



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:52 PM EST

PDB ID : 5I7F
Title : Crystal structure of B. pseudomallei FabI in complex with NAD and PT405
Authors : Eltschkner, S.; Tonge, P.J.; Kisker, C.
Deposited on : 2016-02-17
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

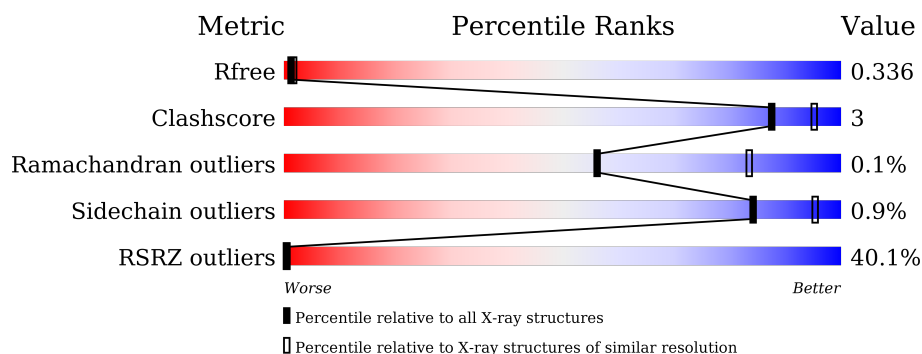
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	276	<div> <div>35%</div> <div>86% 7% 7%</div> </div>
1	B	276	<div> <div>36%</div> <div>86% 7% 7%</div> </div>
1	C	276	<div> <div>51%</div> <div>88% 5% 7%</div> </div>
1	D	276	<div> <div>37%</div> <div>87% 7% 7%</div> </div>
1	E	276	<div> <div>48%</div> <div>89% • 7%</div> </div>
1	F	276	<div> <div>39%</div> <div>89% • 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	276	<div><div></div><div>38%86%7%7%</div></div>
1	H	276	<div><div></div><div>36%84%9%7%</div></div>
1	I	276	<div><div></div><div>30%90%•7%</div></div>
1	J	276	<div><div></div><div>35%88%5%7%</div></div>
1	K	276	<div><div></div><div>32%89%•7%</div></div>
1	L	276	<div><div></div><div>31%86%7%7%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46664 atoms, of which 22715 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	257	Total	C	H	N	O	S	0	0	0
			3754	1218	1842	325	363	6			
1	E	257	Total	C	H	N	O	S	0	1	0
			3765	1221	1848	325	365	6			
1	H	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	C	257	Total	C	H	N	O	S	0	0	0
			3754	1218	1842	325	363	6			
1	A	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	F	257	Total	C	H	N	O	S	19	1	0
			3777	1223	1859	326	363	6			
1	G	257	Total	C	H	N	O	S	0	1	0
			3766	1221	1849	325	365	6			
1	D	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	I	257	Total	C	H	N	O	S	0	0	0
			3772	1218	1860	325	363	6			
1	K	257	Total	C	H	N	O	S	0	1	0
			3771	1223	1853	326	363	6			
1	L	257	Total	C	H	N	O	S	0	0	0
			3774	1218	1862	325	363	6			
1	J	257	Total	C	H	N	O	S	19	1	0
			3809	1223	1891	326	363	6			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	LYS	-	expression tag	UNP A0A069B9A4
B	265	LEU	-	expression tag	UNP A0A069B9A4
B	266	ALA	-	expression tag	UNP A0A069B9A4
B	267	ALA	-	expression tag	UNP A0A069B9A4
B	268	ALA	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	269	LEU	-	expression tag	UNP A0A069B9A4
B	270	GLU	-	expression tag	UNP A0A069B9A4
B	271	HIS	-	expression tag	UNP A0A069B9A4
B	272	HIS	-	expression tag	UNP A0A069B9A4
B	273	HIS	-	expression tag	UNP A0A069B9A4
B	274	HIS	-	expression tag	UNP A0A069B9A4
B	275	HIS	-	expression tag	UNP A0A069B9A4
B	276	HIS	-	expression tag	UNP A0A069B9A4
E	264	LYS	-	expression tag	UNP A0A069B9A4
E	265	LEU	-	expression tag	UNP A0A069B9A4
E	266	ALA	-	expression tag	UNP A0A069B9A4
E	267	ALA	-	expression tag	UNP A0A069B9A4
E	268	ALA	-	expression tag	UNP A0A069B9A4
E	269	LEU	-	expression tag	UNP A0A069B9A4
E	270	GLU	-	expression tag	UNP A0A069B9A4
E	271	HIS	-	expression tag	UNP A0A069B9A4
E	272	HIS	-	expression tag	UNP A0A069B9A4
E	273	HIS	-	expression tag	UNP A0A069B9A4
E	274	HIS	-	expression tag	UNP A0A069B9A4
E	275	HIS	-	expression tag	UNP A0A069B9A4
E	276	HIS	-	expression tag	UNP A0A069B9A4
H	264	LYS	-	expression tag	UNP A0A069B9A4
H	265	LEU	-	expression tag	UNP A0A069B9A4
H	266	ALA	-	expression tag	UNP A0A069B9A4
H	267	ALA	-	expression tag	UNP A0A069B9A4
H	268	ALA	-	expression tag	UNP A0A069B9A4
H	269	LEU	-	expression tag	UNP A0A069B9A4
H	270	GLU	-	expression tag	UNP A0A069B9A4
H	271	HIS	-	expression tag	UNP A0A069B9A4
H	272	HIS	-	expression tag	UNP A0A069B9A4
H	273	HIS	-	expression tag	UNP A0A069B9A4
H	274	HIS	-	expression tag	UNP A0A069B9A4
H	275	HIS	-	expression tag	UNP A0A069B9A4
H	276	HIS	-	expression tag	UNP A0A069B9A4
C	264	LYS	-	expression tag	UNP A0A069B9A4
C	265	LEU	-	expression tag	UNP A0A069B9A4
C	266	ALA	-	expression tag	UNP A0A069B9A4
C	267	ALA	-	expression tag	UNP A0A069B9A4
C	268	ALA	-	expression tag	UNP A0A069B9A4
C	269	LEU	-	expression tag	UNP A0A069B9A4
C	270	GLU	-	expression tag	UNP A0A069B9A4
C	271	HIS	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	272	HIS	-	expression tag	UNP A0A069B9A4
C	273	HIS	-	expression tag	UNP A0A069B9A4
C	274	HIS	-	expression tag	UNP A0A069B9A4
C	275	HIS	-	expression tag	UNP A0A069B9A4
C	276	HIS	-	expression tag	UNP A0A069B9A4
A	264	LYS	-	expression tag	UNP A0A069B9A4
A	265	LEU	-	expression tag	UNP A0A069B9A4
A	266	ALA	-	expression tag	UNP A0A069B9A4
A	267	ALA	-	expression tag	UNP A0A069B9A4
A	268	ALA	-	expression tag	UNP A0A069B9A4
A	269	LEU	-	expression tag	UNP A0A069B9A4
A	270	GLU	-	expression tag	UNP A0A069B9A4
A	271	HIS	-	expression tag	UNP A0A069B9A4
A	272	HIS	-	expression tag	UNP A0A069B9A4
A	273	HIS	-	expression tag	UNP A0A069B9A4
A	274	HIS	-	expression tag	UNP A0A069B9A4
A	275	HIS	-	expression tag	UNP A0A069B9A4
A	276	HIS	-	expression tag	UNP A0A069B9A4
F	264	LYS	-	expression tag	UNP A0A069B9A4
F	265	LEU	-	expression tag	UNP A0A069B9A4
F	266	ALA	-	expression tag	UNP A0A069B9A4
F	267	ALA	-	expression tag	UNP A0A069B9A4
F	268	ALA	-	expression tag	UNP A0A069B9A4
F	269	LEU	-	expression tag	UNP A0A069B9A4
F	270	GLU	-	expression tag	UNP A0A069B9A4
F	271	HIS	-	expression tag	UNP A0A069B9A4
F	272	HIS	-	expression tag	UNP A0A069B9A4
F	273	HIS	-	expression tag	UNP A0A069B9A4
F	274	HIS	-	expression tag	UNP A0A069B9A4
F	275	HIS	-	expression tag	UNP A0A069B9A4
F	276	HIS	-	expression tag	UNP A0A069B9A4
G	264	LYS	-	expression tag	UNP A0A069B9A4
G	265	LEU	-	expression tag	UNP A0A069B9A4
G	266	ALA	-	expression tag	UNP A0A069B9A4
G	267	ALA	-	expression tag	UNP A0A069B9A4
G	268	ALA	-	expression tag	UNP A0A069B9A4
G	269	LEU	-	expression tag	UNP A0A069B9A4
G	270	GLU	-	expression tag	UNP A0A069B9A4
G	271	HIS	-	expression tag	UNP A0A069B9A4
G	272	HIS	-	expression tag	UNP A0A069B9A4
G	273	HIS	-	expression tag	UNP A0A069B9A4
G	274	HIS	-	expression tag	UNP A0A069B9A4

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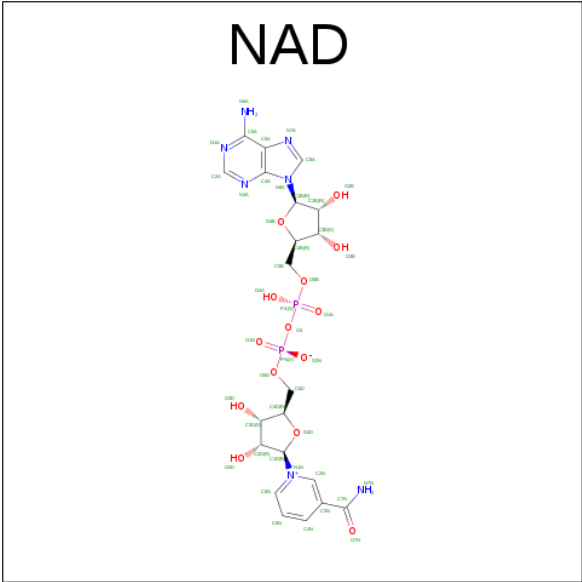
Chain	Residue	Modelled	Actual	Comment	Reference
G	275	HIS	-	expression tag	UNP A0A069B9A4
G	276	HIS	-	expression tag	UNP A0A069B9A4
D	264	LYS	-	expression tag	UNP A0A069B9A4
D	265	LEU	-	expression tag	UNP A0A069B9A4
D	266	ALA	-	expression tag	UNP A0A069B9A4
D	267	ALA	-	expression tag	UNP A0A069B9A4
D	268	ALA	-	expression tag	UNP A0A069B9A4
D	269	LEU	-	expression tag	UNP A0A069B9A4
D	270	GLU	-	expression tag	UNP A0A069B9A4
D	271	HIS	-	expression tag	UNP A0A069B9A4
D	272	HIS	-	expression tag	UNP A0A069B9A4
D	273	HIS	-	expression tag	UNP A0A069B9A4
D	274	HIS	-	expression tag	UNP A0A069B9A4
D	275	HIS	-	expression tag	UNP A0A069B9A4
D	276	HIS	-	expression tag	UNP A0A069B9A4
I	264	LYS	-	expression tag	UNP A0A069B9A4
I	265	LEU	-	expression tag	UNP A0A069B9A4
I	266	ALA	-	expression tag	UNP A0A069B9A4
I	267	ALA	-	expression tag	UNP A0A069B9A4
I	268	ALA	-	expression tag	UNP A0A069B9A4
I	269	LEU	-	expression tag	UNP A0A069B9A4
I	270	GLU	-	expression tag	UNP A0A069B9A4
I	271	HIS	-	expression tag	UNP A0A069B9A4
I	272	HIS	-	expression tag	UNP A0A069B9A4
I	273	HIS	-	expression tag	UNP A0A069B9A4
I	274	HIS	-	expression tag	UNP A0A069B9A4
I	275	HIS	-	expression tag	UNP A0A069B9A4
I	276	HIS	-	expression tag	UNP A0A069B9A4
K	264	LYS	-	expression tag	UNP A0A069B9A4
K	265	LEU	-	expression tag	UNP A0A069B9A4
K	266	ALA	-	expression tag	UNP A0A069B9A4
K	267	ALA	-	expression tag	UNP A0A069B9A4
K	268	ALA	-	expression tag	UNP A0A069B9A4
K	269	LEU	-	expression tag	UNP A0A069B9A4
K	270	GLU	-	expression tag	UNP A0A069B9A4
K	271	HIS	-	expression tag	UNP A0A069B9A4
K	272	HIS	-	expression tag	UNP A0A069B9A4
K	273	HIS	-	expression tag	UNP A0A069B9A4
K	274	HIS	-	expression tag	UNP A0A069B9A4
K	275	HIS	-	expression tag	UNP A0A069B9A4
K	276	HIS	-	expression tag	UNP A0A069B9A4
L	264	LYS	-	expression tag	UNP A0A069B9A4

