



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:41 PM UTC

PDB ID : 7QW4 / pdb_00007qw4
Title : Pden_5119 protein
Authors : Kryl, M.; Sedlacek, V.
Deposited on : 2022-01-24
Resolution : 3.10 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 ⓘ 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

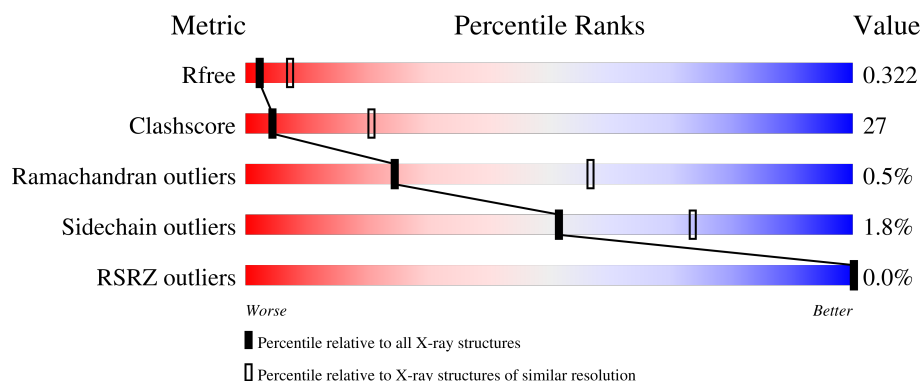
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



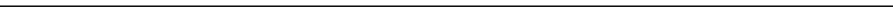
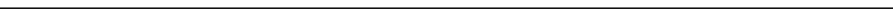
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	193	
1	B	193	
1	C	193	
1	D	193	
1	E	193	

