



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:02 PM UTC

PDB ID : 5D80 / pdb_00005d80
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 : 2015-08-14
Resolution : 6.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

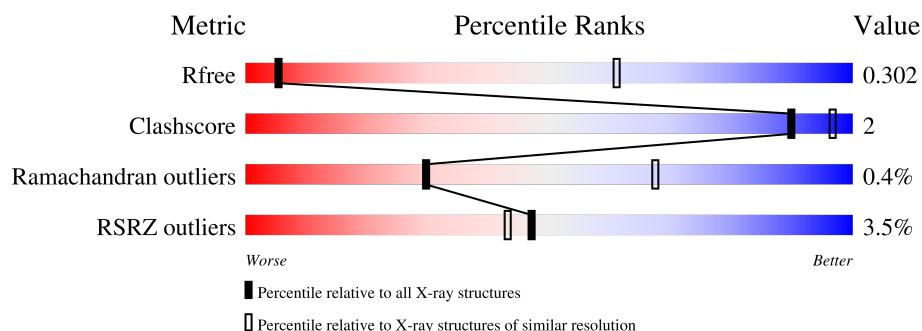
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.20 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}	180053	1148 (8.40-4.00)
Clashscore	190562	1008 (8.30-4.02)
Ramachandran outliers	187476	1037 (8.40-4.00)
RSRZ outliers	180081	1141 (8.40-4.00)

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 $\leq 5\%$. 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	617	3% 91% 5% .
1	B	617	5% 91% 6% .
1	C	617	4% 90% 5% 5%
1	a	617	4% 91% . .
1	b	617	3% 91% 6% .
1	c	617	4% 90% 5% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	517	
2	E	517	
2	F	517	
2	d	517	
2	e	517	
2	f	517	
3	H	478	
3	h	478	
4	J	122	
4	L	122	
4	N	122	
4	j	122	
4	l	122	
4	n	122	
5	I	233	
5	K	233	
5	M	233	
5	i	233	
5	k	233	
5	m	233	
6	G	256	
6	g	256	
7	O	118	
7	o	118	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47363 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 proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	0	0	0
			2905	1723	591	591			
1	B	598	Total	C	N	O	0	0	0
			2940	1744	598	598			
1	C	589	Total	C	N	O	0	0	0
			2895	1717	589	589			
1	a	591	Total	C	N	O	0	0	0
			2905	1723	591	591			
1	b	598	Total	C	N	O	0	0	0
			2940	1744	598	598			
1	c	589	Total	C	N	O	0	0	0
			2895	1717	589	589			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	457	Total	C	N	O	0	0	0
			2250	1336	457	457			
2	E	453	Total	C	N	O	0	0	0
			2231	1325	453	453			
2	F	447	Total	C	N	O	0	0	0
			2201	1307	447	447			
2	d	456	Total	C	N	O	0	0	0
			2245	1333	456	456			
2	e	453	Total	C	N	O	0	0	0
			2231	1325	453	453			
2	f	449	Total	C	N	O	0	0	0
			2211	1313	449	449			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	445	Total	C	N	O	0	0	0
			2212	1322	445	445			
3	h	445	Total	C	N	O	0	0	0
			2212	1322	445	445			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	104	Total	C	N	O	0	0	0
			514	306	104	104			
4	L	88	Total	C	N	O	0	0	0
			435	259	88	88			
4	N	81	Total	C	N	O	0	0	0
			400	238	81	81			
4	j	104	Total	C	N	O	0	0	0
			514	306	104	104			
4	l	68	Total	C	N	O	0	0	0
			335	199	68	68			
4	n	105	Total	C	N	O	0	0	0
			519	309	105	105			

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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
l	-7	MET	-	initiating methionine	UNP P48836
l	-6	ASP	-	expression tag	UNP P48836
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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	216	Total	C	N	O	0	0	0
			1073	641	216	216			
5	K	203	Total	C	N	O	0	0	0
			1008	602	203	203			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	203	Total	C	N	O	0	0	0
			1008	602	203	203			
5	i	216	Total	C	N	O	0	0	0
			1073	641	216	216			
5	k	178	Total	C	N	O	0	0	0
			883	527	178	178			
5	m	208	Total	C	N	O	0	0	0
			1033	617	208	208			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	223	Total	C	N	O	0	0	0
			1104	658	223	223			
6	g	212	Total	C	N	O	0	0	0
			1049	625	212	212			

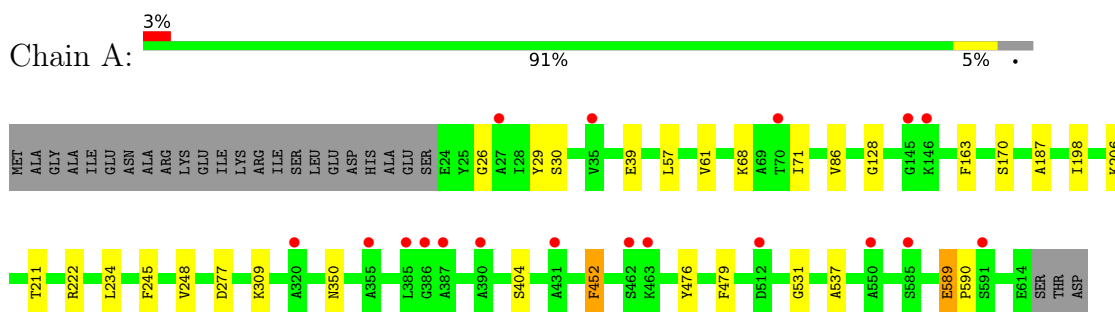
- Molecule 7 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	o	115	Total	C	N	O	0	0	0
			571	341	115	115			
7	O	115	Total	C	N	O	0	0	0
			571	341	115	115			

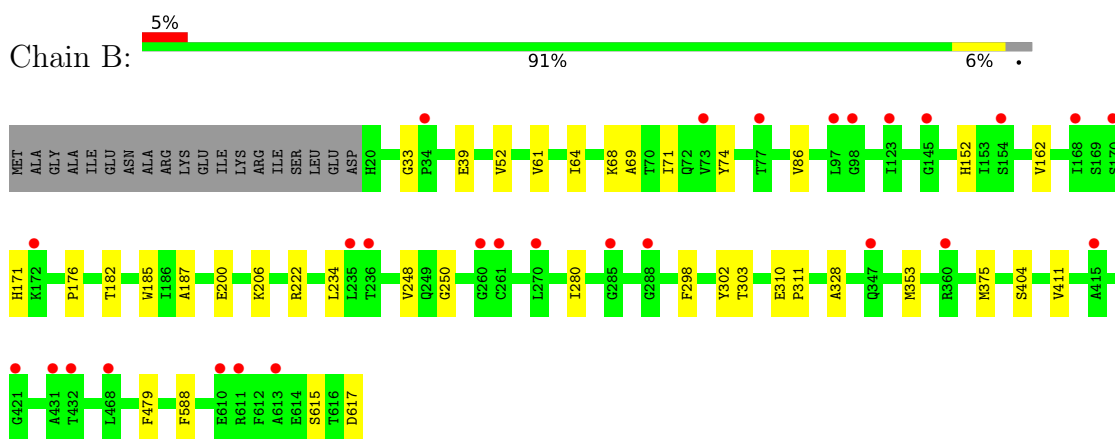
3 Residue-property plots [i](#)

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.

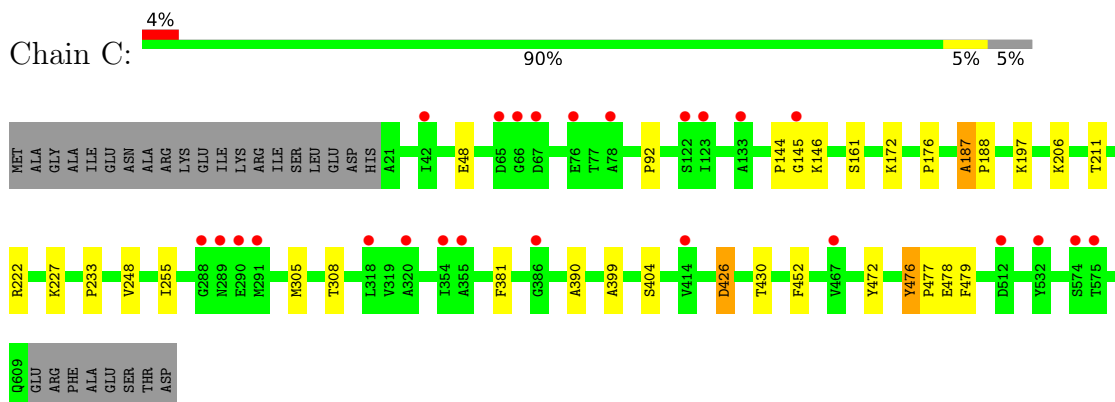
- Molecule 1: V-type proton ATPase catalytic subunit A



