

wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 10:11 PM EDT

PDB ID	:	5BW9
Title	:	Crystal Structure of Yeast V1-ATPase in the Autoinhibited Form
Authors	:	Oot, R.A.; Kane, P.M.; Berry, E.A.; Wilkens, S.
Deposited on	:	2015-06-06
Resolution	:	7.00 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 7.00 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.



Motric	Whole archive	Similar resolution
IVIEU IC	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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		017	15%	
	А	617	92%	• •
			11%	
1	В	617	93%	• •
			10%	
1	C	617	93%	• 5%
			17%	
1	a	617	95%	• •
			10%	
1	b	617	95%	5%
			8%	
1	С	617	94%	• 5%



 Continued from previous page...

 Mol
 Chain
 Length

Mol	Chain	Length	Quality of chain	
2	D	517	86%	• 12%
2	Е	517	3% 	• 12%
			5%	• 1270
2	F,	517	84%	• 13%
2	d	517	89%	11%
2	е	517	88%	12%
2	f	517	<u>6%</u> 87%	13%
3	Н	478	92%	• 7%
3	h	478	93%	7%
4	G	256	54%	46%
4	g	256	55%	45%
5	J	122	3% 85%	15%
5	L	122	8%	44%
5	Ν	122	66%	34%
5	j	122	83%	17%
5	l	122	54%	46%
5	n	122	48% 52'	%
6	Ι	233	9%	7%
6	К	233	10%	• 24%
6	М	233	21%	• 13%
6	i	233	93%	7%
6	k	233	18%	28%
6	m	233	11%	22%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 44760 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.

Mol	Chain	Residues		Ator	ns		ZeroOcc	AltConf	Trace
1	Δ	501	Total	С	Ν	Ο	0	0	0
1	Л	591	2905	1723	591	591	0	0	0
1	В	504	Total	С	Ν	Ο	0	0	0
1	D	554	2920	1732	594	594	0	0	0
1	С	580	Total	С	Ν	Ο	0	0	0
1		009	2895	1717	589	589	0		0
1	0	501	Total	С	Ν	Ο	0	0	0
1	a	591	2905	1723	591	591	0	0	0
1	h	580	Total	С	Ν	Ο	0	0	0
1	U	009	2895	1717	589	589	0	0	0
1		586	Total	С	Ν	Ο	0	0	0
	C	500	2880	1708	586	586	0		U

• Molecule 1 is a protein called V-type proton ATPase catalytic subunit A.

• Molecule 2 is a protein called V-type proton ATPase subunit B.

Mol	Chain	Residues		Ator	ns		ZeroOcc	AltConf	Trace
2	Л	457	Total	С	Ν	Ο	0	0 0	0
	D	407	2250	1336	457	457	0	0	0
2	F	453	Total	С	Ν	Ο	0	0	0
	Ľ	400	2231	1325	453	453	0	0	0
2	F	440	Total	С	Ν	Ο	0	0	0
	Г	449	2211	1313	449	449	0		
2	d	460	Total	С	Ν	Ο	0	0	0
	u	400	2265	1345	460	460	0	0	
9	0	456	Total	С	Ν	Ο	0	0	0
	е	450	2245	1333	456	456	U	0	0
2	f	440	Total	С	Ν	Ο	0	0	0
	1	449	2212	1314	449	449	0		U

• Molecule 3 is a protein called V-type proton ATPase subunit H.