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Mol	Chain	Length	Quality of chain
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	
1	O	193	
1	P	193	
1	Q	193	
1	R	193	
1	S	193	
1	T	193	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26343 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 NADPH-dependent FMN reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1282	818	233	230	1			
1	B	168	Total	C	N	O	S	0	0	0
			1262	811	231	219	1			
1	C	178	Total	C	N	O		0	0	0
			1291	825	237	229				
1	D	182	Total	C	N	O	S	0	0	0
			1334	848	244	241	1			
1	E	180	Total	C	N	O	S	0	0	0
			1302	834	232	235	1			
1	F	177	Total	C	N	O		0	0	0
			1296	825	240	231				
1	G	181	Total	C	N	O	S	0	0	0
			1336	851	244	240	1			
1	H	184	Total	C	N	O	S	0	0	0
			1342	855	243	243	1			
1	I	184	Total	C	N	O		0	0	0
			1340	859	240	241				
1	J	181	Total	C	N	O		0	0	0
			1336	859	244	233				
1	K	181	Total	C	N	O	S	0	0	0
			1348	859	247	241	1			
1	L	188	Total	C	N	O		0	0	0
			1346	850	251	245				
1	M	179	Total	C	N	O		0	0	0
			1292	823	234	235				
1	N	174	Total	C	N	O	S	0	0	0
			1283	820	229	233	1			
1	O	184	Total	C	N	O	S	0	0	0
			1393	886	260	246	1			
1	P	187	Total	C	N	O	S	0	0	0
			1402	891	263	247	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	170	Total	C	N	O	S	0	0	0
			1257	803	228	225	1			
1	R	176	Total	C	N	O	S	0	0	0
			1291	825	233	232	1			
1	S	181	Total	C	N	O		0	0	0
			1304	829	238	237				
1	T	182	Total	C	N	O	S	0	0	0
			1306	830	239	236	1			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	-	expression tag	UNP A1BCD5
A	189	GLU	-	expression tag	UNP A1BCD5
A	190	HIS	-	expression tag	UNP A1BCD5
A	191	HIS	-	expression tag	UNP A1BCD5
A	192	HIS	-	expression tag	UNP A1BCD5
A	193	HIS	-	expression tag	UNP A1BCD5
A	194	HIS	-	expression tag	UNP A1BCD5
A	195	HIS	-	expression tag	UNP A1BCD5
B	379	LEU	-	expression tag	UNP A1BCD5
B	380	GLU	-	expression tag	UNP A1BCD5
B	381	HIS	-	expression tag	UNP A1BCD5
B	382	HIS	-	expression tag	UNP A1BCD5
B	383	HIS	-	expression tag	UNP A1BCD5
B	384	HIS	-	expression tag	UNP A1BCD5
B	385	HIS	-	expression tag	UNP A1BCD5
B	386	HIS	-	expression tag	UNP A1BCD5
C	572	LEU	-	expression tag	UNP A1BCD5
C	573	GLU	-	expression tag	UNP A1BCD5
C	574	HIS	-	expression tag	UNP A1BCD5
C	575	HIS	-	expression tag	UNP A1BCD5
C	576	HIS	-	expression tag	UNP A1BCD5
C	577	HIS	-	expression tag	UNP A1BCD5
C	578	HIS	-	expression tag	UNP A1BCD5
C	579	HIS	-	expression tag	UNP A1BCD5
D	766	LEU	-	expression tag	UNP A1BCD5
D	767	GLU	-	expression tag	UNP A1BCD5
D	768	HIS	-	expression tag	UNP A1BCD5
D	769	HIS	-	expression tag	UNP A1BCD5
D	770	HIS	-	expression tag	UNP A1BCD5
D	771	HIS	-	expression tag	UNP A1BCD5
D	772	HIS	-	expression tag	UNP A1BCD5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	773	HIS	-	expression tag	UNP A1BCD5
E	958	LEU	-	expression tag	UNP A1BCD5
E	959	GLU	-	expression tag	UNP A1BCD5
E	960	HIS	-	expression tag	UNP A1BCD5
E	961	HIS	-	expression tag	UNP A1BCD5
E	962	HIS	-	expression tag	UNP A1BCD5
E	963	HIS	-	expression tag	UNP A1BCD5
E	964	HIS	-	expression tag	UNP A1BCD5
E	965	HIS	-	expression tag	UNP A1BCD5
F	1154	LEU	-	expression tag	UNP A1BCD5
F	1155	GLU	-	expression tag	UNP A1BCD5
F	1156	HIS	-	expression tag	UNP A1BCD5
F	1157	HIS	-	expression tag	UNP A1BCD5
F	1158	HIS	-	expression tag	UNP A1BCD5
F	1159	HIS	-	expression tag	UNP A1BCD5
F	1160	HIS	-	expression tag	UNP A1BCD5
F	1161	HIS	-	expression tag	UNP A1BCD5
G	1345	LEU	-	expression tag	UNP A1BCD5
G	1346	GLU	-	expression tag	UNP A1BCD5
G	1347	HIS	-	expression tag	UNP A1BCD5
G	1348	HIS	-	expression tag	UNP A1BCD5
G	1349	HIS	-	expression tag	UNP A1BCD5
G	1350	HIS	-	expression tag	UNP A1BCD5
G	1351	HIS	-	expression tag	UNP A1BCD5
G	1352	HIS	-	expression tag	UNP A1BCD5
H	1537	LEU	-	expression tag	UNP A1BCD5
H	1538	GLU	-	expression tag	UNP A1BCD5
H	1539	HIS	-	expression tag	UNP A1BCD5
H	1540	HIS	-	expression tag	UNP A1BCD5
H	1541	HIS	-	expression tag	UNP A1BCD5
H	1542	HIS	-	expression tag	UNP A1BCD5
H	1543	HIS	-	expression tag	UNP A1BCD5
H	1544	HIS	-	expression tag	UNP A1BCD5
I	1730	LEU	-	expression tag	UNP A1BCD5
I	1731	GLU	-	expression tag	UNP A1BCD5
I	1732	HIS	-	expression tag	UNP A1BCD5
I	1733	HIS	-	expression tag	UNP A1BCD5
I	1734	HIS	-	expression tag	UNP A1BCD5
I	1735	HIS	-	expression tag	UNP A1BCD5
I	1736	HIS	-	expression tag	UNP A1BCD5
I	1737	HIS	-	expression tag	UNP A1BCD5
J	1923	LEU	-	expression tag	UNP A1BCD5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1924	GLU	-	expression tag	UNP A1BCD5
J	1925	HIS	-	expression tag	UNP A1BCD5
J	1926	HIS	-	expression tag	UNP A1BCD5
J	1927	HIS	-	expression tag	UNP A1BCD5
J	1928	HIS	-	expression tag	UNP A1BCD5
J	1929	HIS	-	expression tag	UNP A1BCD5
J	1930	HIS	-	expression tag	UNP A1BCD5
K	2116	LEU	-	expression tag	UNP A1BCD5
K	2117	GLU	-	expression tag	UNP A1BCD5
K	2118	HIS	-	expression tag	UNP A1BCD5
K	2119	HIS	-	expression tag	UNP A1BCD5
K	2120	HIS	-	expression tag	UNP A1BCD5
K	2121	HIS	-	expression tag	UNP A1BCD5
K	2122	HIS	-	expression tag	UNP A1BCD5
K	2123	HIS	-	expression tag	UNP A1BCD5
L	2309	LEU	-	expression tag	UNP A1BCD5
L	2310	GLU	-	expression tag	UNP A1BCD5
L	2311	HIS	-	expression tag	UNP A1BCD5
L	2312	HIS	-	expression tag	UNP A1BCD5
L	2313	HIS	-	expression tag	UNP A1BCD5
L	2314	HIS	-	expression tag	UNP A1BCD5
L	2315	HIS	-	expression tag	UNP A1BCD5
L	2316	HIS	-	expression tag	UNP A1BCD5
M	2502	LEU	-	expression tag	UNP A1BCD5
M	2503	GLU	-	expression tag	UNP A1BCD5
M	2504	HIS	-	expression tag	UNP A1BCD5
M	2505	HIS	-	expression tag	UNP A1BCD5
M	2506	HIS	-	expression tag	UNP A1BCD5
M	2507	HIS	-	expression tag	UNP A1BCD5
M	2508	HIS	-	expression tag	UNP A1BCD5
M	2509	HIS	-	expression tag	UNP A1BCD5
N	2695	LEU	-	expression tag	UNP A1BCD5
N	2696	GLU	-	expression tag	UNP A1BCD5
N	2697	HIS	-	expression tag	UNP A1BCD5
N	2698	HIS	-	expression tag	UNP A1BCD5
N	2699	HIS	-	expression tag	UNP A1BCD5
N	2700	HIS	-	expression tag	UNP A1BCD5
N	2701	HIS	-	expression tag	UNP A1BCD5
N	2702	HIS	-	expression tag	UNP A1BCD5
O	2888	LEU	-	expression tag	UNP A1BCD5
O	2889	GLU	-	expression tag	UNP A1BCD5
O	2890	HIS	-	expression tag	UNP A1BCD5