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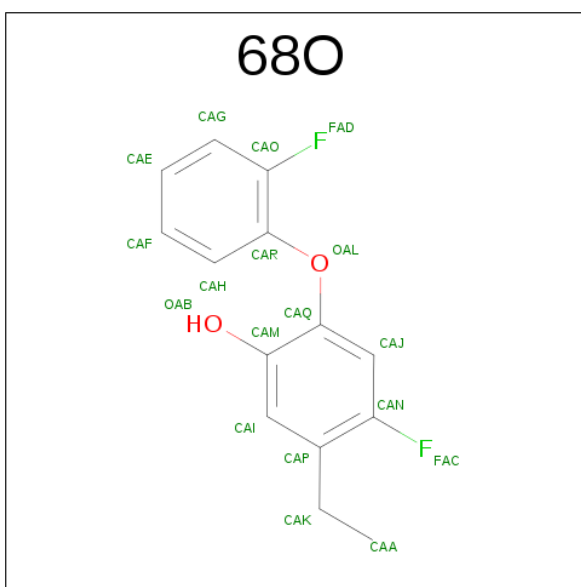
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L	265	LEU	-	expression tag	UNP A0A069B9A4
L	266	ALA	-	expression tag	UNP A0A069B9A4
L	267	ALA	-	expression tag	UNP A0A069B9A4
L	268	ALA	-	expression tag	UNP A0A069B9A4
L	269	LEU	-	expression tag	UNP A0A069B9A4
L	270	GLU	-	expression tag	UNP A0A069B9A4
L	271	HIS	-	expression tag	UNP A0A069B9A4
L	272	HIS	-	expression tag	UNP A0A069B9A4
L	273	HIS	-	expression tag	UNP A0A069B9A4
L	274	HIS	-	expression tag	UNP A0A069B9A4
L	275	HIS	-	expression tag	UNP A0A069B9A4
L	276	HIS	-	expression tag	UNP A0A069B9A4
J	264	LYS	-	expression tag	UNP A0A069B9A4
J	265	LEU	-	expression tag	UNP A0A069B9A4
J	266	ALA	-	expression tag	UNP A0A069B9A4
J	267	ALA	-	expression tag	UNP A0A069B9A4
J	268	ALA	-	expression tag	UNP A0A069B9A4
J	269	LEU	-	expression tag	UNP A0A069B9A4
J	270	GLU	-	expression tag	UNP A0A069B9A4
J	271	HIS	-	expression tag	UNP A0A069B9A4
J	272	HIS	-	expression tag	UNP A0A069B9A4
J	273	HIS	-	expression tag	UNP A0A069B9A4
J	274	HIS	-	expression tag	UNP A0A069B9A4
J	275	HIS	-	expression tag	UNP A0A069B9A4
J	276	HIS	-	expression tag	UNP A0A069B9A4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	E	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	H	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	F	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	G	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	I	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	K	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	L	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	J	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

- Molecule 3 is 5-ethyl-4-fluoro-2-(2-fluorophenoxy)phenol (three-letter code: 68O) (formula: C₁₄H₁₂F₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	E	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	H	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	C	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	A	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	F	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	G	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	D	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	I	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	K	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	L	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	J	1	Total	C	F	H	O	0	0
			30	14	2	12	2		

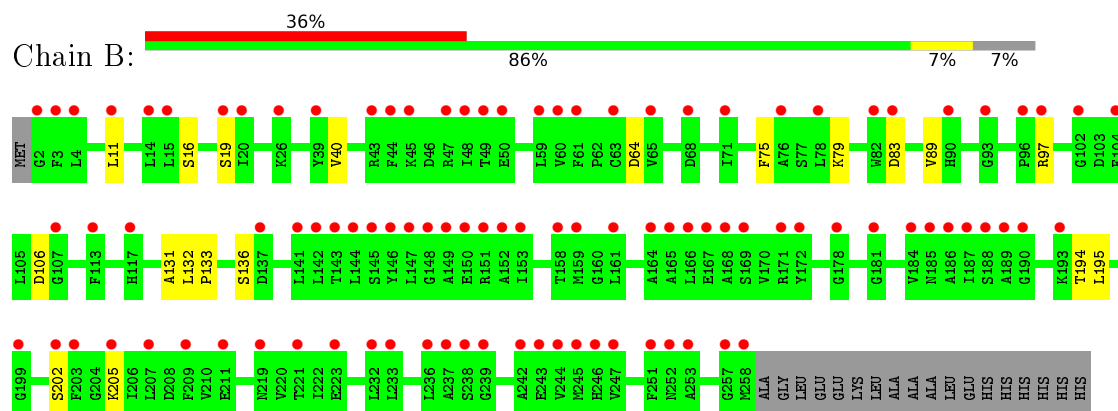
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total 20	O 20	0	0
4	E	22	Total 22	O 22	0	0
4	H	17	Total 17	O 17	0	0
4	C	13	Total 13	O 13	0	0
4	A	22	Total 22	O 22	0	0
4	F	24	Total 24	O 24	0	0
4	G	23	Total 23	O 23	0	0
4	D	32	Total 32	O 32	0	0
4	I	10	Total 10	O 10	0	0
4	K	18	Total 18	O 18	0	0
4	L	12	Total 12	O 12	0	0
4	J	20	Total 20	O 20	0	0

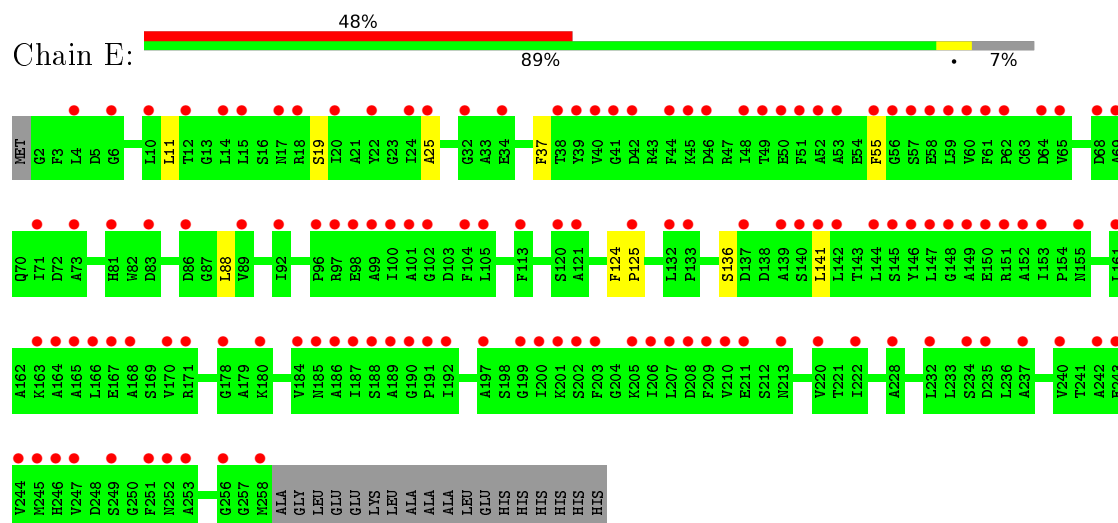
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

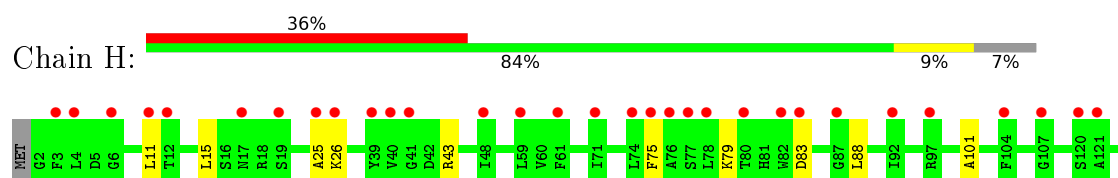
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

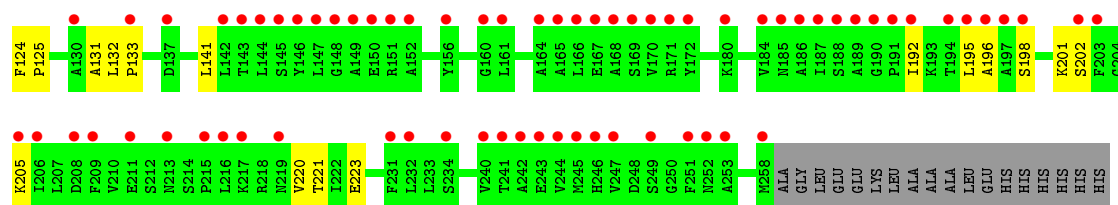


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

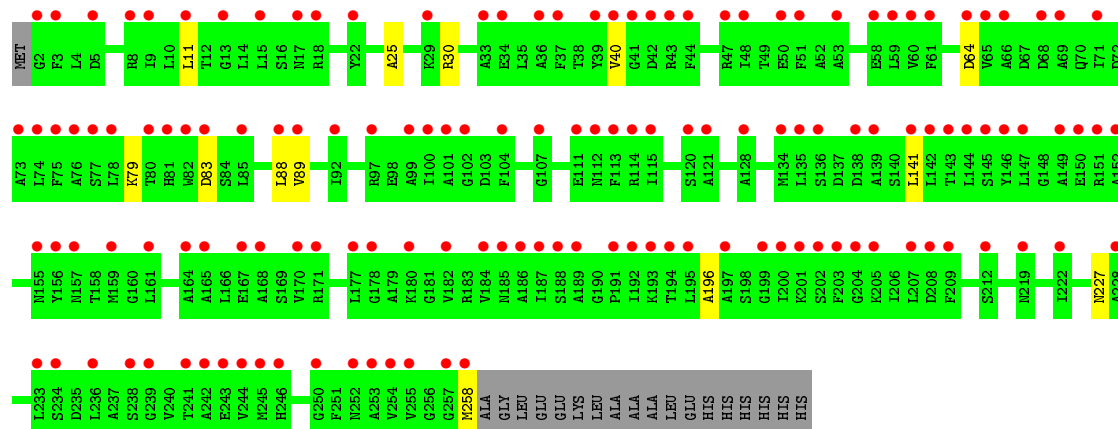
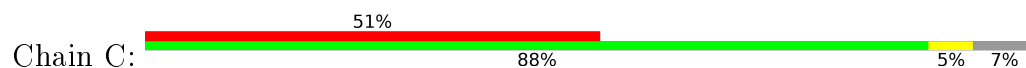


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

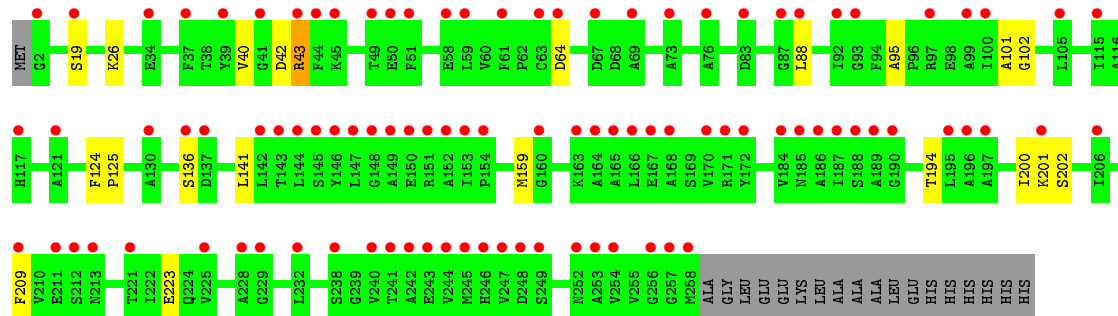
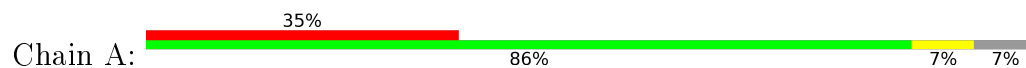




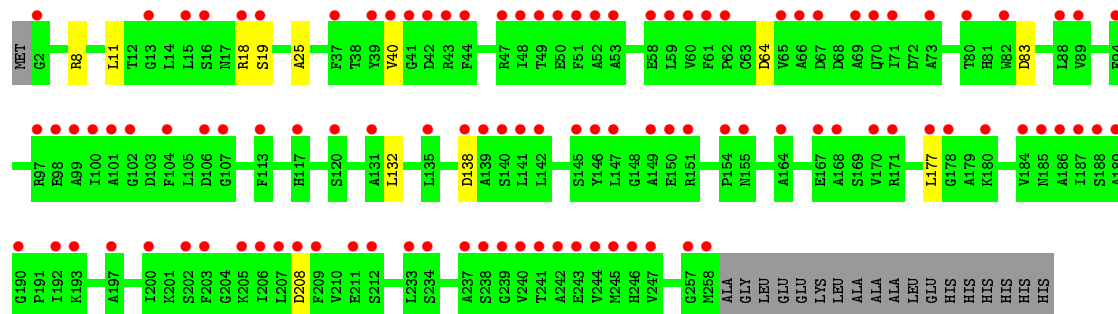
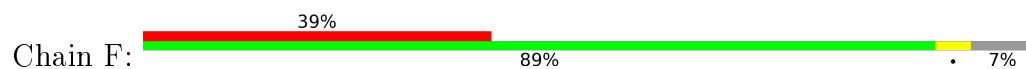
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