Mol	Chain	Residues		Ator	ns		ZeroOcc	AltConf	Trace
3	н	445	Total	С	Ν	Ο	0	0	0
5	11	440	2212	1322	445	445	0	0	0
2	h	444	Total	С	Ν	Ο	0	0	0
່ <u>ວ</u>	11	444	2208	1320	444	444	0		

• Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
4	С	120	Total	С	Ν	Ο	0	0	0
4	G	159	691	413	139	139	0	0	0
4	<i>a</i> r	1 / 1	Total	С	Ν	Ο	0 0	0	0
4	g	141	701	419	141	141	0	0	0

• Molecule 5 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	J	104	Total C N O 514 306 104 104	0	0	0
5	L	68	Total C N O 335 199 68 68	0	0	0
5	Ν	81	Total C N O 400 238 81 81	0	0	0
5	j	101	Total C N O 499 297 101 101	0	0	0
5	1	66	Total C N O 325 193 66 66	0	0	0
5	n	58	Total C N O 288 172 58 58	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-7	MET	-	initiating methionine	UNP P48836
J	-6	ASP	-	expression tag	UNP P48836
J	-5	TYR	-	expression tag	UNP P48836
J	-4	LYS	-	expression tag	UNP P48836
J	-3	ASP	-	expression tag	UNP P48836
J	-2	ASP	-	expression tag	UNP P48836
J	-1	ASP	-	expression tag	UNP P48836
J	0	ASP	-	expression tag	UNP P48836
J	1	LYS	-	expression tag	UNP P48836
L	-7	MET	-	initiating methionine	UNP P48836
L	-6	ASP	-	expression tag	UNP P48836



5BW9

Chain		Modelled	Actual	Comment	Reference
L	-5	TYR	_	expression tag	UNP P48836
L	-4	LYS	_	expression tag	UNP P48836
L	-3	ASP	-	expression tag	UNP P48836
L	-2	ASP	-	expression tag	UNP P48836
L	-1	ASP	-	expression tag	UNP P48836
L	0	ASP	-	expression tag	UNP P48836
L	1	LYS	-	expression tag	UNP P48836
N	-7	MET	-	initiating methionine	UNP P48836
N	-6	ASP	-	expression tag	UNP P48836
N	-5	TYR	-	expression tag	UNP P48836
N	-4	LYS	-	expression tag	UNP P48836
N	-3	ASP	-	expression tag	UNP P48836
N	-2	ASP	-	expression tag	UNP P48836
N	-1	ASP	-	expression tag	UNP P48836
N	0	ASP	-	expression tag	UNP P48836
N	1	LYS	-	expression tag	UNP P48836
j	-7	MET	-	initiating methionine	UNP P48836
j	-6	ASP	-	expression tag	UNP P48836
j	-5	TYR	-	expression tag	UNP P48836
j	-4	LYS	-	expression tag	UNP P48836
j	-3	ASP	-	expression tag	UNP P48836
j	-2	ASP	-	expression tag	UNP P48836
j	-1	ASP	-	expression tag	UNP P48836
j	0	ASP	-	expression tag	UNP P48836
j	1	LYS	-	expression tag	UNP P48836
1	-7	MET	-	initiating methionine	UNP P48836
1	-6	ASP	-	expression tag	UNP P48836
1	-5	TYR	-	expression tag	UNP P48836
1	-4	LYS	-	expression tag	UNP P48836
1	-3	ASP	-	expression tag	UNP P48836
1	-2	ASP	-	expression tag	UNP P48836
1	-1	ASP	-	expression tag	UNP P48836
1	0	ASP	-	expression tag	UNP P48836
1	1	LYS	-	expression tag	UNP P48836
n	-7	MET	-	initiating methionine	UNP P48836
n	-6	ASP	-	expression tag	UNP P48836
n	-5	TYR	-	expression tag	UNP P48836
n	-4	LYS	-	expression tag	UNP P48836
n	-3	ASP	-	expression tag	UNP P48836
n	-2	ASP	-	expression tag	UNP P48836
n	-1	ASP	-	expression tag	UNP P48836
n	0	ASP	-	expression tag	UNP P48836



Chain	Residue	Modelled	Actual	Comment	Reference
n	1	LYS	-	expression tag	UNP P48836

