wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:52 AM GMT

PDB ID	:	3Q2K
Title	:	Crystal structure of the WlbA dehydrogenase from Bordetella pertussis in complex with NADH and UDP-GlcNAcA
Authors	:	Holden, H.M.; Thoden, J.B.
Deposited on	:	2010-12-20
Resolution	:	2.13 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

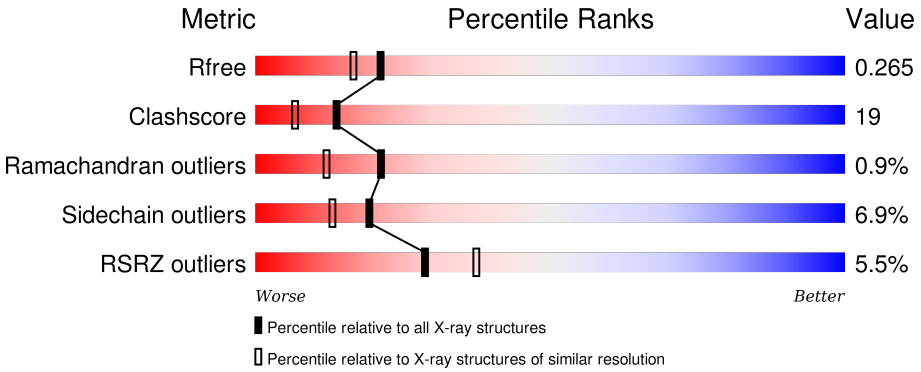
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.13 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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 <=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	370	2% 71% 20% • 6%
1	B	370	5% 58% 26% 5% 11%
1	C	370	2% 72% 19% • 6%
1	D	370	6% 64% 25% • 7%
1	E	370	9% 52% 31% • 13%

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Mol	Chain	Length	Quality of chain
1	F	370	7% 62% 23% 12%
1	G	370	% 67% 22% 8%
1	H	370	3% 64% 25% 8%
1	I	370	6% 66% 21% 8%
1	J	370	8% 64% 26% 6%
1	K	370	5% 57% 26% 13%
1	L	370	11% 54% 26% 7% 13%
1	M	370	2% 67% 23% 6%
1	N	370	5% 66% 21% 8%
1	O	370	2% 64% 24% 10%
1	P	370	5% 58% 25% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43985 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 oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	B	329	Total	C	N	O	S	0	2	0
			2587	1625	476	474	12			
1	C	347	Total	C	N	O	S	0	0	0
			2712	1702	493	505	12			
1	D	343	Total	C	N	O	S	0	1	0
			2693	1689	492	500	12			
1	E	321	Total	C	N	O	S	0	0	0
			2501	1572	457	460	12			
1	F	327	Total	C	N	O	S	0	0	0
			2552	1600	468	472	12			
1	G	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	H	342	Total	C	N	O	S	0	1	0
			2681	1684	488	497	12			
1	I	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	J	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	K	322	Total	C	N	O	S	0	0	0
			2511	1577	461	461	12			
1	L	321	Total	C	N	O	S	0	1	0
			2514	1579	463	460	12			
1	M	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	N	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	O	334	Total	C	N	O	S	0	0	0
			2610	1637	479	482	12			
1	P	322	Total	C	N	O	S	0	0	0
			2511	1577	461	461	12			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q79H45
A	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
A	-17	SER	-	EXPRESSION TAG	UNP Q79H45
A	-16	SER	-	EXPRESSION TAG	UNP Q79H45
A	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-9	SER	-	EXPRESSION TAG	UNP Q79H45
A	-8	SER	-	EXPRESSION TAG	UNP Q79H45
A	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
A	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
A	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
A	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
A	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
A	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
A	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
A	0	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-19	MET	-	EXPRESSION TAG	UNP Q79H45
B	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
B	-17	SER	-	EXPRESSION TAG	UNP Q79H45
B	-16	SER	-	EXPRESSION TAG	UNP Q79H45
B	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-9	SER	-	EXPRESSION TAG	UNP Q79H45
B	-8	SER	-	EXPRESSION TAG	UNP Q79H45
B	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
B	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
B	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
B	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
B	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
B	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
B	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
B	0	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-19	MET	-	EXPRESSION TAG	UNP Q79H45
C	-18	GLY	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	EXPRESSION TAG	UNP Q79H45
C	-16	SER	-	EXPRESSION TAG	UNP Q79H45
C	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-9	SER	-	EXPRESSION TAG	UNP Q79H45
C	-8	SER	-	EXPRESSION TAG	UNP Q79H45
C	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
C	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
C	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
C	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
C	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
C	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
C	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
C	0	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-19	MET	-	EXPRESSION TAG	UNP Q79H45
D	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
D	-17	SER	-	EXPRESSION TAG	UNP Q79H45
D	-16	SER	-	EXPRESSION TAG	UNP Q79H45
D	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-9	SER	-	EXPRESSION TAG	UNP Q79H45
D	-8	SER	-	EXPRESSION TAG	UNP Q79H45
D	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
D	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
D	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
D	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
D	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
D	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
D	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
D	0	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-19	MET	-	EXPRESSION TAG	UNP Q79H45
E	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
E	-17	SER	-	EXPRESSION TAG	UNP Q79H45
E	-16	SER	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-9	SER	-	EXPRESSION TAG	UNP Q79H45
E	-8	SER	-	EXPRESSION TAG	UNP Q79H45
E	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
E	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
E	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
E	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
E	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
E	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
E	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
E	0	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-19	MET	-	EXPRESSION TAG	UNP Q79H45
F	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
F	-17	SER	-	EXPRESSION TAG	UNP Q79H45
F	-16	SER	-	EXPRESSION TAG	UNP Q79H45
F	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-9	SER	-	EXPRESSION TAG	UNP Q79H45
F	-8	SER	-	EXPRESSION TAG	UNP Q79H45
F	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
F	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
F	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
F	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
F	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
F	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
F	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
F	0	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-19	MET	-	EXPRESSION TAG	UNP Q79H45
G	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
G	-17	SER	-	EXPRESSION TAG	UNP Q79H45
G	-16	SER	-	EXPRESSION TAG	UNP Q79H45
G	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-14	HIS	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-9	SER	-	EXPRESSION TAG	UNP Q79H45
G	-8	SER	-	EXPRESSION TAG	UNP Q79H45
G	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
G	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
G	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
G	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
G	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
G	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
G	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
G	0	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-19	MET	-	EXPRESSION TAG	UNP Q79H45
H	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
H	-17	SER	-	EXPRESSION TAG	UNP Q79H45
H	-16	SER	-	EXPRESSION TAG	UNP Q79H45
H	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-9	SER	-	EXPRESSION TAG	UNP Q79H45
H	-8	SER	-	EXPRESSION TAG	UNP Q79H45
H	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
H	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
H	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
H	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
H	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
H	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
H	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
H	0	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-19	MET	-	EXPRESSION TAG	UNP Q79H45
I	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
I	-17	SER	-	EXPRESSION TAG	UNP Q79H45
I	-16	SER	-	EXPRESSION TAG	UNP Q79H45
I	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-12	HIS	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-9	SER	-	EXPRESSION TAG	UNP Q79H45
I	-8	SER	-	EXPRESSION TAG	UNP Q79H45
I	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
I	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
I	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
I	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
I	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
I	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
I	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
I	0	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-19	MET	-	EXPRESSION TAG	UNP Q79H45
J	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
J	-17	SER	-	EXPRESSION TAG	UNP Q79H45
J	-16	SER	-	EXPRESSION TAG	UNP Q79H45
J	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-9	SER	-	EXPRESSION TAG	UNP Q79H45
J	-8	SER	-	EXPRESSION TAG	UNP Q79H45
J	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
J	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
J	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
J	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
J	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
J	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
J	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
J	0	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-19	MET	-	EXPRESSION TAG	UNP Q79H45
K	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
K	-17	SER	-	EXPRESSION TAG	UNP Q79H45
K	-16	SER	-	EXPRESSION TAG	UNP Q79H45
K	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-10	HIS	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	EXPRESSION TAG	UNP Q79H45
K	-8	SER	-	EXPRESSION TAG	UNP Q79H45
K	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
K	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
K	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
K	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
K	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
K	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
K	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
K	0	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-19	MET	-	EXPRESSION TAG	UNP Q79H45
L	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
L	-17	SER	-	EXPRESSION TAG	UNP Q79H45
L	-16	SER	-	EXPRESSION TAG	UNP Q79H45
L	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-9	SER	-	EXPRESSION TAG	UNP Q79H45
L	-8	SER	-	EXPRESSION TAG	UNP Q79H45
L	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
L	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
L	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
L	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
L	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
L	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
L	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
L	0	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-19	MET	-	EXPRESSION TAG	UNP Q79H45
M	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
M	-17	SER	-	EXPRESSION TAG	UNP Q79H45
M	-16	SER	-	EXPRESSION TAG	UNP Q79H45
M	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-9	SER	-	EXPRESSION TAG	UNP Q79H45
M	-8	SER	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
M	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
M	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
M	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
M	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
M	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
M	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
M	0	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-19	MET	-	EXPRESSION TAG	UNP Q79H45
N	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
N	-17	SER	-	EXPRESSION TAG	UNP Q79H45
N	-16	SER	-	EXPRESSION TAG	UNP Q79H45
N	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-9	SER	-	EXPRESSION TAG	UNP Q79H45
N	-8	SER	-	EXPRESSION TAG	UNP Q79H45
N	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
N	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
N	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
N	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
N	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
N	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
N	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
N	0	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-19	MET	-	EXPRESSION TAG	UNP Q79H45
O	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
O	-17	SER	-	EXPRESSION TAG	UNP Q79H45
O	-16	SER	-	EXPRESSION TAG	UNP Q79H45
O	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-9	SER	-	EXPRESSION TAG	UNP Q79H45
O	-8	SER	-	EXPRESSION TAG	UNP Q79H45
O	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
O	-6	ASN	-	EXPRESSION TAG	UNP Q79H45

