wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2023 – 01:22 pm GMT

PDB ID	:	7QW4
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 (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 (i)) were used in the production of this report:

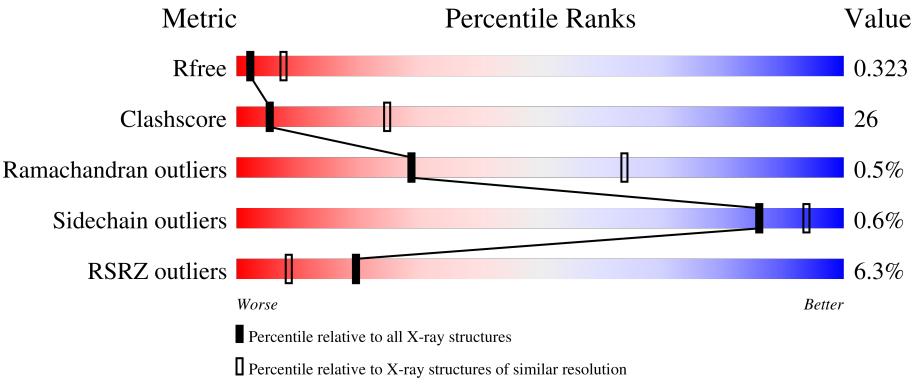
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	5% 60% 31% 10%
1	B	193	5% 53% 34% 13%
1	C	193	4% 64% 28% 8%
1	D	193	5% 63% 31% 6%
1	E	193	3% 71% 21% 7%

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Mol	Chain	Length	Quality of chain
1	F	193	6% 55% 36% 8%
1	G	193	6% 72% 22% 6%
1	H	193	4% 67% 28% 5%
1	I	193	6% 61% 34% 5%
1	J	193	6% 61% 33% 6%
1	K	193	12% 69% 24% 6%
1	L	193	9% 58% 39%
1	M	193	6% 60% 32% 7%
1	N	193	4% 62% 28% 10%
1	O	193	5% 75% 21% 5%
1	P	193	6% 69% 26%
1	Q	193	5% 56% 31% 12%
1	R	193	5% 68% 23% 9%
1	S	193	7% 61% 32% 6%
1	T	193	9% 62% 30% 6%

2 Entry composition (i)

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

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

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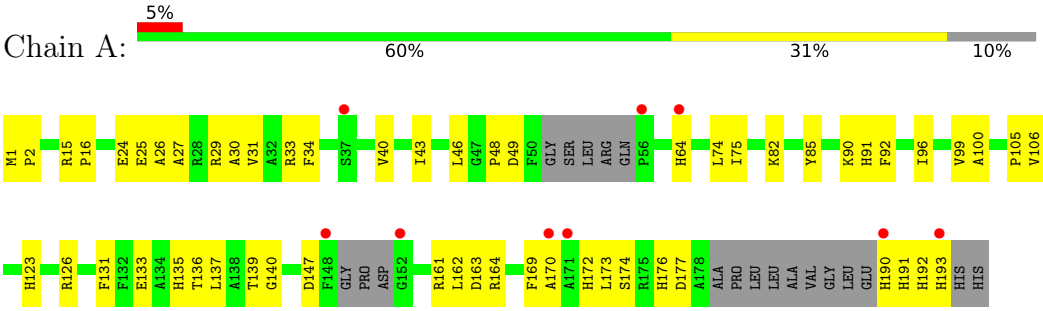
Chain	Residue	Modelled	Actual	Comment	Reference
T	3858	HIS	-	expression tag	UNP A1BCD5
T	3859	HIS	-	expression tag	UNP A1BCD5
T	3860	HIS	-	expression tag	UNP A1BCD5

3 Residue-property plots (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.

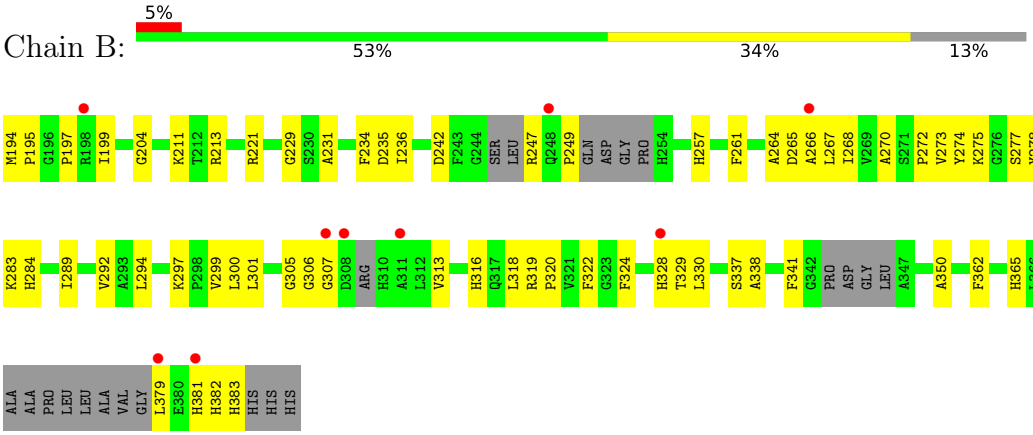
• Molecule 1: NADPH-dependent FMN reductase