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Chain	Residue	Modelled	Actual	Comment	Reference
O	2891	HIS	-	expression tag	UNP A1BCD5
O	2892	HIS	-	expression tag	UNP A1BCD5
O	2893	HIS	-	expression tag	UNP A1BCD5
O	2894	HIS	-	expression tag	UNP A1BCD5
O	2895	HIS	-	expression tag	UNP A1BCD5
P	3081	LEU	-	expression tag	UNP A1BCD5
P	3082	GLU	-	expression tag	UNP A1BCD5
P	3083	HIS	-	expression tag	UNP A1BCD5
P	3084	HIS	-	expression tag	UNP A1BCD5
P	3085	HIS	-	expression tag	UNP A1BCD5
P	3086	HIS	-	expression tag	UNP A1BCD5
P	3087	HIS	-	expression tag	UNP A1BCD5
P	3088	HIS	-	expression tag	UNP A1BCD5
Q	3275	LEU	-	expression tag	UNP A1BCD5
Q	3276	GLU	-	expression tag	UNP A1BCD5
Q	3277	HIS	-	expression tag	UNP A1BCD5
Q	3278	HIS	-	expression tag	UNP A1BCD5
Q	3279	HIS	-	expression tag	UNP A1BCD5
Q	3280	HIS	-	expression tag	UNP A1BCD5
Q	3281	HIS	-	expression tag	UNP A1BCD5
Q	3282	HIS	-	expression tag	UNP A1BCD5
R	3467	LEU	-	expression tag	UNP A1BCD5
R	3468	GLU	-	expression tag	UNP A1BCD5
R	3469	HIS	-	expression tag	UNP A1BCD5
R	3470	HIS	-	expression tag	UNP A1BCD5
R	3471	HIS	-	expression tag	UNP A1BCD5
R	3472	HIS	-	expression tag	UNP A1BCD5
R	3473	HIS	-	expression tag	UNP A1BCD5
R	3474	HIS	-	expression tag	UNP A1BCD5
S	3661	LEU	-	expression tag	UNP A1BCD5
S	3662	GLU	-	expression tag	UNP A1BCD5
S	3663	HIS	-	expression tag	UNP A1BCD5
S	3664	HIS	-	expression tag	UNP A1BCD5
S	3665	HIS	-	expression tag	UNP A1BCD5
S	3666	HIS	-	expression tag	UNP A1BCD5
S	3667	HIS	-	expression tag	UNP A1BCD5
S	3668	HIS	-	expression tag	UNP A1BCD5
T	3853	LEU	-	expression tag	UNP A1BCD5
T	3854	GLU	-	expression tag	UNP A1BCD5
T	3855	HIS	-	expression tag	UNP A1BCD5
T	3856	HIS	-	expression tag	UNP A1BCD5
T	3857	HIS	-	expression tag	UNP A1BCD5

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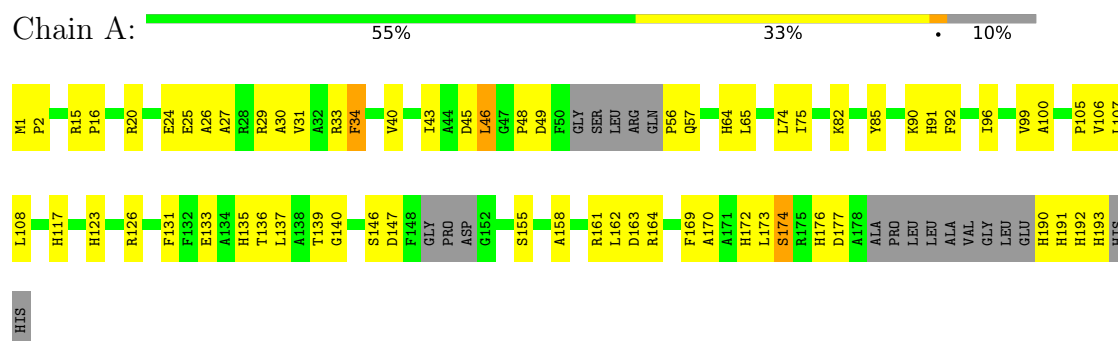
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Chain	Residue	Modelled	Actual	Comment	Reference
T	3858	HIS	-	expression tag	UNP A1BCD5
T	3859	HIS	-	expression tag	UNP A1BCD5
T	3860	HIS	-	expression tag	UNP A1BCD5