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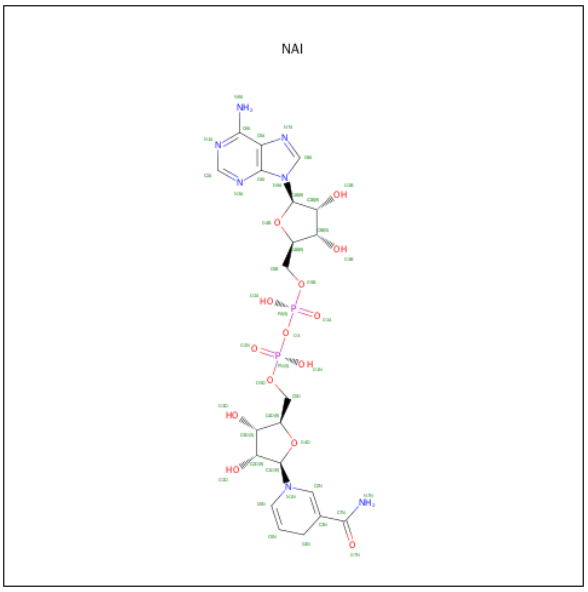
Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
O	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
O	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
O	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
O	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
O	0	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-19	MET	-	EXPRESSION TAG	UNP Q79H45
P	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
P	-17	SER	-	EXPRESSION TAG	UNP Q79H45
P	-16	SER	-	EXPRESSION TAG	UNP Q79H45
P	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-9	SER	-	EXPRESSION TAG	UNP Q79H45
P	-8	SER	-	EXPRESSION TAG	UNP Q79H45
P	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
P	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
P	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
P	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
P	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
P	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
P	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
P	0	HIS	-	EXPRESSION TAG	UNP Q79H45

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	N	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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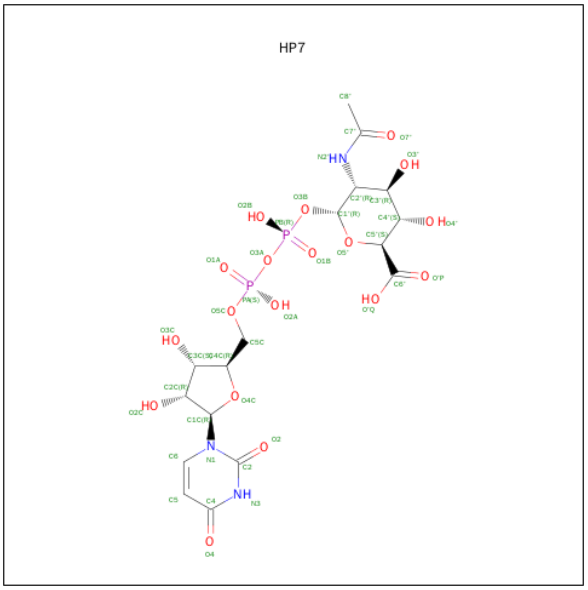
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2S,3S,4R,5R,6R)-5-ACETAMIDO-6-[[[(2R,3S,4R,5R)-5-(2,4-DIOXOPYRIMIDIN-1-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL]OXY-HYDROXY-PHOSPHORYL]OXY-3,4-DIHYDROXY-OXANE-2-CARBOXYLIC ACID (three-letter code: HP7) (formula: $C_{17}H_{25}N_3O_{18}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	B	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	C	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	D	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	E	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	F	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	G	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	H	1	Total	C	N	O	P	0	0
			40	17	3	18	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	I	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	J	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	K	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	L	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	M	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	N	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	O	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	P	1	Total	C	N	O	P	0	0
			40	17	3	18	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	54	Total	O	0	0
			54	54		
4	C	58	Total	O	0	0
			58	58		
4	D	51	Total	O	0	0
			51	51		
4	E	21	Total	O	0	0
			21	21		
4	F	24	Total	O	0	0
			24	24		
4	G	49	Total	O	0	0
			49	49		
4	H	35	Total	O	0	0
			35	35		
4	I	36	Total	O	0	0
			36	36		
4	J	30	Total	O	0	0
			30	30		
4	K	26	Total	O	0	0
			26	26		

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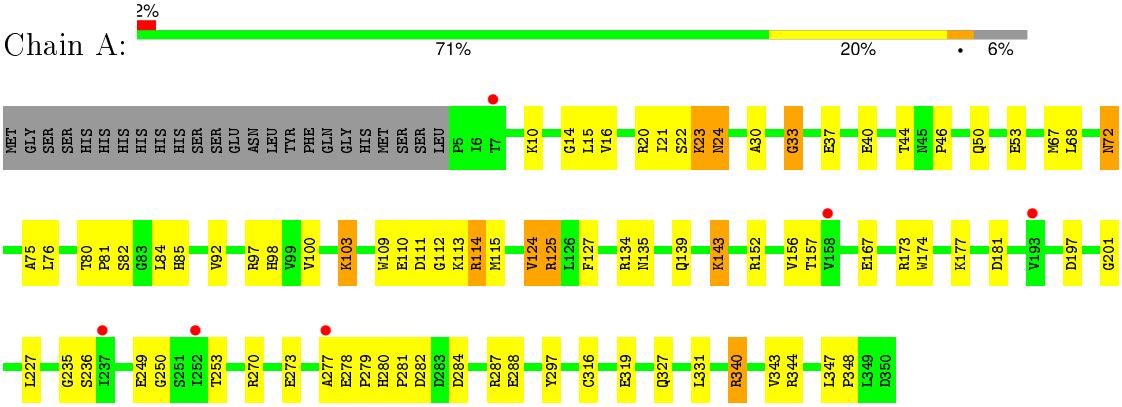
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	37	Total O 37 37	0	0
4	M	36	Total O 36 36	0	0
4	N	34	Total O 34 34	0	0
4	O	17	Total O 17 17	0	0
4	P	24	Total O 24 24	0	0

3 Residue-property plots (i)

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.