Chain A:



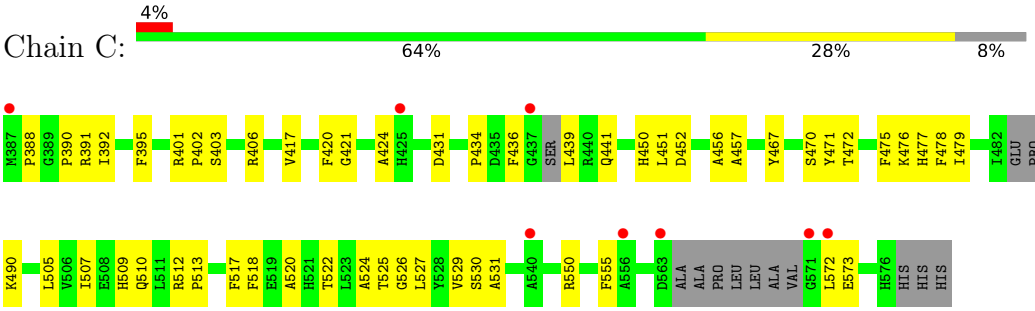
• Molecule 1: NADPH-dependent FMN reductase

Chain B:



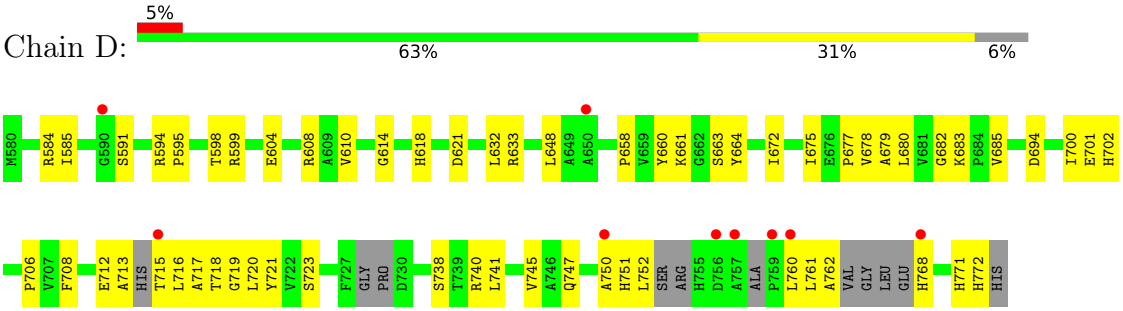
• Molecule 1: NADPH-dependent FMN reductase

Chain C:



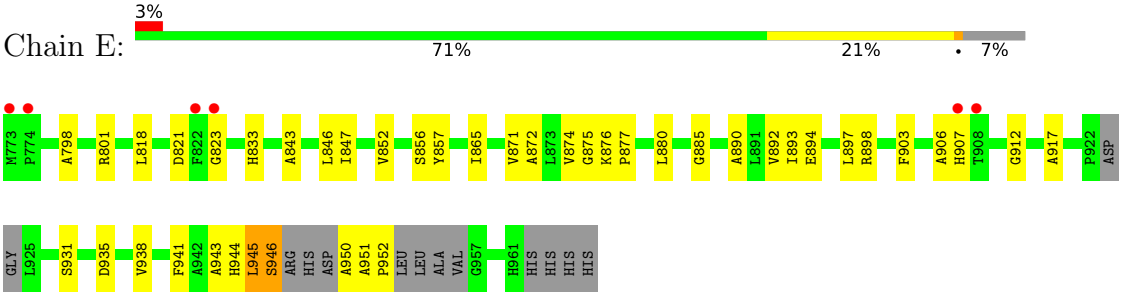
• Molecule 1: NADPH-dependent FMN reductase