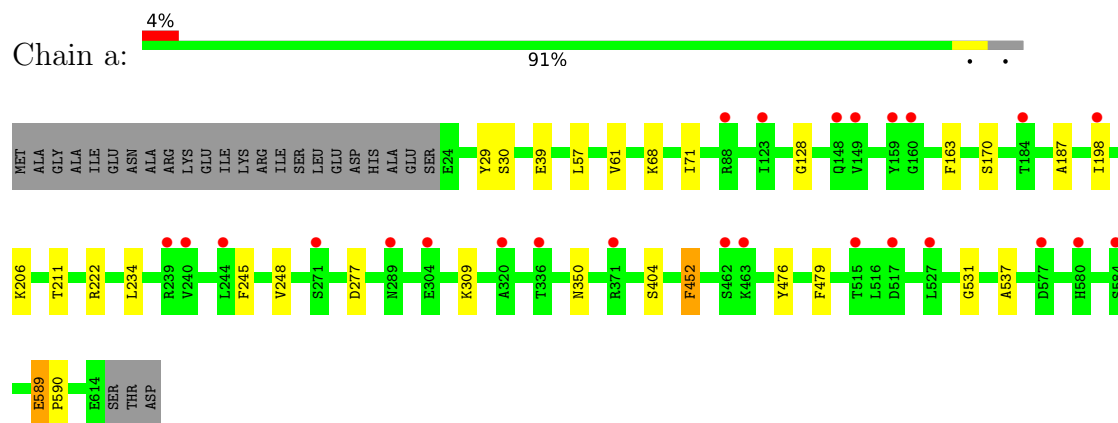
- Molecule 1: V-type proton ATPase catalytic subunit A



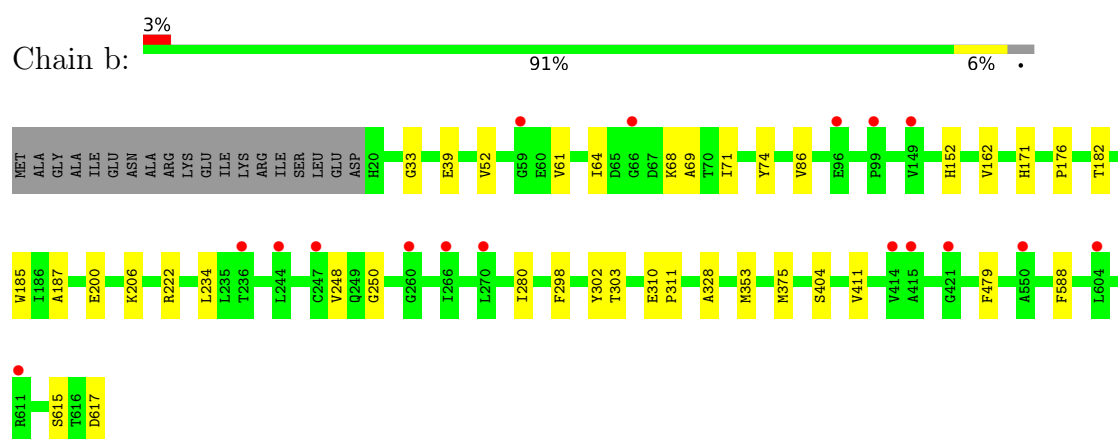
- Molecule 1: V-type proton ATPase catalytic subunit A



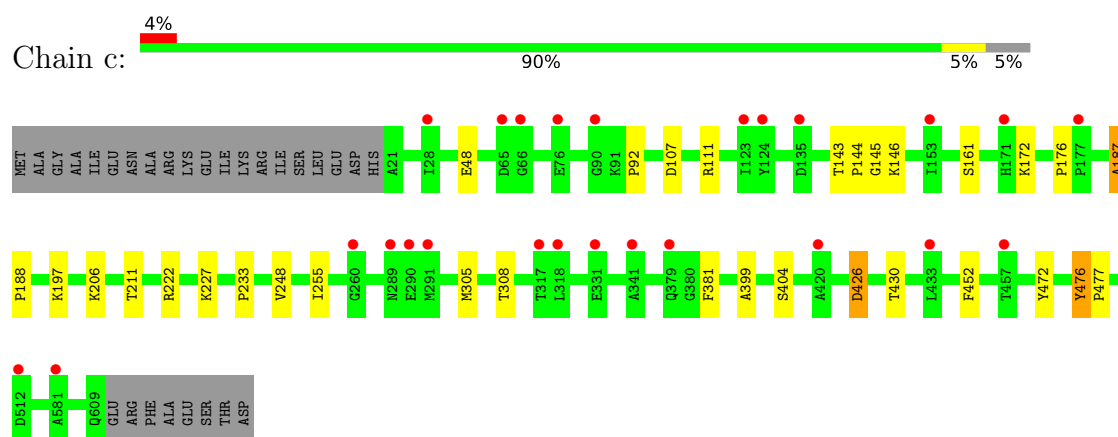
- Molecule 1: V-type proton ATPase catalytic subunit A



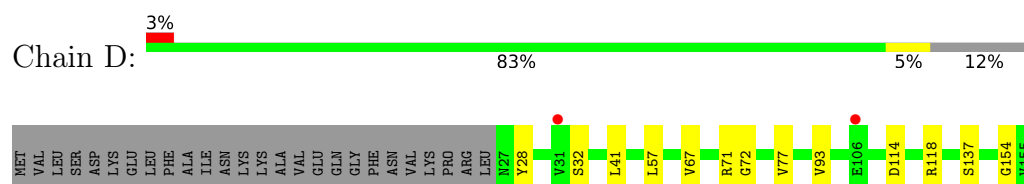
- Molecule 1: V-type proton ATPase catalytic subunit A

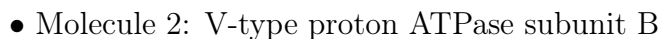


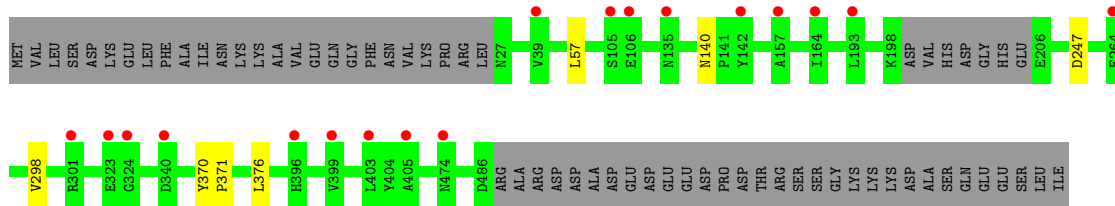
- Molecule 1: V-type proton ATPase catalytic subunit A



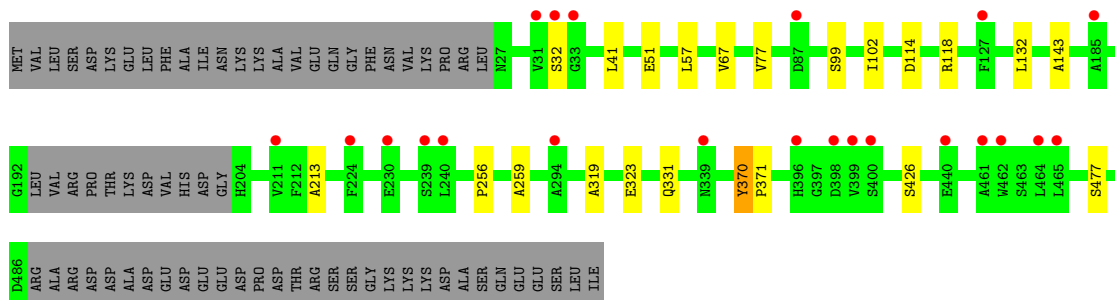
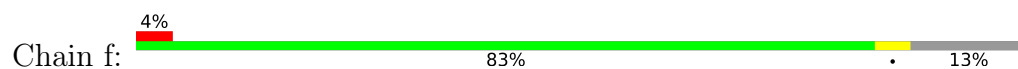
- Molecule 2: V-type proton ATPase subunit B



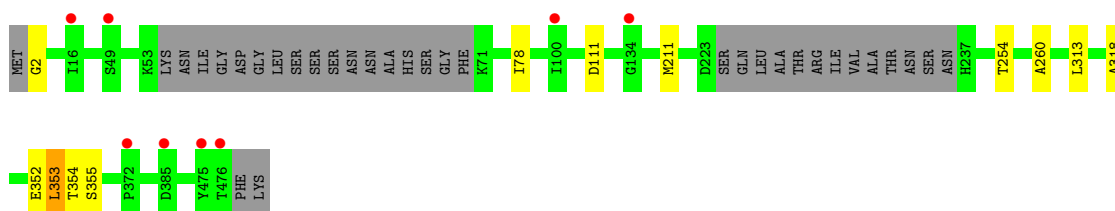




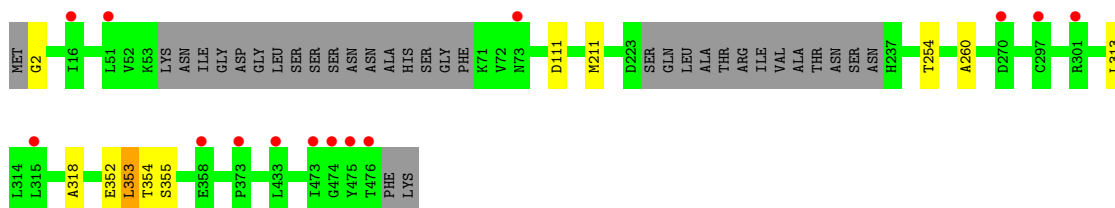
• Molecule 2: V-type proton ATPase subunit B