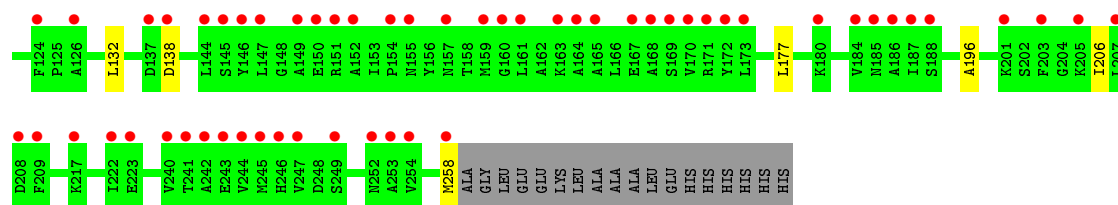


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

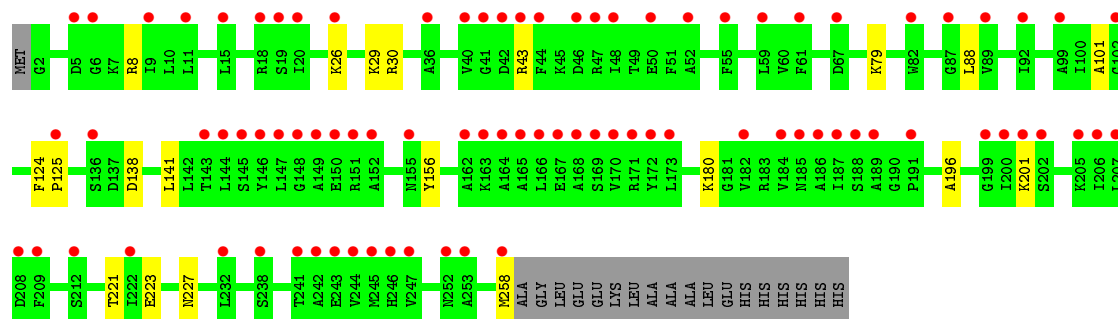
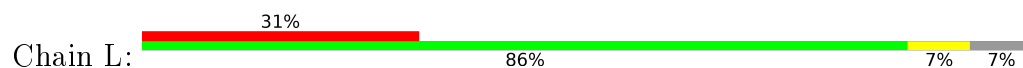


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

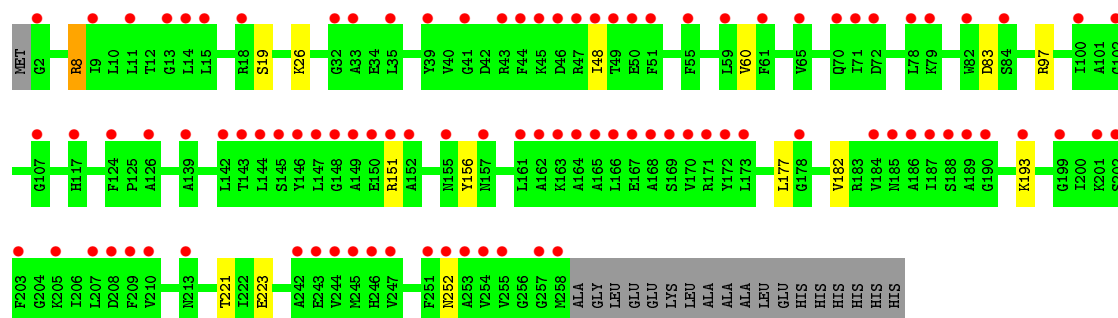
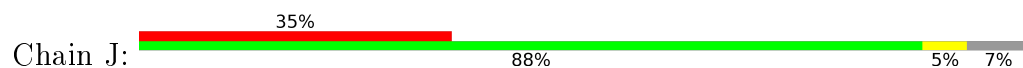




- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.43Å 109.78Å 269.80Å 90.00° 104.51° 90.00°	Depositor
Resolution (Å)	47.17 – 2.70 48.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.17-2.70) 94.6 (48.99-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.192 , 0.223 0.322 , 0.336	Depositor DCC
R_{free} test set	1273 reflections (1.25%)	DCC
Wilson B-factor (Å ²)	115.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.47$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	46664	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 68O, NAD

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	0.36	2/1945 (0.1%)	0.68	2/2631 (0.1%)
1	B	0.27	0/1945	0.45	0/2631
1	C	0.26	0/1945	0.46	0/2631
1	D	0.28	0/1945	0.46	0/2631
1	E	0.28	0/1953	0.46	0/2642
1	F	0.28	0/1954	0.47	0/2642
1	G	0.27	0/1953	0.46	0/2642
1	H	0.27	0/1945	0.47	0/2631
1	I	0.26	0/1945	0.45	0/2631
1	J	0.28	0/1954	0.47	0/2642
1	K	0.29	0/1954	0.49	0/2642
1	L	0.27	0/1945	0.48	0/2631
All	All	0.28	2/23383 (0.0%)	0.49	2/31627 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	ARG	CZ-NH2	-6.43	1.24	1.33
1	A	43	ARG	CD-NE	-5.42	1.37	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-18.27	111.17	120.30
1	A	43	ARG	NE-CZ-NH1	16.36	128.48	120.30

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	1912	1847	1919	15	0
1	B	1912	1842	1919	17	0
1	C	1912	1842	1919	7	0
1	D	1912	1847	1919	10	0
1	E	1917	1848	1923	7	0
1	F	1918	1859	1932	6	0
1	G	1917	1849	1923	10	0
1	H	1912	1847	1919	15	0
1	I	1912	1860	1919	4	0
1	J	1918	1891	1932	12	0
1	K	1918	1853	1932	7	0
1	L	1912	1862	1919	14	0
2	A	44	27	26	3	0
2	B	44	27	26	3	0
2	C	44	27	26	1	0
2	D	44	27	26	0	0
2	E	44	27	26	1	0
2	F	44	27	26	1	0
2	G	44	27	26	2	0
2	H	44	27	26	1	0
2	I	44	27	26	2	0
2	J	44	27	26	1	0
2	K	44	27	26	2	0
2	L	44	27	26	1	0
3	A	18	12	0	1	0
3	B	18	12	0	0	0
3	C	18	12	0	0	0
3	D	18	12	0	0	0
3	E	18	12	0	0	0
3	F	18	12	0	0	0
3	G	18	12	0	0	0
3	H	18	12	0	0	0
3	I	18	12	0	0	0
3	J	18	12	0	1	0
3	K	18	12	0	0	0
3	L	18	12	0	1	0
4	A	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	1	0
4	C	13	0	0	0	0
4	D	32	0	0	0	0
4	E	22	0	0	0	0
4	F	24	0	0	0	0
4	G	23	0	0	0	0
4	H	17	0	0	0	0
4	I	10	0	0	0	0
4	J	20	0	0	1	0
4	K	18	0	0	0	0
4	L	12	0	0	0	0
All	All	23949	22715	23387	120	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 3.