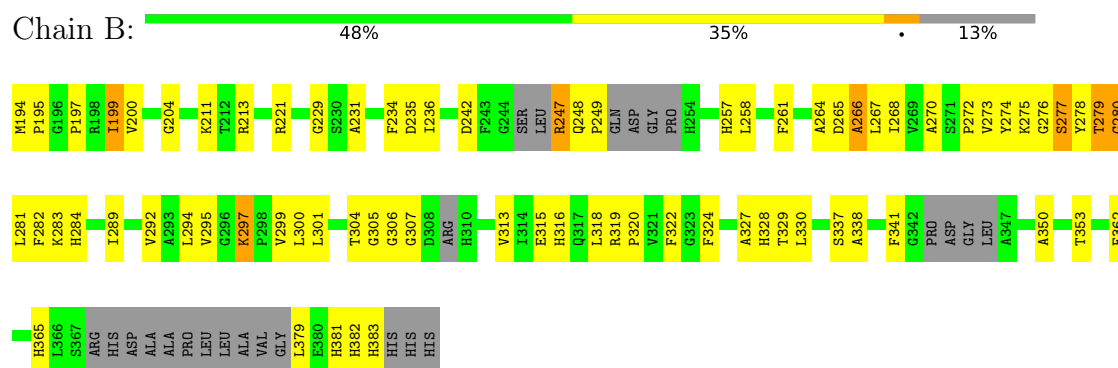
3 Residue-property plots

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.

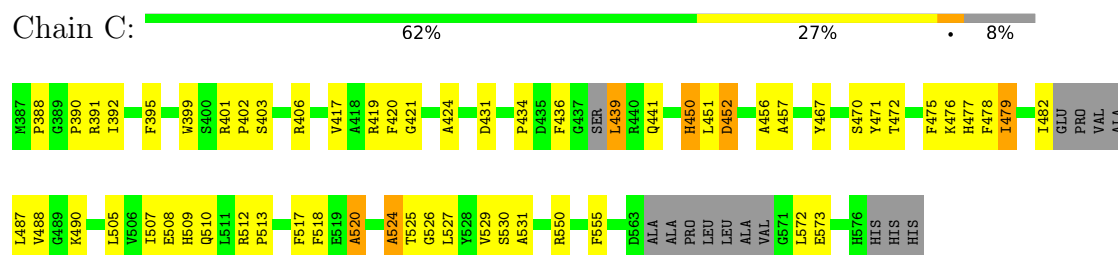
• Molecule 1: NADPH-dependent FMN reductase



• Molecule 1: NADPH-dependent FMN reductase

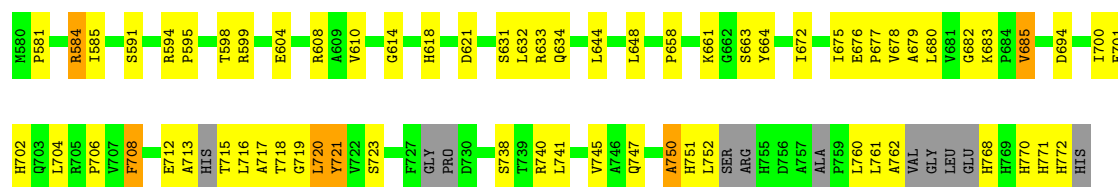


• Molecule 1: NADPH-dependent FMN reductase



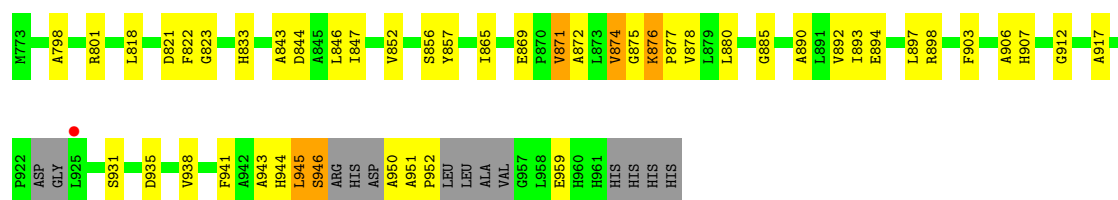
• Molecule 1: NADPH-dependent FMN reductase

Chain D:  60% 31% 6%



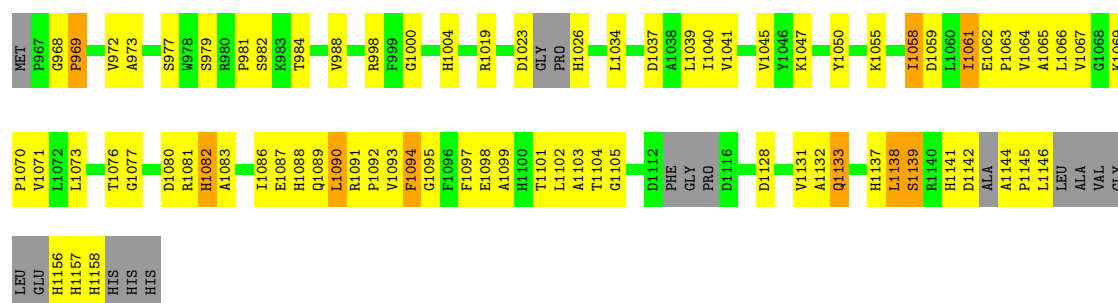
• Molecule 1: NADPH-dependent FMN reductase