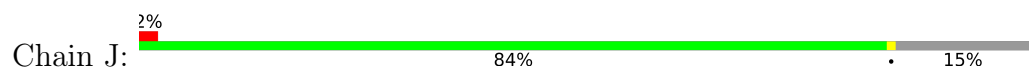
• Molecule 3: V-type proton ATPase subunit H



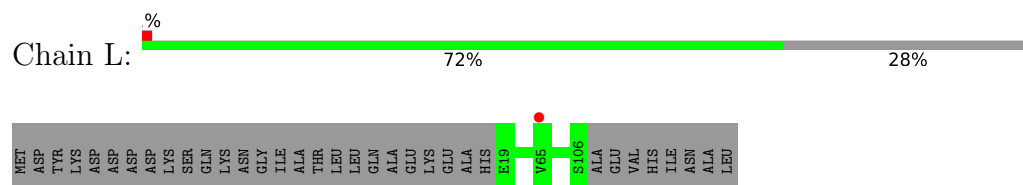
• Molecule 3: V-type proton ATPase subunit H



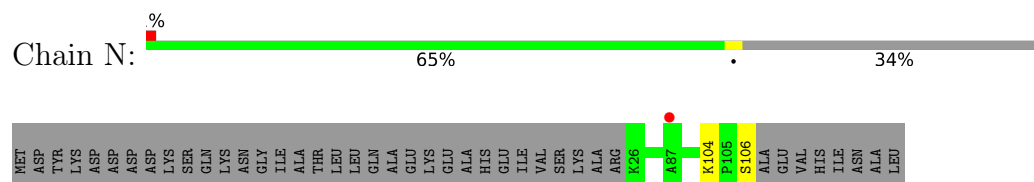
• Molecule 4: V-type proton ATPase subunit G



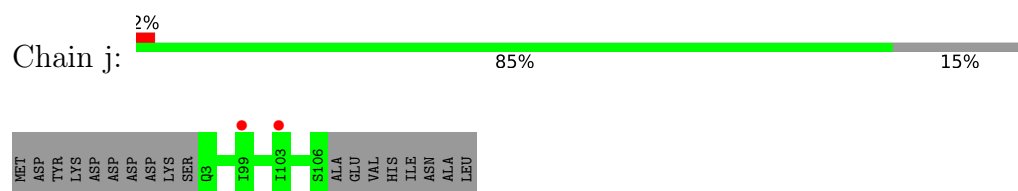
- Molecule 4: V-type proton ATPase subunit G



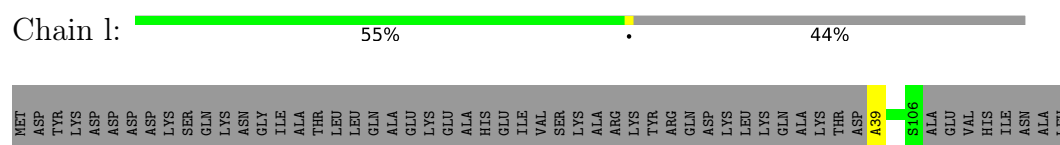
- Molecule 4: V-type proton ATPase subunit G



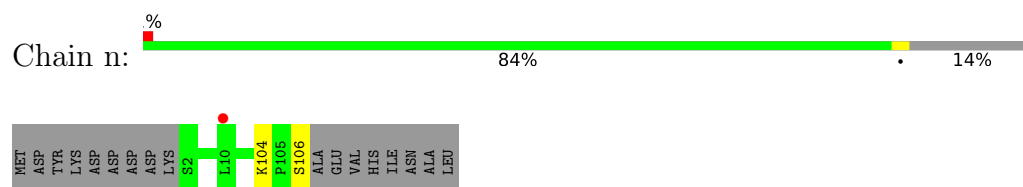
- Molecule 4: V-type proton ATPase subunit G



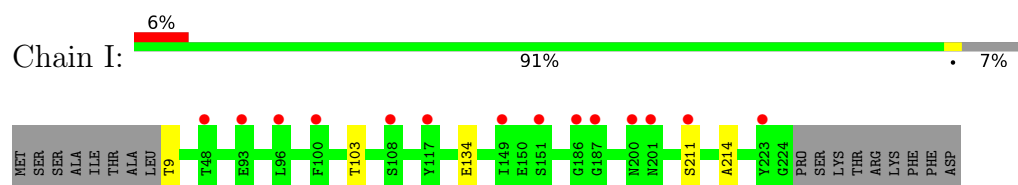
- Molecule 4: V-type proton ATPase subunit G



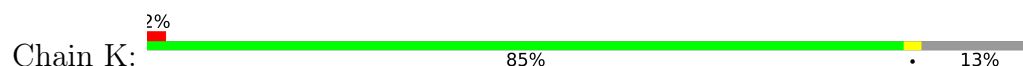
- Molecule 4: V-type proton ATPase subunit G

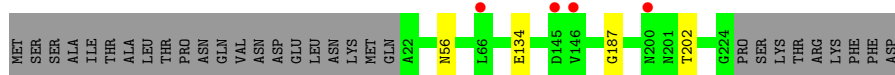


- Molecule 5: V-type proton ATPase subunit E

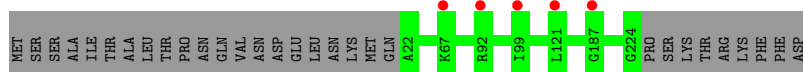
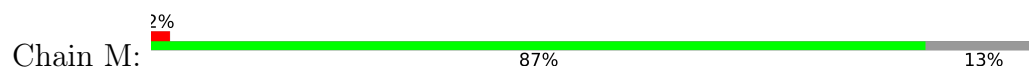


- Molecule 5: V-type proton ATPase subunit E

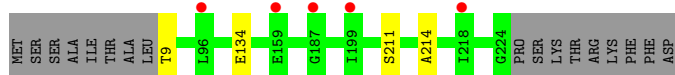
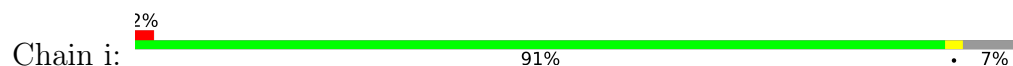




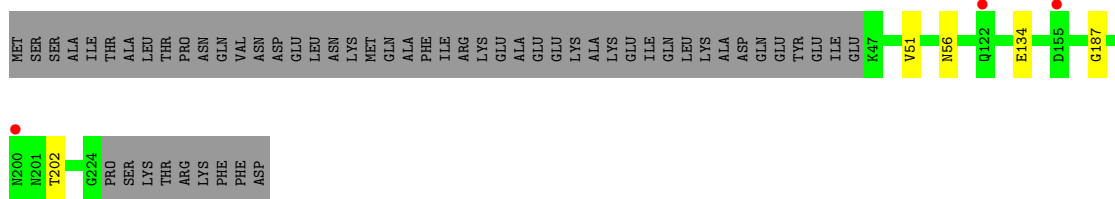
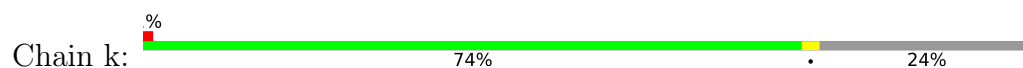
- Molecule 5: V-type proton ATPase subunit E



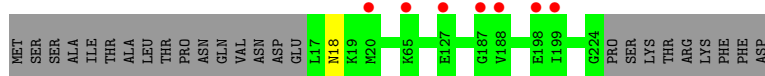
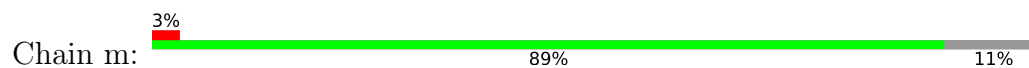
- Molecule 5: V-type proton ATPase subunit E



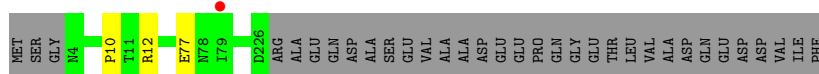
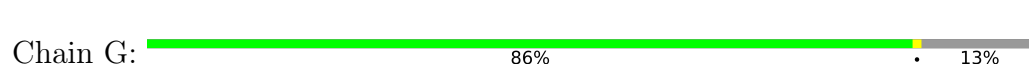
- Molecule 5: V-type proton ATPase subunit E



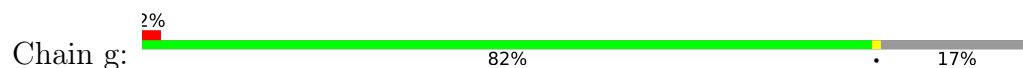
- Molecule 5: V-type proton ATPase subunit E

