wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:18 AM GMT

PDB ID	:	3A5C
Title	:	Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors	:	Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on	:	2009-08-06
Resolution	:	4.51 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

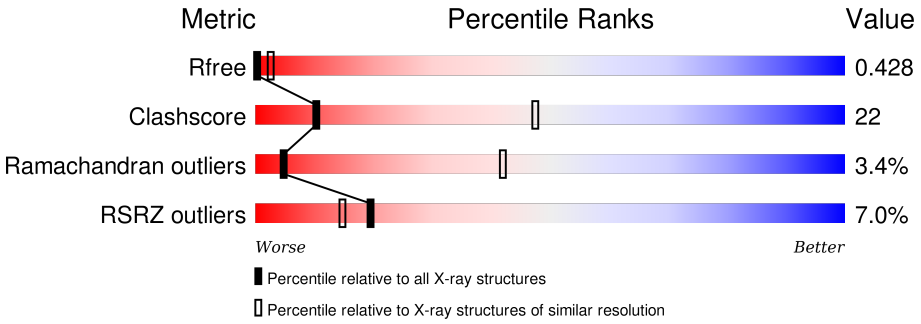
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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	1071 (5.40-3.60)
Clashscore	102246	1004 (5.40-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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 <=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	578	8% 83% 12%
1	B	578	2% 85% 11%
1	C	578	8% 84% 11%
1	I	578	12% 81% 13%
1	J	578	% 84% 11%
1	K	578	10% 83% 12%
2	D	478	5% 83% 9% 6%

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Mol	Chain	Length	Quality of chain
2	E	478	7% 81% 11% 6%
2	F	478	8% 83% 10% 6%
2	L	478	4% 83% 10% 6%
2	M	478	5% 83% 10% 6%
2	N	478	12% 82% 11% 6%
3	G	223	24% 23% 7% 42%
3	O	223	23% 24% 8% 42%
4	H	104	6% 79% 18%
4	P	104	7% 77% 16% 7%

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	ADP	K	600	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32188 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	B	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	C	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	I	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	J	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	K	561	Total 2752	C 1630	N 561	O 561	0	0	0

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	E	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	F	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	L	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	M	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	N	450	Total 2212	C 1312	N 450	O 450	0	0	0

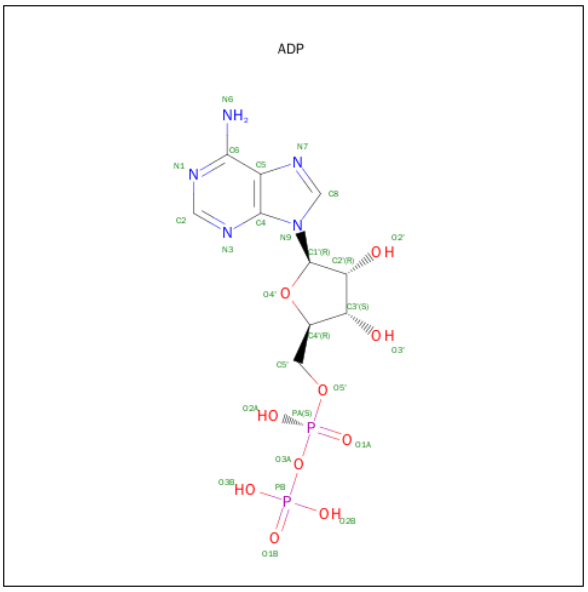
- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total 639	C 381	N 129	O 129	0	0	0
3	O	129	Total 639	C 381	N 129	O 129	0	0	0

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total 509	C 301	N 104	O 104	0	0	0
4	P	104	Total 509	C 301	N 104	O 104	0	0	0