Chain D:



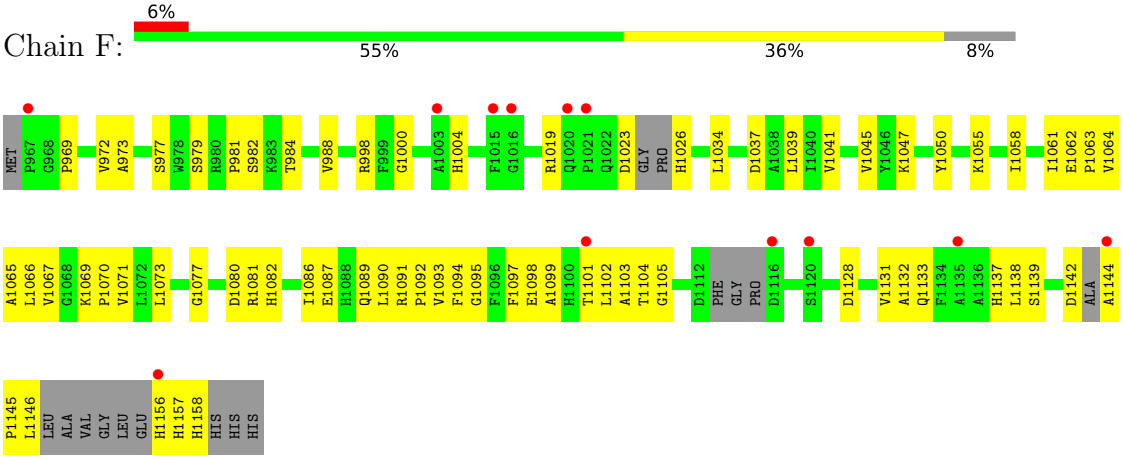
• Molecule 1: NADPH-dependent FMN reductase

Chain E:



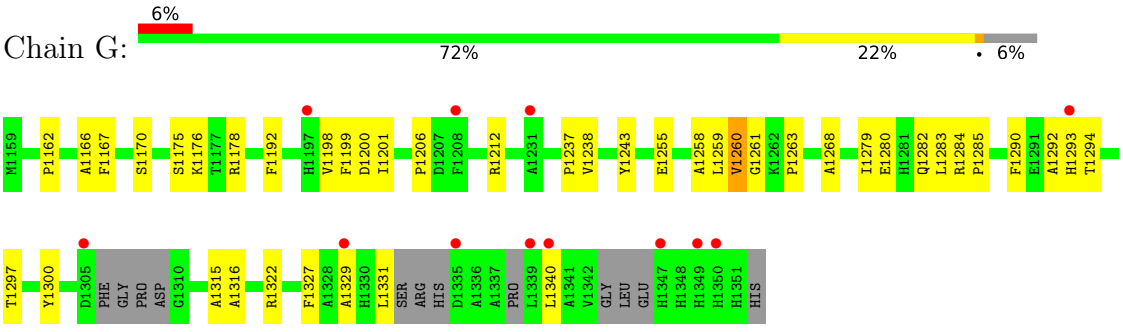
• Molecule 1: NADPH-dependent FMN reductase

Chain F:



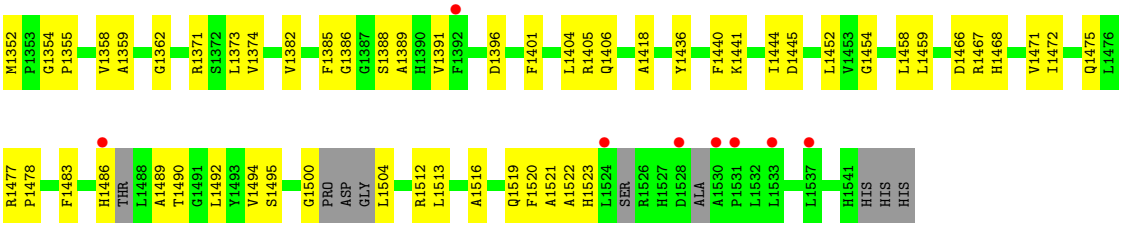
• Molecule 1: NADPH-dependent FMN reductase

Chain G:

