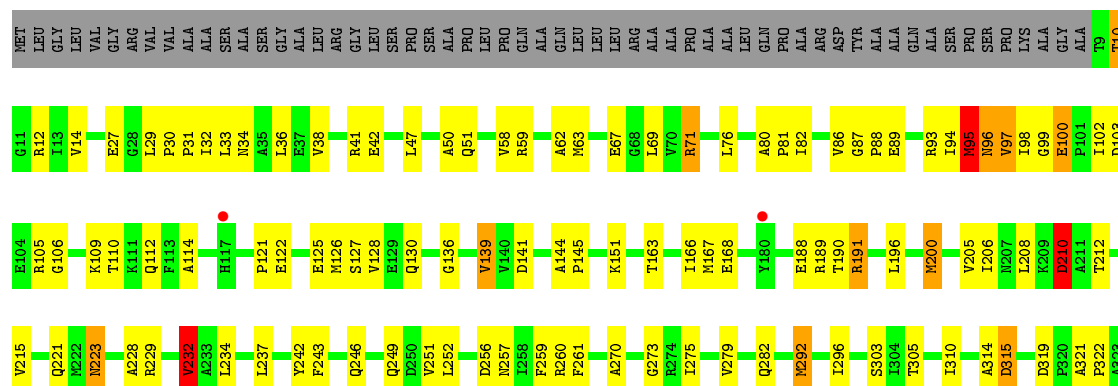




• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

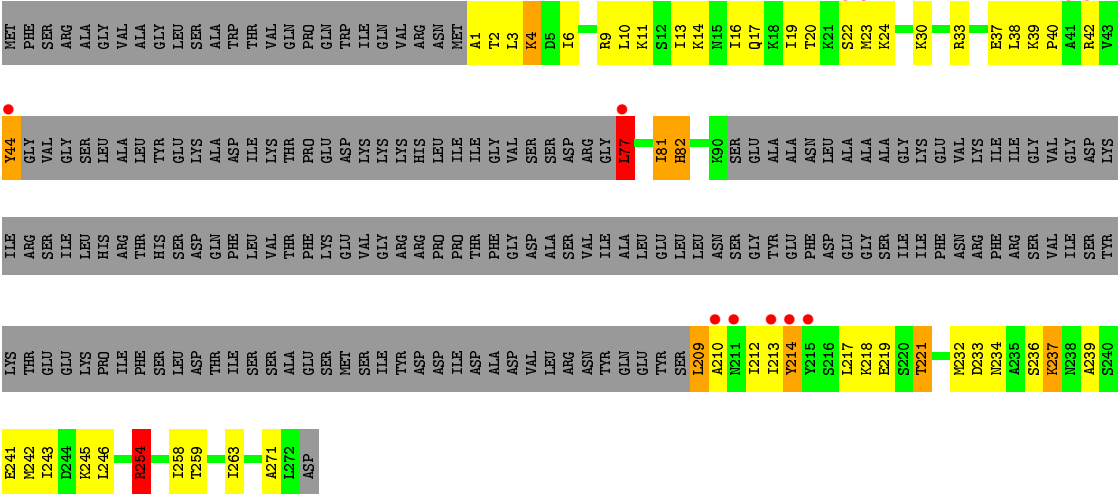


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





● Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.49Å 141.15Å 285.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 6.50 50.70 – 6.50	Depositor EDS
% Data completeness (in resolution range)	86.9 (30.00-6.50) 86.8 (50.70-6.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.290 , 0.285 0.299 , 0.295	Depositor DCC
R_{free} test set	373 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	176.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 7889 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	22690	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: 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	0.60	0/3766	1.31	29/5080 (0.6%)
1	B	0.61	0/3704	1.36	33/4995 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	28/4867 (0.6%)
3	G	0.52	0/949	1.15	5/1266 (0.4%)
All	All	0.61	0/22988	1.34	160/31080 (0.5%)

There are no bond length outliers.