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



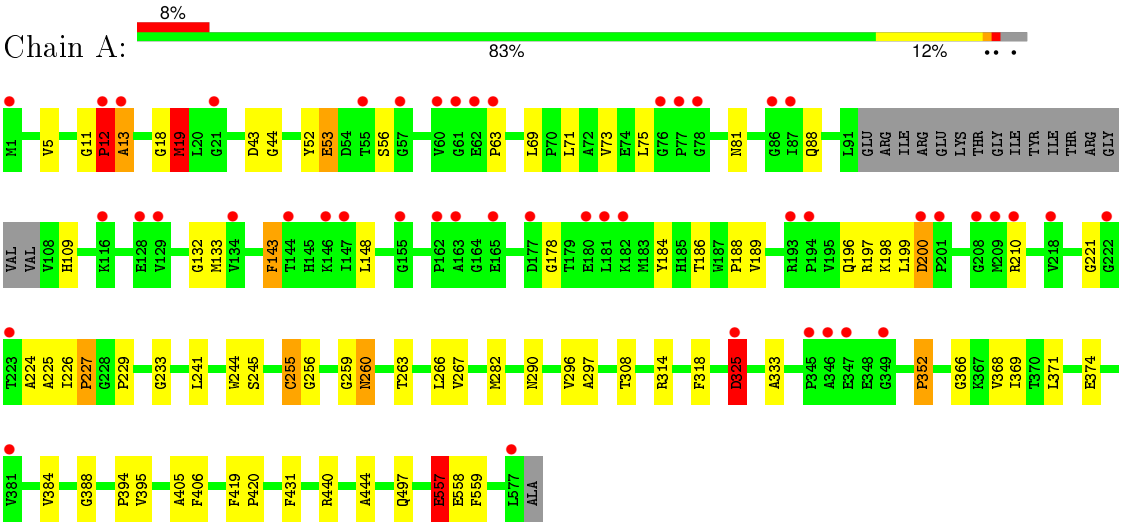
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	K	1	Total 27	C 10	N 5	O 10	P 2	0	0

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.

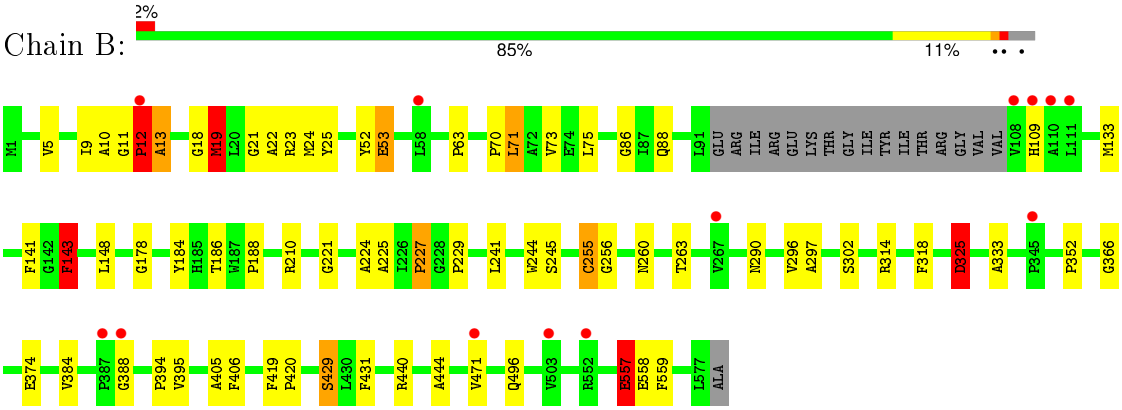
- Molecule 1: V-type ATP synthase alpha chain

Chain A:



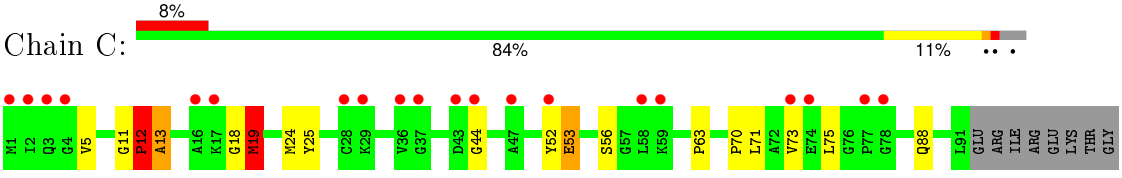
- Molecule 1: V-type ATP synthase alpha chain

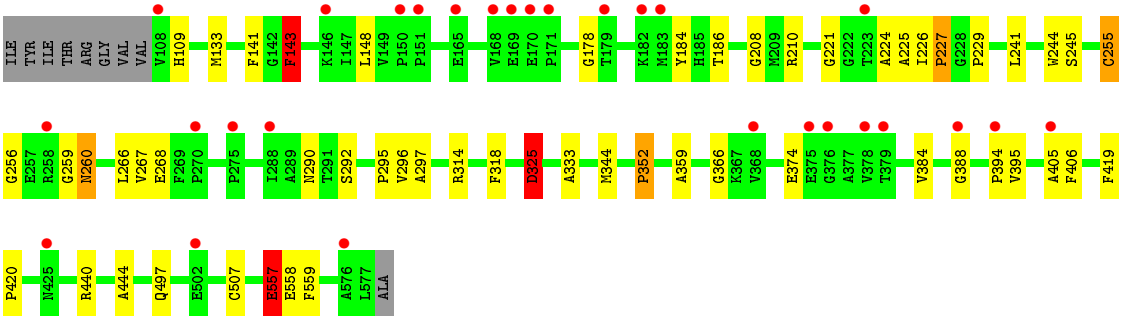
Chain B:



- Molecule 1: V-type ATP synthase alpha chain

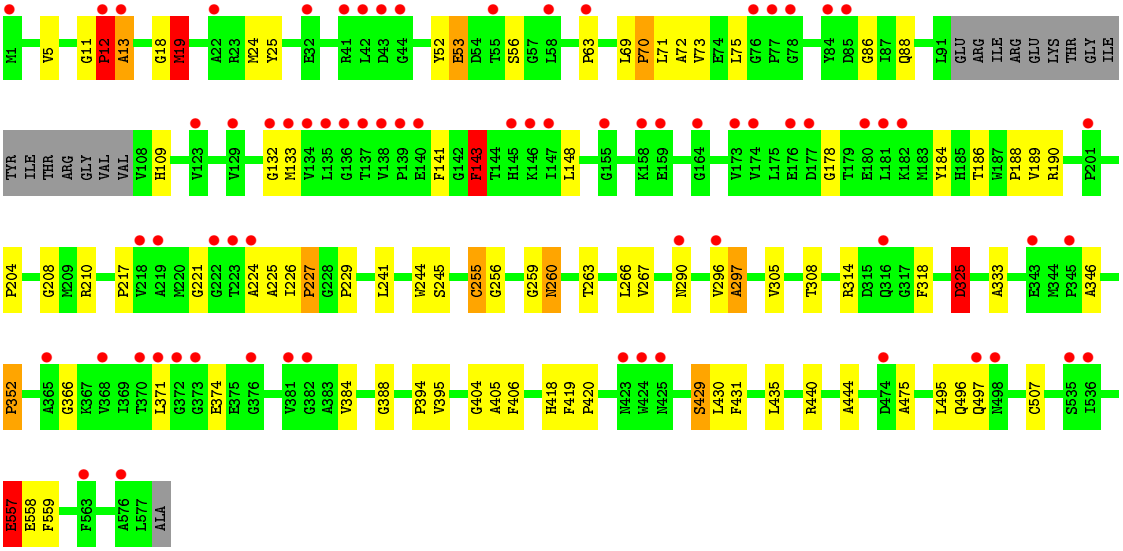
Chain C:





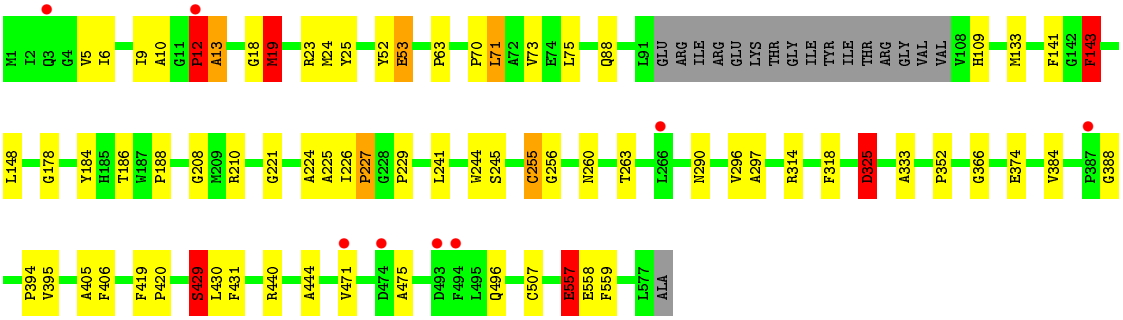
• Molecule 1: V-type ATP synthase alpha chain

Chain I:



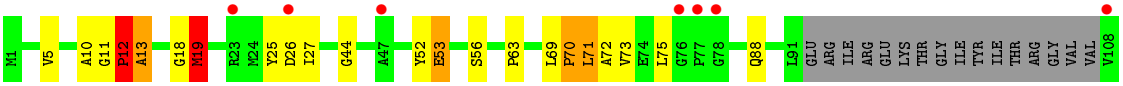
• Molecule 1: V-type ATP synthase alpha chain