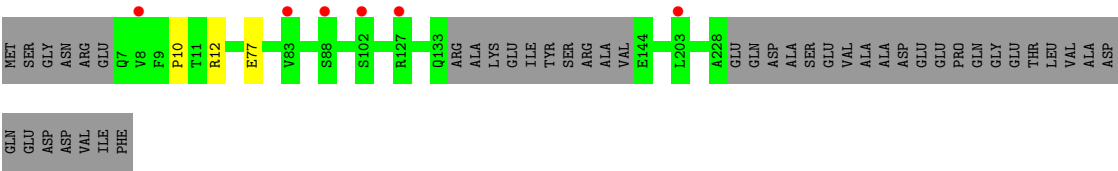


- Molecule 6: V-type proton ATPase subunit D

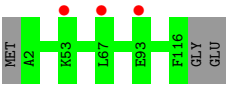


- Molecule 6: V-type proton ATPase subunit D

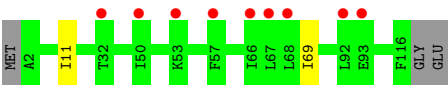
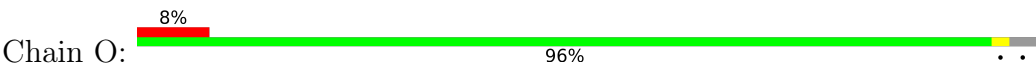




● Molecule 7: V-type proton ATPase subunit F



● Molecule 7: V-type proton ATPase subunit F



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	468.02Å 159.65Å 248.27Å 90.00° 113.75° 90.00°	Depositor
Resolution (Å)	39.72 – 6.20 39.72 – 6.20	Depositor EDS
% Data completeness (in resolution range)	87.6 (39.72-6.20) 87.4 (39.72-6.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 6.13Å)	Xtriage
Refinement program	PHENIX dev-1957	Depositor
R, R_{free}	0.255 , 0.302 0.259 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å ²)	422.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	47363	wwPDB-VP
Average B, all atoms (Å ²)	320.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.333 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	0.31	0/2904	0.94	13/4034 (0.3%)
1	B	0.32	0/2939	0.94	18/4083 (0.4%)
1	C	0.33	0/2894	0.99	20/4020 (0.5%)
1	a	0.31	0/2904	0.94	13/4034 (0.3%)
1	b	0.32	0/2939	0.94	18/4083 (0.4%)
1	c	0.32	0/2894	0.99	22/4020 (0.5%)
2	D	0.33	0/2248	0.95	10/3123 (0.3%)
2	E	0.32	0/2229	0.94	12/3097 (0.4%)
2	F	0.31	0/2199	0.93	9/3055 (0.3%)
2	d	0.33	0/2243	0.95	10/3116 (0.3%)
2	e	0.32	0/2229	0.94	14/3097 (0.5%)
2	f	0.32	0/2209	0.93	9/3069 (0.3%)
3	H	0.34	0/2209	0.94	6/3080 (0.2%)
3	h	0.34	0/2209	0.94	4/3080 (0.1%)
4	J	0.30	0/513	0.84	0/713
4	L	0.31	0/434	0.86	0/603
4	N	0.31	0/399	0.84	0/554
4	j	0.30	0/513	0.84	0/713
4	l	0.29	0/334	0.85	0/463
4	n	0.30	0/518	0.83	0/720
5	I	0.31	0/1072	0.89	4/1495 (0.3%)
5	K	0.29	0/1007	0.85	3/1404 (0.2%)
5	M	0.29	0/1007	0.82	0/1404
5	i	0.31	0/1072	0.89	4/1495 (0.3%)
5	k	0.30	0/882	0.86	3/1229 (0.2%)
5	m	0.30	0/1032	0.82	0/1439
6	G	0.30	0/1103	0.88	0/1536
6	g	0.32	0/1047	0.87	0/1456
7	O	0.32	0/570	0.89	0/794
7	o	0.31	0/570	0.90	0/794
All	All	0.32	0/47322	0.93	192/65803 (0.3%)

There are no bond length outliers.