Chain E:  68% 22% 7%



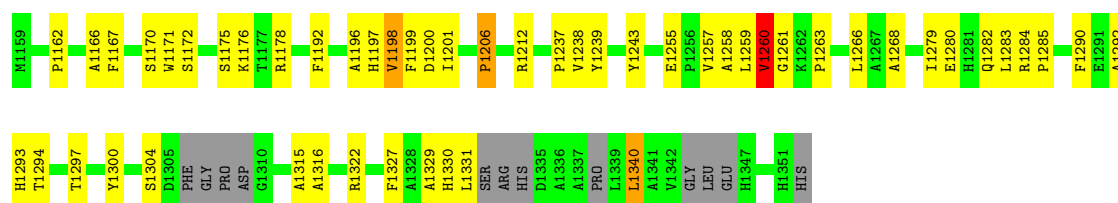
• Molecule 1: NADPH-dependent FMN reductase

Chain F:  52% 35% 5% 8%



• Molecule 1: NADPH-dependent FMN reductase

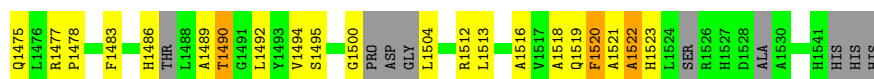
Chain G:  67% 25% 6%



• Molecule 1: NADPH-dependent FMN reductase

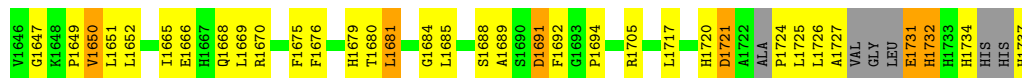
Chain H:  65% 27% 5%





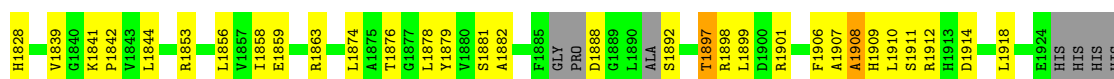
- Molecule 1: NADPH-dependent FMN reductase

Chain I: 59% 31% 6% 5%



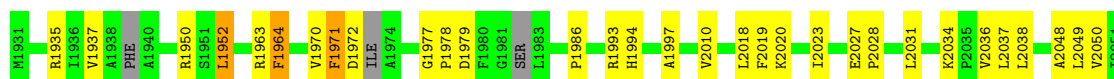
- Molecule 1: NADPH-dependent FMN reductase

Chain J: 58% 34% 6%



- Molecule 1: NADPH-dependent FMN reductase

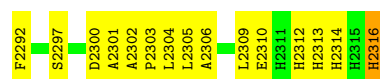
Chain K: 66% 26% 6%



- Molecule 1: NADPH-dependent FMN reductase

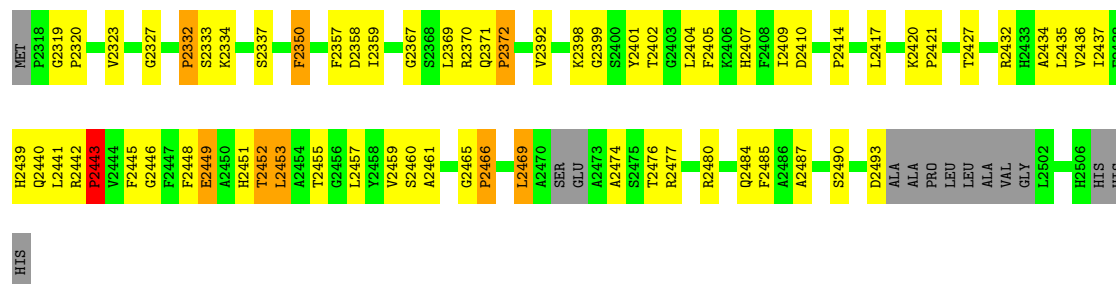
Chain L: 52% 42% 6%





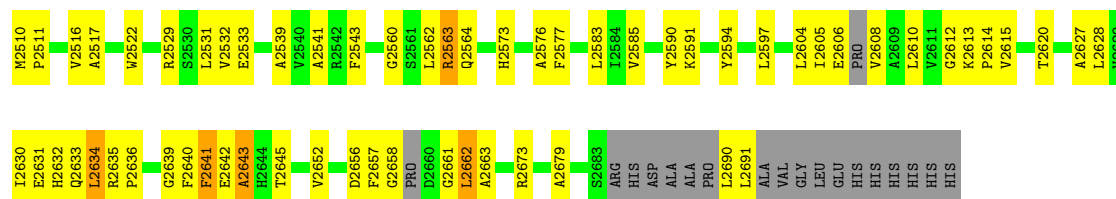
• Molecule 1: NADPH-dependent FMN reductase