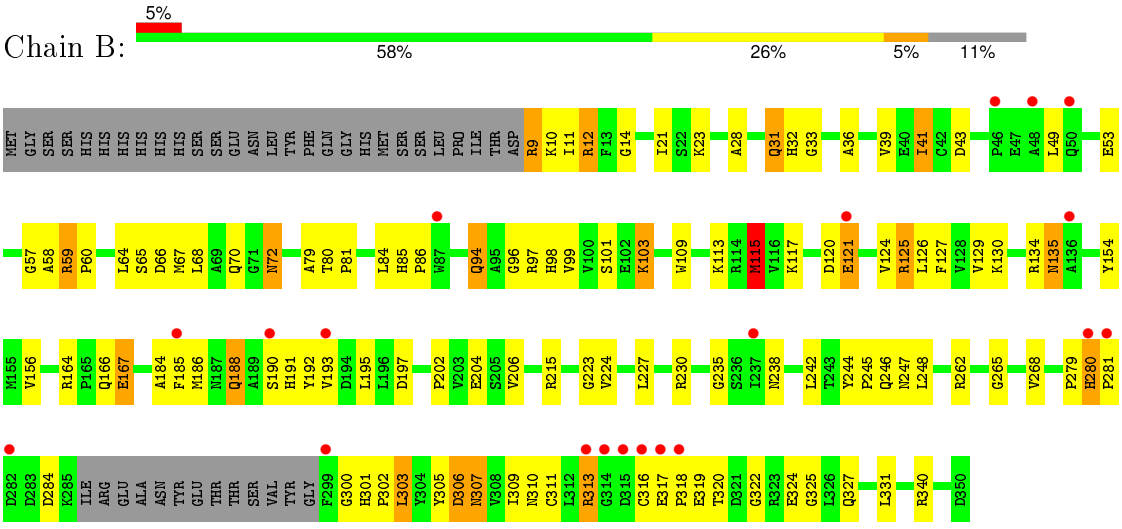
- Molecule 1: oxidoreductase

Chain A:



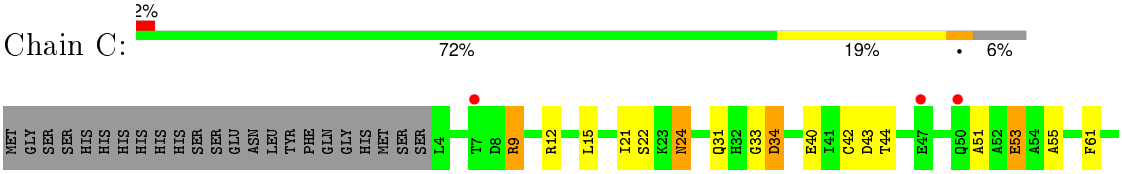
- Molecule 1: oxidoreductase

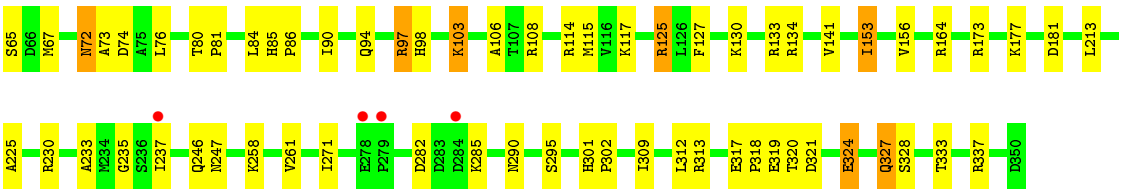
Chain B:



- Molecule 1: oxidoreductase

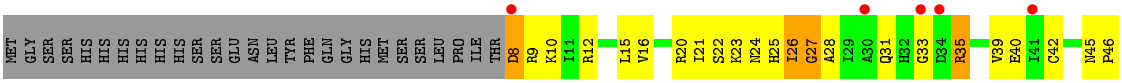
Chain C:

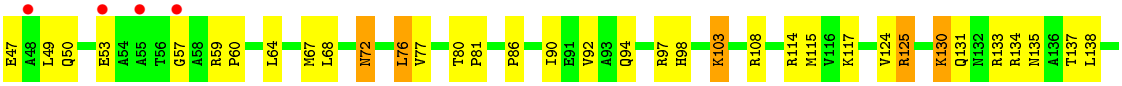


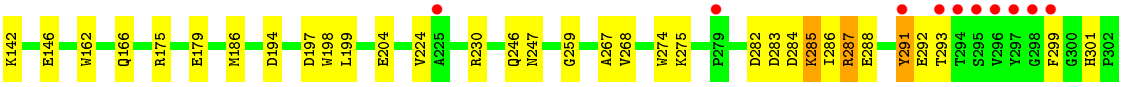


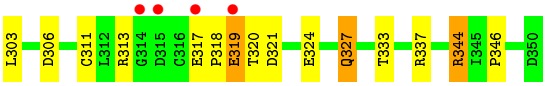
• Molecule 1: oxidoreductase

Chain D:



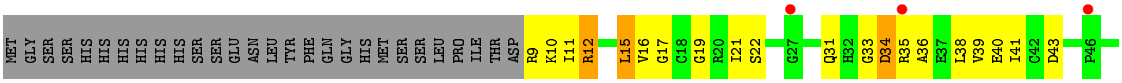


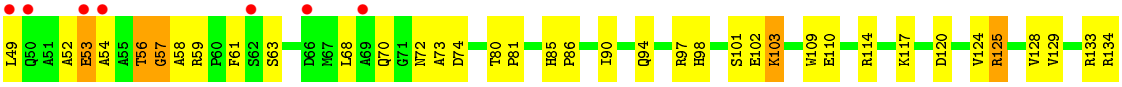


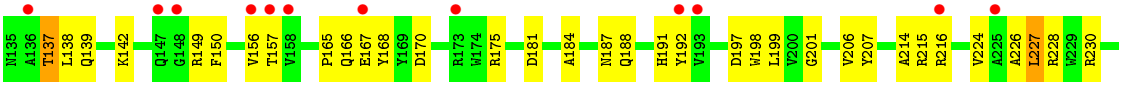


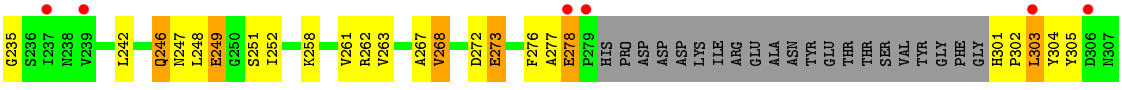
• Molecule 1: oxidoreductase

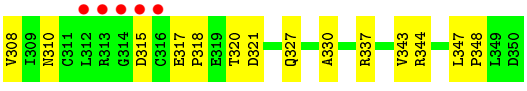
Chain E:





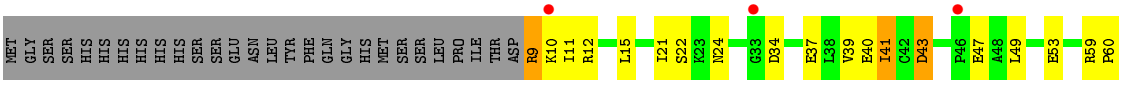


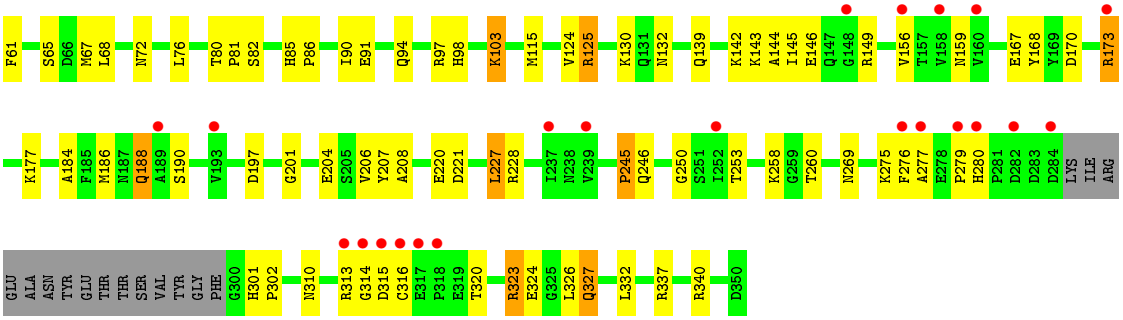




• Molecule 1: oxidoreductase

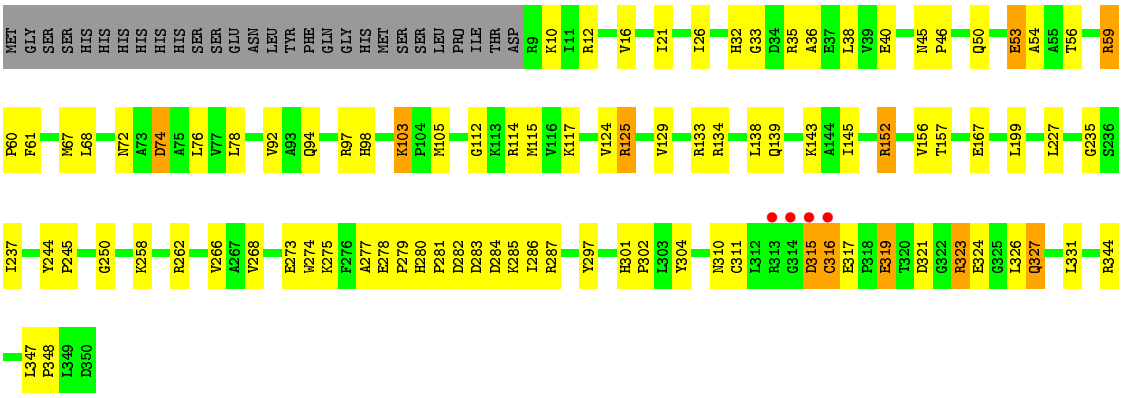
Chain F:





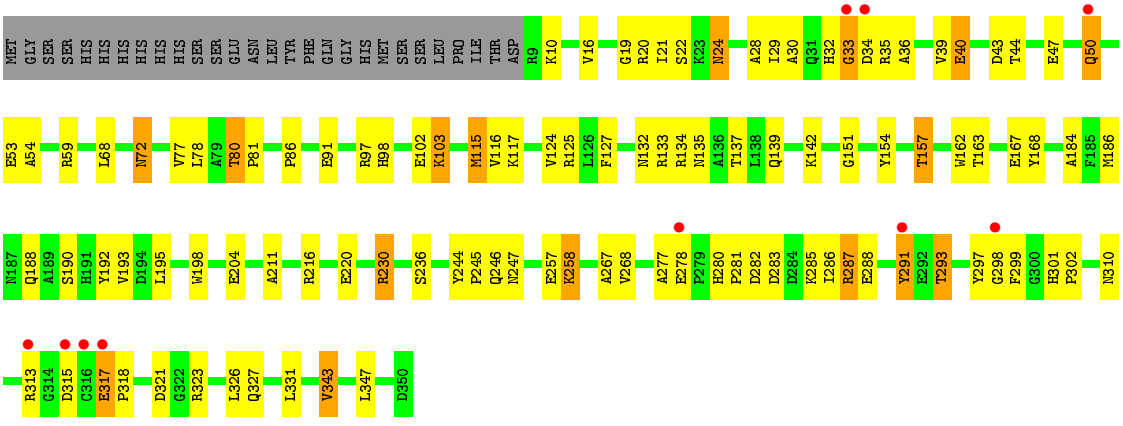
• Molecule 1: oxidoreductase

Chain G:



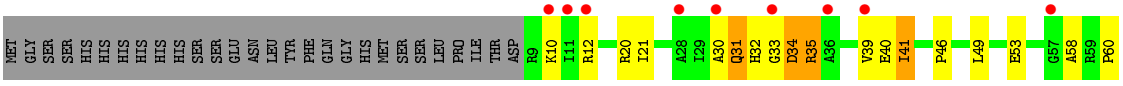
• Molecule 1: oxidoreductase

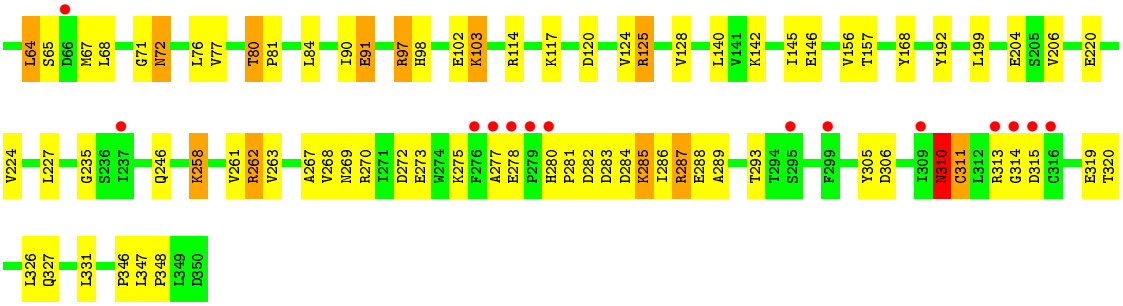
Chain H:



• Molecule 1: oxidoreductase

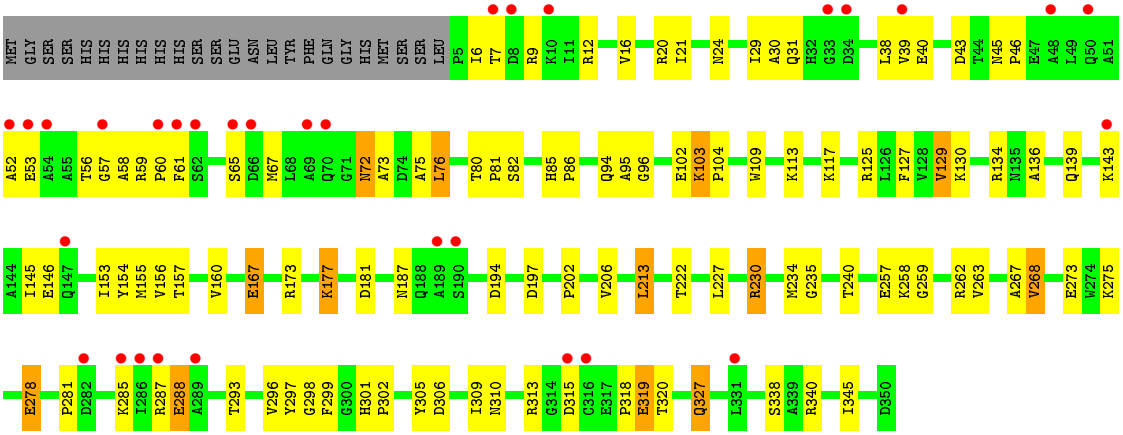
Chain I:





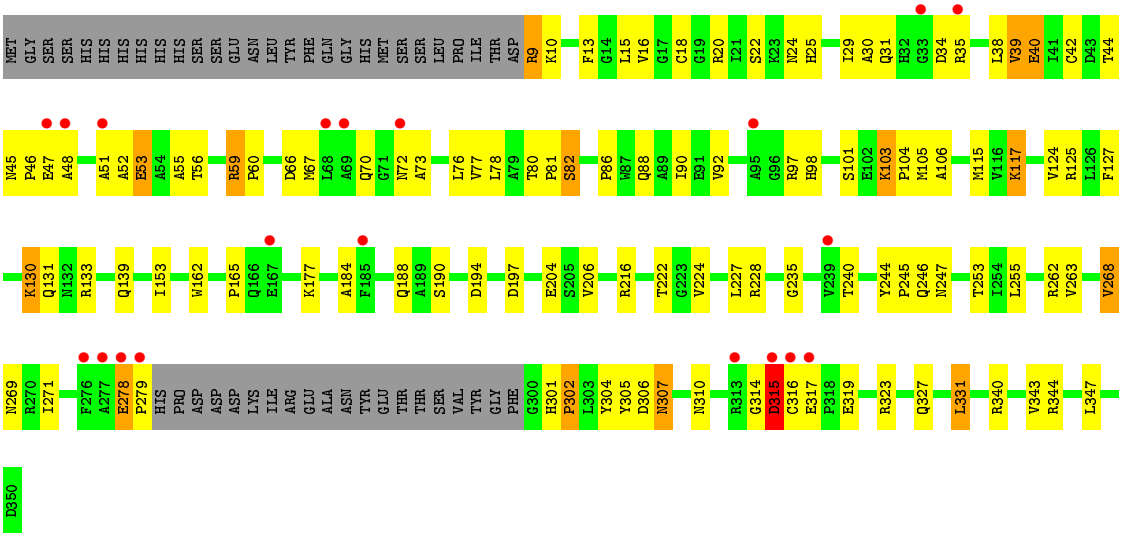
• Molecule 1: oxidoreductase

Chain J:



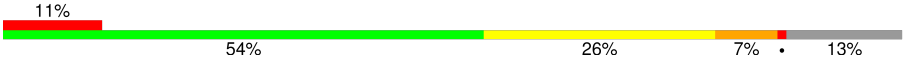
• Molecule 1: oxidoreductase

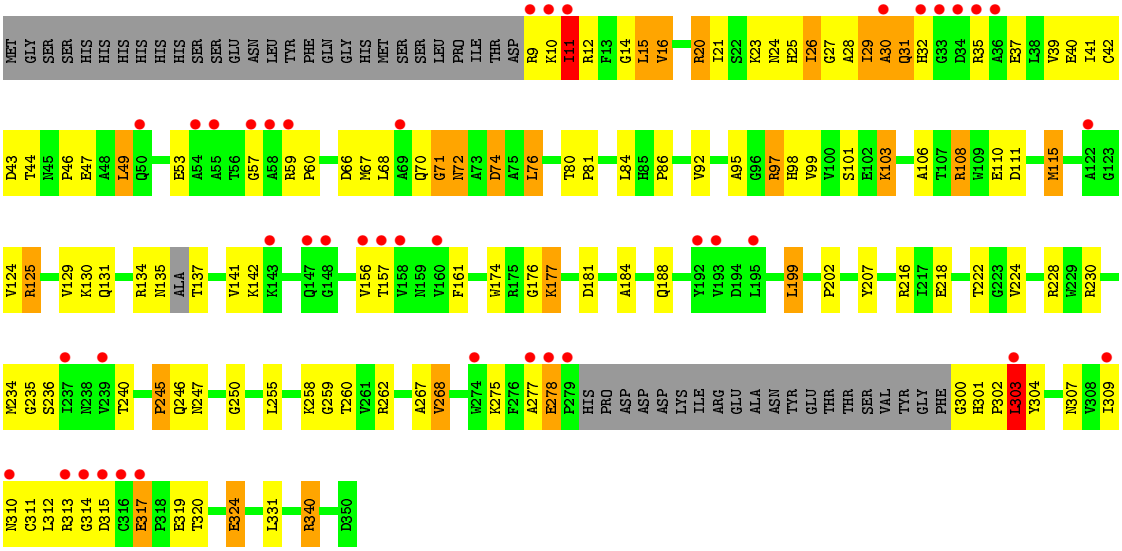
Chain K:



• Molecule 1: oxidoreductase

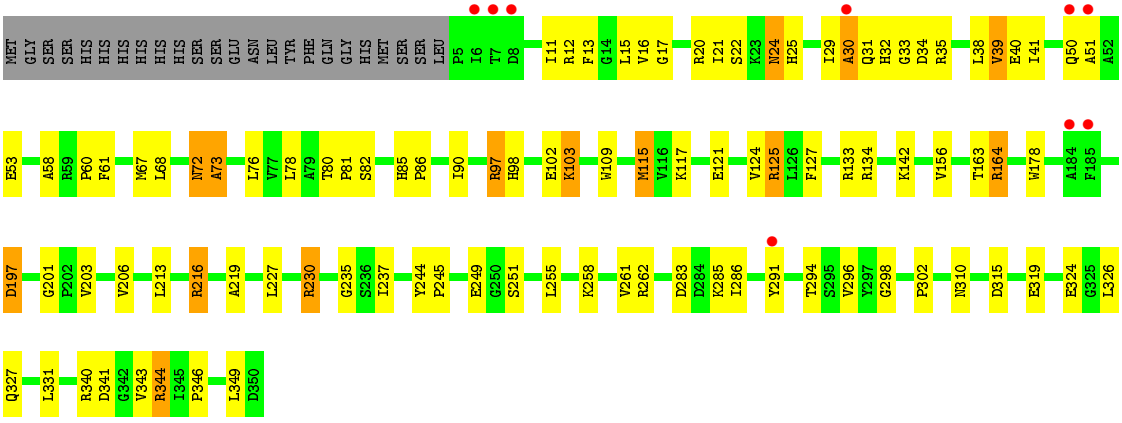
Chain L:





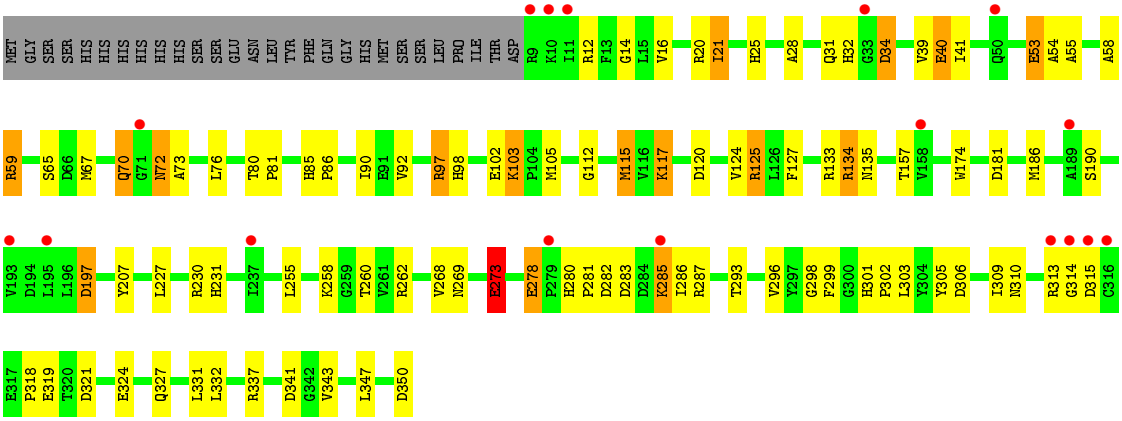
• Molecule 1: oxidoreductase

Chain M:



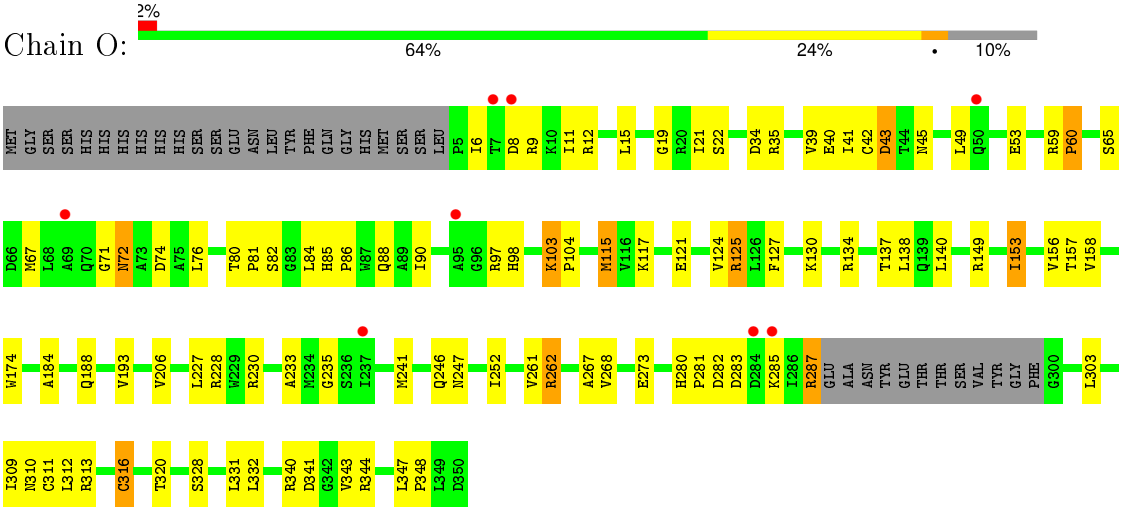
• Molecule 1: oxidoreductase

Chain N:



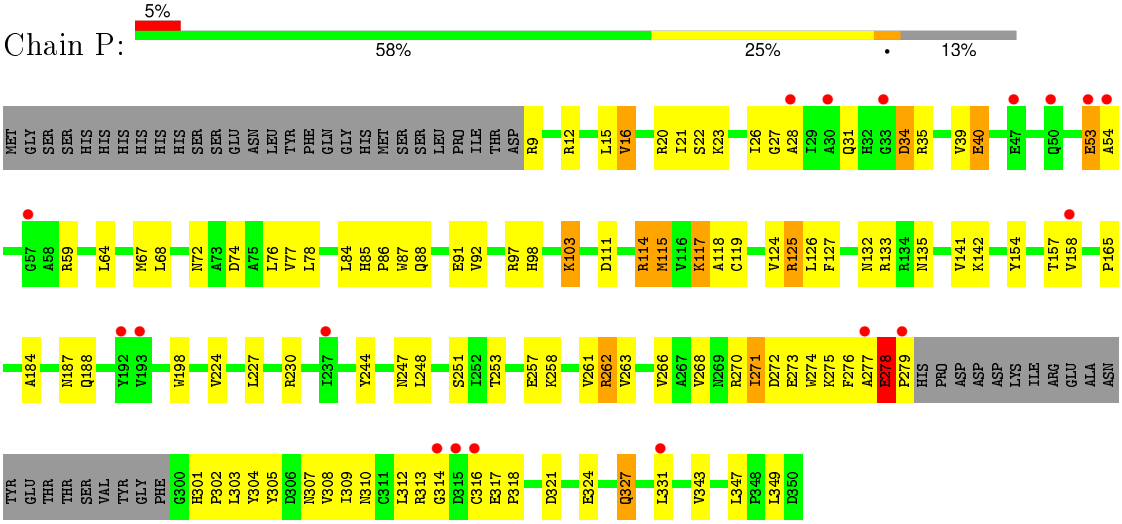
• Molecule 1: oxidoreductase

Chain O:



- Molecule 1: oxidoreductase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.26Å 319.98Å 103.80Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	30.00 – 2.13 34.28 – 2.13	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-2.13) 92.6 (34.28-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.54 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.269 0.184 , 0.265	Depositor DCC
R_{free} test set	15037 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.4	EDS
Estimated twinning fraction	0.007 for -h-l,k,h 0.007 for l,k,-h-l 0.026 for h,-k,-h-l 0.024 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 297987 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	43985	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, HP7

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	0.32	0/2767	1.16	14/3755 (0.4%)
1	B	0.28	0/2650	1.07	7/3593 (0.2%)
1	C	0.28	0/2772	1.08	5/3763 (0.1%)
1	D	0.27	0/2755	1.06	2/3737 (0.1%)
1	E	0.27	0/2554	1.06	6/3464 (0.2%)
1	F	0.28	0/2607	1.09	10/3536 (0.3%)
1	G	0.29	0/2736	1.11	8/3712 (0.2%)
1	H	0.28	0/2743	1.08	6/3722 (0.2%)
1	I	0.27	0/2736	1.05	1/3712 (0.0%)
1	J	0.27	0/2767	1.06	7/3755 (0.2%)
1	K	0.27	0/2564	1.06	7/3476 (0.2%)
1	L	0.26	0/2569	1.02	8/3480 (0.2%)
1	M	0.29	0/2767	1.16	14/3755 (0.4%)
1	N	0.30	0/2736	1.10	8/3712 (0.2%)
1	O	0.27	0/2666	1.19	7/3615 (0.2%)
1	P	0.26	0/2564	1.05	3/3476 (0.1%)
All	All	0.28	0/42953	1.09	113/58263 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

There are no bond length outliers.

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	230	ARG	NE-CZ-NH2	-20.32	110.14	120.30
1	O	230	ARG	NE-CZ-NH1	19.79	130.20	120.30
1	M	230	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	K	340	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	F	221	ASP	CB-CG-OD1	9.39	126.75	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	315	ASP	Peptide

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	2707	0	2654	65	0
1	B	2587	0	2547	122	0
1	C	2712	0	2655	72	0
1	D	2693	0	2641	133	0
1	E	2501	0	2465	136	0
1	F	2552	0	2505	82	0
1	G	2677	0	2624	71	0
1	H	2681	0	2633	110	2
1	I	2677	0	2624	108	1
1	J	2707	0	2654	80	1
1	K	2511	0	2479	104	0
1	L	2514	0	2486	130	0
1	M	2707	0	2654	85	0
1	N	2677	0	2624	98	0
1	O	2610	0	2572	87	0
1	P	2511	0	2479	98	0
2	A	44	0	27	1	0
2	B	44	0	27	6	0
2	C	44	0	27	6	0
2	D	44	0	27	7	0
2	E	44	0	27	7	0
2	F	44	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	44	0	27	4	0
2	H	44	0	27	8	0
2	I	44	0	27	12	0
2	J	44	0	27	7	0
2	K	44	0	27	4	0
2	L	44	0	27	6	0
2	M	44	0	27	4	0
2	N	44	0	27	4	0
2	O	44	0	27	3	0
2	P	44	0	27	5	0
3	A	40	0	22	2	0
3	B	40	0	22	1	0
3	C	40	0	22	1	0
3	D	40	0	22	1	0
3	E	40	0	22	5	0
3	F	40	0	22	2	0
3	G	40	0	22	2	0
3	H	40	0	22	3	0
3	I	40	0	22	3	0
3	J	40	0	22	3	0
3	K	40	0	22	6	0
3	L	40	0	22	0	0
3	M	40	0	22	4	0
3	N	40	0	22	1	0
3	O	40	0	22	2	0
3	P	40	0	22	1	0
4	A	85	0	0	8	0
4	B	54	0	0	6	0
4	C	58	0	0	3	0
4	D	51	0	0	3	0
4	E	21	0	0	2	0
4	F	24	0	0	0	0
4	G	49	0	0	4	0
4	H	35	0	0	2	0
4	I	36	0	0	2	0
4	J	30	0	0	1	0
4	K	26	0	0	2	0
4	L	37	0	0	3	0
4	M	36	0	0	1	0
4	N	34	0	0	4	0
4	O	17	0	0	1	0
4	P	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	43985	0	42080	1583	2

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 19.