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	589	GLU	CA-C-N	11.99	134.82	119.84
1	a	589	GLU	C-N-CA	11.99	134.82	119.84
1	A	589	GLU	CA-C-N	11.92	134.74	119.84
1	A	589	GLU	C-N-CA	11.92	134.74	119.84
2	d	376	LEU	CA-C-N	11.24	131.11	119.19
2	d	376	LEU	C-N-CA	11.24	131.11	119.19
2	D	376	LEU	CA-C-N	11.08	130.94	119.19
2	D	376	LEU	C-N-CA	11.08	130.94	119.19
1	C	255	ILE	CA-C-N	8.85	128.87	119.76
1	C	255	ILE	C-N-CA	8.85	128.87	119.76
1	c	255	ILE	CA-C-N	8.75	128.77	119.76
1	c	255	ILE	C-N-CA	8.75	128.77	119.76
2	f	57	LEU	CA-C-N	8.70	128.34	119.56
2	f	57	LEU	C-N-CA	8.70	128.34	119.56
2	F	57	LEU	CA-C-N	8.59	128.24	119.56
2	F	57	LEU	C-N-CA	8.59	128.24	119.56
5	i	9	THR	CA-C-N	8.22	127.94	119.56
5	i	9	THR	C-N-CA	8.22	127.94	119.56
5	I	9	THR	CA-C-N	8.05	127.77	119.56
5	I	9	THR	C-N-CA	8.05	127.77	119.56
1	A	479	PHE	CA-C-N	7.87	129.67	119.84
1	A	479	PHE	C-N-CA	7.87	129.67	119.84
1	a	479	PHE	CA-C-N	7.85	129.65	119.84
1	a	479	PHE	C-N-CA	7.85	129.65	119.84
1	C	381	PHE	CA-C-N	7.35	127.52	120.31
1	C	381	PHE	C-N-CA	7.35	127.52	120.31
1	b	187	ALA	CA-C-N	7.35	127.79	119.92
1	b	187	ALA	C-N-CA	7.35	127.79	119.92
1	B	187	ALA	CA-C-N	7.33	127.76	119.92
1	B	187	ALA	C-N-CA	7.33	127.76	119.92
2	d	370	TYR	CA-C-N	7.31	127.91	120.38
2	d	370	TYR	C-N-CA	7.31	127.91	120.38
3	h	211	MET	CA-C-N	7.30	126.57	118.97
3	h	211	MET	C-N-CA	7.30	126.57	118.97
2	D	370	TYR	CA-C-N	7.29	127.89	120.38
2	D	370	TYR	C-N-CA	7.29	127.89	120.38
3	H	211	MET	CA-C-N	7.27	126.53	118.97
3	H	211	MET	C-N-CA	7.27	126.53	118.97
1	B	298	PHE	CA-C-N	7.25	126.88	119.19
1	B	298	PHE	C-N-CA	7.25	126.88	119.19
1	b	298	PHE	CA-C-N	7.22	126.84	119.19
1	b	298	PHE	C-N-CA	7.22	126.84	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ALA	CA-C-N	7.18	128.82	119.84
1	C	187	ALA	C-N-CA	7.18	128.82	119.84
1	c	381	PHE	CA-C-N	7.15	127.31	120.31
1	c	381	PHE	C-N-CA	7.15	127.31	120.31
1	c	187	ALA	CA-C-N	7.10	128.72	119.84
1	c	187	ALA	C-N-CA	7.10	128.72	119.84
1	B	375	MET	CA-C-N	7.09	127.26	120.31
1	B	375	MET	C-N-CA	7.09	127.26	120.31
1	C	452	PHE	CA-C-N	7.05	128.65	119.84
1	C	452	PHE	C-N-CA	7.05	128.65	119.84
1	C	404	SER	CA-C-N	7.01	127.60	119.47
1	C	404	SER	C-N-CA	7.01	127.60	119.47
1	c	404	SER	CA-C-N	6.99	127.58	119.47
1	c	404	SER	C-N-CA	6.99	127.58	119.47
2	D	255	THR	CA-C-N	6.97	126.22	118.97
2	D	255	THR	C-N-CA	6.97	126.22	118.97
1	b	375	MET	CA-C-N	6.97	127.14	120.31
1	b	375	MET	C-N-CA	6.97	127.14	120.31
1	c	452	PHE	CA-C-N	6.95	128.53	119.84
1	c	452	PHE	C-N-CA	6.95	128.53	119.84
2	d	255	THR	CA-C-N	6.91	126.16	118.97
2	d	255	THR	C-N-CA	6.91	126.16	118.97
1	c	426	ASP	CA-C-N	6.61	126.55	119.28
1	c	426	ASP	C-N-CA	6.61	126.55	119.28
1	a	404	SER	CA-C-N	6.59	126.83	119.32
1	a	404	SER	C-N-CA	6.59	126.83	119.32
1	c	176	PRO	CA-C-N	6.57	126.95	119.92
1	c	176	PRO	C-N-CA	6.57	126.95	119.92
1	C	176	PRO	CA-C-N	6.57	126.95	119.92
1	C	176	PRO	C-N-CA	6.57	126.95	119.92
2	f	477	SER	CA-C-N	6.57	126.34	119.05
2	f	477	SER	C-N-CA	6.57	126.34	119.05
2	f	370	TYR	CA-C-N	6.52	127.10	120.38
2	f	370	TYR	C-N-CA	6.52	127.10	120.38
1	A	404	SER	CA-C-N	6.46	126.69	119.32
1	A	404	SER	C-N-CA	6.46	126.69	119.32
2	F	370	TYR	CA-C-N	6.45	127.02	120.38
2	F	370	TYR	C-N-CA	6.45	127.02	120.38
1	A	222	ARG	CA-C-N	6.44	126.40	119.76
1	A	222	ARG	C-N-CA	6.44	126.40	119.76
2	e	370	TYR	CA-C-N	6.43	127.00	120.38
2	e	370	TYR	C-N-CA	6.43	127.00	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ASP	CA-C-N	6.40	126.32	119.28
1	C	426	ASP	C-N-CA	6.40	126.32	119.28
2	F	477	SER	CA-C-N	6.39	126.15	119.05
2	F	477	SER	C-N-CA	6.39	126.15	119.05
1	a	222	ARG	CA-C-N	6.30	126.25	119.76
1	a	222	ARG	C-N-CA	6.30	126.25	119.76
2	E	370	TYR	CA-C-N	6.25	126.82	120.38
2	E	370	TYR	C-N-CA	6.25	126.82	120.38
2	E	140	ASN	CA-C-N	6.24	126.43	119.32
2	E	140	ASN	C-N-CA	6.24	126.43	119.32
2	e	140	ASN	CA-C-N	6.21	126.41	119.32
2	e	140	ASN	C-N-CA	6.21	126.41	119.32
3	h	353	LEU	CA-C-N	6.05	132.59	121.70
3	h	353	LEU	C-N-CA	6.05	132.59	121.70
2	f	426	SER	CB-CA-C	-6.01	109.66	116.63
2	F	426	SER	CB-CA-C	-5.99	109.68	116.63
2	E	57	LEU	CA-C-N	5.96	125.51	119.19
2	E	57	LEU	C-N-CA	5.96	125.51	119.19
3	H	353	LEU	CA-C-N	5.96	132.42	121.70
3	H	353	LEU	C-N-CA	5.96	132.42	121.70
2	e	247	ASP	CA-C-N	5.85	126.18	119.92
2	e	247	ASP	C-N-CA	5.85	126.18	119.92
1	b	479	PHE	CA-C-N	5.83	125.53	119.05
1	b	479	PHE	C-N-CA	5.83	125.53	119.05
2	E	247	ASP	CA-C-N	5.82	126.15	119.92
2	E	247	ASP	C-N-CA	5.82	126.15	119.92
2	F	371	PRO	CA-C-N	5.81	127.10	119.84
2	F	371	PRO	C-N-CA	5.81	127.10	119.84
1	b	404	SER	CA-C-N	5.80	125.93	119.32
1	b	404	SER	C-N-CA	5.80	125.93	119.32
2	e	57	LEU	CA-C-N	5.80	125.34	119.19
2	e	57	LEU	C-N-CA	5.80	125.34	119.19
1	B	404	SER	CA-C-N	5.80	125.93	119.32
1	B	404	SER	C-N-CA	5.80	125.93	119.32
1	b	222	ARG	CA-C-N	5.78	126.10	119.92
1	b	222	ARG	C-N-CA	5.78	126.10	119.92
1	B	479	PHE	CA-C-N	5.77	125.45	119.05
1	B	479	PHE	C-N-CA	5.77	125.45	119.05
5	k	56	ASN	N-CA-C	-5.76	106.79	113.88
5	K	56	ASN	N-CA-C	-5.75	106.81	113.88
5	I	134	GLU	CA-C-N	5.71	125.39	119.05
5	I	134	GLU	C-N-CA	5.71	125.39	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	i	134	GLU	CA-C-N	5.63	125.30	119.05
5	i	134	GLU	C-N-CA	5.63	125.30	119.05
1	b	33	GLY	CA-C-N	5.62	125.23	119.56
1	b	33	GLY	C-N-CA	5.62	125.23	119.56
1	B	588	PHE	CB-CA-C	-5.61	110.12	116.63
1	A	206	LYS	CB-CA-C	-5.59	110.14	116.63
1	c	222	ARG	CA-C-N	5.59	126.03	119.99
1	c	222	ARG	C-N-CA	5.59	126.03	119.99
1	C	222	ARG	CA-C-N	5.59	126.02	119.99
1	C	222	ARG	C-N-CA	5.59	126.02	119.99
1	a	206	LYS	CB-CA-C	-5.59	110.15	116.63
2	f	371	PRO	CA-C-N	5.58	126.81	119.84
2	f	371	PRO	C-N-CA	5.58	126.81	119.84
1	b	588	PHE	CB-CA-C	-5.57	110.17	116.63
1	a	452	PHE	CA-C-N	5.50	126.71	119.84
1	a	452	PHE	C-N-CA	5.50	126.71	119.84
1	B	222	ARG	CA-C-N	5.50	125.80	119.92
1	B	222	ARG	C-N-CA	5.50	125.80	119.92
5	k	134	GLU	CA-C-N	5.46	124.92	119.24
5	k	134	GLU	C-N-CA	5.46	124.92	119.24
1	B	33	GLY	CA-C-N	5.45	125.06	119.56
1	B	33	GLY	C-N-CA	5.45	125.06	119.56
1	B	206	LYS	CB-CA-C	-5.44	110.32	116.63
1	c	206	LYS	CB-CA-C	-5.44	110.32	116.63
1	C	206	LYS	CB-CA-C	-5.42	110.34	116.63
1	b	206	LYS	CB-CA-C	-5.42	110.34	116.63
1	A	452	PHE	CA-C-N	5.42	126.61	119.84
1	A	452	PHE	C-N-CA	5.42	126.61	119.84
5	K	134	GLU	CA-C-N	5.37	124.82	119.24
5	K	134	GLU	C-N-CA	5.37	124.82	119.24
2	D	137	SER	CA-C-N	5.36	125.33	120.03
2	D	137	SER	C-N-CA	5.36	125.33	120.03
1	C	476	TYR	CA-C-N	5.34	126.52	119.84
1	C	476	TYR	C-N-CA	5.34	126.52	119.84
1	c	476	TYR	CA-C-N	5.32	126.49	119.84
1	c	476	TYR	C-N-CA	5.32	126.49	119.84
2	d	137	SER	CA-C-N	5.29	125.27	120.03
2	d	137	SER	C-N-CA	5.29	125.27	120.03
2	e	371	PRO	CA-C-N	5.23	133.72	120.53
2	e	371	PRO	C-N-CA	5.23	133.72	120.53
2	E	371	PRO	CA-C-N	5.21	133.67	120.53
2	E	371	PRO	C-N-CA	5.21	133.67	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	143	THR	CA-C-N	5.14	126.27	119.84
1	c	143	THR	C-N-CA	5.14	126.27	119.84
2	E	298	VAL	CA-C-N	5.13	125.34	120.31
2	E	298	VAL	C-N-CA	5.13	125.34	120.31
2	e	298	VAL	CA-C-N	5.13	125.33	120.31
2	e	298	VAL	C-N-CA	5.13	125.33	120.31
1	a	245	PHE	CA-C-N	5.12	125.28	119.90
1	a	245	PHE	C-N-CA	5.12	125.28	119.90
2	e	376	LEU	CA-C-N	5.12	124.62	119.19
2	e	376	LEU	C-N-CA	5.12	124.62	119.19
3	H	78	ILE	CA-C-N	5.11	124.42	118.85
3	H	78	ILE	C-N-CA	5.11	124.42	118.85
1	b	176	PRO	CA-C-N	5.09	125.37	119.92
1	b	176	PRO	C-N-CA	5.09	125.37	119.92
2	D	57	LEU	CA-C-N	5.08	124.87	119.28
2	D	57	LEU	C-N-CA	5.08	124.87	119.28
2	d	57	LEU	CA-C-N	5.07	124.85	119.28
2	d	57	LEU	C-N-CA	5.07	124.85	119.28
1	A	245	PHE	CA-C-N	5.06	125.21	119.90
1	A	245	PHE	C-N-CA	5.06	125.21	119.90
1	c	308	THR	CB-CA-C	-5.04	109.24	115.89
1	C	308	THR	CB-CA-C	-5.02	109.27	115.89
1	B	176	PRO	CA-C-N	5.01	125.28	119.92
1	B	176	PRO	C-N-CA	5.01	125.28	119.92

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	2905	0	1339	11	0
1	B	2940	0	1356	15	0
1	C	2895	0	1335	9	0
1	a	2905	0	1339	10	0
1	b	2940	0	1356	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	2895	0	1335	8	0
2	D	2250	0	1015	14	0
2	E	2231	0	1006	0	0
2	F	2201	0	995	10	0
2	d	2245	0	1013	13	0
2	e	2231	0	1006	0	0
2	f	2211	0	999	9	0
3	H	2212	0	951	5	0
3	h	2212	0	951	6	0
4	J	514	0	248	1	0
4	L	435	0	206	0	0
4	N	400	0	189	1	0
4	j	514	0	248	0	0
4	l	335	0	160	1	0
4	n	519	0	250	1	0
5	I	1073	0	481	2	0
5	K	1008	0	456	1	0
5	M	1008	0	456	0	0
5	i	1073	0	481	1	0
5	k	883	0	394	2	0
5	m	1033	0	466	0	0
6	G	1104	0	504	0	0
6	g	1049	0	478	0	0
7	O	571	0	255	1	0
7	o	571	0	255	0	0
All	All	47363	0	21523	127	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 2.