Chain M: 59% 30% 7%



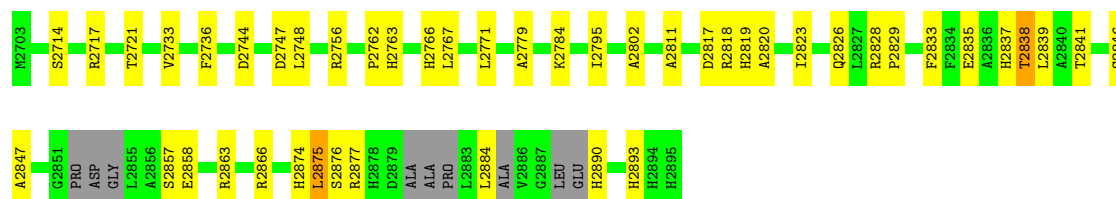
• Molecule 1: NADPH-dependent FMN reductase

Chain N: 59% 29% 10%



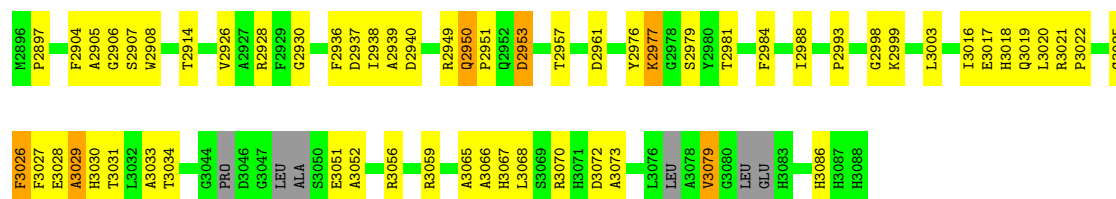
• Molecule 1: NADPH-dependent FMN reductase

Chain O: 72% 23% 5%



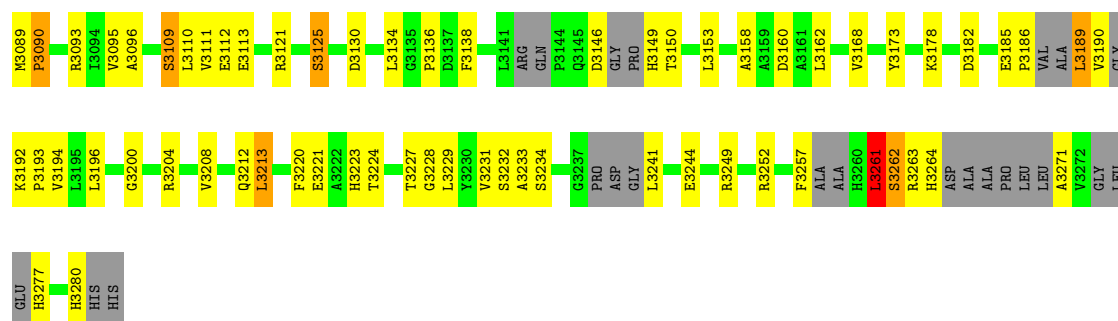
• Molecule 1: NADPH-dependent FMN reductase

Chain P: 66% 28% 6%



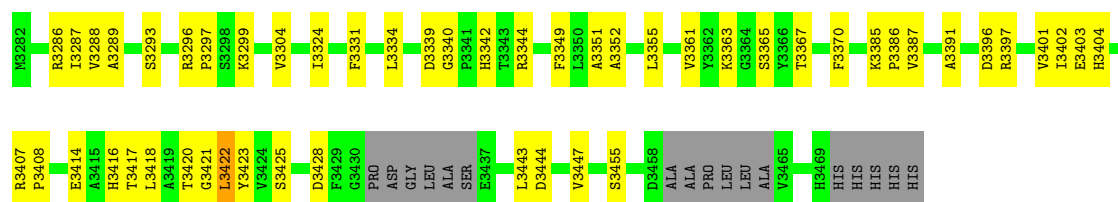
• Molecule 1: NADPH-dependent FMN reductase

Chain Q: 



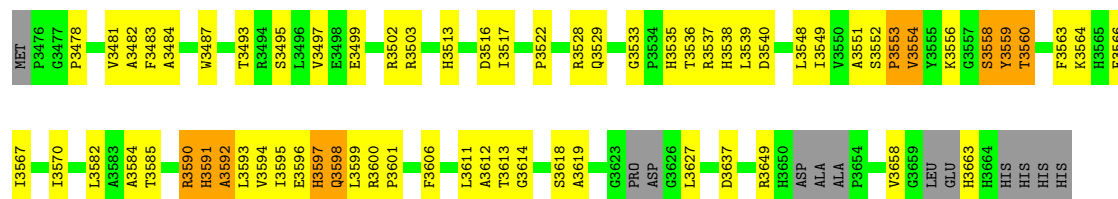
• Molecule 1: NADPH-dependent FMN reductase