The worst 5 of 1583 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:K:39:VAL:HG12	1:K:40:GLU:CG	1.49	1.43
1:I:64:LEU:HD23	1:I:67:MET:CE	1.59	1.31
1:B:12:ARG:HG2	1:B:39:VAL:CG2	1.61	1.28
1:B:12:ARG:CG	1:B:39:VAL:HG21	1.64	1.27
1:N:12:ARG:NH1	1:N:72:ASN:OD1	1.70	1.25

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:TYR:CE2	1:I:287:ARG:CD[2_746]	1.84	0.36
1:H:287:ARG:NH2	1:J:273:GLU:OE2[2_746]	2.12	0.08

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	344/370 (93%)	323 (94%)	20 (6%)	1 (0%)	46 41
1	B	327/370 (88%)	306 (94%)	20 (6%)	1 (0%)	46 41
1	C	345/370 (93%)	322 (93%)	21 (6%)	2 (1%)	30 21
1	D	342/370 (92%)	309 (90%)	29 (8%)	4 (1%)	16 8
1	E	317/370 (86%)	278 (88%)	34 (11%)	5 (2%)	12 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	323/370 (87%)	297 (92%)	25 (8%)	1 (0%)	46 41
1	G	340/370 (92%)	317 (93%)	20 (6%)	3 (1%)	21 12
1	H	341/370 (92%)	317 (93%)	23 (7%)	1 (0%)	46 41
1	I	340/370 (92%)	306 (90%)	28 (8%)	6 (2%)	11 3
1	J	344/370 (93%)	309 (90%)	31 (9%)	4 (1%)	16 8
1	K	318/370 (86%)	287 (90%)	26 (8%)	5 (2%)	12 4
1	L	316/370 (85%)	281 (89%)	27 (8%)	8 (2%)	7 1
1	M	344/370 (93%)	321 (93%)	20 (6%)	3 (1%)	21 12
1	N	340/370 (92%)	313 (92%)	26 (8%)	1 (0%)	46 41
1	O	330/370 (89%)	299 (91%)	29 (9%)	2 (1%)	30 21
1	P	318/370 (86%)	291 (92%)	24 (8%)	3 (1%)	21 12
All	All	5329/5920 (90%)	4876 (92%)	403 (8%)	50 (1%)	21 12

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	30	ALA
1	L	26	ILE
1	L	30	ALA
1	M	30	ALA
1	M	31	GLN

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	277/299 (93%)	261 (94%)	16 (6%)	25 19
1	B	264/299 (88%)	242 (92%)	22 (8%)	14 8
1	C	277/299 (93%)	262 (95%)	15 (5%)	27 21
1	D	275/299 (92%)	259 (94%)	16 (6%)	25 19
1	E	254/299 (85%)	238 (94%)	16 (6%)	22 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	260/299 (87%)	244 (94%)	16 (6%)	23 17
1	G	273/299 (91%)	257 (94%)	16 (6%)	24 18
1	H	274/299 (92%)	251 (92%)	23 (8%)	14 8
1	I	273/299 (91%)	256 (94%)	17 (6%)	23 17
1	J	277/299 (93%)	259 (94%)	18 (6%)	21 15
1	K	255/299 (85%)	233 (91%)	22 (9%)	13 7
1	L	256/299 (86%)	231 (90%)	25 (10%)	10 5
1	M	277/299 (93%)	262 (95%)	15 (5%)	27 21
1	N	273/299 (91%)	250 (92%)	23 (8%)	14 8
1	O	267/299 (89%)	251 (94%)	16 (6%)	24 18
1	P	255/299 (85%)	233 (91%)	22 (9%)	13 7
All	All	4287/4784 (90%)	3989 (93%)	298 (7%)	19 13

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	278	GLU
1	J	167	GLU
1	O	343	VAL
1	H	317	GLU
1	I	285	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	139	GLN
1	H	188	GLN
1	P	31	GLN
1	F	188	GLN
1	H	24	ASN

5.3.3 RNA

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 (i)

32 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	NAI	A	500	-	38,48,48	1.33	4 (10%)	48,73,73	2.66	12 (25%)
3	HP7	A	550	-	30,42,42	0.58	0	44,64,64	1.84	10 (22%)
2	NAI	B	500	-	38,48,48	1.37	4 (10%)	48,73,73	2.82	16 (33%)
3	HP7	B	550	-	30,42,42	0.56	0	44,64,64	1.65	9 (20%)
2	NAI	C	500	-	38,48,48	1.30	3 (7%)	48,73,73	2.76	16 (33%)
3	HP7	C	550	-	30,42,42	0.63	0	44,64,64	1.92	16 (36%)
2	NAI	D	500	-	38,48,48	1.34	5 (13%)	48,73,73	2.73	14 (29%)
3	HP7	D	550	-	30,42,42	0.58	0	44,64,64	1.81	5 (11%)
2	NAI	E	500	-	38,48,48	1.35	4 (10%)	48,73,73	2.61	10 (20%)
3	HP7	E	550	-	30,42,42	0.60	0	44,64,64	1.68	8 (18%)
2	NAI	F	500	-	38,48,48	1.32	3 (7%)	48,73,73	2.72	20 (41%)
3	HP7	F	550	-	30,42,42	0.54	0	44,64,64	1.83	7 (15%)
2	NAI	G	500	-	38,48,48	1.33	4 (10%)	48,73,73	2.94	19 (39%)
3	HP7	G	550	-	30,42,42	0.58	0	44,64,64	1.74	8 (18%)
2	NAI	H	500	-	38,48,48	1.34	5 (13%)	48,73,73	2.71	18 (37%)
3	HP7	H	550	-	30,42,42	0.59	0	44,64,64	2.02	10 (22%)
2	NAI	I	500	-	38,48,48	1.31	4 (10%)	48,73,73	2.59	13 (27%)
3	HP7	I	550	-	30,42,42	0.58	0	44,64,64	2.29	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAI	J	500	-	38,48,48	1.35	4 (10%)	48,73,73	2.80	18 (37%)
3	HP7	J	550	-	30,42,42	0.58	0	44,64,64	1.82	13 (29%)
2	NAI	K	500	-	38,48,48	1.32	4 (10%)	48,73,73	3.14	17 (35%)
3	HP7	K	550	-	30,42,42	0.59	0	44,64,64	2.08	12 (27%)
2	NAI	L	500	-	38,48,48	1.34	4 (10%)	48,73,73	2.84	16 (33%)
3	HP7	L	550	-	30,42,42	0.58	0	44,64,64	2.09	7 (15%)
2	NAI	M	500	-	38,48,48	1.36	4 (10%)	48,73,73	2.60	14 (29%)
3	HP7	M	550	-	30,42,42	0.61	0	44,64,64	2.08	9 (20%)
2	NAI	N	500	-	38,48,48	1.34	4 (10%)	48,73,73	2.86	14 (29%)
3	HP7	N	550	-	30,42,42	0.57	0	44,64,64	1.79	8 (18%)
2	NAI	O	500	-	38,48,48	1.31	4 (10%)	48,73,73	2.87	15 (31%)
3	HP7	O	550	-	30,42,42	0.59	0	44,64,64	1.85	8 (18%)
2	NAI	P	500	-	38,48,48	1.30	4 (10%)	48,73,73	2.36	16 (33%)
3	HP7	P	550	-	30,42,42	0.57	0	44,64,64	2.22	9 (20%)