All (127) 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:B:74:TYR:HA	1:B:328:ALA:HB3	1.69	0.74
3:H:353:LEU:H	3:H:354:THR:C	1.96	0.74
1:b:74:TYR:HA	1:b:328:ALA:HB3	1.69	0.73
3:h:353:LEU:H	3:h:354:THR:C	1.97	0.71
1:a:531:GLY:HA2	1:a:537:ALA:HA	1.75	0.69
1:A:531:GLY:HA2	1:A:537:ALA:HA	1.75	0.69
2:F:213:ALA:HB1	2:F:256:PRO:HA	1.77	0.67
2:f:213:ALA:HB1	2:f:256:PRO:HA	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:352:GLU:HA	3:H:355:SER:HA	1.78	0.66
3:h:352:GLU:HA	3:h:355:SER:HA	1.79	0.65
1:b:302:TYR:HA	1:b:311:PRO:HA	1.79	0.64
1:B:302:TYR:HA	1:B:311:PRO:HA	1.79	0.63
2:f:51:GLU:HA	2:f:99:SER:HA	1.81	0.62
2:F:319:ALA:HB2	2:F:331:GLN:H	1.64	0.62
2:f:319:ALA:HB2	2:f:331:GLN:H	1.64	0.62
2:F:51:GLU:HA	2:F:99:SER:HA	1.81	0.62
2:F:67:VAL:HA	2:F:77:VAL:HA	1.83	0.59
1:b:64:ILE:HA	1:b:69:ALA:HA	1.84	0.59
2:f:67:VAL:HA	2:f:77:VAL:HA	1.83	0.59
2:F:102:ILE:N	2:F:132:LEU:O	2.36	0.58
1:c:233:PRO:HA	1:c:248:VAL:HA	1.85	0.58
2:d:214:ALA:HB3	2:d:242:LEU:HA	1.85	0.58
1:B:64:ILE:HA	1:B:69:ALA:HA	1.84	0.58
1:C:233:PRO:HA	1:C:248:VAL:HA	1.85	0.58
2:d:114:ASP:N	2:d:118:ARG:O	2.35	0.58
2:D:214:ALA:HB3	2:D:242:LEU:HA	1.85	0.58
2:f:102:ILE:N	2:f:132:LEU:O	2.36	0.58
2:D:114:ASP:N	2:D:118:ARG:O	2.36	0.58
1:b:39:GLU:HA	1:b:68:LYS:HA	1.86	0.57
1:B:39:GLU:HA	1:B:68:LYS:HA	1.86	0.56
5:k:187:GLY:HA3	5:k:202:THR:HA	1.86	0.56
5:K:187:GLY:HA3	5:K:202:THR:HA	1.86	0.56
1:a:198:ILE:H	1:a:211:THR:HA	1.71	0.56
2:d:28:TYR:H	2:d:93:VAL:H	1.53	0.55
2:D:28:TYR:H	2:D:93:VAL:H	1.53	0.55
2:D:165:ALA:HB2	2:D:386:ALA:HB2	1.89	0.55
1:B:303:THR:N	1:B:310:GLU:O	2.33	0.54
2:d:165:ALA:HB2	2:d:386:ALA:HB2	1.89	0.54
1:a:39:GLU:HA	1:a:68:LYS:HA	1.91	0.53
1:B:64:ILE:O	2:F:34:VAL:N	2.41	0.53
2:D:67:VAL:HA	2:D:77:VAL:HA	1.91	0.53
1:A:198:ILE:H	1:A:211:THR:HA	1.73	0.53
2:d:67:VAL:HA	2:d:77:VAL:HA	1.90	0.53
1:A:39:GLU:HA	1:A:68:LYS:HA	1.90	0.52
1:C:390:ALA:HB1	2:D:245:ALA:HB1	1.91	0.52
2:D:167:GLY:HA2	2:D:320:GLY:HA2	1.91	0.52
2:D:28:TYR:N	2:D:93:VAL:O	2.43	0.52
1:B:61:VAL:HA	1:B:71:ILE:HA	1.92	0.51
1:b:52:VAL:HA	1:b:86:VAL:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:48:GLU:HA	1:c:92:PRO:HA	1.92	0.51
2:d:167:GLY:HA2	2:d:320:GLY:HA2	1.92	0.51
2:d:28:TYR:N	2:d:93:VAL:O	2.43	0.51
1:B:52:VAL:HA	1:B:86:VAL:HA	1.92	0.51
1:b:61:VAL:HA	1:b:71:ILE:HA	1.93	0.50
1:b:185:TRP:O	1:b:200:GLU:N	2.45	0.50
1:B:162:VAL:O	1:B:171:HIS:N	2.34	0.50
1:C:48:GLU:HA	1:C:92:PRO:HA	1.93	0.50
1:b:303:THR:N	1:b:310:GLU:O	2.33	0.49
2:F:114:ASP:N	2:F:118:ARG:O	2.43	0.49
1:A:30:SER:HA	2:D:71:ARG:HA	1.94	0.49
1:b:162:VAL:O	1:b:171:HIS:N	2.34	0.49
1:A:163:PHE:HA	1:A:170:SER:HA	1.94	0.49
1:a:163:PHE:HA	1:a:170:SER:HA	1.94	0.48
1:B:185:TRP:O	1:B:200:GLU:N	2.45	0.48
1:A:29:TYR:O	2:D:72:GLY:N	2.47	0.48
2:D:173:PHE:N	2:D:358:ILE:O	2.33	0.48
2:f:114:ASP:N	2:f:118:ARG:O	2.44	0.47
1:b:250:GLY:HA2	1:b:411:VAL:O	2.15	0.46
2:D:154:GLY:HA3	2:D:190:GLN:CB	2.45	0.46
1:B:250:GLY:HA2	1:B:411:VAL:O	2.15	0.46
1:C:161:SER:HA	1:C:172:LYS:HA	1.97	0.46
5:i:211:SER:HA	5:i:214:ALA:HB3	1.97	0.46
1:a:234:LEU:H	1:a:248:VAL:HA	1.81	0.46
1:C:426:ASP:O	1:C:430:THR:N	2.46	0.45
1:c:472:TYR:O	1:c:476:TYR:N	2.49	0.45
1:c:161:SER:HA	1:c:172:LYS:HA	1.97	0.45
5:I:211:SER:HA	5:I:214:ALA:HB3	1.98	0.45
2:d:370:TYR:CB	2:d:445:THR:HA	2.46	0.45
1:a:57:LEU:HA	1:a:128:GLY:HA2	1.99	0.45
1:C:472:TYR:O	1:C:476:TYR:N	2.50	0.45
2:d:154:GLY:HA3	2:d:190:GLN:CB	2.47	0.44
2:D:370:TYR:CB	2:D:445:THR:HA	2.47	0.44
1:A:234:LEU:H	1:A:248:VAL:HA	1.81	0.44
2:F:143:ALA:O	2:F:323:GLU:N	2.50	0.44
3:H:254:THR:HA	3:H:260:ALA:HB2	2.00	0.44
1:A:57:LEU:HA	1:A:128:GLY:HA2	1.99	0.44
1:C:197:LYS:HA	1:C:211:THR:HA	1.99	0.44
1:c:426:ASP:O	1:c:430:THR:N	2.46	0.44
2:d:173:PHE:N	2:d:358:ILE:O	2.34	0.44
2:f:143:ALA:O	2:f:323:GLU:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:SER:H	2:D:41:LEU:HA	1.83	0.43
1:A:61:VAL:HA	1:A:71:ILE:HA	2.01	0.43
1:C:227:LYS:HA	1:C:399:ALA:HB2	1.99	0.43
1:a:61:VAL:HA	1:a:71:ILE:HA	2.01	0.43
1:A:277:ASP:N	1:A:350:ASN:O	2.43	0.43
1:a:30:SER:HA	2:d:71:ARG:HA	2.00	0.43
1:c:227:LYS:HA	1:c:399:ALA:HB2	2.00	0.43
1:B:234:LEU:H	1:B:248:VAL:HA	1.84	0.43
2:f:32:SER:H	2:f:41:LEU:HA	1.83	0.43
1:b:280:ILE:O	1:b:353:MET:HA	2.19	0.42
1:c:197:LYS:HA	1:c:211:THR:HA	1.99	0.42
2:d:32:SER:H	2:d:41:LEU:HA	1.84	0.42
1:a:29:TYR:O	2:d:72:GLY:N	2.52	0.42
1:B:280:ILE:O	1:B:353:MET:HA	2.19	0.42
4:J:95:VAL:HA	5:I:103:THR:HA	2.02	0.42
1:C:478:GLU:HA	1:C:479:PHE:HA	1.74	0.42
3:H:313:LEU:HA	3:H:318:ALA:HB3	2.01	0.42
1:a:277:ASP:N	1:a:350:ASN:O	2.43	0.42
1:b:234:LEU:H	1:b:248:VAL:HA	1.85	0.42
3:h:2:GLY:HA3	3:h:111:ASP:H	1.83	0.42
1:A:26:GLY:O	1:A:86:VAL:N	2.32	0.42
2:F:32:SER:H	2:F:41:LEU:HA	1.84	0.42
1:c:107:ASP:N	1:c:111:ARG:O	2.41	0.42
3:h:313:LEU:HA	3:h:318:ALA:HB3	2.02	0.42
1:b:615:SER:C	1:b:617:ASP:HA	2.45	0.41
4:N:104:LYS:O	4:N:106:SER:N	2.53	0.41
3:h:254:THR:HA	3:h:260:ALA:HB2	2.01	0.41
4:n:104:LYS:O	4:n:106:SER:N	2.52	0.41
1:B:152:HIS:HA	1:B:182:THR:HA	2.02	0.41
1:B:615:SER:C	1:B:617:ASP:HA	2.45	0.41
2:f:213:ALA:HB2	2:f:259:ALA:HB3	2.02	0.41
2:F:213:ALA:HB2	2:F:259:ALA:HB3	2.02	0.41
3:H:2:GLY:HA3	3:H:111:ASP:H	1.85	0.41
3:h:2:GLY:HA3	3:h:111:ASP:N	2.36	0.41
7:O:11:ILE:O	7:O:69:ILE:HA	2.21	0.41
5:k:51:VAL:CB	4:l:39:ALA:HB1	2.51	0.40
1:b:152:HIS:HA	1:b:182:THR:HA	2.02	0.40

There are no symmetry-related clashes.