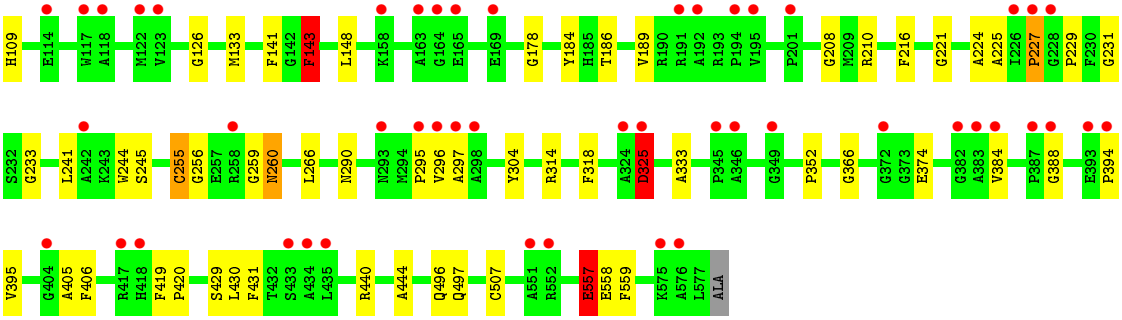
Chain J:



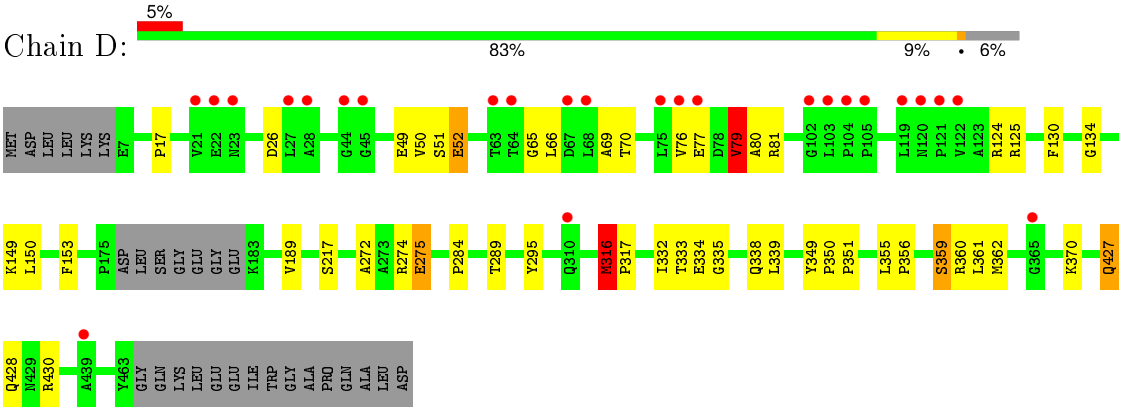
• Molecule 1: V-type ATP synthase alpha chain

Chain K:

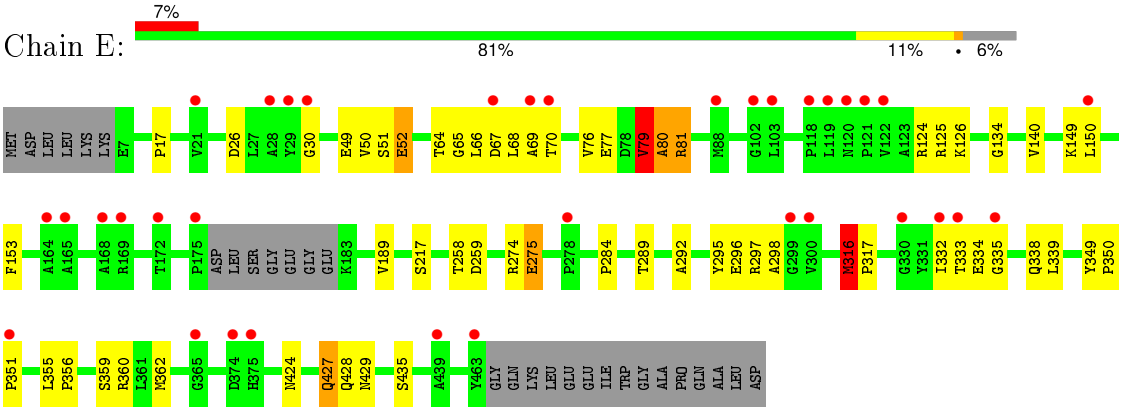




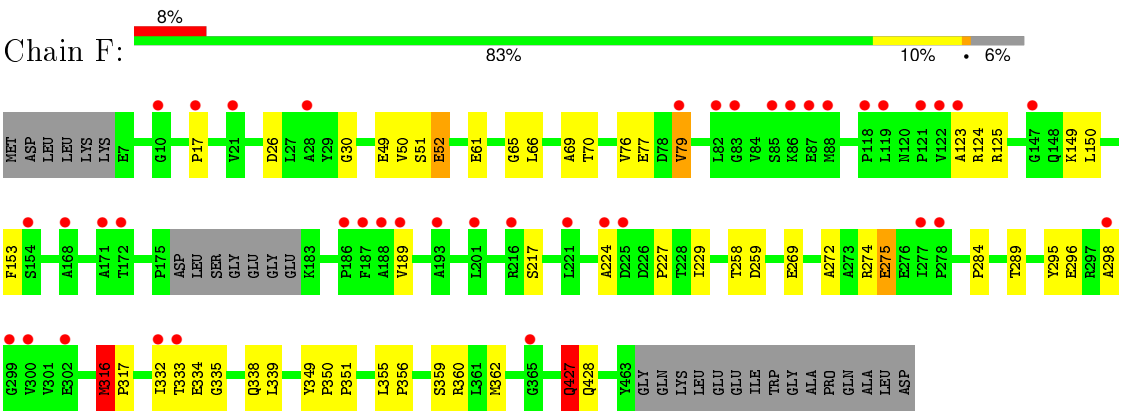
• Molecule 2: V-type ATP synthase beta chain



• Molecule 2: V-type ATP synthase beta chain

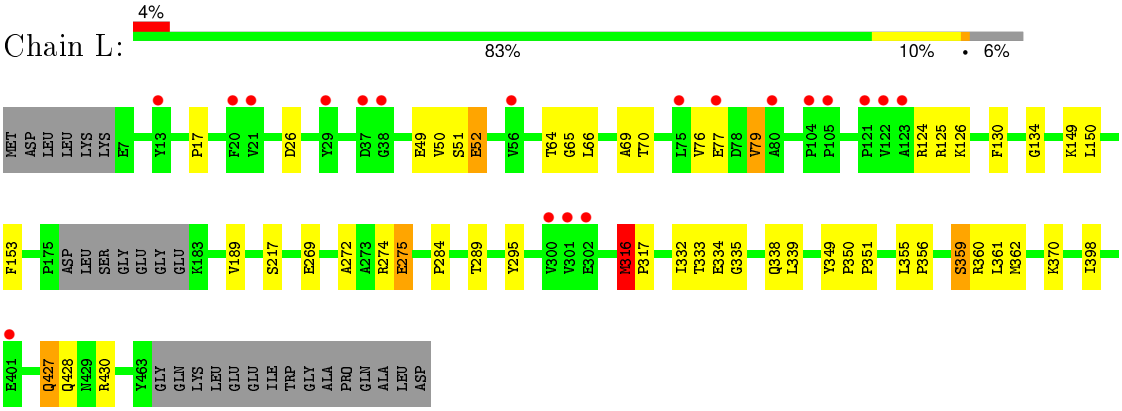


• Molecule 2: V-type ATP synthase beta chain



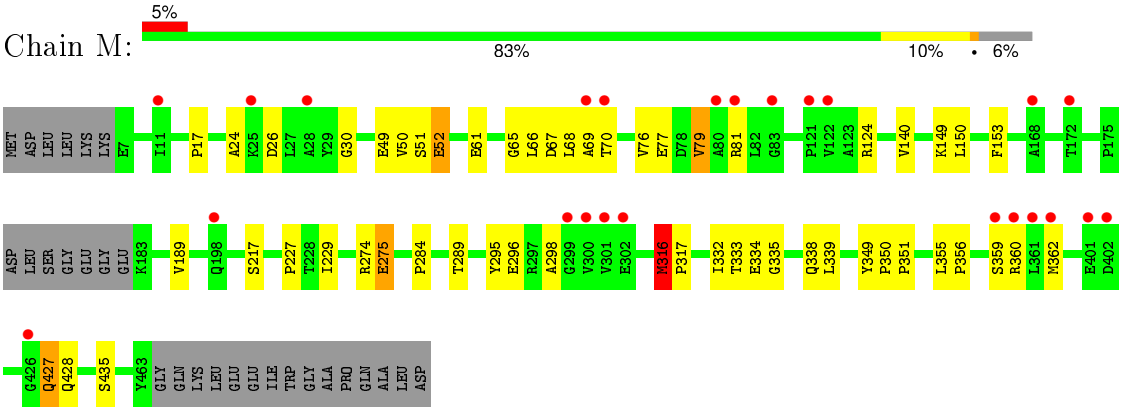
• Molecule 2: V-type ATP synthase beta chain