• Molecule 6 is a protein called V-type proton ATPase subunit E.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
6	6 I	916	Total	С	Ν	Ο	0	0	0
0		210	1073	641	216	216	0	0	0
6	V	170	Total	С	Ν	0	0	0	0
0	n	178	883	527	178	178	0	0	0
6	м	203	Total	С	Ν	0	0	0	0
0	1/1		1008	602	203	203	0		
6	:	217	Total	С	Ν	0	0	0	0
0	1		1078	644	217	217	0	0	U
6	1.	168	Total	С	Ν	0	0	0	0
0	K		833	497	168	168	0	0	U
6	m	181	Total	С	Ν	Ο	0	0	0
6	m		898	536	181	181		U	U



3 Residue-property plots (i)

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: V-type proton ATPase catalytic subunit A















G303 G303 E322 E323 E323 ARG ARG ARG ARG ARG ARG ARG ARG ARD ARD ARD ARD ARD ARD ARD ARD ARD ARD
• Molecule 2: V-type proton ATPase subunit B
Chain f: 87% 13%
MET WALT NALT SER ASP LUS CLU LUS CLU LUS LUS LUS LUS LUS LUS CLU CLN CLU CLN CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
HIS 011 112 1206 1211 1226 1226 1324 1321 144 1321 144 1322 1324 1324 1
• Molecule 3: V-type proton ATPase subunit H
Chain H: 92% • 7%
MET MET KA3 LYS LYS LYS LYS LIJE CLY ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN
• Molecule 3: V-type proton ATPase subunit H
Chain h: 93% 7%
Chain h: 93% 7%
Ohain h: 93% 7% Image: Ima
Chain h: 93% 7% Image: State of the st
Chain h: 93% 7% Molecule 4: V-type proton ATPase subunit D Chain G: 54% 46%
Chain h: 93% 7% • 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Chain h: 93% 7% • Molecule 4: V-type proton ATPase subunit D Chain G: 54% 46% • Molecule 4: V-type proton ATPase subunit D • Molecule 5: 54% 46% • Molecule 4: V-type proton ATPase subunit D 46% • Molecule 5: 54% 6 6 • Molecule 4: V-type proton ATPase subunit D 6 6 • Molecule 4: V-type proton ATPase subunit D 6 6 • Molecule 5: 6 6 6 • Molecule 4: V-type proton ATPase subunit D 6 6 • Molecule 5: 6 6 6 6 • Molecule 5: 6 6 6 6 6 • Molecule 5: 6 6 6 6 6 6 • Molecule 5: 6 6 6 6 6 6 6 6 • Molecule 5: 6 6 6
Chain h: 93% 7% Weile at the set of th
Chain h: 93% 7% 93% 7% 93% 7% 93% 7% 93% 7% 93% 9% 93% 7% 93% 7% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 94% 9% 93% 9% 93% 9% 93% 9% 93% 9% 93% 9% 9% 9% 9% 9% 9% 9% 9% 9% 9% 9% 9% 9%





V65 K90 S106 GLU VAL HIS ALA ALA LEU
• Molecule 5: V-type proton ATPase subunit G
Chain n: 48% 52%
MET ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
ST 06 GLU GLU GLU GLU GLU GLU ASN LEU
• Molecule 6: V-type proton ATPase subunit E
Chain I: 93% 7%
MET SER SER ALA LLEU LLEU LEU AL1 AL1 AL1 CL29 CL29 CL29 CL29 CL29 CL29 CL29 CL29
• Molecule 6: V-type proton ATPase subunit E
Chain K: 76% • 24%
MET MET ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
R140 A141 E143 E144 B145 B146 F171 E170 E100
• Molecule 6: V-type proton ATPase subunit E
Chain M: 86% • 13%
MET MET ALA ALA ALA ALA ALA ALA ALA ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS
E102 T103 K104 E105 E105 E121 Q122 Q122 A137 A137 A137 A137 A137 A137 A137 A137
• Molecule 6: V-type proton ATPase subunit E
Chain i: 93% 7%
MET SER SER ALA ALA ALA ALA ALA L8 C F68 C F68 D59 D59 D59 D59 D59 D59 D59 D59 C F62 C F62 C F62 C F62 C F62 C F62 C F62 C F62 C F63 C C F63 C C C C C C C C C C C C C C C C C C C
VORLDWIDE FROTEIN DATA BANK