All (120) 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:L:101:ALA:HB1	1:L:201:LYS:HD2	1.50	0.91
1:H:101:ALA:HB1	1:H:201:LYS:HD2	1.56	0.87
1:G:97:ARG:NH1	1:L:138:ASP:OD2	2.15	0.79
1:C:30:ARG:NH2	1:C:227:ASN:OD1	2.18	0.76
1:A:101:ALA:HB1	1:A:201:LYS:HD2	1.67	0.76
1:B:202:SER:HB3	1:B:205:LYS:HD2	1.68	0.75
1:H:79:LYS:NZ	1:H:83:ASP:O	2.23	0.72
1:C:79:LYS:NZ	1:C:83:ASP:O	2.25	0.69
1:G:79:LYS:NZ	1:G:83:ASP:O	2.27	0.67
1:L:101:ALA:CB	1:L:201:LYS:HD2	2.24	0.65
1:D:95:ALA:HB2	1:D:159:MET:HE2	1.80	0.64
1:B:11:LEU:HD23	1:B:89:VAL:HB	1.80	0.63
1:D:79:LYS:NZ	1:D:83:ASP:O	2.32	0.63
1:D:155:ASN:ND2	1:D:201:LYS:O	2.32	0.62
2:I:301:NAD:H2N	2:I:301:NAD:O1N	1.99	0.62
1:B:97:ARG:NE	4:B:401:HOH:O	2.33	0.60
1:J:193:LYS:NZ	4:J:401:HOH:O	2.34	0.60
2:B:301:NAD:O1N	2:B:301:NAD:H2N	2.02	0.59
1:B:194:THR:HG21	2:B:301:NAD:O2N	2.04	0.58
1:A:194:THR:HG21	2:A:301:NAD:O2N	2.04	0.57
1:K:19:SER:OG	2:K:301:NAD:O1A	2.19	0.57
1:B:106:ASP:OD2	1:L:26:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HG	1:J:83:ASP:OD2	2.06	0.56
1:C:11:LEU:HD23	1:C:89:VAL:HB	1.88	0.56
2:A:301:NAD:H2N	2:A:301:NAD:O1N	2.05	0.56
1:A:102:GLY:H	1:A:201:LYS:HD3	1.70	0.55
1:H:101:ALA:CB	1:H:201:LYS:HD2	2.33	0.55
1:F:19:SER:OG	2:F:301:NAD:O1A	2.21	0.55
1:H:202:SER:HB2	1:H:205:LYS:HD2	1.88	0.55
1:E:19:SER:OG	2:E:301:NAD:O1A	2.26	0.53
1:B:79:LYS:NZ	1:B:83:ASP:O	2.40	0.53
1:D:2:GLY:N	1:D:5:ASP:OD2	2.42	0.52
1:A:95:ALA:HB2	1:A:159:MET:CE	2.40	0.51
1:H:221:THR:HB	1:H:223:GLU:OE1	2.11	0.51
1:B:19:SER:OG	2:B:301:NAD:O1A	2.20	0.50
1:B:40:VAL:HG23	1:B:64:ASP:HB2	1.94	0.50
1:K:42:ASP:N	1:K:42:ASP:OD1	2.44	0.50
1:L:196:ALA:HB2	2:L:301:NAD:O2A	2.12	0.50
1:G:9:ILE:HG22	1:G:11:LEU:HD12	1.94	0.50
1:G:88:LEU:HB3	1:G:141:LEU:HD22	1.94	0.49
1:I:194:THR:HG21	2:I:301:NAD:O2N	2.12	0.49
1:J:156:TYR:OH	3:J:302:68O:OAB	2.23	0.49
1:K:138:ASP:N	1:K:138:ASP:OD1	2.45	0.49
1:L:88:LEU:HB3	1:L:141:LEU:HD22	1.94	0.49
1:J:8:ARG:HH12	1:J:83:ASP:HB3	1.76	0.49
1:L:221:THR:HB	1:L:223:GLU:OE1	2.14	0.48
1:C:11:LEU:HD13	1:C:25:ALA:HB2	1.96	0.47
1:G:47:ARG:CZ	1:L:79:LYS:HE2	2.44	0.47
1:F:11:LEU:CD2	1:F:25:ALA:HB2	2.45	0.47
1:J:151:ARG:NH2	1:J:252:ASN:O	2.47	0.47
1:G:192:ILE:HD11	1:G:220:VAL:HG23	1.97	0.47
1:H:88:LEU:HB3	1:H:141:LEU:HD22	1.96	0.47
1:F:8:ARG:HH22	1:F:83:ASP:H	1.63	0.47
1:D:88:LEU:HB3	1:D:141:LEU:HD22	1.97	0.47
1:B:16:SER:HB2	1:J:83:ASP:OD1	2.14	0.47
1:H:195:LEU:O	1:H:198:SER:OG	2.28	0.47
1:H:196:ALA:HB2	2:H:301:NAD:O2A	2.15	0.47
1:A:40:VAL:HG23	1:A:64:ASP:HB2	1.98	0.46
1:C:40:VAL:HG23	1:C:64:ASP:HB2	1.98	0.46
1:J:48:ILE:HG23	1:J:60:VAL:HG11	1.96	0.46
1:K:196:ALA:HB2	2:K:301:NAD:O2A	2.15	0.46
1:L:156:TYR:OH	3:L:302:68O:OAB	2.26	0.46
1:A:26:LYS:NZ	1:A:223:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:SER:CB	1:J:83:ASP:OD1	2.64	0.46
2:G:301:NAD:O1N	2:G:301:NAD:H2N	2.16	0.46
1:E:25:ALA:HB1	1:E:55:PHE:CE2	2.51	0.46
1:J:19:SER:OG	2:J:301:NAD:O1A	2.18	0.45
1:D:151:ARG:NH2	1:D:252:ASN:O	2.46	0.45
1:H:26:LYS:NZ	1:H:223:GLU:HG3	2.30	0.45
1:D:132:LEU:HD13	1:D:177:LEU:HD22	1.98	0.45
1:H:192:ILE:HD11	1:H:220:VAL:HG23	1.99	0.45
1:B:11:LEU:HD23	1:B:89:VAL:CB	2.46	0.45
1:G:34:GLU:HG2	1:G:82:TRP:HZ2	1.81	0.45
1:A:101:ALA:CB	1:A:201:LYS:HD2	2.43	0.44
1:B:202:SER:HB3	1:B:205:LYS:CD	2.44	0.44
1:C:196:ALA:HB2	2:C:301:NAD:O2A	2.17	0.44
1:A:42:ASP:O	1:A:43:ARG:HB3	2.18	0.44
1:G:196:ALA:HB2	2:G:301:NAD:O2A	2.17	0.44
1:I:88:LEU:HB3	1:I:141:LEU:HD22	1.99	0.44
1:F:40:VAL:HG23	1:F:64:ASP:HB2	1.99	0.44
1:F:132:LEU:HD13	1:F:177:LEU:HD22	2.01	0.43
1:E:88:LEU:HB3	1:E:141:LEU:HD22	1.99	0.43
1:A:26:LYS:NZ	1:A:223:GLU:HG3	2.34	0.43
1:B:11:LEU:HD23	1:B:89:VAL:CG2	2.48	0.43
1:J:221:THR:HB	1:J:223:GLU:OE1	2.19	0.43
1:H:11:LEU:CD2	1:H:25:ALA:HB2	2.49	0.42
1:A:64:ASP:OD1	2:A:301:NAD:N6A	2.49	0.42
1:L:30:ARG:NH2	1:L:227:ASN:OD1	2.46	0.42
1:A:201:LYS:HE3	1:A:201:LYS:HB3	1.86	0.42
1:B:11:LEU:CD2	1:B:89:VAL:HG21	2.49	0.42
1:A:88:LEU:HB3	1:A:141:LEU:HD22	2.02	0.42
1:C:88:LEU:HB3	1:C:141:LEU:HD22	2.00	0.42
1:H:75:PHE:CZ	1:H:131:ALA:HB2	2.55	0.41
1:K:8:ARG:HH12	1:K:83:ASP:HB3	1.85	0.41
1:L:101:ALA:HA	1:L:201:LYS:HD3	2.01	0.41
1:E:124:PHE:HB3	1:E:125:PRO:CD	2.50	0.41
1:E:37:PHE:HZ	1:E:55:PHE:HD2	1.68	0.41
1:I:40:VAL:O	1:I:44:PHE:HD2	2.03	0.41
1:L:124:PHE:HB3	1:L:125:PRO:CD	2.49	0.41
1:G:194:THR:O	1:G:197:ALA:HB3	2.20	0.41
1:K:132:LEU:HD13	1:K:177:LEU:HD22	2.01	0.41
1:K:206:ILE:HG12	1:L:258:MET:SD	2.61	0.41
1:H:15:LEU:HD23	1:H:195:LEU:HD12	2.02	0.41
1:B:132:LEU:N	1:B:133:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:223:GLU:N	1:J:223:GLU:OE1	2.47	0.41
1:A:209:PHE:CG	1:D:258:MET:HG2	2.56	0.41
1:B:75:PHE:CZ	1:B:131:ALA:HB2	2.56	0.41
1:D:95:ALA:HB2	1:D:159:MET:CE	2.49	0.41
1:L:138:ASP:N	1:L:138:ASP:OD1	2.50	0.41
1:A:124:PHE:HB3	1:A:125:PRO:CD	2.51	0.41
1:E:37:PHE:CZ	1:E:55:PHE:HD2	2.39	0.41
1:A:200:ILE:HD12	3:A:302:68O:CAN	2.50	0.41
1:D:124:PHE:HB3	1:D:125:PRO:CD	2.51	0.41
1:H:124:PHE:HB3	1:H:125:PRO:CD	2.51	0.41
1:F:138:ASP:OD1	1:F:138:ASP:N	2.53	0.40
1:I:177:LEU:HB3	1:I:182:VAL:HB	2.03	0.40
1:E:11:LEU:HD13	1:E:25:ALA:HB2	2.04	0.40
1:J:177:LEU:HB3	1:J:182:VAL:HB	2.03	0.40
1:G:124:PHE:HB3	1:G:125:PRO:CD	2.52	0.40
1:H:132:LEU:HB3	1:H:133:PRO:HD3	2.04	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	255/276 (92%)	241 (94%)	13 (5%)	1 (0%)	39	69
1	B	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	C	255/276 (92%)	241 (94%)	14 (6%)	0	100	100
1	D	255/276 (92%)	244 (96%)	11 (4%)	0	100	100
1	E	256/276 (93%)	244 (95%)	12 (5%)	0	100	100
1	F	256/276 (93%)	243 (95%)	13 (5%)	0	100	100
1	G	256/276 (93%)	242 (94%)	13 (5%)	1 (0%)	39	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	I	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	J	256/276 (93%)	245 (96%)	11 (4%)	0	100	100
1	K	256/276 (93%)	245 (96%)	11 (4%)	0	100	100
1	L	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
All	All	3065/3312 (92%)	2917 (95%)	146 (5%)	2 (0%)	56	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	202	SER
1	A	202	SER

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	195/209 (93%)	193 (99%)	2 (1%)	82	94
1	B	195/209 (93%)	194 (100%)	1 (0%)	92	98
1	C	195/209 (93%)	194 (100%)	1 (0%)	92	98
1	D	195/209 (93%)	194 (100%)	1 (0%)	92	98
1	E	196/209 (94%)	195 (100%)	1 (0%)	92	98
1	F	196/209 (94%)	194 (99%)	2 (1%)	82	94
1	G	196/209 (94%)	194 (99%)	2 (1%)	82	94
1	H	195/209 (93%)	194 (100%)	1 (0%)	92	98
1	I	195/209 (93%)	194 (100%)	1 (0%)	92	98
1	J	196/209 (94%)	193 (98%)	3 (2%)	72	91
1	K	196/209 (94%)	194 (99%)	2 (1%)	82	94
1	L	195/209 (93%)	191 (98%)	4 (2%)	61	87
All	All	2345/2508 (94%)	2324 (99%)	21 (1%)	84	95