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	NAI	A	500	-	-	0/25/72/72	0/5/5/5
3	HP7	A	550	-	-	0/20/65/65	0/3/3/3
2	NAI	B	500	-	-	0/25/72/72	0/5/5/5
3	HP7	B	550	-	-	0/20/65/65	0/3/3/3
2	NAI	C	500	-	-	0/25/72/72	0/5/5/5
3	HP7	C	550	-	-	0/20/65/65	0/3/3/3
2	NAI	D	500	-	-	0/25/72/72	0/5/5/5
3	HP7	D	550	-	-	0/20/65/65	0/3/3/3
2	NAI	E	500	-	-	0/25/72/72	0/5/5/5
3	HP7	E	550	-	-	0/20/65/65	0/3/3/3
2	NAI	F	500	-	-	0/25/72/72	0/5/5/5
3	HP7	F	550	-	-	0/20/65/65	0/3/3/3
2	NAI	G	500	-	-	0/25/72/72	0/5/5/5
3	HP7	G	550	-	-	0/20/65/65	0/3/3/3
2	NAI	H	500	-	-	0/25/72/72	0/5/5/5
3	HP7	H	550	-	-	0/20/65/65	0/3/3/3
2	NAI	I	500	-	-	0/25/72/72	0/5/5/5
3	HP7	I	550	-	-	0/20/65/65	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	J	500	-	-	0/25/72/72	0/5/5/5
3	HP7	J	550	-	-	0/20/65/65	0/3/3/3
2	NAI	K	500	-	-	0/25/72/72	0/5/5/5
3	HP7	K	550	-	-	0/20/65/65	0/3/3/3
2	NAI	L	500	-	-	0/25/72/72	0/5/5/5
3	HP7	L	550	-	-	0/20/65/65	0/3/3/3
2	NAI	M	500	-	-	0/25/72/72	0/5/5/5
3	HP7	M	550	-	-	0/20/65/65	0/3/3/3
2	NAI	N	500	-	-	0/25/72/72	0/5/5/5
3	HP7	N	550	-	-	0/20/65/65	0/3/3/3
2	NAI	O	500	-	-	0/25/72/72	0/5/5/5
3	HP7	O	550	-	-	0/20/65/65	0/3/3/3
2	NAI	P	500	-	-	0/25/72/72	0/5/5/5
3	HP7	P	550	-	-	0/20/65/65	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	NAI	C4N-C5N	-4.87	1.38	1.49
2	C	500	NAI	C4N-C5N	-4.83	1.38	1.49
2	L	500	NAI	C4N-C5N	-4.83	1.38	1.49
2	F	500	NAI	C4N-C5N	-4.82	1.38	1.49
2	E	500	NAI	C4N-C5N	-4.77	1.38	1.49

The worst 5 of 401 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	500	NAI	N3A-C2A-N1A	-12.73	119.15	128.89
2	N	500	NAI	N3A-C2A-N1A	-12.29	119.48	128.89
2	K	500	NAI	N3A-C2A-N1A	-11.78	119.88	128.89
2	L	500	NAI	N3A-C2A-N1A	-11.57	120.04	128.89
2	O	500	NAI	N3A-C2A-N1A	-11.23	120.29	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAI	1	0
3	A	550	HP7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	NAI	6	0
3	B	550	HP7	1	0
2	C	500	NAI	6	0
3	C	550	HP7	1	0
2	D	500	NAI	7	0
3	D	550	HP7	1	0
2	E	500	NAI	7	0
3	E	550	HP7	5	0
2	F	500	NAI	4	0
3	F	550	HP7	2	0
2	G	500	NAI	4	0
3	G	550	HP7	2	0
2	H	500	NAI	8	0
3	H	550	HP7	3	0
2	I	500	NAI	12	0
3	I	550	HP7	3	0
2	J	500	NAI	7	0
3	J	550	HP7	3	0
2	K	500	NAI	4	0
3	K	550	HP7	6	0
2	L	500	NAI	6	0
2	M	500	NAI	4	0
3	M	550	HP7	4	0
2	N	500	NAI	4	0
3	N	550	HP7	1	0
2	O	500	NAI	3	0
3	O	550	HP7	2	0
2	P	500	NAI	5	0
3	P	550	HP7	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	346/370 (93%)	-0.03	6 (1%) 73 79	16, 29, 45, 62	0
1	B	329/370 (88%)	0.24	20 (6%) 25 32	15, 37, 68, 94	0
1	C	347/370 (93%)	-0.01	7 (2%) 68 75	13, 34, 62, 82	0
1	D	343/370 (92%)	0.19	23 (6%) 21 28	17, 39, 75, 90	0
1	E	321/370 (86%)	0.40	33 (10%) 9 13	16, 46, 74, 89	0
1	F	327/370 (88%)	0.15	25 (7%) 17 22	16, 38, 69, 87	0
1	G	342/370 (92%)	-0.02	4 (1%) 81 85	13, 31, 59, 75	0
1	H	342/370 (92%)	0.03	10 (2%) 55 64	16, 36, 72, 88	0
1	I	342/370 (92%)	0.24	23 (6%) 21 28	17, 39, 72, 91	0
1	J	346/370 (93%)	0.28	31 (8%) 12 17	20, 40, 73, 86	0
1	K	322/370 (87%)	0.32	20 (6%) 24 31	15, 42, 75, 97	0
1	L	321/370 (86%)	0.48	41 (12%) 5 7	18, 47, 83, 93	0
1	M	346/370 (93%)	-0.08	9 (2%) 59 67	12, 31, 61, 84	0
1	N	342/370 (92%)	0.12	17 (4%) 32 42	13, 34, 69, 80	0
1	O	334/370 (90%)	0.03	8 (2%) 62 69	16, 39, 64, 86	0
1	P	322/370 (87%)	0.29	18 (5%) 28 36	16, 40, 74, 93	0
All	All	5372/5920 (90%)	0.16	295 (5%) 29 37	12, 37, 72, 97	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	30	ALA	7.4
1	L	316	CYS	7.3
1	P	30	ALA	7.3
1	L	33	GLY	6.8
1	P	279	PRO	6.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
2	NAI	C	500	44/44	0.96	0.11	-0.04	14,28,44,71	0
3	HP7	O	550	40/40	0.91	0.12	-0.07	22,56,100,100	0
2	NAI	H	500	44/44	0.96	0.10	-0.13	21,34,60,100	0
2	NAI	A	500	44/44	0.95	0.10	-0.20	19,25,31,45	0
2	NAI	F	500	44/44	0.96	0.10	-0.21	15,28,43,64	0
3	HP7	J	550	40/40	0.94	0.11	-0.25	14,36,75,100	0
3	HP7	L	550	40/40	0.91	0.13	-0.30	20,56,100,100	0
3	HP7	P	550	40/40	0.91	0.12	-0.33	28,48,100,100	0
3	HP7	E	550	40/40	0.90	0.13	-0.36	32,64,100,100	0
3	HP7	A	550	40/40	0.97	0.11	-0.36	11,25,50,100	0
2	NAI	O	500	44/44	0.97	0.10	-0.40	19,35,52,63	0
2	NAI	M	500	44/44	0.97	0.11	-0.40	15,32,49,84	0
3	HP7	F	550	40/40	0.92	0.11	-0.43	24,43,100,100	0
2	NAI	G	500	44/44	0.96	0.10	-0.43	17,28,38,57	0
3	HP7	K	550	40/40	0.92	0.12	-0.43	17,53,100,100	0
3	HP7	D	550	40/40	0.94	0.10	-0.51	23,47,99,100	0
3	HP7	B	550	40/40	0.93	0.11	-0.51	25,45,100,100	0
2	NAI	J	500	44/44	0.96	0.10	-0.55	18,37,60,78	0
2	NAI	N	500	44/44	0.95	0.10	-0.55	17,32,48,63	0
2	NAI	K	500	44/44	0.96	0.10	-0.55	18,33,53,100	0
2	NAI	L	500	44/44	0.95	0.10	-0.57	23,40,63,100	0
2	NAI	E	500	44/44	0.95	0.10	-0.60	23,43,87,98	0
2	NAI	I	500	44/44	0.97	0.09	-0.64	20,35,46,59	0
3	HP7	N	550	40/40	0.97	0.09	-0.65	15,27,50,56	0
2	NAI	D	500	44/44	0.97	0.09	-0.72	20,36,52,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAI	P	500	44/44	0.96	0.09	-0.75	24,37,54,73	0
3	HP7	C	550	40/40	0.95	0.10	-0.76	17,30,76,100	0
2	NAI	B	500	44/44	0.96	0.09	-0.78	21,36,58,79	0
3	HP7	G	550	40/40	0.97	0.09	-0.83	14,32,77,100	0
3	HP7	H	550	40/40	0.96	0.10	-0.86	21,34,59,90	0
3	HP7	M	550	40/40	0.97	0.09	-0.88	17,31,42,59	0
3	HP7	I	550	40/40	0.96	0.09	-0.89	19,40,82,100	0

6.5 Other polymers

There are no such residues in this entry.