Chain L:



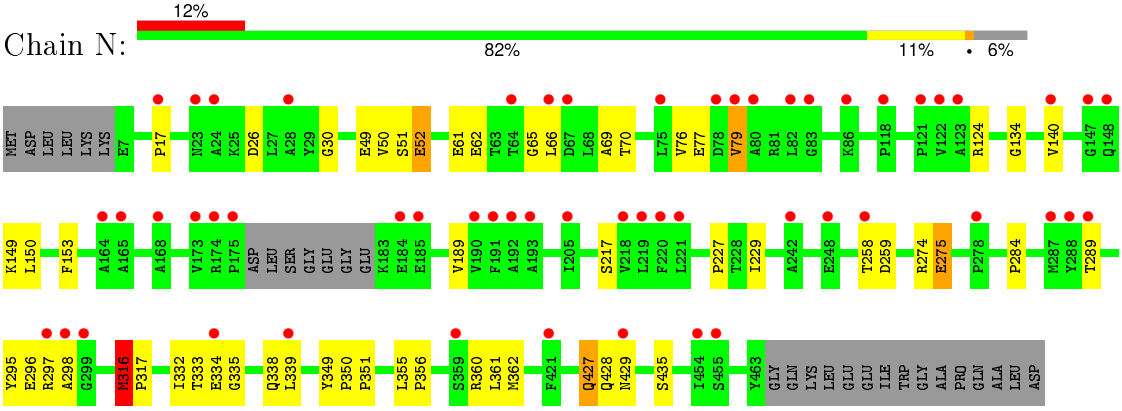
• Molecule 2: V-type ATP synthase beta chain

Chain M:



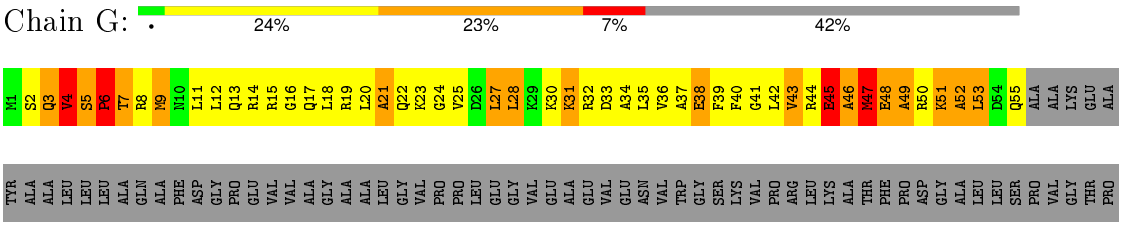
• Molecule 2: V-type ATP synthase beta chain

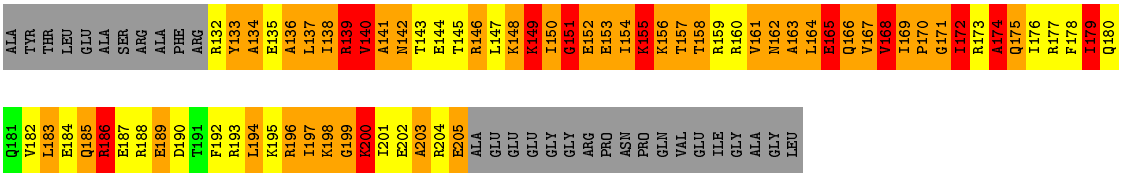
Chain N:



• Molecule 3: V-type ATP synthase subunit D

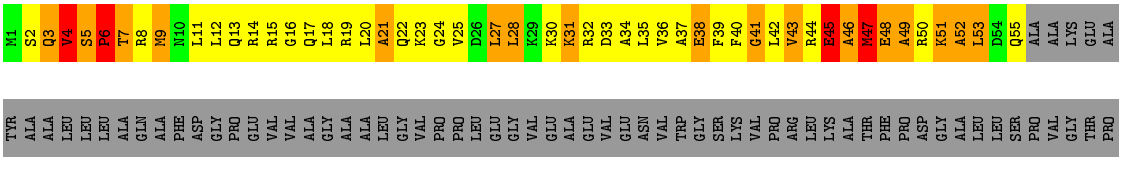
Chain G:

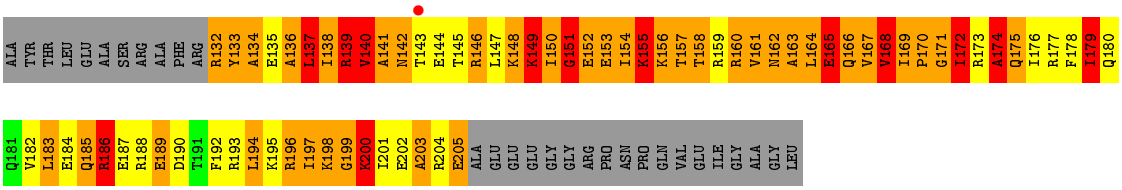




- Molecule 3: V-type ATP synthase subunit D

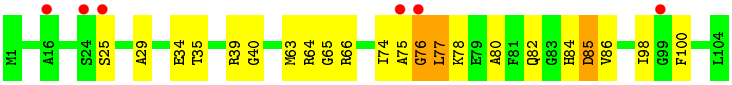
Chain O:





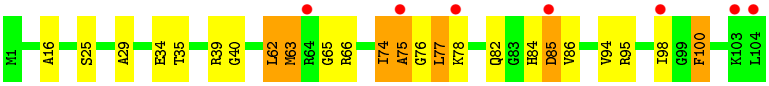
- Molecule 4: V-type ATP synthase subunit F

Chain H:



- Molecule 4: V-type ATP synthase subunit F

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	381.58Å 381.58Å 147.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.51 49.81 – 4.51	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.92-4.51) 96.8 (49.81-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.429 , 0.437 0.421 , 0.428	Depositor DCC
R_{free} test set	3582 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	145.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.01 , -10.0	EDS
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.28$, $< L^2 > = 0.13$	Xtriage
Outliers	1 of 70593 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	32188	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.59	3/2750 (0.1%)	1.20	9/3815 (0.2%)
1	B	0.59	3/2750 (0.1%)	1.21	12/3815 (0.3%)
1	C	0.59	3/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	J	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	K	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.80	7/2210 (0.3%)	1.03	13/3068 (0.4%)
2	E	0.85	7/2210 (0.3%)	1.04	10/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	M	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	N	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	122/637 (19.2%)	2.62	48/885 (5.4%)
3	O	4.09	126/637 (19.8%)	2.63	50/885 (5.6%)
4	H	1.48	6/508 (1.2%)	1.43	9/703 (1.3%)
4	P	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
All	All	1.08	308/32050 (1.0%)	1.27	244/44474 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	5
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	3
2	L	0	4
2	M	0	3
2	N	0	3
4	H	0	3
4	P	0	2
All	All	0	60

The worst 5 of 308 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-25.00	0.98	1.53
3	G	47	MET	CA-CB	-24.93	0.99	1.53
3	O	27	LEU	CA-CB	14.81	1.87	1.53
3	G	27	LEU	CA-CB	14.78	1.87	1.53
4	P	75	ALA	N-CA	13.48	1.73	1.46

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	325	ASP	O-C-N	-39.90	58.86	122.70
1	J	325	ASP	O-C-N	-39.89	58.87	122.70
1	C	325	ASP	O-C-N	-39.89	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.89	122.70
1	K	325	ASP	O-C-N	-39.85	58.94	122.70

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	69	LEU	Peptide

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	2752	0	1302	92	0
1	B	2752	0	1303	65	0
1	C	2752	0	1303	100	0
1	I	2752	0	1300	122	0
1	J	2752	0	1303	61	2
1	K	2752	0	1302	94	0
2	D	2212	0	1009	66	0
2	E	2212	0	1008	80	0
2	F	2212	0	1009	94	0
2	L	2212	0	1009	80	0
2	M	2212	0	1009	59	2
2	N	2212	0	1009	76	0
3	G	639	0	299	131	0
3	O	639	0	299	136	0
4	H	509	0	255	12	0
4	P	509	0	255	23	0
5	A	27	0	12	2	0
5	C	27	0	12	1	0
5	I	27	0	12	0	0
5	K	27	0	12	5	0
All	All	32188	0	15022	1021	2

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 22.