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	136	SER
1	E	136	SER
1	H	43	ARG
1	C	258	MET
1	A	19	SER
1	A	136	SER
1	F	18	ARG
1	F	208	ASP
1	G	43	ARG
1	G	176	SER
1	D	47	ARG
1	I	137	ASP
1	K	42	ASP
1	K	258	MET
1	L	8	ARG
1	L	29	LYS
1	L	43	ARG
1	L	180	LYS
1	J	8	ARG
1	J	26	LYS
1	J	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	A	301	-	42,48,48	0.81	2 (4%)	46,73,73	0.96	1 (2%)
3	68O	A	302	-	19,19,19	1.15	1 (5%)	26,26,26	1.42	3 (11%)
2	NAD	B	301	-	42,48,48	0.81	2 (4%)	46,73,73	0.80	1 (2%)
3	68O	B	302	-	19,19,19	1.17	1 (5%)	26,26,26	1.40	3 (11%)
2	NAD	C	301	-	42,48,48	0.87	2 (4%)	46,73,73	0.85	1 (2%)
3	68O	C	302	-	19,19,19	1.29	2 (10%)	26,26,26	1.36	3 (11%)
2	NAD	D	301	-	42,48,48	0.80	2 (4%)	46,73,73	0.80	1 (2%)
3	68O	D	302	-	19,19,19	1.31	2 (10%)	26,26,26	1.48	5 (19%)
2	NAD	E	301	-	42,48,48	0.87	2 (4%)	46,73,73	0.82	1 (2%)
3	68O	E	302	-	19,19,19	1.15	2 (10%)	26,26,26	1.40	4 (15%)
2	NAD	F	301	-	42,48,48	0.87	2 (4%)	46,73,73	0.81	1 (2%)
3	68O	F	302	-	19,19,19	1.14	1 (5%)	26,26,26	1.45	3 (11%)
2	NAD	G	301	-	42,48,48	0.77	2 (4%)	46,73,73	0.76	1 (2%)
3	68O	G	302	-	19,19,19	1.16	1 (5%)	26,26,26	1.48	3 (11%)
2	NAD	H	301	-	42,48,48	0.90	2 (4%)	46,73,73	0.97	2 (4%)
3	68O	H	302	-	19,19,19	1.18	1 (5%)	26,26,26	1.45	3 (11%)
2	NAD	I	301	-	42,48,48	0.79	2 (4%)	46,73,73	0.86	1 (2%)
3	68O	I	302	-	19,19,19	1.12	1 (5%)	26,26,26	1.45	3 (11%)
2	NAD	J	301	-	42,48,48	0.87	2 (4%)	46,73,73	0.77	0
3	68O	J	302	-	19,19,19	1.15	1 (5%)	26,26,26	1.33	3 (11%)
2	NAD	K	301	-	42,48,48	0.85	2 (4%)	46,73,73	0.82	1 (2%)
3	68O	K	302	-	19,19,19	1.17	1 (5%)	26,26,26	1.74	7 (26%)
2	NAD	L	301	-	42,48,48	0.77	2 (4%)	46,73,73	0.81	1 (2%)
3	68O	L	302	-	19,19,19	1.11	1 (5%)	26,26,26	1.46	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	301	-	-	0/22/62/62	0/5/5/5
3	68O	A	302	-	-	0/6/6/6	0/2/2/2
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
3	68O	B	302	-	-	0/6/6/6	0/2/2/2
2	NAD	C	301	-	-	0/22/62/62	0/5/5/5
3	68O	C	302	-	-	0/6/6/6	0/2/2/2
2	NAD	D	301	-	-	0/22/62/62	0/5/5/5
3	68O	D	302	-	-	0/6/6/6	0/2/2/2
2	NAD	E	301	-	-	0/22/62/62	0/5/5/5
3	68O	E	302	-	-	0/6/6/6	0/2/2/2
2	NAD	F	301	-	-	0/22/62/62	0/5/5/5
3	68O	F	302	-	-	0/6/6/6	0/2/2/2
2	NAD	G	301	-	-	0/22/62/62	0/5/5/5
3	68O	G	302	-	-	0/6/6/6	0/2/2/2
2	NAD	H	301	-	-	0/22/62/62	0/5/5/5
3	68O	H	302	-	-	0/6/6/6	0/2/2/2
2	NAD	I	301	-	-	0/22/62/62	0/5/5/5
3	68O	I	302	-	-	0/6/6/6	0/2/2/2
2	NAD	J	301	-	-	0/22/62/62	0/5/5/5
3	68O	J	302	-	-	0/6/6/6	0/2/2/2
2	NAD	K	301	-	-	0/22/62/62	0/5/5/5
3	68O	K	302	-	-	0/6/6/6	0/2/2/2
2	NAD	L	301	-	-	0/22/62/62	0/5/5/5
3	68O	L	302	-	-	0/6/6/6	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	68O	CAK-CAP	-4.17	1.39	1.51
3	I	302	68O	CAK-CAP	-4.05	1.39	1.51
3	D	302	68O	CAK-CAP	-4.04	1.39	1.51
3	H	302	68O	CAK-CAP	-4.03	1.39	1.51
3	A	302	68O	CAK-CAP	-4.00	1.39	1.51
3	B	302	68O	CAK-CAP	-3.97	1.39	1.51
3	L	302	68O	CAK-CAP	-3.96	1.39	1.51
3	J	302	68O	CAK-CAP	-3.92	1.39	1.51
2	H	301	NAD	O4D-C1D	-3.86	1.35	1.41
3	F	302	68O	CAK-CAP	-3.86	1.39	1.51
3	E	302	68O	CAK-CAP	-3.75	1.40	1.51
3	K	302	68O	CAK-CAP	-3.72	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	68O	CAK-CAP	-3.70	1.40	1.51
2	F	301	NAD	O4D-C1D	-3.56	1.36	1.41
2	C	301	NAD	O4D-C1D	-3.34	1.36	1.41
2	E	301	NAD	O4D-C1D	-3.30	1.36	1.41
2	J	301	NAD	O4D-C1D	-3.08	1.36	1.41
3	C	302	68O	FAC-CAN	-2.95	1.28	1.35
2	K	301	NAD	O4D-C1D	-2.77	1.37	1.41
3	D	302	68O	FAC-CAN	-2.76	1.28	1.35
2	B	301	NAD	O4D-C1D	-2.72	1.37	1.41
2	A	301	NAD	O4D-C1D	-2.35	1.37	1.41
2	I	301	NAD	O4D-C1D	-2.33	1.37	1.41
2	G	301	NAD	O4D-C1D	-2.25	1.38	1.41
2	L	301	NAD	O4D-C1D	-2.23	1.38	1.41
2	D	301	NAD	O4D-C1D	-2.17	1.38	1.41
3	E	302	68O	FAC-CAN	-2.01	1.30	1.35
2	G	301	NAD	C2N-N1N	2.67	1.38	1.35
2	F	301	NAD	C2N-N1N	2.87	1.39	1.35
2	L	301	NAD	C2N-N1N	2.88	1.39	1.35
2	H	301	NAD	C2N-N1N	2.97	1.39	1.35
2	B	301	NAD	C2N-N1N	3.03	1.39	1.35
2	I	301	NAD	C2N-N1N	3.04	1.39	1.35
2	E	301	NAD	C2N-N1N	3.05	1.39	1.35
2	C	301	NAD	C2N-N1N	3.14	1.39	1.35
2	A	301	NAD	C2N-N1N	3.26	1.39	1.35
2	D	301	NAD	C2N-N1N	3.26	1.39	1.35
2	J	301	NAD	C2N-N1N	3.35	1.39	1.35
2	K	301	NAD	C2N-N1N	3.36	1.39	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C4B-O4B-C1B	-4.76	104.60	109.64
2	H	301	NAD	C4B-O4B-C1B	-4.64	104.72	109.64
2	I	301	NAD	C4B-O4B-C1B	-4.14	105.25	109.64
2	C	301	NAD	C4B-O4B-C1B	-4.10	105.30	109.64
2	F	301	NAD	C4B-O4B-C1B	-3.93	105.47	109.64
2	B	301	NAD	C4B-O4B-C1B	-3.83	105.58	109.64
2	L	301	NAD	C4B-O4B-C1B	-3.66	105.77	109.64
2	K	301	NAD	C4B-O4B-C1B	-3.61	105.82	109.64
2	G	301	NAD	C4B-O4B-C1B	-3.60	105.83	109.64
2	E	301	NAD	C4B-O4B-C1B	-3.50	105.94	109.64
2	D	301	NAD	C4B-O4B-C1B	-3.44	106.00	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	68O	CAJ-CAN-CAP	-3.24	120.04	124.19
3	L	302	68O	CAJ-CAN-CAP	-3.09	120.23	124.19
3	B	302	68O	CAJ-CAN-CAP	-2.96	120.40	124.19
3	I	302	68O	CAJ-CAN-CAP	-2.93	120.44	124.19
3	G	302	68O	CAJ-CAN-CAP	-2.91	120.46	124.19
3	H	302	68O	CAJ-CAN-CAP	-2.91	120.46	124.19
3	J	302	68O	CAJ-CAN-CAP	-2.87	120.51	124.19
3	A	302	68O	CAJ-CAN-CAP	-2.82	120.58	124.19
3	F	302	68O	CAJ-CAN-CAP	-2.80	120.61	124.19
3	E	302	68O	CAJ-CAN-CAP	-2.78	120.63	124.19
3	A	302	68O	OAL-CAR-CAO	-2.68	114.22	119.51
3	L	302	68O	OAL-CAR-CAO	-2.60	114.37	119.51
3	B	302	68O	OAL-CAR-CAO	-2.55	114.48	119.51
3	K	302	68O	CAQ-OAL-CAR	-2.54	111.48	117.84
3	I	302	68O	OAL-CAR-CAO	-2.52	114.54	119.51
3	C	302	68O	CAJ-CAN-CAP	-2.52	120.97	124.19
3	G	302	68O	OAL-CAR-CAO	-2.41	114.75	119.51
3	F	302	68O	OAL-CAR-CAO	-2.41	114.76	119.51
3	H	302	68O	OAL-CAR-CAO	-2.40	114.77	119.51
3	C	302	68O	OAL-CAR-CAO	-2.38	114.81	119.51
3	D	302	68O	OAL-CAR-CAO	-2.35	114.87	119.51
3	D	302	68O	CAJ-CAN-CAP	-2.35	121.19	124.19
3	E	302	68O	OAL-CAR-CAO	-2.34	114.89	119.51
3	K	302	68O	CAK-CAP-CAI	-2.31	114.85	119.53
2	H	301	NAD	O2D-C2D-C1D	-2.27	104.52	111.61
3	K	302	68O	OAL-CAR-CAO	-2.24	115.09	119.51
3	J	302	68O	OAL-CAR-CAO	-2.24	115.09	119.51
3	D	302	68O	CAM-CAI-CAP	-2.03	118.52	121.46
3	L	302	68O	FAC-CAN-CAP	2.02	120.89	117.92
3	D	302	68O	FAD-CAO-CAR	2.02	120.87	118.28
3	E	302	68O	FAC-CAN-CAP	2.19	121.14	117.92
3	K	302	68O	CAI-CAP-CAN	3.06	119.01	116.50
3	E	302	68O	CAI-CAP-CAN	3.40	119.29	116.50
3	K	302	68O	CAK-CAP-CAN	3.47	126.12	121.66
3	C	302	68O	CAI-CAP-CAN	3.54	119.41	116.50
3	K	302	68O	FAC-CAN-CAP	3.63	123.27	117.92
3	J	302	68O	CAI-CAP-CAN	3.78	119.60	116.50
3	F	302	68O	CAI-CAP-CAN	4.04	119.82	116.50
3	D	302	68O	CAI-CAP-CAN	4.05	119.83	116.50
3	A	302	68O	CAI-CAP-CAN	4.07	119.84	116.50
3	L	302	68O	CAI-CAP-CAN	4.11	119.88	116.50
3	H	302	68O	CAI-CAP-CAN	4.14	119.90	116.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	68O	CAI-CAP-CAN	4.15	119.91	116.50
3	I	302	68O	CAI-CAP-CAN	4.21	119.96	116.50
3	G	302	68O	CAI-CAP-CAN	4.38	120.10	116.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	3	0
3	A	302	68O	1	0
2	B	301	NAD	3	0
2	C	301	NAD	1	0
2	E	301	NAD	1	0
2	F	301	NAD	1	0
2	G	301	NAD	2	0
2	H	301	NAD	1	0
2	I	301	NAD	2	0
2	J	301	NAD	1	0
3	J	302	68O	1	0
2	K	301	NAD	2	0
2	L	301	NAD	1	0
3	L	302	68O	1	0

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	257/276 (93%)	1.88	97 (37%) 0 0	34, 50, 73, 150	0
1	B	257/276 (93%)	1.86	99 (38%) 0 0	38, 53, 76, 102	0
1	C	257/276 (93%)	2.41	141 (54%) 0 0	36, 55, 78, 127	0
1	D	257/276 (93%)	1.94	102 (39%) 0 0	31, 46, 63, 103	0
1	E	257/276 (93%)	2.34	132 (51%) 0 0	41, 55, 82, 121	0
1	F	257/276 (93%)	2.00	107 (41%) 0 0	33, 46, 69, 103	0
1	G	257/276 (93%)	1.87	104 (40%) 0 0	36, 49, 72, 97	0
1	H	257/276 (93%)	1.91	100 (38%) 0 0	40, 56, 78, 90	0
1	I	257/276 (93%)	1.71	83 (32%) 1 0	41, 52, 73, 93	0
1	J	257/276 (93%)	1.78	97 (37%) 0 0	39, 51, 70, 103	0
1	K	257/276 (93%)	1.78	89 (34%) 0 0	36, 50, 73, 108	0
1	L	257/276 (93%)	1.86	86 (33%) 0 0	42, 55, 80, 111	0
All	All	3084/3312 (93%)	1.94	1237 (40%) 0 0	31, 52, 75, 150	0