• Molecule 6: V-type proton ATPase subunit E

Chain k:	72%	28%
MET SER SER ALA ALA THR THR THR THR THR THR THR ASN	GLN VAL ASP ASP ASP ASP CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	TYR CLU TLE CLU CLU CLU CLU CLU CLU CLU CLU ASN ASN ASN ASN ASN CLU ASN ASN CLU ASN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
F62 K63 S64 K65 K65 T103 T103 C109 C109 T110	N112 1125 1125 1125 1125 1128 1128 1129 1129 1138 1138 1138 1138 1138 1142 1142 1142 1142 1143 1144 1142 1143 1144 1142 1142	8191 N192 A193 E198 E198 1199 N200 N201 P2016 P216 P216 P216 P216 P216 P216 P216 P2
LYS PHE ASP ASP		
• Molecule 6: 7	V-type proton ATPase subunit E	
Chain m:	78%	22%
MET SER SER ALA ILE THR ALA LEU THR PRO ASN	CLN VAL ASP ASP ASP ASP CLU ASN ASN ASN ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	TYR E44 E46 E166 E115 E115 E115 A137 A137 A137 A141 A141 L142
Y160 L169 S185 G185 C187 V188 V189	8191 K195 1197 1197 1198 1198 N200 N200 C198 C178 C178 C178 ARG C178 ARG C178 ARG ARG ARG	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	468.48Å 159.74Å 245.04Å	Deperitor
a, b, c, α , β , γ	90.00° 113.88° 90.00°	Depositor
Bosolution(A)	40.10 - 7.00	Depositor
Resolution (A)	40.10 - 7.00	EDS
% Data completeness	99.3 (40.10-7.00)	Depositor
(in resolution range)	90.4 (40.10-7.00)	EDS
R_{merge}	0.19	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 7.33 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1957)	Depositor
B B.	0.260 , 0.309	Depositor
Π, Π_{free}	0.268 , 0.313	DCC
R_{free} test set	2000 reflections $(7.66%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	321.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40, 999.0	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	0.80	EDS
Total number of atoms	44760	wwPDB-VP
Average B, all atoms $(Å^2)$	290.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.18	0/2904	0.31	0/4034	
1	В	0.18	0/2919	0.31	0/4055	
1	С	0.19	0/2894	0.32	0/4020	
1	a	0.18	0/2904	0.31	0/4034	
1	b	0.18	0/2894	0.30	0/4020	
1	с	0.18	0/2879	0.32	0/3999	
2	D	0.18	0/2248	0.30	0/3123	
2	Е	0.18	0/2229	0.30	0/3097	
2	F	0.18	0/2209	0.30	0/3069	
2	d	0.18	0/2264	0.30	0/3147	
2	е	0.18	0/2243	0.30	0/3116	
2	f	0.18	0/2210	0.30	0/3071	
3	Н	0.19	0/2209	0.32	0/3080	
3	h	0.19	0/2205	0.32	0/3075	
4	G	0.18	0/689	0.31	0/959	
4	g	0.18	0/699	0.30	0/973	
5	J	0.18	0/513	0.30	0/713	
5	L	0.19	0/334	0.30	0/463	
5	N	0.18	0/399	0.30	0/554	
5	j	0.18	0/498	0.30	0/692	
5	1	0.19	0/324	0.30	0/449	
5	n	0.18	0/286	0.29	0/396	
6	Ι	0.18	0/1072	0.29	0/1495	
6	К	0.18	0/882	0.29	0/1229	
6	М	0.18	0/1007	0.28	0/1404	
6	i	0.18	0/1077	0.29	0/1502	
6	k	0.18	0/832	0.28	0/1159	
6	m	0.18	0/897	0.28	0/1250	
All	All	0.18	0/44720	0.31	0/62178	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2905	0	1339	12	0
1	В	2920	0	1348	11	0
1	С	2895	0	1335	6	0
1	a	2905	0	1339	0	0
1	b	2895	0	1335	0	0
1	с	2880	0	1326	0	0
2	D	2250	0	1015	8	0
2	Е	2231	0	1006	7	0
2	F	2211	0	999	9	0
2	d	2265	0	1022	0	0
2	е	2245	0	1013	0	0
2	f	2212	0	998	0	0
3	Н	2212	0	951	2	0
3	h	2208	0	948	0	0
4	G	691	0	311	0	0
4	g	701	0	312	0	0
5	J	514	0	248	0	0
5	L	335	0	160	0	0
5	N	400	0	189	0	0
5	j	499	0	243	0	0
5	1	325	0	150	0	0
5	n	288	0	136	0	0
6	Ι	1073	0	481	0	0
6	K	883	0	394	1	0
6	М	1008	0	456	1	0
6	i	1078	0	483	0	0
6	k	833	0	374	0	0
6	m	898	0	400	0	0
All	All	44760	0	20311	52	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 1.