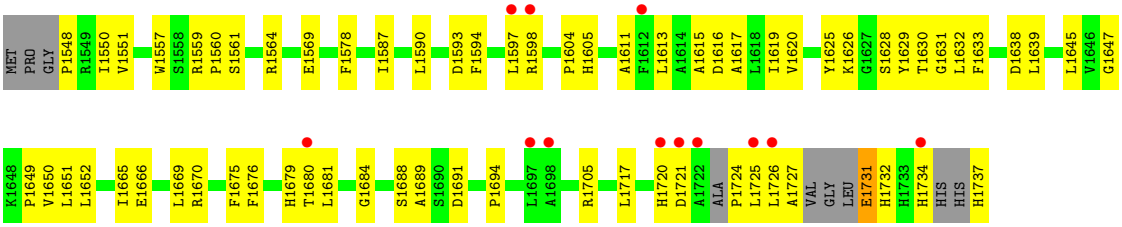


• Molecule 1: NADPH-dependent FMN reductase

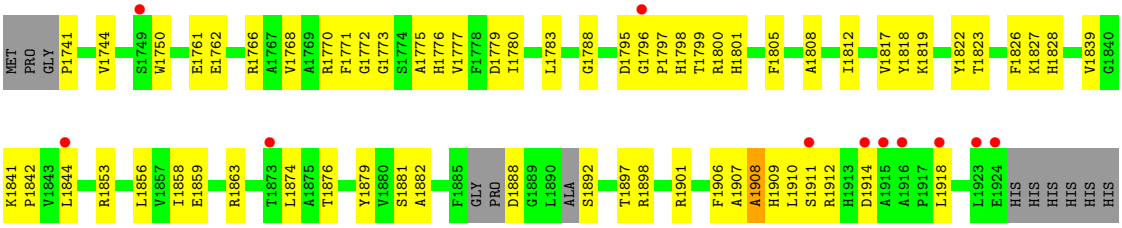
Chain H:



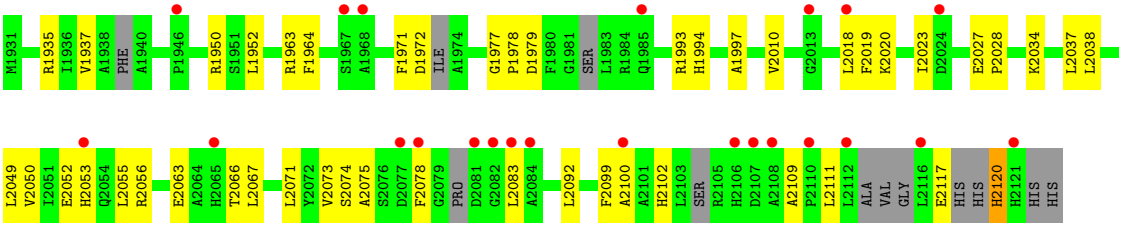
• Molecule 1: NADPH-dependent FMN reductase



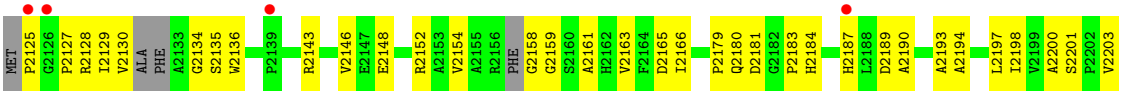
• Molecule 1: NADPH-dependent FMN reductase