All (1237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	2	GLY	9.1
1	E	60	VAL	8.9
1	D	199	GLY	8.9
1	B	244	VAL	7.8
1	C	43	ARG	7.3
1	D	202	SER	7.1
1	F	244	VAL	6.9
1	E	69	ALA	6.9
1	L	150	GLU	6.9
1	F	100	ILE	6.8
1	H	244	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	K	150	GLU	6.5
1	K	244	VAL	6.5
1	E	244	VAL	6.4
1	A	244	VAL	6.4
1	A	243	GLU	6.4
1	F	243	GLU	6.4
1	B	242	ALA	6.3
1	A	258	MET	6.3
1	F	193	LYS	6.3
1	G	150	GLU	6.3
1	C	245	MET	6.3
1	D	244	VAL	6.2
1	E	186	ALA	6.2
1	E	104	PHE	6.2
1	G	244	VAL	6.2
1	G	245	MET	6.1
1	E	150	GLU	6.0
1	E	44	PHE	6.0
1	J	258	MET	6.0
1	D	150	GLU	6.0
1	A	245	MET	6.0
1	B	137	ASP	6.0
1	E	246	HIS	5.9
1	L	244	VAL	5.9
1	F	209	PHE	5.9
1	C	150	GLU	5.8
1	F	245	MET	5.8
1	E	188	SER	5.8
1	K	258	MET	5.8
1	E	57	SER	5.7
1	C	199	GLY	5.7
1	I	242	ALA	5.7
1	J	244	VAL	5.7
1	J	150	GLU	5.7
1	L	43	ARG	5.7
1	E	206	ILE	5.6
1	C	69	ALA	5.6
1	J	246	HIS	5.6
1	I	150	GLU	5.6
1	C	82	TRP	5.6
1	E	18	ARG	5.6
1	B	150	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	49	THR	5.5
1	H	167	GLU	5.5
1	B	149	ALA	5.5
1	B	245	MET	5.5
1	G	186	ALA	5.5
1	I	149	ALA	5.5
1	B	243	GLU	5.5
1	H	245	MET	5.5
1	D	245	MET	5.4
1	F	186	ALA	5.4
1	I	244	VAL	5.4
1	H	243	GLU	5.4
1	K	245	MET	5.4
1	I	44	PHE	5.4
1	E	243	GLU	5.3
1	D	200	ILE	5.3
1	L	82	TRP	5.3
1	C	207	LEU	5.3
1	A	213	ASN	5.3
1	G	243	GLU	5.2
1	H	150	GLU	5.2
1	E	200	ILE	5.2
1	C	202	SER	5.2
1	B	246	HIS	5.2
1	C	243	GLU	5.1
1	G	202	SER	5.1
1	I	167	GLU	5.1
1	A	150	GLU	5.1
1	J	242	ALA	5.1
1	C	100	ILE	5.1
1	L	245	MET	5.1
1	E	142	LEU	5.1
1	D	203	PHE	5.1
1	K	149	ALA	5.1
1	L	243	GLU	5.0
1	F	202	SER	5.0
1	C	59	LEU	5.0
1	C	99	ALA	5.0
1	G	164	ALA	5.0
1	C	51	PHE	5.0
1	D	188	SER	5.0
1	A	151	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	K	242	ALA	5.0
1	A	186	ALA	5.0
1	C	61	PHE	5.0
1	F	59	LEU	5.0
1	C	186	ALA	4.9
1	J	47	ARG	4.9
1	L	167	GLU	4.9
1	I	245	MET	4.9
1	H	242	ALA	4.9
1	K	164	ALA	4.9
1	L	149	ALA	4.9
1	D	187	ILE	4.9
1	K	168	ALA	4.9
1	E	203	PHE	4.9
1	C	244	VAL	4.9
1	D	201	LYS	4.9
1	B	186	ALA	4.9
1	A	43	ARG	4.8
1	C	171	ARG	4.8
1	F	102	GLY	4.8
1	L	145	SER	4.8
1	J	145	SER	4.8
1	J	245	MET	4.8
1	E	167	GLU	4.8
1	F	187	ILE	4.7
1	L	188	SER	4.7
1	B	167	GLU	4.7
1	C	246	HIS	4.7
1	L	189	ALA	4.7
1	H	151	ARG	4.7
1	C	102	GLY	4.7
1	L	187	ILE	4.7
1	C	145	SER	4.7
1	F	167	GLU	4.7
1	L	151	ARG	4.6
1	D	99	ALA	4.6
1	C	107	GLY	4.6
1	F	41	GLY	4.6
1	D	207	LEU	4.6
1	D	97	ARG	4.6
1	D	48	ILE	4.6
1	H	186	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	K	188	SER	4.6
1	D	167	GLU	4.6
1	E	25	ALA	4.5
1	J	203	PHE	4.5
1	J	243	GLU	4.5
1	F	47	ARG	4.5
1	E	45	LYS	4.5
1	F	99	ALA	4.5
1	L	164	ALA	4.5
1	I	246	HIS	4.5
1	E	48	ILE	4.5
1	E	189	ALA	4.5
1	H	130	ALA	4.5
1	I	43	ARG	4.5
1	F	101	ALA	4.5
1	F	50	GLU	4.5
1	K	246	HIS	4.5
1	G	167	GLU	4.4
1	D	186	ALA	4.4
1	I	186	ALA	4.4
1	C	155	ASN	4.4
1	E	209	PHE	4.4
1	A	149	ALA	4.4
1	L	171	ARG	4.4
1	J	151	ARG	4.4
1	L	258	MET	4.4
1	F	188	SER	4.4
1	C	208	ASP	4.4
1	I	168	ALA	4.4
1	H	188	SER	4.4
1	C	120	SER	4.4
1	E	207	LEU	4.4
1	A	147	LEU	4.4
1	C	80	THR	4.4
1	C	203	PHE	4.4
1	E	199	GLY	4.4
1	H	97	ARG	4.4
1	G	62	PRO	4.4
1	I	2	GLY	4.4
1	E	245	MET	4.3
1	G	185	ASN	4.3
1	E	197	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	197	ALA	4.3
1	D	211	GLU	4.3
1	H	164	ALA	4.3
1	C	44	PHE	4.3
1	C	188	SER	4.3
1	A	148	GLY	4.3
1	K	201	LYS	4.3
1	J	149	ALA	4.3
1	D	151	ARG	4.3
1	A	144	LEU	4.3
1	K	167	GLU	4.3
1	A	59	LEU	4.3
1	E	149	ALA	4.3
1	J	164	ALA	4.2
1	G	151	ARG	4.2
1	I	171	ARG	4.2
1	C	78	LEU	4.2
1	B	97	ARG	4.2
1	G	203	PHE	4.2
1	D	142	LEU	4.2
1	I	151	ARG	4.2
1	L	47	ARG	4.2
1	L	186	ALA	4.2
1	E	61	PHE	4.2
1	A	146	TYR	4.2
1	C	151	ARG	4.1
1	C	185	ASN	4.1
1	K	186	ALA	4.1
1	C	167	GLU	4.1
1	H	195	LEU	4.1
1	L	202	SER	4.1
1	A	197	ALA	4.1
1	B	102	GLY	4.1
1	H	185	ASN	4.1
1	J	166	LEU	4.1
1	C	40	VAL	4.1
1	J	188	SER	4.1
1	E	58	GLU	4.1
1	L	206	ILE	4.1
1	I	165	ALA	4.1
1	G	143	THR	4.1
1	B	151	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	97	ARG	4.0
1	G	246	HIS	4.0
1	H	48	ILE	4.0
1	E	220	VAL	4.0
1	A	167	GLU	4.0
1	H	205	LYS	4.0
1	A	252	ASN	4.0
1	A	41	GLY	4.0
1	D	171	ARG	4.0
1	L	162	ALA	4.0
1	H	246	HIS	4.0
1	B	211	GLU	4.0
1	K	243	GLU	4.0
1	G	240	VAL	4.0
1	F	189	ALA	4.0
1	C	81	HIS	4.0
1	F	150	GLU	4.0
1	F	151	ARG	4.0
1	L	184	VAL	4.0
1	H	149	ALA	4.0
1	J	162	ALA	4.0
1	E	185	ASN	4.0
1	C	71	ILE	4.0
1	E	164	ALA	4.0
1	H	165	ALA	4.0
1	J	146	TYR	4.0
1	C	157	ASN	4.0
1	L	246	HIS	4.0
1	K	207	LEU	4.0
1	G	149	ALA	4.0
1	I	39	TYR	4.0
1	H	240	VAL	4.0
1	A	145	SER	3.9
1	F	238	SER	3.9
1	G	188	SER	3.9
1	E	100	ILE	3.9
1	C	58	GLU	3.9
1	L	209	PHE	3.9
1	F	242	ALA	3.9
1	G	148	GLY	3.9
1	B	171	ARG	3.9
1	A	185	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	L	48	ILE	3.9
1	I	188	SER	3.9
1	H	171	ARG	3.9
1	D	185	ASN	3.9
1	B	145	SER	3.9
1	G	171	ARG	3.9
1	C	178	GLY	3.9
1	H	197	ALA	3.9
1	A	152	ALA	3.9
1	C	74	LEU	3.9
1	K	45	LYS	3.9
1	E	55	PHE	3.9
1	C	253	ALA	3.8
1	I	202	SER	3.8
1	L	15	LEU	3.8
1	E	139	ALA	3.8
1	K	165	ALA	3.8
1	K	35	LEU	3.8
1	L	170	VAL	3.8
1	I	148	GLY	3.8
1	B	185	ASN	3.8
1	E	20	ILE	3.8
1	D	243	GLU	3.8
1	I	145	SER	3.8
1	I	164	ALA	3.8
1	J	186	ALA	3.8
1	E	17	ASN	3.8
1	J	252	ASN	3.8
1	F	246	HIS	3.8
1	B	205	LYS	3.8
1	E	151	ARG	3.7
1	J	171	ARG	3.7
1	F	184	VAL	3.7
1	H	107	GLY	3.7
1	C	149	ALA	3.7
1	G	170	VAL	3.7
1	F	185	ASN	3.7
1	C	205	LYS	3.7
1	I	41	GLY	3.7
1	C	209	PHE	3.7
1	I	243	GLU	3.7
1	H	145	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	55	PHE	3.7
1	L	44	PHE	3.7
1	E	213	ASN	3.7
1	B	45	LYS	3.7
1	J	167	GLU	3.7
1	D	190	GLY	3.7
1	B	142	LEU	3.7
1	L	42	ASP	3.7
1	C	242	ALA	3.7
1	B	71	ILE	3.7
1	L	168	ALA	3.7
1	H	148	GLY	3.7
1	C	77	SER	3.7
1	D	43	ARG	3.6
1	I	97	ARG	3.6
1	D	246	HIS	3.6
1	C	168	ALA	3.6
1	F	107	GLY	3.6
1	C	258	MET	3.6
1	D	242	ALA	3.6
1	C	204	GLY	3.6
1	C	192	ILE	3.6
1	F	15	LEU	3.6
1	F	257	GLY	3.6
1	A	246	HIS	3.6
1	B	189	ALA	3.6
1	C	164	ALA	3.6
1	F	171	ARG	3.6
1	K	100	ILE	3.6
1	K	151	ARG	3.6
1	F	205	LYS	3.6
1	A	187	ILE	3.6
1	K	5	ASP	3.6
1	F	40	VAL	3.6
1	A	188	SER	3.6
1	C	239	GLY	3.6
1	J	165	ALA	3.6
1	E	202	SER	3.6
1	A	209	PHE	3.6
1	C	66	ALA	3.6
1	B	146	TYR	3.6
1	E	105	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	142	LEU	3.6
1	B	61	PHE	3.5
1	A	44	PHE	3.5
1	G	69	ALA	3.5
1	G	152	ALA	3.5
1	L	99	ALA	3.5
1	E	62	PRO	3.5
1	E	187	ILE	3.5
1	H	170	VAL	3.5
1	H	241	THR	3.5
1	C	142	LEU	3.5
1	E	51	PHE	3.5
1	D	137	ASP	3.5
1	L	212	SER	3.5
1	C	48	ILE	3.5
1	B	143	THR	3.5
1	E	32	GLY	3.5
1	G	87	GLY	3.5
1	I	172	TYR	3.5
1	E	42	ASP	3.5
1	B	168	ALA	3.5
1	H	187	ILE	3.5
1	E	4	LEU	3.5
1	C	135	LEU	3.5
1	C	64	ASP	3.5
1	F	203	PHE	3.5
1	L	36	ALA	3.5
1	K	47	ARG	3.5
1	E	41	GLY	3.5
1	A	93	GLY	3.5
1	L	166	LEU	3.5
1	L	148	GLY	3.5
1	I	187	ILE	3.5
1	H	208	ASP	3.5
1	F	177	LEU	3.5
1	C	156	TYR	3.5
1	D	256	GLY	3.5
1	L	201	LYS	3.5
1	E	12	THR	3.5
1	E	92	ILE	3.5
1	C	180	LYS	3.5
1	F	164	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	136	SER	3.5
1	E	40	VAL	3.5
1	B	207	LEU	3.5
1	C	128	ALA	3.4
1	C	252	ASN	3.4
1	B	165	ALA	3.4
1	H	146	TYR	3.4
1	C	138	ASP	3.4
1	E	211	GLU	3.4
1	J	255	VAL	3.4
1	B	148	GLY	3.4
1	B	239	GLY	3.4
1	D	145	SER	3.4
1	J	18	ARG	3.4
1	D	170	VAL	3.4
1	B	187	ILE	3.4
1	D	189	ALA	3.4
1	A	211	GLU	3.4
1	A	143	THR	3.4
1	F	212	SER	3.4
1	F	149	ALA	3.4
1	C	159	MET	3.4
1	F	146	TYR	3.4
1	B	193	LYS	3.4
1	A	142	LEU	3.4
1	I	82	TRP	3.4
1	K	82	TRP	3.4
1	K	171	ARG	3.4
1	A	168	ALA	3.4
1	J	35	LEU	3.4
1	F	37	PHE	3.4
1	E	253	ALA	3.4
1	H	76	ALA	3.4
1	E	102	GLY	3.4
1	C	97	ARG	3.4
1	C	194	THR	3.3
1	H	206	ILE	3.3
1	B	164	ALA	3.3
1	F	142	LEU	3.3
1	J	59	LEU	3.3
1	G	241	THR	3.3
1	L	241	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	75	PHE	3.3
