wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 7, 2023 – 11:20 pm GMT

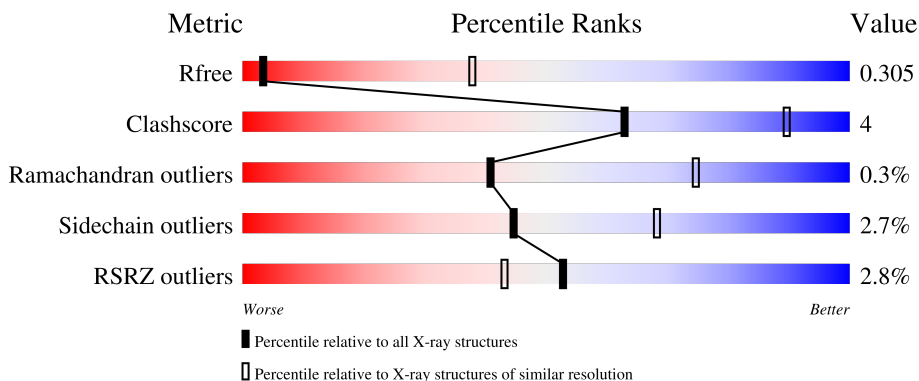|		
PDB ID	:	2W6J
Title	:	Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 5.
Authors	:	Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.
Deposited on	:	2008-12-18
Resolution	:	3.84 Å(reported)

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 3.84 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	Percentile Ranks	Value
Rfree		0.305
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		2.7%
RSRZ outliers		2.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures
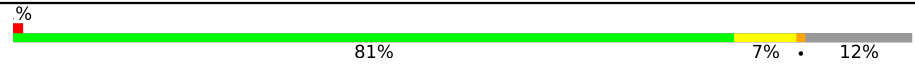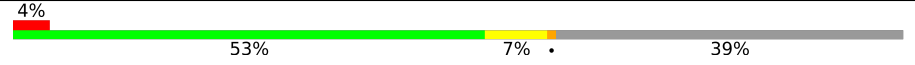
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	2% / 76% 11% · 12%
1	B	553	2% / 81% 5% · 13%
1	C	553	% / 80% 8% · 11%
2	D	528	% / 80% 8% · 12%
2	E	528	4% / 77% 8% · 13%

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Mol	Chain	Length	Quality of chain
2	F	528	81% 7% · 12%
3	G	298	4% 53% 7% · 39%
4	H	168	7% 38% 9% · 51%
5	I	51	10% 39% 10% 51%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 23874 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	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	490	Total	C	N	O	S	0	0	0
			3735	2353	659	711	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	458	Total	C	N	O	S	0	0	0
			3472	2201	592	669	10			
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	182	Total	C	N	O	S	0	0	1
			1397	881	250	260	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	83	Total	C	N	O	S	0	0	0
			620	391	102	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	I	25	203	130	38	34	1	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

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

GLY ALA ASP T21 S22 V23 E26 R45 N78 D79 K80 I94 V95 D96 V99 V107 D116 K124 R128 L131 S141 V142 R143 G160 Q163 R164 A179 I180 Y200 L216 M253 A264 I267 Y278 L283 R287 P288 P289

P295 V334 N341 Q349 I350 F351 E355 K359 G360 I361 R362 P363 A364 S419 R420 G421 V422 R423 K455 Q475 L479 L497 V501 L505 A510

• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:

%

80%　　8%　·　12%

MET LEU GLY LEU VAL GLY ARG VAL VAL ALA ALA SER ALA SER GLY ALA LEU ARG GLY LEU SER PRO SER ALA PRO LEU PRO ALA GLN ALA GLN LEU LEU LEU ARG ALA ALA PRO ALA LEU GLN PRO ALA ARG ASP TYR ALA ALA GLN ALA SER PRO SER PRO LYS ALA GLY ALA T9