The worst 5 of 1021 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)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.65
3:O:189:GLU:CA	3:O:189:GLU:CB	1.76	1.64
3:G:205:GLU:CA	3:G:205:GLU:CB	1.78	1.62
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
3:G:189:GLU:CB	3:G:189:GLU:CA	1.76	1.58

All (2) 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:J:6:ILE:CB	2:M:24:ALA:O[5_555]	2.04	0.16
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	2.10	0.10

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	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	5	43
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	43
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	5	44
1	I	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	6	45
1	J	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	43
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	5	44
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	53
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	9	53
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	9	53
2	L	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	53
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	9	53
2	N	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	8	51
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	89 (87%)	11 (11%)	2 (2%)	9	53
4	P	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	9	53
All	All	6472/6990 (93%)	5808 (90%)	443 (7%)	221 (3%)	5	42

5 of 221 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

4 ligands are 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	$\#\|Z\| > 2$
5	ADP	A	600	-	22,29,29	1.17	3 (13%)	27,45,45	0.88	1 (3%)
5	ADP	C	600	-	22,29,29	1.04	2 (9%)	27,45,45	1.15	3 (11%)
5	ADP	I	600	-	22,29,29	1.16	3 (13%)	27,45,45	0.88	1 (3%)
5	ADP	K	600	-	22,29,29	1.04	2 (9%)	27,45,45	1.15	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
5	ADP	A	600	-	-	0/12/32/32	0/3/3/3
5	ADP	C	600	-	-	0/12/32/32	0/3/3/3
5	ADP	I	600	-	-	0/12/32/32	0/3/3/3
5	ADP	K	600	-	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	600	ADP	PB-O2B	-2.58	1.45	1.54
5	C	600	ADP	PB-O2B	-2.58	1.45	1.54
5	A	600	ADP	PB-O2B	-2.49	1.45	1.54
5	I	600	ADP	PB-O2B	-2.47	1.45	1.54
5	C	600	ADP	PA-O1A	-2.33	1.42	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	600	ADP	C2'-C1'-N9	-3.03	109.66	114.29
5	K	600	ADP	C2'-C1'-N9	-3.03	109.66	114.29
5	I	600	ADP	C2'-C1'-N9	-2.32	110.75	114.29
5	A	600	ADP	C2'-C1'-N9	-2.29	110.79	114.29
5	K	600	ADP	O4'-C4'-C3'	-2.02	101.08	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ADP	2	0
5	C	600	ADP	1	0
5	K	600	ADP	5	0

5.7 Other polymers (i)

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, 95^{th} 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	561/578 (97%)	0.24	47 (8%) 14 11	103, 162, 214, 214	0
1	B	561/578 (97%)	-0.14	13 (2%) 64 54	79, 130, 144, 144	0
1	C	561/578 (97%)	0.28	48 (8%) 13 11	137, 189, 210, 210	0
1	I	561/578 (97%)	0.48	72 (12%) 5 6	172, 172, 232, 232	0
1	J	561/578 (97%)	-0.33	8 (1%) 78 69	50, 58, 104, 104	0
1	K	561/578 (97%)	0.39	55 (9%) 10 8	146, 177, 189, 189	0
2	D	450/478 (94%)	0.05	25 (5%) 28 21	118, 118, 188, 188	0
2	E	450/478 (94%)	0.18	35 (7%) 16 12	122, 130, 162, 162	0
2	F	450/478 (94%)	0.28	40 (8%) 12 9	109, 217, 217, 217	0
2	L	450/478 (94%)	0.00	19 (4%) 40 31	98, 98, 158, 158	0
2	M	450/478 (94%)	0.07	24 (5%) 30 23	99, 99, 148, 148	0
2	N	450/478 (94%)	0.54	55 (12%) 5 6	158, 250, 250, 250	0
3	G	129/223 (57%)	-0.68	0 100 100	34, 34, 49, 49	0
3	O	129/223 (57%)	-0.60	1 (0%) 87 82	84, 85, 85, 85	0
4	H	104/104 (100%)	0.14	6 (5%) 26 20	110, 110, 134, 134	0
4	P	104/104 (100%)	0.03	7 (6%) 21 15	94, 94, 141, 141	0
All	All	6532/6990 (93%)	0.13	455 (6%) 19 15	34, 137, 232, 250	0

The worst 5 of 455 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	10.8
2	N	191	PHE	9.9
1	I	372	GLY	9.6
2	N	192	ALA	9.3
1	C	379	THR	8.8

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ADP	K	600	27/27	0.63	0.47	0.17	112,112,112,112	0
5	ADP	C	600	27/27	0.79	0.28	-0.27	116,116,116,116	0
5	ADP	A	600	27/27	0.82	0.26	-0.38	109,109,109,109	0
5	ADP	I	600	27/27	0.80	0.28	-0.96	110,110,110,110	0

6.5 Other polymers (i)

There are no such residues in this entry.