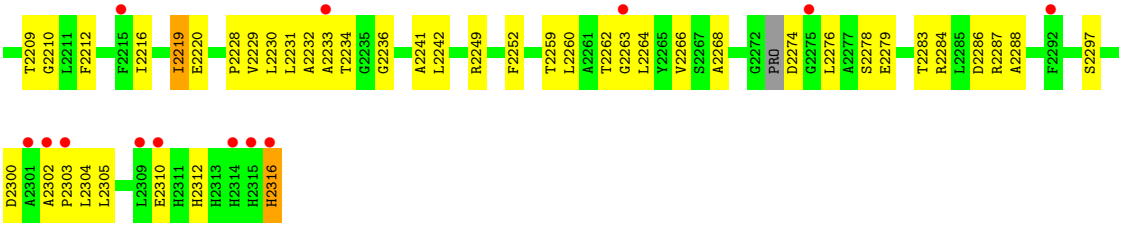


• Molecule 1: NADPH-dependent FMN reductase



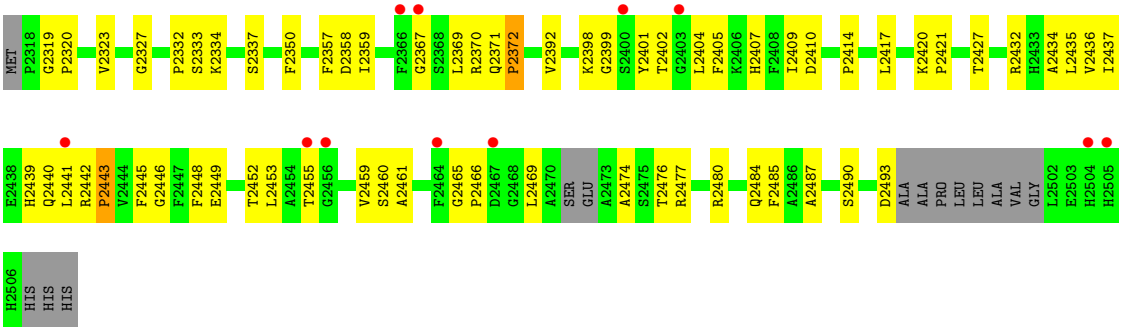
• Molecule 1: NADPH-dependent FMN reductase





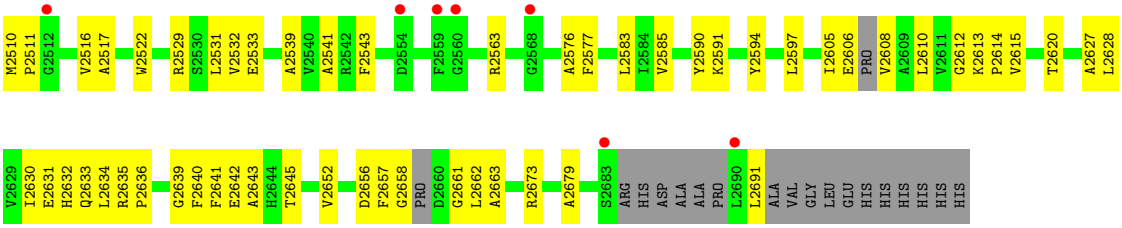
• Molecule 1: NADPH-dependent FMN reductase

Chain M:



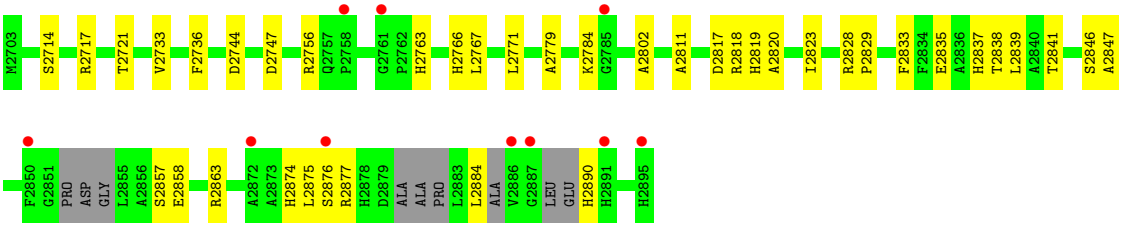
• Molecule 1: NADPH-dependent FMN reductase

Chain N:



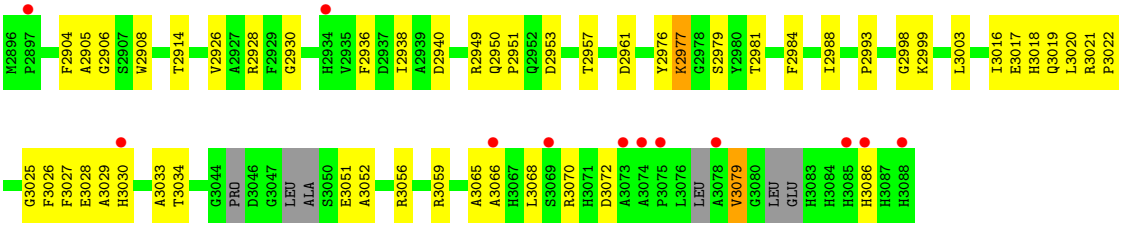
• Molecule 1: NADPH-dependent FMN reductase

Chain O:

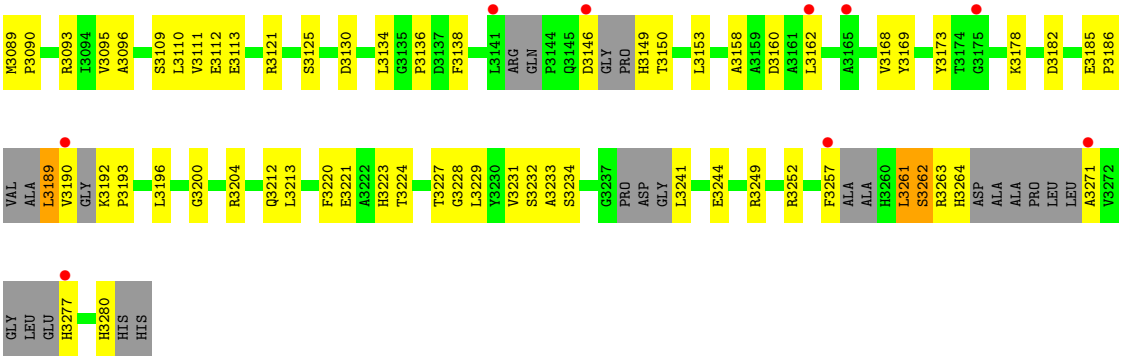


• Molecule 1: NADPH-dependent FMN reductase

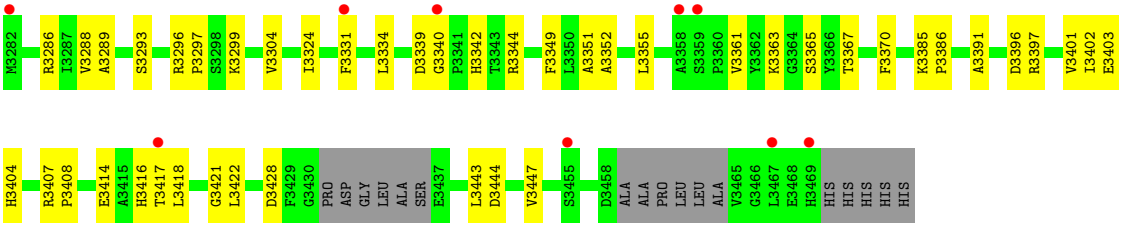
Chain P:



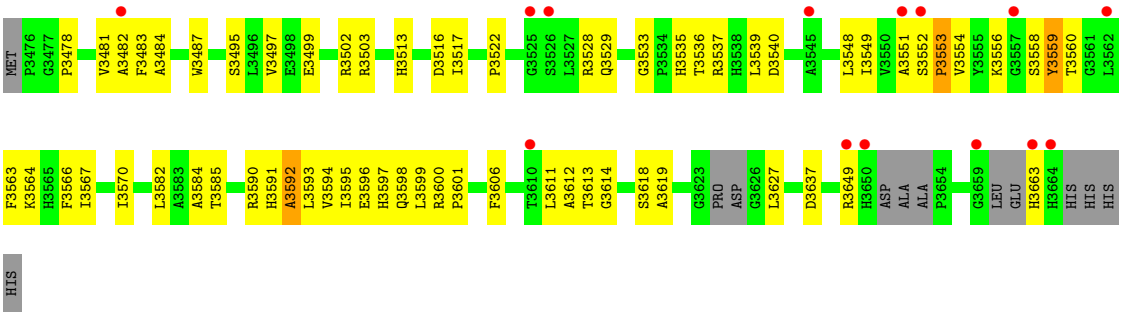
• Molecule 1: NADPH-dependent FMN reductase



• Molecule 1: NADPH-dependent FMN reductase

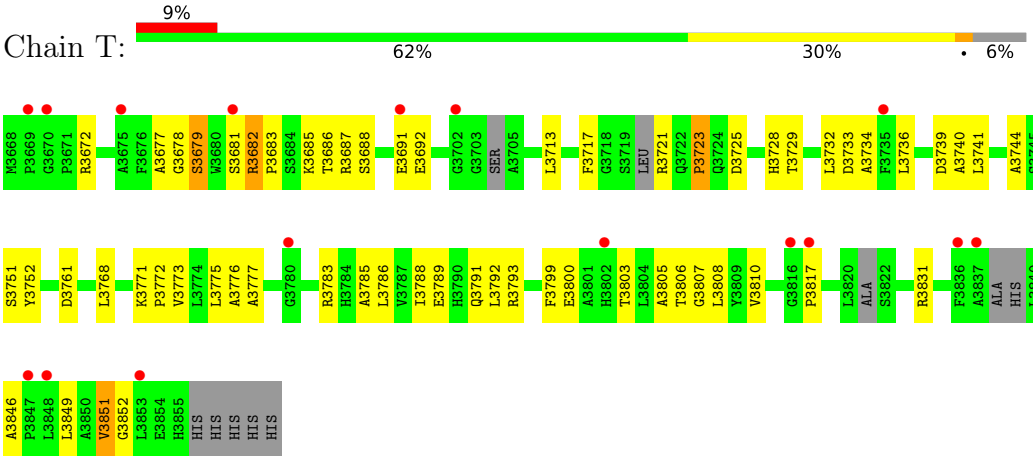


• Molecule 1: NADPH-dependent FMN reductase



• Molecule 1: NADPH-dependent FMN reductase

Chain T:


9%
62%
30%
6%
M3668 P3669 G3670 P3671 R3672 A3675 P3676 A3677 G3678 S3679 W3680 S3681 R3682 P3683 S3684 K3685 T3686 R3687 S3688 E3691 E3692 G3702 G3703 SER A3705 L3713 F3717 G3718 S3719 LEU R3721 Q3722 P3723 Q3724 D3725 H3728 T3729 L3732 D3733 A3734 F3735 L3736 D3739 A3740 L3741 A3744 S3745 P3746 K3749 G3750
S3751 Y3752 D3761 L3768 K3771 P3772 V3773 L3774 L3775 A3776 A3777 G3780 R3783 H3784 A3785 L3786 V3787 I3788 E3789 H3790 Q3791 L3792 R3793 F3799 E3800 A3801 H3802 T3803 L3804 A3805 T3806 G3807 L3808 Y3809 V3810 G3816 P3817 L3820 ALA S3822 R3831 F3836 A3837 ALA HIS L3840 SER H3842 H3843
A3846 P3847 L3848 L3849 A3850 V3851 G3852 L3853 E3854 H3855 HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.320 , 0.321 0.319 , 0.323	Depositor DCC
R_{free} test set	2005 reflections (3.11%)	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)	0.28 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.064 for k,h,-l	Xtriage
F_o,F_c correlation	0.87	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.63	0/1312	1.09	0/1781
1	B	0.67	0/1293	1.03	0/1750
1	C	0.62	0/1323	1.07	0/1798
1	D	0.65	0/1363	1.09	0/1848
1	E	0.69	0/1335	1.04	0/1817
1	F	0.69	0/1324	1.09	0/1796
1	G	0.65	0/1367	1.04	0/1856
1	H	0.64	0/1373	1.07	0/1865
1	I	0.64	0/1374	1.07	0/1868
1	J	0.62	0/1369	1.02	0/1860
1	K	0.61	0/1375	1.11	0/1858
1	L	0.62	0/1376	1.10	0/1870
1	M	0.65	0/1323	1.12	0/1799
1	N	0.63	0/1311	1.05	0/1779
1	O	0.64	0/1428	1.06	0/1933
1	P	0.61	1/1439 (0.1%)	1.05	0/1950
1	Q	0.63	0/1282	1.07	0/1731
1	R	0.61	0/1323	1.04	0/1799
1	S	0.69	0/1333	1.07	0/1811
1	T	0.66	0/1333	1.14	0/1811
All	All	0.64	1/26956 (0.0%)	1.07	0/36580

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	2977	LYS	C-N	-6.10	1.22	1.33

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	A	1282	0	1233	119	0
1	B	1262	0	1234	101	0
1	C	1291	0	1225	89	0
1	D	1334	0	1278	101	0
1	E	1302	0	1247	64	0
1	F	1296	0	1249	130	0
1	G	1336	0	1282	48	0
1	H	1342	0	1277	69	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	81	0
1	M	1292	0	1220	83	0
1	N	1283	0	1254	74	0
1	O	1393	0	1357	50	0
1	P	1402	0	1347	93	0
1	Q	1257	0	1208	92	0
1	R	1291	0	1244	33	0
1	S	1304	0	1251	80	0
1	T	1306	0	1245	93	0
All	All	26343	0	25308	1349	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 26.

The worst 5 of 1349 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%)	25	59
1	F	167/193 (86%)	151 (90%)	16 (10%)	0	100	100
1	G	171/193 (89%)	148 (86%)	21 (12%)	2 (1%)	13	44
1	H	174/193 (90%)	158 (91%)	15 (9%)	1 (1%)	25	59
1	I	177/193 (92%)	161 (91%)	16 (9%)	0	100	100
1	J	175/193 (91%)	152 (87%)	21 (12%)	2 (1%)	14	46
1	K	165/193 (86%)	144 (87%)	21 (13%)	0	100	100
1	L	180/193 (93%)	148 (82%)	30 (17%)	2 (1%)	14	46
1	M	173/193 (90%)	139 (80%)	31 (18%)	3 (2%)	9	36
1	N	166/193 (86%)	147 (89%)	19 (11%)	0	100	100
1	O	174/193 (90%)	155 (89%)	19 (11%)	0	100	100
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%)	9	36
1	T	171/193 (89%)	134 (78%)	34 (20%)	3 (2%)	8	34
All	All	3399/3860 (88%)	2965 (87%)	417 (12%)	17 (0%)	29	64