1	D	61	PHE	3.3
1	H	258	MET	3.3
1	J	205	LYS	3.3
1	J	170	VAL	3.3
1	C	104	PHE	3.3
1	K	241	THR	3.3
1	D	155	ASN	3.3
1	H	6	GLY	3.3
1	K	253	ALA	3.3
1	L	242	ALA	3.3
1	A	247	VAL	3.3
1	F	240	VAL	3.3
1	E	99	ALA	3.3
1	D	253	ALA	3.3
1	L	205	LYS	3.3
1	H	169	SER	3.3
1	A	97	ARG	3.3
1	G	187	ILE	3.3
1	I	155	ASN	3.3
1	L	172	TYR	3.3
1	E	148	GLY	3.3
1	A	253	ALA	3.3
1	I	152	ALA	3.3
1	J	189	ALA	3.3
1	E	97	ARG	3.3
1	G	97	ARG	3.3
1	F	155	ASN	3.2
1	K	252	ASN	3.2
1	L	20	ILE	3.2
1	A	34	GLU	3.2
1	L	67	ASP	3.2
1	A	170	VAL	3.2
1	B	3	PHE	3.2
1	K	209	PHE	3.2
1	A	99	ALA	3.2
1	I	5	ASP	3.2
1	J	84	SER	3.2
1	D	206	ILE	3.2
1	E	52	ALA	3.2
1	A	242	ALA	3.2
1	E	205	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	142	LEU	3.2
1	K	59	LEU	3.2
1	J	82	TRP	3.2
1	J	163	LYS	3.2
1	E	258	MET	3.2
1	F	98	GLU	3.2
1	F	258	MET	3.2
1	E	165	ALA	3.2
1	C	42	ASP	3.2
1	C	53	ALA	3.2
1	G	242	ALA	3.2
1	E	59	LEU	3.2
1	H	144	LEU	3.2
1	L	87	GLY	3.2
1	G	53	ALA	3.2
1	B	107	GLY	3.2
1	G	157	ASN	3.2
1	F	168	ALA	3.2
1	F	207	LEU	3.2
1	L	199	GLY	3.2
1	J	199	GLY	3.2
1	C	201	LYS	3.2
1	K	187	ILE	3.2
1	A	171	ARG	3.2
1	G	194	THR	3.1
1	L	165	ALA	3.1
1	J	178	GLY	3.1
1	F	145	SER	3.1
1	L	125	PRO	3.1
1	J	46	ASP	3.1
1	J	209	PHE	3.1
1	C	101	ALA	3.1
1	C	257	GLY	3.1
1	D	100	ILE	3.1
1	J	78	LEU	3.1
1	J	202	SER	3.1
1	I	159	MET	3.1
1	I	201	LYS	3.1
1	A	257	GLY	3.1
1	F	18	ARG	3.1
1	C	39	TYR	3.1
1	B	252	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	168	ALA	3.1
1	E	242	ALA	3.1
1	K	9	ILE	3.1
1	A	64	ASP	3.1
1	E	170	VAL	3.1
1	H	184	VAL	3.1
1	E	152	ALA	3.1
1	A	212	SER	3.1
1	E	251	PHE	3.1
1	H	40	VAL	3.1
1	G	27	ALA	3.1
1	L	152	ALA	3.1
1	J	201	LYS	3.1
1	F	61	PHE	3.1
1	F	82	TRP	3.1
1	J	55	PHE	3.1
1	A	69	ALA	3.1
1	F	66	ALA	3.1
1	J	161	LEU	3.1
1	J	193	LYS	3.1
1	E	39	TYR	3.0
1	F	178	GLY	3.0
1	E	247	VAL	3.0
1	H	120	SER	3.0
1	A	137	ASP	3.0
1	F	42	ASP	3.0
1	B	48	ILE	3.0
1	C	200	ILE	3.0
1	B	2	GLY	3.0
1	E	38	THR	3.0
1	L	185	ASN	3.0
1	B	202	SER	3.0
1	I	42	ASP	3.0
1	I	142	LEU	3.0
1	E	252	ASN	3.0
1	I	258	MET	3.0
1	C	212	SER	3.0
1	F	106	ASP	3.0
1	C	41	GLY	3.0
1	F	113	PHE	3.0
1	K	146	TYR	3.0
1	J	44	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	63	CYS	3.0
1	C	177	LEU	3.0
1	G	85	LEU	3.0
1	J	168	ALA	3.0
1	F	190	GLY	3.0
1	J	102	GLY	3.0
1	A	92	ILE	3.0
1	C	8	ARG	3.0
1	K	145	SER	3.0
1	H	59	LEU	3.0
1	J	207	LEU	3.0
1	A	73	ALA	3.0
1	K	203	PHE	3.0
1	H	147	LEU	3.0
1	I	207	LEU	3.0
1	A	164	ALA	3.0
1	K	152	ALA	3.0
1	C	50	GLU	2.9
1	I	170	VAL	2.9
1	K	184	VAL	2.9
1	A	189	ALA	2.9
1	K	180	LYS	2.9
1	B	59	LEU	2.9
1	B	181	GLY	2.9
1	H	156	TYR	2.9
1	G	257	GLY	2.9
1	L	252	ASN	2.9
1	E	120	SER	2.9
1	J	43	ARG	2.9
1	D	254	VAL	2.9
1	B	223	GLU	2.9
1	I	211	GLU	2.9
1	J	208	ASP	2.9
1	L	26	LYS	2.9
1	C	189	ALA	2.9
1	C	37	PHE	2.9
1	A	37	PHE	2.9
1	K	94	PHE	2.9
1	D	59	LEU	2.9
1	K	154	PRO	2.9
1	K	155	ASN	2.9
1	B	43	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	187	ILE	2.9
1	L	55	PHE	2.9
1	C	141	LEU	2.9
1	G	233	LEU	2.9
1	K	240	VAL	2.9
1	I	208	ASP	2.9
1	C	2	GLY	2.9
1	F	206	ILE	2.9
1	C	241	THR	2.9
1	H	83	ASP	2.9
1	B	39	TYR	2.9
1	H	196	ALA	2.9
1	C	146	TYR	2.9
1	G	146	TYR	2.9
1	D	146	TYR	2.9
1	D	149	ALA	2.9
1	I	121	ALA	2.9
1	C	234	SER	2.8
1	D	234	SER	2.8
1	I	205	LYS	2.8
1	F	88	LEU	2.8
1	J	155	ASN	2.8
1	A	172	TYR	2.8
1	D	75	PHE	2.8
1	C	76	ALA	2.8
1	C	254	VAL	2.8
1	A	240	VAL	2.8
1	F	237	ALA	2.8
1	E	146	TYR	2.8
1	L	146	TYR	2.8
1	J	172	TYR	2.8
1	E	24	ILE	2.8
1	G	44	PHE	2.8
1	E	147	LEU	2.8
1	K	173	LEU	2.8
1	G	213	ASN	2.8
1	E	56	GLY	2.8
1	E	113	PHE	2.8
1	F	51	PHE	2.8
1	E	68	ASP	2.8
1	H	78	LEU	2.8
1	L	50	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	139	ALA	2.8
1	B	83	ASP	2.8
1	H	4	LEU	2.8
1	G	144	LEU	2.8
1	J	61	PHE	2.8
1	A	254	VAL	2.8
1	L	247	VAL	2.8
1	E	145	SER	2.8
1	H	202	SER	2.8
1	D	147	LEU	2.8
1	L	155	ASN	2.8
1	E	125	PRO	2.8
1	K	36	ALA	2.8
1	J	253	ALA	2.8
1	E	34	GLU	2.8
1	E	140	SER	2.8
1	K	223	GLU	2.8
1	F	200	ILE	2.8
1	L	200	ILE	2.8
1	E	190	GLY	2.8
1	B	221	THR	2.8
1	G	43	ARG	2.8
1	H	25	ALA	2.7
1	F	170	VAL	2.7
1	J	184	VAL	2.7
1	B	188	SER	2.7
1	L	5	ASP	2.7
1	E	22	TYR	2.7
1	D	156	TYR	2.7
1	L	11	LEU	2.7
1	H	19	SER	2.7
1	G	11	LEU	2.7
1	D	82	TRP	2.7
1	J	39	TYR	2.7
1	B	47	ARG	2.7
1	K	98	GLU	2.7
1	B	184	VAL	2.7
1	F	60	VAL	2.7
1	F	234	SER	2.7
1	D	91	SER	2.7
1	G	10	LEU	2.7
1	D	252	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	44	PHE	2.7
1	K	50	GLU	2.7
1	H	192	ILE	2.7
1	B	19	SER	2.7
1	F	247	VAL	2.7
1	G	58	GLU	2.7
1	H	203	PHE	2.7
1	D	205	LYS	2.7
1	D	143	THR	2.7
1	A	165	ALA	2.7
1	D	21	ALA	2.7
1	D	247	VAL	2.7
1	H	252	ASN	2.7
1	A	61	PHE	2.7
1	K	161	LEU	2.7
1	J	173	LEU	2.7
1	J	100	ILE	2.7
1	B	68	ASP	2.7
1	E	208	ASP	2.7
1	E	237	ALA	2.7
1	D	249	SER	2.7
1	I	60	VAL	2.7
1	E	201	LYS	2.7
1	H	209	PHE	2.7
1	I	37	PHE	2.7
1	K	144	LEU	2.7
1	F	241	THR	2.7
1	G	199	GLY	2.7
1	I	252	ASN	2.7
1	K	147	LEU	2.7
1	L	144	LEU	2.7
1	L	207	LEU	2.7
1	I	50	GLU	2.7
1	H	71	ILE	2.7
1	G	100	ILE	2.7
1	K	172	TYR	2.7
1	E	234	SER	2.7
1	A	190	GLY	2.6
1	E	210	VAL	2.6
1	L	182	VAL	2.6
1	B	219	ASN	2.6
1	A	195	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	251	PHE	2.6
1	E	171	ARG	2.6
1	B	172	TYR	2.6
1	E	64	ASP	2.6
1	C	68	ASP	2.6
1	K	137	ASP	2.6
1	I	123	SER	2.6
1	J	9	ILE	2.6
1	B	199	GLY	2.6
1	H	121	ALA	2.6
1	A	87	GLY	2.6
1	G	23	GLY	2.6
1	D	237	ALA	2.6
1	J	2	GLY	2.6
1	I	90	HIS	2.6
1	C	3	PHE	2.6
1	G	256	GLY	2.6
1	J	41	GLY	2.6
1	J	48	ILE	2.6
1	H	253	ALA	2.6
1	A	196	ALA	2.6
1	E	184	VAL	2.6
1	G	184	VAL	2.6
1	G	252	ASN	2.6
1	E	14	LEU	2.6
1	F	208	ASP	2.6
1	K	138	ASP	2.6
1	B	169	SER	2.6
1	C	136	SER	2.6
1	C	191	PRO	2.6
1	A	163	LYS	2.6
1	G	168	ALA	2.6
1	G	247	VAL	2.6
1	J	144	LEU	2.6
1	A	67	ASP	2.6
1	C	238	SER	2.6
1	G	6	GLY	2.6
1	I	238	SER	2.6
1	G	92	ILE	2.6
1	H	17	ASN	2.6
1	H	11	LEU	2.6
1	C	11	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	208	ASP	2.6
1	I	138	ASP	2.6
1	L	46	ASP	2.6
1	B	209	PHE	2.6
1	C	29	LYS	2.6
1	F	44	PHE	2.6
1	L	41	GLY	2.6
1	J	45	LYS	2.6
1	J	107	GLY	2.6
1	H	191	PRO	2.6
1	F	49	THR	2.6
1	L	143	THR	2.6
1	C	139	ALA	2.6
1	F	67	ASP	2.6
1	H	3	PHE	2.6
1	C	60	VAL	2.6
1	B	50	GLU	2.6
1	E	137[A]	ASP	2.6
1	C	13	GLY	2.6
1	F	2	GLY	2.6
1	D	37	PHE	2.6
1	F	43	ARG	2.6
1	G	19	SER	2.6
1	D	213	ASN	2.5
1	D	101	ALA	2.5
1	I	162	ALA	2.5
1	E	232	LEU	2.5
1	D	141	LEU	2.5
1	I	87	GLY	2.5
1	C	222	ILE	2.5
1	I	253	ALA	2.5
1	B	166	LEU	2.5
1	E	178	GLY	2.5
1	K	170	VAL	2.5
1	B	258	MET	2.5
1	H	198	SER	2.5
1	E	121	ALA	2.5
1	F	138	ASP	2.5
1	J	139	ALA	2.5
1	H	166	LEU	2.5
1	F	65	VAL	2.5
1	D	14	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	161	LEU	2.5
1	K	39	TYR	2.5
1	L	102	GLY	2.5
1	K	163	LYS	2.5
1	L	147	LEU	2.5
1	F	19	SER	2.5
1	G	219	ASN	2.5
1	L	253	ALA	2.5
1	J	187	ILE	2.5
1	F	13	GLY	2.5
1	B	233	LEU	2.5
1	E	141	LEU	2.5
1	H	161	LEU	2.5
1	C	144	LEU	2.5
1	D	4	LEU	2.5
1	J	65	VAL	2.5
1	J	147	LEU	2.5
1	L	169	SER	2.5
1	J	157	ASN	2.5
1	G	205	LYS	2.5
1	F	197	ALA	2.5
1	G	49	THR	2.5
1	G	165	ALA	2.5
1	G	207	LEU	2.5
1	B	247	VAL	2.5
1	D	94	PHE	2.5
1	D	136	SER	2.5
1	H	87	GLY	2.5
1	A	256	GLY	2.5
1	L	52	ALA	2.5
1	J	32	GLY	2.5
1	F	71	ILE	2.5
1	L	222	ILE	2.5
1	I	173	LEU	2.5
1	K	11	LEU	2.5
1	H	231	PHE	2.5
1	K	208	ASP	2.5
1	B	257	GLY	2.5
1	E	96	PRO	2.5
1	H	143	THR	2.5
1	C	115	ILE	2.5
1	B	144	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	45	LYS	2.5
1	A	184	VAL	2.5
1	I	169	SER	2.5
1	H	61	PHE	2.5
1	A	58	GLU	2.4
1	K	56	GLY	2.4
1	D	69	ALA	2.4
1	D	90	HIS	2.4
1	D	164	ALA	2.4
1	J	143	THR	2.4
1	E	153	ILE	2.4
1	E	192	ILE	2.4
1	F	192	ILE	2.4
1	G	74	LEU	2.4
1	J	15	LEU	2.4
1	H	247	VAL	2.4
1	J	251	PHE	2.4
1	C	83	ASP	2.4
1	E	256	GLY	2.4
1	C	121	ALA	2.4
1	F	139	ALA	2.4
1	G	99	ALA	2.4