Chain R: 



• Molecule 1: NADPH-dependent FMN reductase

Chain S: 



• Molecule 1: NADPH-dependent FMN reductase

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.51Å 136.38Å 212.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.10 48.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.2 (48.75-3.10) 86.7 (48.75-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.320 , 0.321 0.320 , 0.322	Depositor DCC
R_{free} test set	2005 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 167.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.064 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26343	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.92% 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	0.88	0/1312	1.36	8/1781 (0.4%)
1	B	0.96	3/1293 (0.2%)	1.29	12/1750 (0.7%)
1	C	0.86	0/1323	1.32	7/1798 (0.4%)
1	D	0.90	1/1363 (0.1%)	1.38	10/1848 (0.5%)
1	E	0.95	0/1335	1.37	9/1817 (0.5%)
1	F	0.96	2/1324 (0.2%)	1.42	15/1796 (0.8%)
1	G	0.93	0/1367	1.33	13/1856 (0.7%)
1	H	0.90	0/1373	1.33	7/1865 (0.4%)
1	I	0.94	1/1374 (0.1%)	1.39	14/1868 (0.7%)
1	J	0.90	0/1369	1.31	7/1860 (0.4%)
1	K	0.86	0/1375	1.37	11/1858 (0.6%)
1	L	0.88	0/1376	1.39	15/1870 (0.8%)
1	M	0.90	0/1323	1.40	9/1799 (0.5%)
1	N	0.92	0/1311	1.29	6/1779 (0.3%)
1	O	0.88	0/1428	1.27	6/1933 (0.3%)
1	P	0.91	1/1439 (0.1%)	1.35	12/1950 (0.6%)
1	Q	0.90	0/1282	1.31	5/1731 (0.3%)
1	R	0.88	1/1323 (0.1%)	1.30	5/1799 (0.3%)
1	S	0.98	2/1333 (0.2%)	1.35	9/1811 (0.5%)
1	T	0.95	2/1333 (0.2%)	1.48	15/1811 (0.8%)
All	All	0.91	13/26956 (0.0%)	1.35	195/36580 (0.5%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	2977	LYS	C-N	-7.83	1.22	1.33
1	S	3554	VAL	CA-CB	7.33	1.64	1.54
1	I	1691	ASP	N-CA	-7.27	1.38	1.46
1	T	3752	TYR	C-O	-6.80	1.16	1.23
1	S	3591	HIS	CA-C	6.18	1.63	1.52

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ALA	N-CA-C	-10.87	100.29	114.31
1	S	3590	ARG	N-CA-C	-10.57	102.57	114.62
1	J	1899	LEU	N-CA-C	-10.46	101.07	114.04
1	E	844	ASP	N-CA-C	-10.38	100.69	113.97
1	S	3591	HIS	N-CA-C	9.54	124.50	113.15

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	1282	0	1233	121	0
1	B	1262	0	1234	102	0
1	C	1291	0	1225	91	0
1	D	1334	0	1278	102	0
1	E	1302	0	1247	65	0
1	F	1296	0	1249	130	0
1	G	1336	0	1282	49	0
1	H	1342	0	1277	71	0
1	I	1340	0	1277	97	0
1	J	1336	0	1304	86	0
1	K	1348	0	1307	49	0
1	L	1346	0	1269	83	0
1	M	1292	0	1220	88	0
1	N	1283	0	1254	80	0
1	O	1393	0	1357	51	0
1	P	1402	0	1348	92	0
1	Q	1257	0	1208	95	0
1	R	1291	0	1244	33	0
1	S	1304	0	1251	81	0
1	T	1306	0	1245	94	0
All	All	26343	0	25309	1372	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 27.

The worst 5 of 1372 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:266:ALA:HB1	1:B:362:PHE:CE2	1.36	1.58
1:P:2998:GLY:HA2	1:P:3030:HIS:CD2	1.64	1.31
1:L:2198:ILE:HG22	1:L:2230:LEU:CB	1.64	1.27
1:D:719:GLY:O	1:D:720:LEU:HD12	1.31	1.27
1:K:2049:LEU:HD12	1:K:2049:LEU:O	1.28	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/193 (86%)	150 (90%)	16 (10%)	0	100	100
1	B	156/193 (81%)	144 (92%)	12 (8%)	0	100	100
1	C	170/193 (88%)	153 (90%)	17 (10%)	0	100	100
1	D	170/193 (88%)	142 (84%)	28 (16%)	0	100	100
1	E	172/193 (89%)	158 (92%)	13 (8%)	1 (1%)	21	52
1	F	167/193 (86%)	151 (90%)	16 (10%)	0	100	100
1	G	171/193 (89%)	148 (86%)	21 (12%)	2 (1%)	10	37
1	H	174/193 (90%)	158 (91%)	15 (9%)	1 (1%)	21	52
1	I	177/193 (92%)	161 (91%)	16 (9%)	0	100	100
1	J	175/193 (91%)	152 (87%)	21 (12%)	2 (1%)	11	39
1	K	165/193 (86%)	144 (87%)	21 (13%)	0	100	100
1	L	180/193 (93%)	148 (82%)	30 (17%)	2 (1%)	11	39
1	M	173/193 (90%)	139 (80%)	31 (18%)	3 (2%)	7	30
1	N	166/193 (86%)	147 (89%)	19 (11%)	0	100	100
1	O	174/193 (90%)	155 (89%)	19 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	177/193 (92%)	145 (82%)	32 (18%)	0	100	100
1	Q	152/193 (79%)	141 (93%)	11 (7%)	0	100	100
1	R	170/193 (88%)	149 (88%)	21 (12%)	0	100	100
1	S	173/193 (90%)	146 (84%)	24 (14%)	3 (2%)	7	30
1	T	171/193 (89%)	134 (78%)	34 (20%)	3 (2%)	6	28
All	All	3399/3860 (88%)	2965 (87%)	417 (12%)	17 (0%)	24	57