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	408	ARG	CD-NE-CZ	23.29	156.21	123.60
2	E	408	ARG	CD-NE-CZ	14.03	143.24	123.60
1	C	291	ARG	NE-CZ-NH2	-13.33	113.64	120.30
1	B	40	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	B	279	ARG	NE-CZ-NH1	12.94	126.77	120.30

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	3813	162	0
1	B	3656	0	3764	143	0
1	C	3748	0	3843	145	0
2	D	3539	0	3593	150	0
2	E	3530	0	3587	184	0
2	F	3530	0	3586	117	0
3	G	945	0	1019	43	0
4	D	27	0	12	1	0
All	All	22690	0	23217	908	0

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

The worst 5 of 908 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	1.07
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.35	1.05
2:E:223:ASN:H	2:E:223:ASN:HD22	1.00	0.95
2:F:223:ASN:HD22	2:F:223:ASN:H	1.07	0.94
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.92

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	485/553 (88%)	442 (91%)	36 (7%)	7 (1%)	14 58
1	B	475/553 (86%)	426 (90%)	42 (9%)	7 (2%)	13 57
1	C	490/553 (89%)	445 (91%)	37 (8%)	8 (2%)	12 56
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	30 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	464/528 (88%)	408 (88%)	47 (10%)	9 (2%)	10	52
2	F	464/528 (88%)	432 (93%)	30 (6%)	2 (0%)	39	80
3	G	116/298 (39%)	97 (84%)	18 (16%)	1 (1%)	21	67
All	All	2959/3541 (84%)	2669 (90%)	253 (9%)	37 (1%)	15	60

5 of 37 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%)	8	36
1	B	388/444 (87%)	342 (88%)	46 (12%)	6	31
1	C	397/444 (89%)	369 (93%)	28 (7%)	18	55
2	D	377/417 (90%)	346 (92%)	31 (8%)	14	49
2	E	376/417 (90%)	344 (92%)	32 (8%)	13	48
2	F	376/417 (90%)	354 (94%)	22 (6%)	24	61
3	G	102/251 (41%)	92 (90%)	10 (10%)	10	39
All	All	2409/2834 (85%)	2198 (91%)	211 (9%)	12	45

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	164	ARG
2	D	56	SER

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Mol	Chain	Res	Type
2	F	386	ASP
1	C	208	GLN
1	C	406	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	221	GLN
2	D	442	GLN
2	F	282	GLN
2	D	223	ASN
2	E	39	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	D	1476	-	22,29,29	0.95	1 (4%)	27,45,45	1.27	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	D	1476	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1476	ADP	O4'-C1'	2.06	1.43	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1476	ADP	O3'-C3'-C2'	-2.11	104.97	111.83
4	D	1476	ADP	N6-C6-N1	2.32	124.19	119.20
4	D	1476	ADP	C4-C5-N7	3.00	112.24	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1476	ADP	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 [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, 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	487/553 (88%)	-0.01	6 (1%) 81 75	20, 20, 20, 20	0
1	B	479/553 (86%)	0.01	4 (0%) 87 83	20, 20, 20, 20	0
1	C	492/553 (88%)	-0.04	3 (0%) 90 87	20, 20, 20, 20	0
2	D	467/528 (88%)	0.07	1 (0%) 95 94	20, 20, 20, 20	0
2	E	466/528 (88%)	0.10	6 (1%) 79 73	20, 20, 20, 20	0
2	F	466/528 (88%)	-0.05	2 (0%) 93 90	20, 20, 20, 20	0
3	G	122/298 (40%)	0.35	11 (9%) 12 16	20, 20, 20, 20	0
All	All	2979/3541 (84%)	0.03	33 (1%) 82 78	20, 20, 20, 20	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ASP	3.6
3	G	77	LEU	2.9
1	A	173	THR	2.8
3	G	211	ASN	2.6
1	A	269	ASP	2.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ADP	D	1476	27/27	0.64	0.43	1.61	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.