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	589/617 (96%)	551 (94%)	32 (5%)	6 (1%)	12	48
1	B	596/617 (97%)	557 (94%)	39 (6%)	0	100	100
1	C	587/617 (95%)	546 (93%)	34 (6%)	7 (1%)	10	43
1	a	589/617 (96%)	551 (94%)	32 (5%)	6 (1%)	12	48
1	b	596/617 (97%)	557 (94%)	39 (6%)	0	100	100
1	c	587/617 (95%)	546 (93%)	34 (6%)	7 (1%)	10	43
2	D	453/517 (88%)	424 (94%)	29 (6%)	0	100	100
2	E	449/517 (87%)	424 (94%)	25 (6%)	0	100	100
2	F	443/517 (86%)	416 (94%)	26 (6%)	1 (0%)	43	78
2	d	452/517 (87%)	423 (94%)	29 (6%)	0	100	100
2	e	449/517 (87%)	424 (94%)	25 (6%)	0	100	100
2	f	445/517 (86%)	418 (94%)	26 (6%)	1 (0%)	43	78
3	H	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
3	h	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
4	J	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
4	L	86/122 (70%)	85 (99%)	1 (1%)	0	100	100
4	N	79/122 (65%)	76 (96%)	3 (4%)	0	100	100
4	j	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
4	l	66/122 (54%)	65 (98%)	1 (2%)	0	100	100
4	n	103/122 (84%)	100 (97%)	3 (3%)	0	100	100
5	I	214/233 (92%)	214 (100%)	0	0	100	100
5	K	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
5	M	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
5	i	214/233 (92%)	214 (100%)	0	0	100	100
5	k	176/233 (76%)	175 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	m	206/233 (88%)	204 (99%)	1 (0%)	1 (0%)	24	63
6	G	221/256 (86%)	211 (96%)	7 (3%)	3 (1%)	9	40
6	g	208/256 (81%)	199 (96%)	6 (3%)	3 (1%)	9	40
7	O	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
7	o	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
All	All	9518/10638 (90%)	9024 (95%)	459 (5%)	35 (0%)	30	67

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ALA
1	C	188	PRO
1	c	187	ALA
1	c	188	PRO
6	G	10	PRO
6	G	12	ARG
6	G	77	GLU
6	g	10	PRO
6	g	12	ARG
6	g	77	GLU
1	A	476	TYR
1	A	589	GLU
1	C	144	PRO
1	a	476	TYR
1	a	589	GLU
1	c	144	PRO
1	A	590	PRO
1	C	305	MET
1	a	590	PRO
1	c	305	MET
1	C	146	LYS
1	c	146	LYS
5	m	18	ASN
1	A	187	ALA
1	A	309	LYS
1	a	187	ALA
1	a	309	LYS
1	C	145	GLY
1	c	145	GLY
1	C	477	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	370	TYR
1	c	477	PRO
2	f	370	TYR
1	A	452	PHE
1	a	452	PHE

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 oligosaccharides 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 ⓘ