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	3679	SER
1	G	1176	LYS
1	G	1260	VAL
1	J	1908	ALA
1	S	3553	PRO

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	121/145 (83%)	120 (99%)	1 (1%)	73	81
1	B	123/145 (85%)	121 (98%)	2 (2%)	55	75
1	C	119/145 (82%)	116 (98%)	3 (2%)	42	69
1	D	127/145 (88%)	125 (98%)	2 (2%)	55	75
1	E	123/145 (85%)	121 (98%)	2 (2%)	55	75
1	F	122/145 (84%)	119 (98%)	3 (2%)	42	69
1	G	127/145 (88%)	126 (99%)	1 (1%)	73	81
1	H	126/145 (87%)	124 (98%)	2 (2%)	55	75
1	I	126/145 (87%)	120 (95%)	6 (5%)	23	54
1	J	126/145 (87%)	124 (98%)	2 (2%)	55	75
1	K	129/145 (89%)	127 (98%)	2 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	123/145 (85%)	120 (98%)	3 (2%)	43	69
1	M	118/145 (81%)	118 (100%)	0	100	100
1	N	125/145 (86%)	122 (98%)	3 (2%)	43	69
1	O	138/145 (95%)	136 (99%)	2 (1%)	59	76
1	P	136/145 (94%)	135 (99%)	1 (1%)	76	82
1	Q	122/145 (84%)	117 (96%)	5 (4%)	27	59
1	R	124/145 (86%)	122 (98%)	2 (2%)	55	75
1	S	121/145 (83%)	120 (99%)	1 (1%)	73	81
1	T	121/145 (83%)	118 (98%)	3 (2%)	42	69
All	All	2497/2900 (86%)	2451 (98%)	46 (2%)	51	73

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2316	HIS
1	Q	3189	LEU
1	N	2590	TYR
1	O	2795	ILE
1	Q	3208	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1282	GLN
1	K	2053	HIS
1	P	3012	HIS
1	J	1860	HIS
1	K	2102	HIS

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 [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	174/193 (90%)	-1.11	0 100 100	30, 62, 98, 135	0
1	B	168/193 (87%)	-1.14	0 100 100	30, 64, 101, 117	0
1	C	178/193 (92%)	-1.09	0 100 100	33, 65, 113, 149	0
1	D	182/193 (94%)	-1.07	0 100 100	30, 72, 105, 123	0
1	E	180/193 (93%)	-1.10	1 (0%) 85 70	30, 58, 98, 148	0
1	F	177/193 (91%)	-1.02	0 100 100	30, 67, 114, 151	0
1	G	181/193 (93%)	-1.10	0 100 100	30, 70, 114, 149	0
1	H	184/193 (95%)	-1.04	0 100 100	30, 69, 117, 175	0
1	I	184/193 (95%)	-1.12	0 100 100	30, 64, 108, 133	0
1	J	181/193 (93%)	-1.05	0 100 100	30, 69, 113, 155	0
1	K	181/193 (93%)	-0.99	0 100 100	44, 86, 118, 144	0
1	L	188/193 (97%)	-1.01	0 100 100	30, 86, 135, 177	0
1	M	179/193 (92%)	-1.07	0 100 100	30, 68, 114, 151	0
1	N	174/193 (90%)	-1.08	0 100 100	42, 69, 107, 153	0
1	O	184/193 (95%)	-1.13	0 100 100	43, 71, 117, 153	0
1	P	187/193 (96%)	-1.11	0 100 100	30, 77, 115, 159	0
1	Q	170/193 (88%)	-1.09	0 100 100	30, 83, 130, 137	0
1	R	176/193 (91%)	-1.15	0 100 100	46, 76, 123, 175	0
1	S	181/193 (93%)	-1.07	0 100 100	45, 78, 116, 137	0
1	T	182/193 (94%)	-1.07	0 100 100	30, 94, 131, 169	0
All	All	3591/3860 (93%)	-1.08	1 (0%) 100 100	30, 72, 119, 177	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	925	LEU	2.2

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.