F25 G28 I32 L33 S56 P85 V86 G87 P88 E89 M95 N96 V97 T110 K111 V124 Q130 T163 I166 S181 V186 G187 E188 V215 G220 Q221 A228 V232 Y242 Q249 D256 N257 S266 R274 I275 Q282 T287

T291 R356 D359 V363 E366 V370 D386 L396 D400 R412 Q442 Q455 E475 GLU HIS SER

• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:

4%

77%　　8%　·　13%

MET LEU GLY LEU VAL GLY ARG VAL VAL ALA ALA SER ALA SER GLY ALA LEU ARG GLY LEU SER PRO SER ALA PRO LEU PRO GLN ALA GLN LEU LEU LEU ARG ALA ALA PRO ALA LEU ALA LEU GLN PRO ALA ARG ASP TYR ALA ALA GLN ALA GLY ALA T9

I17 M63 G68 R71 G87 I94 V97 M126 G136 V139 I170 S181 R189 N194 Y197 V215 N223 R229 Y242 N257 I258 F259 R260 E267 R274 V279 G280 Y281 Q282 Q293 T298 K301 G302 S303

Q308 D316 L317 T318 D330 Y345 P346 R356 L384 I387 ILE ALA ILE LEU GLY MET ASP GLU L396 S397 E398 E399 D400 Y403 A407 R408 K409 R412 F413 L414 V423 H427 L428 L431 K439 Y449 D450 H451 L452 P453 E454 Q455 A456 F457 Y458

G461 P462 A468 D471 K472 L473 A474 GLU GLU HIS SER

• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:

%

81%　　7%　·　12%

MET LEU GLY LEU VAL GLY ARG VAL VAL ALA ALA SER ALA SER GLY ALA LEU ARG GLY LEU SER PRO SER ALA PRO LEU PRO GLN ALA GLN LEU LEU LEU ARG ALA ALA PRO ALA LEU GLN PRO ALA ARG ASP TYR ALA ALA GLN ALA SER PRO SER PRO LYS ALA GLY ALA T9 T10

G11 R12 I13 E27 V70 Q73 G87 P88 E89 N96 V97 E104 T110 K111 Q112 V139 L142 N172 K175 E188 Q221 M222 N223 V232 A233 L237 Y242 D256 N257 R274 V279 Q282 T287 T291 H367 Q385

D386 I387 I390 L391 E395 E398 L414 Q419 L434 I438 A474 GLU GLU HIS SER

• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL
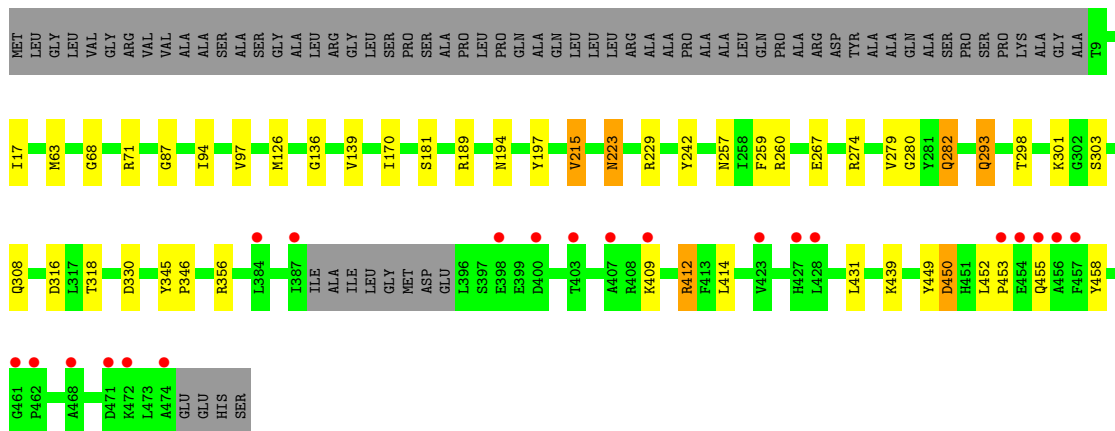
Chain G:

4%

53%   7% •   39%

MET PHE SER ARG ALA GLY VAL ALA GLY LEU SER ALA TRP THR VAL GLN PRO GLN TRP ILE GLN VAL ARG ASN MET A1 R8 I13 T20 R33 V43 G47 SER LEU ALA LEU TYR GLU LYS ALA ASP ILE LYS THR PRO GLU ASP LYS LYS HIS L67 I68 I69

S73 I81 A86 LYS GLN MET LYS SER GLU GLU ALA ALA ASN LEU ALA ALA GLY LYS VAL LYS I105 I106 G107 L116 HIS ARG THR HIS SER ASP GLN PHE LEU VAL T127 E130 V131 P136 T137 F138 G139 D140 I144 L148 LEU ASN SER GLY TYR GLU PHE

ASP GLU GLY S159 I160 N163 R166 S167 V168 I169 S170 Y171 K172 T173 GLU GLU LYS PRO ILE PHE SER LEU ASP THR ILE SER SER ALA GLU SER MET SER ILE TYR ASP ASP ILE ASP ALA ASP VAL LEU ARG ASN TYR GLN E206 N211 I212 S216 L217 K218 T221 M232

M242 I243 R254 Q255 L262 A271 LEU ASP

• Molecule 4: F1-ATPASE DELTA SUBUNIT

Chain H:

7%

38%   9% •   51%

MET LEU PRO SER ALA LEU LEU ARG ARG PRO GLY LEU GLY LEU VAL ARG GLN VAL ARG LEU ARG TYR ALA GLU ALA ALA ALA GLN ALA PRO ALA ALA GLY PRO GLY GLN MET S17 F18 V26 F27 F28 N29 SER ALA ASN VAL ARG Q35 T40 GLN THR GLY ALA PHE GLY ILE

LEU ALA ALA HIS VAL PRO THR LEU GLN VAL L58 V65 HIS ALA GLU ASP GLY THR THR SER LYS TYR F76 S79 G80 S81 VAL THR VAL ASN ALA ASP SER SER VAL Q91 A94 E95 E96 A97 V98 T99 L100 D101 M102 L103 D104 L105 G106 A107 L112 A115 E118

G121 A122 A123 D124 E125 A126 T127 R128 N138 E139 A140 LEU VAL LYS ALA LEU GLU

• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:

10%

39%   10%   51%

MET V1 Q6 A7 S10 Y11 I12 R13 Q16 A19 A25 LEU LYS THR GLU PHE LYS SER ALA ASN ALA MET LYS THR SER GLY SER THR ILE LYS ILE VAL LYS VAL LYS LYS GLU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.93Å 124.07Å 264.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	132.45 – 3.84 71.86 – 3.84	Depositor EDS
% Data completeness (in resolution range)	95.3 (132.45-3.84) 95.3 (71.86-3.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.305 , (Not available) 0.307 , 0.305	Depositor DCC
R_{free} test set	1665 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 3.6	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	23874	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 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	0.37	1/3766 (0.0%)	0.53	0/5080
1	B	0.38	0/3711	0.52	0/5005
1	C	0.35	0/3786	0.51	0/5108
2	D	0.36	0/3596	0.54	0/4879
2	E	0.35	0/3528	0.52	0/4786
2	F	0.39	0/3587	0.54	0/4867
3	G	0.37	0/1406	0.47	0/1880
4	H	0.39	0/623	0.62	0/840
5	I	0.41	0/207	0.59	0/279
All	All	0.37	1/24210 (0.0%)	0.53	0/32724

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	VAL	CA-CB	5.47	1.66	1.54

There are no bond angle outliers.

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	42	1
1	B	3663	0	3773	15	0
1	C	3735	0	3834	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3539	0	3593	37	1
2	E	3472	0	3526	39	0
2	F	3530	0	3587	25	0
3	G	1397	0	1481	16	0
4	H	620	0	614	30	0
5	I	203	0	205	4	0
All	All	23874	0	24426	209	1

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 4.