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	591/617 (95%)	0.01	18 (3%)	52	46	153, 336, 460, 561	0
1	B	598/617 (96%)	0.12	28 (4%)	36	37	112, 322, 468, 647	0
1	C	589/617 (95%)	0.10	25 (4%)	40	40	148, 325, 484, 591	0
1	a	591/617 (95%)	0.04	25 (4%)	40	40	155, 335, 460, 557	0
1	b	598/617 (96%)	0.04	17 (2%)	55	48	109, 321, 465, 650	0
1	c	589/617 (95%)	0.14	25 (4%)	40	40	146, 323, 481, 593	0
2	D	457/517 (88%)	0.13	18 (3%)	43	41	93, 267, 414, 596	0
2	E	453/517 (87%)	-0.01	10 (2%)	62	53	149, 285, 407, 560	0
2	F	447/517 (86%)	0.11	23 (5%)	33	35	138, 312, 463, 552	0
2	d	456/517 (88%)	0.14	22 (4%)	35	36	91, 265, 408, 553	0
2	e	453/517 (87%)	-0.03	18 (3%)	42	41	145, 285, 408, 566	0
2	f	449/517 (86%)	0.20	22 (4%)	35	35	137, 313, 467, 570	0
3	H	445/478 (93%)	-0.21	8 (1%)	67	57	85, 192, 339, 469	0
3	h	445/478 (93%)	-0.08	14 (3%)	51	45	79, 193, 337, 470	0
4	J	104/122 (85%)	-0.33	2 (1%)	66	56	140, 258, 401, 458	0
4	L	88/122 (72%)	-0.03	1 (1%)	78	66	281, 427, 520, 540	0
4	N	81/122 (66%)	-0.06	1 (1%)	76	65	244, 400, 519, 569	0
4	j	104/122 (85%)	-0.35	2 (1%)	66	56	140, 260, 398, 459	0
4	l	68/122 (55%)	-0.02	0	100	100	282, 414, 487, 535	0
4	n	105/122 (86%)	0.00	1 (0%)	79	68	229, 409, 525, 572	0
5	I	216/233 (92%)	0.23	14 (6%)	25	29	103, 383, 522, 578	0
5	K	203/233 (87%)	-0.07	4 (1%)	65	55	255, 380, 542, 600	0
5	M	203/233 (87%)	0.21	5 (2%)	58	50	235, 422, 520, 578	0
5	i	216/233 (92%)	0.04	5 (2%)	61	52	99, 382, 522, 573	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
5	k	178/233 (76%)	0.11	3 (1%)	69 59	254, 366, 478, 548	0
5	m	208/233 (89%)	0.10	7 (3%)	48 43	239, 415, 520, 577	0
6	G	223/256 (87%)	-0.36	1 (0%)	88 79	114, 325, 538, 586	0
6	g	212/256 (82%)	-0.30	6 (2%)	55 48	112, 316, 539, 581	0
7	O	115/118 (97%)	0.12	9 (7%)	19 25	260, 414, 524, 579	0
7	o	115/118 (97%)	0.07	3 (2%)	57 49	260, 416, 526, 577	0
All	All	9600/10638 (90%)	0.03	337 (3%)	47 43	79, 317, 487, 650	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	290	GLU	12.0
3	h	476	THR	9.2
1	A	462	SER	8.5
3	h	475	TYR	7.8
1	a	240	VAL	7.6
2	F	126	VAL	7.3
1	C	66	GLY	6.4
4	j	103	ILE	6.3
3	H	475	TYR	6.2
2	D	319	ALA	6.2
2	D	318	ARG	6.1
5	m	199	ILE	6.0
3	h	474	GLY	5.9
1	C	355	ALA	5.8
2	D	239	SER	5.8
5	M	187	GLY	5.8
2	d	399	VAL	5.6
1	a	304	GLU	5.4
2	f	399	VAL	5.4
7	O	67	LEU	5.3
2	E	324	GLY	5.3
2	F	127	PHE	5.3
2	f	398	ASP	5.1
2	f	230	GLU	4.9
2	e	323	GLU	4.9
1	c	177	PRO	4.8
1	c	581	ALA	4.8
2	F	464	LEU	4.8
2	E	164	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	157	ALA	4.6
2	f	239	SER	4.6
1	b	414	VAL	4.6
1	A	463	LYS	4.6
2	d	318	ARG	4.5
1	a	88	ARG	4.5
1	b	236	THR	4.4
1	a	159	TYR	4.4
1	B	123	ILE	4.4
1	B	613	ALA	4.4
2	f	400	SER	4.3
6	g	102	SER	4.2
1	b	415	ALA	4.2
5	m	187	GLY	4.2
2	d	396	HIS	4.2
2	d	156	SER	4.2
1	B	421	GLY	4.2
2	F	139	ILE	4.2
1	a	123	ILE	4.2
1	B	260	GLY	4.1
4	J	103	ILE	4.1
2	f	224	PHE	4.1
1	a	577	ASP	4.1
1	b	270	LEU	4.0
3	h	51	LEU	4.0
2	F	399	VAL	4.0
3	H	385	ASP	3.9
5	K	66	LEU	3.9
2	D	299	PRO	3.9
3	h	473	ILE	3.8
1	A	386	GLY	3.8
5	I	187	GLY	3.8
2	D	294	ALA	3.8
2	E	323	GLU	3.8
7	O	50	ILE	3.8
1	C	288	GLY	3.7
2	f	464	LEU	3.7
3	H	476	THR	3.7
1	b	421	GLY	3.7
2	d	319	ALA	3.7
7	O	92	LEU	3.7
1	B	172	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	O	53	LYS	3.6
2	F	83	THR	3.6
5	I	117	TYR	3.6
5	k	200	ASN	3.5
2	F	402	GLN	3.5
5	i	218	ILE	3.5
1	A	355	ALA	3.5
3	H	134	GLY	3.5
2	F	230	GLU	3.4
1	B	432	THR	3.4
2	E	163	SER	3.4
1	C	289	ASN	3.4
2	F	138	PRO	3.3
1	a	149	VAL	3.3
2	d	157	ALA	3.3
1	C	467	VAL	3.3
2	f	396	HIS	3.3
5	M	99	ILE	3.3
2	e	324	GLY	3.3
1	B	168	ILE	3.3
1	A	145	GLY	3.3
1	A	387	ALA	3.3
1	c	260	GLY	3.2
2	d	294	ALA	3.2
1	a	580	HIS	3.2
1	C	290	GLU	3.2
1	b	96	GLU	3.2
3	H	100	ILE	3.2
2	F	89	LYS	3.2
7	O	57	PHE	3.2
2	e	340	ASP	3.2
1	c	289	ASN	3.2
4	n	10	LEU	3.1
1	b	550	ALA	3.1
1	c	318	LEU	3.1
2	e	474	ASN	3.1
1	B	415	ALA	3.1
5	I	93	GLU	3.0
1	B	236	THR	3.0
2	e	157	ALA	3.0
2	D	238	THR	3.0
5	m	65	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	e	135	ASN	3.0
3	h	73	ASN	3.0
2	e	264	GLU	3.0
5	i	199	ILE	3.0
1	c	90	GLY	3.0
3	h	373	PRO	3.0
5	I	200	ASN	3.0
7	O	66	ILE	2.9
2	e	105	SER	2.9
1	c	171	HIS	2.9
3	h	315	LEU	2.9
5	I	149	ILE	2.9
3	h	358	GLU	2.9
1	B	285	GLY	2.9
5	I	96	LEU	2.9
1	a	463	LYS	2.8
1	B	235	LEU	2.8
1	A	146	LYS	2.8
5	K	200	ASN	2.8
2	e	106	GLU	2.8
5	k	122	GLN	2.8
2	F	461	ALA	2.8
2	f	294	ALA	2.8
7	o	93	GLU	2.8
2	d	461	ALA	2.8
2	f	87	ASP	2.8
1	a	198	ILE	2.8
2	f	462	TRP	2.8
1	B	270	LEU	2.7
1	C	318	LEU	2.7
1	b	99	PRO	2.7
1	B	347	GLN	2.7
2	D	156	SER	2.7
1	B	73	VAL	2.7
2	d	452	ARG	2.7
2	D	221	THR	2.7
2	d	239	SER	2.7
2	e	142	TYR	2.7
1	c	28	ILE	2.7
2	E	139	ILE	2.7
1	C	414	VAL	2.7
2	E	39	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	31	VAL	2.7
1	B	360	ARG	2.7
2	F	152	SER	2.7
1	a	527	LEU	2.6
5	m	198	GLU	2.6
1	C	42	ILE	2.6
3	h	16	ILE	2.6
1	B	170	SER	2.6
2	F	183	ILE	2.6
2	e	164	ILE	2.6
1	c	65	ASP	2.6
3	h	297	CYS	2.6
2	d	476	ILE	2.6
2	D	452	ARG	2.6
2	E	454	VAL	2.6
1	A	70	THR	2.6
1	C	575	THR	2.6
5	I	108	SER	2.6
2	d	395	ASP	2.6
5	i	187	GLY	2.6
1	A	320	ALA	2.6
2	F	107	ASP	2.6
1	B	97	LEU	2.6
1	A	27	ALA	2.6
1	a	515	THR	2.6
1	C	386	GLY	2.5
1	c	135	ASP	2.5
1	B	431	ALA	2.5
1	c	76	GLU	2.5
2	f	339	ASN	2.5
1	B	154	SER	2.5
1	C	67	ASP	2.5
2	d	398	ASP	2.5
2	f	185	ALA	2.5
2	D	324	GLY	2.5
2	F	137	SER	2.5
1	a	289	ASN	2.5
1	c	512	ASP	2.5
2	f	33	GLY	2.5
1	C	574	SER	2.5
2	f	240	LEU	2.5
2	e	39	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	m	188	VAL	2.5
1	c	331	GLU	2.4
1	A	431	ALA	2.4
1	C	123	ILE	2.4
5	K	146	VAL	2.4
5	I	186	GLY	2.4
2	e	405	ALA	2.4
5	I	211	SER	2.4
5	m	20	MET	2.4
1	b	260	GLY	2.4
5	M	121	LEU	2.4
1	B	611	ARG	2.4
1	c	433	LEU	2.4
2	F	231	GLU	2.4
5	i	96	LEU	2.4
2	E	343	THR	2.4
1	B	288	GLY	2.3
1	A	35	VAL	2.3
1	c	291	MET	2.3
2	e	301	ARG	2.3
1	b	604	LEU	2.3
2	D	316	TYR	2.3
3	h	433	LEU	2.3
2	E	236	GLU	2.3
5	k	155	ASP	2.3
2	d	317	GLU	2.3
5	M	67	LYS	2.3
1	B	468	LEU	2.3
3	H	49	SER	2.3
2	f	440	GLU	2.3
1	c	317	THR	2.3
2	f	465	LEU	2.3
1	b	66	GLY	2.3
2	D	300	GLY	2.3
2	e	399	VAL	2.3
7	O	32	THR	2.3
1	c	124	TYR	2.3
2	d	203	GLY	2.3
1	A	550	ALA	2.3
1	a	239	ARG	2.3
1	b	244	LEU	2.3
5	M	92	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	336	THR	2.3
2	d	158	ILE	2.3
6	G	79	ILE	2.3
2	F	88	VAL	2.3
2	e	403	LEU	2.3
1	a	371	ARG	2.3
2	D	280	ASP	2.3
2	F	398	ASP	2.3
1	B	610	GLU	2.2
5	I	201	ASN	2.2
2	f	461	ALA	2.2
5	I	100	PHE	2.2
1	a	148	GLN	2.2
1	B	261	CYS	2.2
1	b	247	CYS	2.2
6	g	88	SER	2.2
1	b	266	ILE	2.2
2	F	87	ASP	2.2
2	F	465	LEU	2.2
1	c	379	GLN	2.2
4	J	34	GLN	2.2
1	C	532	TYR	2.2
2	F	451	ASP	2.2
2	f	211	VAL	2.2
1	c	123	ILE	2.2
4	j	99	ILE	2.2
7	o	53	LYS	2.2
7	o	67	LEU	2.2
1	b	149	VAL	2.2
2	D	399	VAL	2.2
1	c	420	ALA	2.2
1	B	77	THR	2.2
1	C	354	ILE	2.2
2	d	106	GLU	2.2
2	d	188	CYS	2.2
1	b	59	GLY	2.1
1	A	385	LEU	2.1
7	O	68	LEU	2.1
1	A	585	SER	2.1
1	a	584	SER	2.1
1	C	291	MET	2.1
6	g	127	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	390	ALA	2.1
1	a	160	GLY	2.1
1	C	65	ASP	2.1
1	a	517	ASP	2.1
2	d	322	VAL	2.1
6	g	8	VAL	2.1
1	a	462	SER	2.1
1	C	320	ALA	2.1
1	a	320	ALA	2.1
2	E	306	GLY	2.1
2	F	316	TYR	2.1
5	I	223	TYR	2.1
1	C	78	ALA	2.1
1	c	66	GLY	2.1
2	D	283	SER	2.1
5	m	127	GLU	2.1
2	f	31	VAL	2.1
1	b	611	ARG	2.1
5	I	48	THR	2.1
1	C	133	ALA	2.1
2	d	75	ALA	2.1
2	f	32	SER	2.1
4	N	87	ALA	2.1
2	f	127	PHE	2.1
6	g	203	LEU	2.1
1	c	153	ILE	2.1
3	H	372	PRO	2.1
1	C	145	GLY	2.1
1	c	341	ALA	2.1
1	C	76	GLU	2.1
5	i	159	GLU	2.1
7	O	93	GLU	2.1
3	h	270	ASP	2.1
1	a	184	THR	2.1
1	c	457	THR	2.1
1	A	591	SER	2.1
2	D	106	GLU	2.1
2	F	86	ILE	2.0
1	B	34	PRO	2.0
1	C	122	SER	2.0
4	L	65	VAL	2.0
5	I	151	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	h	301	ARG	2.0
1	A	512	ASP	2.0
1	B	98	GLY	2.0
1	B	145	GLY	2.0
1	C	512	ASP	2.0
5	K	145	ASP	2.0
6	g	83	VAL	2.0
1	a	244	LEU	2.0
2	d	234	SER	2.0
2	d	332	ILE	2.0
3	H	16	ILE	2.0
2	e	396	HIS	2.0
2	e	193	LEU	2.0
1	a	271	SER	2.0

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 oligosaccharides 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.