The worst 5 of 52 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:H:352:GLU:HA	3:H:355:SER:HA	1.72	0.72
2:D:28:TYR:H	2:D:93:VAL:H	1.39	0.69
3:H:353:LEU:H	3:H:354:THR:C	1.97	0.68
1:A:383:ALA:HB1	2:E:290:GLU:HA	1.95	0.63
2:D:31:VAL:HA	2:D:41:LEU:HA	1.80	0.63

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	Percer	ntiles
1	А	589/617~(96%)	550~(93%)	34~(6%)	5 (1%)	19	60
1	В	592/617~(96%)	557 (94%)	35~(6%)	0	100	100
1	С	587/617~(95%)	548 (93%)	33~(6%)	6 (1%)	15	54
1	a	589/617~(96%)	550~(93%)	33~(6%)	6 (1%)	15	54
1	b	587/617~(95%)	552 (94%)	35~(6%)	0	100	100
1	с	584/617~(95%)	545 (93%)	33 (6%)	6 (1%)	15	54
2	D	453/517~(88%)	425 (94%)	28 (6%)	0	100	100
2	Е	449/517~(87%)	428 (95%)	21 (5%)	0	100	100
2	F	445/517~(86%)	420 (94%)	25~(6%)	0	100	100
2	d	458/517~(89%)	429 (94%)	28 (6%)	1 (0%)	47	81
2	е	452/517~(87%)	431 (95%)	21 (5%)	0	100	100
2	f	445/517~(86%)	421 (95%)	23~(5%)	1 (0%)	47	81
3	Н	439/478~(92%)	412 (94%)	27~(6%)	0	100	100
3	h	438/478~(92%)	412 (94%)	25 (6%)	1 (0%)	47	81
4	G	135/256~(53%)	130 (96%)	4 (3%)	1 (1%)	22	63
4	g	137/256~(54%)	134 (98%)	3 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
5	J	102/122~(84%)	100 (98%)	2(2%)	0	100	100
5	L	66/122~(54%)	65~(98%)	1 (2%)	0	100	100
5	Ν	79/122~(65%)	75~(95%)	4 (5%)	0	100	100
5	j	99/122~(81%)	97~(98%)	2(2%)	0	100	100
5	1	64/122~(52%)	63~(98%)	1 (2%)	0	100	100
5	n	54/122~(44%)	51 (94%)	3~(6%)	0	100	100
6	Ι	214/233~(92%)	213 (100%)	1 (0%)	0	100	100
6	Κ	176/233~(76%)	175~(99%)	1 (1%)	0	100	100
6	М	201/233~(86%)	200 (100%)	1 (0%)	0	100	100
6	i	215/233~(92%)	213~(99%)	2 (1%)	0	100	100
6	k	166/233~(71%)	165~(99%)	1 (1%)	0	100	100
6	m	179/233~(77%)	178 (99%)	1 (1%)	0	100	100
All	All	$899\overline{4/10402}$ (86%)	8539 (95%)	428 (5%)	27~(0%)	41	77