1	I	36	ALA	2.4
1	J	33	ALA	2.4
1	F	147	LEU	2.4
1	D	144	LEU	2.4
1	G	136	SER	2.4
1	L	40	VAL	2.4
1	B	113	PHE	2.4
1	D	68	ASP	2.4
1	J	257	GLY	2.4
1	I	96	PRO	2.4
1	A	49	THR	2.4
1	A	130	ALA	2.4
1	E	10	LEU	2.4
1	E	166	LEU	2.4
1	B	82	TRP	2.4
1	E	86	ASP	2.4
1	D	87	GLY	2.4
1	B	117	HIS	2.4
1	B	237	ALA	2.4
1	E	161	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	152	ALA	2.4
1	H	249	SER	2.4
1	K	249	SER	2.4
1	B	44	PHE	2.4
1	H	41	GLY	2.4
1	F	104	PHE	2.4
1	D	44	PHE	2.4
1	I	185	ASN	2.4
1	D	257	GLY	2.4
1	I	209	PHE	2.4
1	A	39	TYR	2.4
1	B	96	PRO	2.4
1	A	154	PRO	2.4
1	F	62	PRO	2.4
1	B	152	ALA	2.4
1	C	228	ALA	2.4
1	A	63	CYS	2.4
1	A	201	LYS	2.4
1	A	166	LEU	2.4
1	F	73	ALA	2.4
1	F	211	GLU	2.4
1	G	45	LYS	2.4
1	I	53	ALA	2.4
1	K	205	LYS	2.4
1	I	200	ILE	2.4
1	L	9	ILE	2.4
1	J	169	SER	2.4
1	H	219	ASN	2.4
1	C	170	VAL	2.4
1	G	51	PHE	2.4
1	I	94	PHE	2.4
1	G	217	LYS	2.4
1	E	73	ALA	2.4
1	H	74	LEU	2.4
1	A	241	THR	2.4
1	G	76	ALA	2.4
1	F	16	SER	2.4
1	K	120	SER	2.4
1	A	51	PHE	2.4
1	G	254	VAL	2.4
1	K	247	VAL	2.4
1	J	210	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	45	LYS	2.4
1	D	47	ARG	2.4
1	F	154	PRO	2.4
1	B	141	LEU	2.4
1	B	232	LEU	2.4
1	H	216	LEU	2.4
1	E	235	ASP	2.4
1	H	77	SER	2.4
1	C	143	THR	2.4
1	G	73	ALA	2.4
1	G	237	ALA	2.4
1	G	239	GLY	2.4
1	K	48	ILE	2.4
1	K	160	GLY	2.4
1	C	113	PHE	2.4
1	F	94	PHE	2.4
1	D	225	VAL	2.4
1	K	22	TYR	2.3
1	E	132	LEU	2.3
1	H	189	ALA	2.3
1	A	249	SER	2.3
1	G	138[A]	ASP	2.3
1	I	49	THR	2.3
1	A	229	GLY	2.3
1	I	199	GLY	2.3
1	H	104	PHE	2.3
1	L	61	PHE	2.3
1	G	96	PRO	2.3
1	E	101	ALA	2.3
1	A	238	SER	2.3
1	F	131	ALA	2.3
1	E	155	ASN	2.3
1	C	47	ARG	2.3
1	F	58	GLU	2.3
1	G	98	GLU	2.3
1	C	92	ILE	2.3
1	I	255	VAL	2.3
1	J	51	PHE	2.3
1	C	34	GLU	2.3
1	C	233	LEU	2.3
1	G	160	GLY	2.3
1	B	49	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	49	THR	2.3
1	L	18	ARG	2.3
1	A	153	ILE	2.3
1	K	222	ILE	2.3
1	B	203	PHE	2.3
1	E	163	LYS	2.3
1	H	180	LYS	2.3
1	C	184	VAL	2.3
1	H	133	PRO	2.3
1	H	137	ASP	2.3
1	H	215	PRO	2.3
1	C	15	LEU	2.3
1	J	13	GLY	2.3
1	C	73	ALA	2.3
1	J	185	ASN	2.3
1	C	193	LYS	2.3
1	B	60	VAL	2.3
1	I	184	VAL	2.3
1	K	89	VAL	2.3
1	F	239	GLY	2.3
1	C	112	ASN	2.3
1	C	165	ALA	2.3
1	C	219	ASN	2.3
1	G	39	TYR	2.3
1	H	92	ILE	2.3
1	J	247	VAL	2.3
1	J	72	ASP	2.3
1	B	11	LEU	2.3
1	C	85	LEU	2.3
1	D	81	HIS	2.3
1	J	14	LEU	2.3
1	B	253	ALA	2.3
1	I	143	THR	2.3
1	J	126	ALA	2.3
1	E	71	ILE	2.3
1	D	92	ILE	2.3
1	E	240	VAL	2.3
1	J	254	VAL	2.3
1	L	208	ASP	2.3
1	H	160	GLY	2.3
1	B	161	LEU	2.3
1	E	249	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	238	SER	2.3
1	J	213	ASN	2.3
1	A	76	ALA	2.3
1	F	39	TYR	2.3
1	E	222	ILE	2.3
1	G	209	PHE	2.3
1	C	5	ASP	2.3
1	L	89	VAL	2.3
1	H	234	SER	2.2
1	G	145	SER	2.2
1	C	147	LEU	2.2
1	K	14	LEU	2.2
1	G	34	GLU	2.2
1	J	50	GLU	2.2
1	I	63	CYS	2.2
1	B	20	ILE	2.2
1	C	9	ILE	2.2
1	K	55	PHE	2.2
1	A	160	GLY	2.2
1	E	15	LEU	2.2
1	F	117	HIS	2.2
1	D	62	PRO	2.2
1	I	120	SER	2.2
1	G	147	LEU	2.2
1	I	127	LEU	2.2
1	K	62	PRO	2.2
1	B	159	MET	2.2
1	D	129	LYS	2.2
1	H	39	TYR	2.2
1	B	93	GLY	2.2
1	B	153	ILE	2.2
1	I	247	VAL	2.2
1	F	140	SER	2.2
1	F	180	LYS	2.2
1	I	141	LEU	2.2
1	C	114	ARG	2.2
1	B	76	ALA	2.2
1	E	53	ALA	2.2
1	H	168	ALA	2.2
1	F	53	ALA	2.2
1	G	189	ALA	2.2
1	G	41	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	107	GLY	2.2
1	H	217	LYS	2.2
1	J	79	LYS	2.2
1	G	120	SER	2.2
1	D	57	SER	2.2
1	C	161	LEU	2.2
1	A	105	LEU	2.2
1	D	132	LEU	2.2
1	A	2	GLY	2.2
1	G	193	LYS	2.2
1	A	225	VAL	2.2
1	D	60	VAL	2.2
1	L	19	SER	2.2
1	E	191	PRO	2.2
1	C	36	ALA	2.2
1	H	194	THR	2.2
1	F	70	GLN	2.2
1	K	159	MET	2.2
1	C	75	PHE	2.2
1	D	39	TYR	2.2
1	J	124	PHE	2.2
1	B	238	SER	2.2
1	H	213	ASN	2.2
1	C	17	ASN	2.2
1	A	100	ILE	2.2
1	D	220	VAL	2.2
1	E	144	LEU	2.2
1	L	232	LEU	2.2
1	B	158	THR	2.2
1	B	190	GLY	2.2
1	C	65	VAL	2.2
1	C	88	LEU	2.2
1	L	163	LYS	2.2
1	L	173	LEU	2.2
1	J	70	GLN	2.2
1	A	83	ASP	2.2
1	G	208	ASP	2.2
1	H	82	TRP	2.2
1	G	121	ALA	2.2
1	G	258	MET	2.2
1	K	43	ARG	2.2
1	B	26	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	172	TYR	2.1
1	A	19	SER	2.1
1	H	211	GLU	2.1
1	G	40	VAL	2.1
1	D	58	GLU	2.1
1	A	117	HIS	2.1
1	D	125	PRO	2.1
1	J	117	HIS	2.1
1	C	152	ALA	2.1
1	F	52	ALA	2.1
1	G	82	TRP	2.1
1	K	97	ARG	2.1
1	K	121	ALA	2.1
1	J	152	ALA	2.1
1	F	80	THR	2.1
1	B	104	PHE	2.1
1	E	65	VAL	2.1
1	C	255	VAL	2.1
1	B	178	GLY	2.1
1	I	137	ASP	2.1
1	F	69	ALA	2.1
1	G	174	ALA	2.1
1	G	221	THR	2.1
1	D	80	THR	2.1
1	B	65	VAL	2.1
1	A	206	ILE	2.1
1	F	48	ILE	2.1
1	L	92	ILE	2.1
1	J	71	ILE	2.1
1	B	90	HIS	2.1
1	D	138	ASP	2.1
1	I	239	GLY	2.1
1	A	121	ALA	2.1
1	D	12	THR	2.1
1	B	4	LEU	2.1
1	C	195	LEU	2.1
1	F	135	LEU	2.1
1	F	141	LEU	2.1
1	D	65	VAL	2.1
1	I	92	ILE	2.1
1	L	191	PRO	2.1
1	E	50	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	26	LYS	2.1
1	L	238	SER	2.1
1	E	83	ASP	2.1
1	D	42	ASP	2.1
1	H	232	LEU	2.1
1	G	65	VAL	2.1
1	G	232	LEU	2.1
1	D	98	GLU	2.1
1	A	221	THR	2.1
1	A	248	ASP	2.1
1	B	15	LEU	2.1
1	B	78	LEU	2.1
1	B	236	LEU	2.1
1	C	89	VAL	2.1
1	F	89	VAL	2.1
1	F	233	LEU	2.1
1	K	254	VAL	2.1
1	E	228	ALA	2.1
1	G	66	ALA	2.1
1	G	253	ALA	2.1
1	K	126	ALA	2.1
1	C	18	ARG	2.1
1	D	158	THR	2.1
1	D	241	THR	2.1
1	J	49	THR	2.1
1	E	46	ASP	2.1
1	G	42	ASP	2.1
1	D	124	PHE	2.1
1	J	148	GLY	2.1
1	J	190	GLY	2.1
1	B	147	LEU	2.1
1	C	236	LEU	2.1
1	K	15	LEU	2.1
1	I	22	TYR	2.1
1	A	228	ALA	2.1
1	A	50	GLU	2.1
1	G	83	ASP	2.1
1	D	251	PHE	2.1
1	K	51	PHE	2.1
1	K	124	PHE	2.1
1	L	6	GLY	2.1
1	A	88	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	108	LEU	2.0
1	G	90	HIS	2.0
1	K	90	HIS	2.0
1	K	217	LYS	2.0
1	A	115	ILE	2.0
1	C	33	ALA	2.0
1	C	111	GLU	2.0
1	G	126	ALA	2.0
1	H	190	GLY	2.0
1	G	231	PHE	2.0
1	D	209	PHE	2.0
1	B	14	LEU	2.0
1	L	59	LEU	2.0
1	J	11	LEU	2.0
1	E	81	HIS	2.0
1	G	182	VAL	2.0
1	D	71	ILE	2.0
1	E	98	GLU	2.0
1	K	157	ASN	2.0
1	K	185	ASN	2.0
1	G	72	ASP	2.0
1	G	201	LYS	2.0
1	D	16	SER	2.0
1	I	56	GLY	2.0
1	I	204	GLY	2.0
1	K	87	GLY	2.0
1	K	169	SER	2.0
1	H	251	PHE	2.0
1	D	159	MET	2.0
1	E	133	PRO	2.0
1	D	40	VAL	2.0
1	E	180	LYS	2.0
1	C	22	TYR	2.0
1	I	146	TYR	2.0
1	E	6	GLY	2.0
1	C	250	GLY	2.0
1	K	101	ALA	2.0
1	A	136	SER	2.0
1	F	120	SER	2.0
1	I	140	SER	2.0
1	H	12	THR	2.0
1	H	80	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	134	MET	2.0
1	D	104	PHE	2.0
1	K	104	PHE	2.0
1	A	232	LEU	2.0
1	J	142	LEU	2.0
1	E	89	VAL	2.0
1	C	182	VAL	2.0
1	I	154	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	68O	L	302	18/18	0.85	0.39	1.10	53,54,64,65	0
3	68O	I	302	18/18	0.83	0.34	1.01	48,51,61,61	0
3	68O	K	302	18/18	0.84	0.34	0.50	46,47,56,57	0
3	68O	H	302	18/18	0.84	0.35	0.36	42,44,52,53	0
3	68O	F	302	18/18	0.80	0.35	0.11	47,47,57,57	0
3	68O	J	302	18/18	0.90	0.30	-0.03	46,48,58,58	0
3	68O	C	302	18/18	0.76	0.36	-0.21	49,51,61,61	0
3	68O	G	302	18/18	0.90	0.30	-0.28	39,43,52,53	0
3	68O	E	302	18/18	0.82	0.33	-0.35	56,57,69,69	0
2	NAD	I	301	44/44	0.83	0.26	-0.43	44,53,65,65	0
3	68O	D	302	18/18	0.90	0.30	-0.51	40,43,52,53	0
2	NAD	B	301	44/44	0.81	0.28	-0.61	44,50,60,62	0
2	NAD	H	301	44/44	0.81	0.29	-0.63	45,58,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAD	K	301	44/44	0.84	0.25	-0.64	42,51,63,65	0
3	68O	B	302	18/18	0.91	0.27	-0.69	48,49,59,60	0
2	NAD	G	301	44/44	0.83	0.27	-0.70	39,51,71,73	0
2	NAD	J	301	44/44	0.85	0.26	-0.73	50,55,66,69	0
2	NAD	E	301	44/44	0.70	0.27	-0.79	48,54,67,81	0
2	NAD	F	301	44/44	0.81	0.26	-0.80	40,48,58,61	0
2	NAD	A	301	44/44	0.82	0.27	-0.91	46,51,61,63	0
2	NAD	L	301	44/44	0.85	0.23	-1.00	52,55,67,68	0
2	NAD	D	301	44/44	0.83	0.25	-1.00	36,48,58,58	0
2	NAD	C	301	44/44	0.80	0.27	-1.07	44,54,66,67	0
3	68O	A	302	18/18	0.91	0.26	-1.15	43,48,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.