The worst 5 of 209 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)
4:H:122:ALA:HA	4:H:123:ALA:CB	1.74	1.15
3:G:68:ILE:HB	3:G:69:ILE:HA	1.31	1.09
2:D:89:GLU:HG3	2:D:110:THR:HB	1.29	1.08
2:D:228:ALA:O	2:D:232:VAL:HG13	1.52	1.08
4:H:104:ASP:HA	4:H:105:LEU:HB2	1.31	1.06

All (1) 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:A:48:GLN:CD	2:D:111:LYS:NZ[4_545]	2.17	0.03

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%)	469 (97%)	15 (3%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	476/553 (86%)	465 (98%)	10 (2%)	1 (0%)	47	78
1	C	488/553 (88%)	476 (98%)	12 (2%)	0	100	100
2	D	465/528 (88%)	445 (96%)	20 (4%)	0	100	100
2	E	454/528 (86%)	444 (98%)	9 (2%)	1 (0%)	47	78
2	F	464/528 (88%)	450 (97%)	13 (3%)	1 (0%)	47	78
3	G	170/298 (57%)	161 (95%)	8 (5%)	1 (1%)	25	62
4	H	73/168 (44%)	64 (88%)	6 (8%)	3 (4%)	3	26
5	I	23/51 (45%)	22 (96%)	1 (4%)	0	100	100
All	All	3098/3760 (82%)	2996 (97%)	94 (3%)	8 (0%)	41	74

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	123	ALA
4	H	128	ARG
4	H	105	LEU
2	E	279	VAL
1	B	35	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	393/444 (88%)	382 (97%)	11 (3%)	43	67
1	B	389/444 (88%)	380 (98%)	9 (2%)	50	71
1	C	396/444 (89%)	383 (97%)	13 (3%)	38	64
2	D	377/417 (90%)	371 (98%)	6 (2%)	62	79
2	E	370/417 (89%)	362 (98%)	8 (2%)	52	72
2	F	376/417 (90%)	364 (97%)	12 (3%)	39	64
3	G	152/251 (61%)	145 (95%)	7 (5%)	27	56
4	H	66/128 (52%)	64 (97%)	2 (3%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	19/42 (45%)	19 (100%)	0	100	100
All	All	2538/3004 (84%)	2470 (97%)	68 (3%)	44	68

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	398	GLU
3	G	33	ARG
3	G	262	LEU
1	C	99	VAL
1	C	96	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	73	GLN
3	G	211	ASN
2	F	96	ASN
2	F	223	ASN
5	I	16	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	487/553 (88%)	0.20	13 (2%)	54	45	20, 20, 20, 20	4 (0%)
1	B	480/553 (86%)	0.27	13 (2%)	54	45	20, 20, 20, 20	1 (0%)
1	C	490/553 (88%)	0.10	6 (1%)	79	72	20, 20, 20, 20	0
2	D	467/528 (88%)	0.13	3 (0%)	89	85	20, 20, 20, 20	2 (0%)
2	E	458/528 (86%)	0.33	21 (4%)	32	27	20, 20, 20, 20	2 (0%)
2	F	466/528 (88%)	0.16	3 (0%)	89	85	20, 20, 20, 20	3 (0%)
3	G	182/298 (61%)	0.73	13 (7%)	16	12	20, 20, 20, 20	0
4	H	83/168 (49%)	1.13	11 (13%)	3	3	20, 20, 20, 20	0
5	I	25/51 (49%)	1.10	5 (20%)	1	1	20, 20, 20, 20	0
All	All	3138/3760 (83%)	0.26	88 (2%)	53	43	20, 20, 20, 20	12 (0%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	THR	4.6
1	A	501	VAL	4.4
1	C	22	SER	4.4
3	G	163	ASN	3.7
2	E	398	GLU	3.7

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.