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	187	ALA
1	С	188	PRO
4	G	138	ILE
1	с	187	ALA
1	с	188	PRO

5.3.2 Protein sidechains (i)

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

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 monosaccharides 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^{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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
1	А	591/617~(95%)	0.56	92~(15%) 2 5	126, 311, 475, 652	0
1	В	594/617~(96%)	0.34	65 (10%) 5 9	107, 290, 447, 594	0
1	С	589/617~(95%)	0.40	59 (10%) 7 10	111, 281, 475, 610	0
1	a	591/617~(95%)	0.80	102 (17%) 1 4	126, 314, 475, 658	0
1	b	589/617~(95%)	0.34	61 (10%) 6 9	107, 292, 450, 597	0
1	с	586/617~(94%)	0.34	52 (8%) 9 12	111, 282, 473, 614	0
2	D	457/517~(88%)	-0.08	7 (1%) 73 65	92, 239, 384, 587	0
2	Ε	453/517~(87%)	0.07	14 (3%) 49 42	124, 258, 413, 663	0
2	F	449/517~(86%)	0.08	28 (6%) 20 20	146, 287, 414, 584	0
2	d	460/517~(88%)	0.04	19 (4%) 37 34	94, 241, 390, 586	0
2	е	456/517~(88%)	0.12	23 (5%) 28 28	125, 258, 415, 667	0
2	f	449/517~(86%)	0.15	30 (6%) 17 18	145, 288, 416, 573	0
3	Н	445/478~(93%)	-0.55	1 (0%) 95 93	65, 163, 317, 625	0
3	h	444/478~(92%)	-0.48	2 (0%) 91 85	61, 164, 321, 631	0
4	G	139/256~(54%)	-0.19	0 100 100	93, 212, 488, 554	0
4	g	141/256~(55%)	-0.45	0 100 100	97, 213, 493, 560	0
5	J	104/122~(85%)	0.05	4 (3%) 40 36	154, 290, 427, 498	0
5	L	68/122~(55%)	0.75	10 (14%) 2 5	283, 418, 525, 566	0
5	Ν	81/122~(66%)	1.31	23 (28%) 0 2	200, 450, 574, 740	0
5	j	101/122~(82%)	0.23	5 (4%) 28 28	151, 282, 419, 497	0
5	1	66/122~(54%)	0.98	13 (19%) 1 3	279, 422, 522, 566	0
5	n	58/122 (47%)	0.18	2 (3%) 45 40	200, 441, 509, 541	0
6	Ι	216/233 (92%)	0.50	22 (10%) 6 10	112, 345, 497, 643	0
6	K	178/233~(76%)	0.57	24 (13%) 3 6	186, 344, 491, 599	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RSRZ > 2		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
6	М	203/233~(87%)	1.26	50~(24%) 0	2	200, 410, 571, 626	0
6	i	217/233~(93%)	0.55	26~(11%) 4	8	91, 345, 511, 638	0
6	k	168/233~(72%)	1.23	43~(25%) 0	2	187, 331, 466, 514	0
6	m	181/233~(77%)	0.72	25~(13%) 2	6	200, 402, 542, 587	0
All	All	9074/10402~(87%)	0.27	802 (8%) 10	12	61, 281, 479, 740	0

The worst 5 of 802 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	а	149	VAL	18.8
1	a	148	GLN	16.8
1	А	151	ASP	11.9
1	А	148	GLN	11.6
1	а	150	GLY	11.4

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 monosaccharides 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.