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	3679	SER

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

5.3.2 Protein sidechains (i)

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%)	121 (100%)	0	100	100
1	B	123/145 (85%)	123 (100%)	0	100	100
1	C	119/145 (82%)	119 (100%)	0	100	100
1	D	127/145 (88%)	126 (99%)	1 (1%)	81	92
1	E	123/145 (85%)	122 (99%)	1 (1%)	81	92
1	F	122/145 (84%)	122 (100%)	0	100	100
1	G	127/145 (88%)	127 (100%)	0	100	100
1	H	126/145 (87%)	126 (100%)	0	100	100
1	I	126/145 (87%)	123 (98%)	3 (2%)	49	76
1	J	126/145 (87%)	126 (100%)	0	100	100
1	K	129/145 (89%)	128 (99%)	1 (1%)	81	92
1	L	123/145 (85%)	122 (99%)	1 (1%)	81	92
1	M	118/145 (81%)	118 (100%)	0	100	100
1	N	125/145 (86%)	124 (99%)	1 (1%)	81	92
1	O	138/145 (95%)	137 (99%)	1 (1%)	84	93
1	P	136/145 (94%)	135 (99%)	1 (1%)	84	93
1	Q	122/145 (84%)	118 (97%)	4 (3%)	38	69
1	R	124/145 (86%)	124 (100%)	0	100	100
1	S	121/145 (83%)	121 (100%)	0	100	100
1	T	121/145 (83%)	119 (98%)	2 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2497/2900 (86%)	2481 (99%)	16 (1%)	86 94

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	3672	ARG
1	Q	3262	SER
1	O	2890	HIS
1	Q	3261	LEU
1	N	2590	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	2316	HIS
1	M	2440	GLN
1	P	3071	HIS
1	E	896	GLN
1	E	960	HIS

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	174/193 (90%)	0.17	9 (5%) 27 12	30, 62, 98, 135	0
1	B	168/193 (87%)	0.18	9 (5%) 25 12	30, 64, 101, 117	0
1	C	178/193 (92%)	0.22	8 (4%) 33 16	33, 65, 113, 149	0
1	D	182/193 (94%)	0.35	9 (4%) 29 14	30, 72, 105, 123	0
1	E	180/193 (93%)	0.08	6 (3%) 46 24	30, 58, 98, 148	0
1	F	177/193 (91%)	0.31	12 (6%) 17 7	30, 67, 114, 151	0
1	G	181/193 (93%)	0.29	12 (6%) 18 7	30, 70, 114, 149	0
1	H	184/193 (95%)	0.32	8 (4%) 35 17	30, 69, 117, 175	0
1	I	184/193 (95%)	0.25	12 (6%) 18 8	30, 64, 108, 133	0
1	J	181/193 (93%)	0.31	11 (6%) 21 9	30, 69, 113, 155	0
1	K	181/193 (93%)	0.62	23 (12%) 3 1	44, 86, 118, 144	0
1	L	188/193 (97%)	0.59	17 (9%) 9 3	30, 86, 135, 177	0
1	M	179/193 (92%)	0.25	11 (6%) 21 9	30, 68, 114, 151	0
1	N	174/193 (90%)	0.21	7 (4%) 38 19	42, 69, 107, 153	0
1	O	184/193 (95%)	0.34	10 (5%) 25 12	43, 71, 117, 153	0
1	P	187/193 (96%)	0.35	12 (6%) 19 8	30, 77, 115, 159	0
1	Q	170/193 (88%)	0.36	9 (5%) 26 12	30, 83, 130, 137	0
1	R	176/193 (91%)	0.31	9 (5%) 28 13	46, 76, 123, 175	0
1	S	181/193 (93%)	0.41	14 (7%) 13 5	45, 78, 116, 137	0
1	T	182/193 (94%)	0.55	17 (9%) 8 3	30, 94, 131, 169	0
All	All	3591/3860 (93%)	0.33	225 (6%) 20 8	30, 72, 119, 177	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	759	PRO	4.7
1	H	1524	LEU	4.6
1	D	715	THR	4.6
1	L	2303	PRO	4.5
1	R	3331	PHE	4.5

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.