



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:55 PM UTC

PDB ID : 4FFU / pdb\_00004ffu  
Title : CRYSTAL STRUCTURE OF putative MaoC-like (monoamine oxidase-like) protein, similar to NodN from Sinorhizo Bium meliloti 1021  
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)  
Deposited on : 2012-06-01  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)

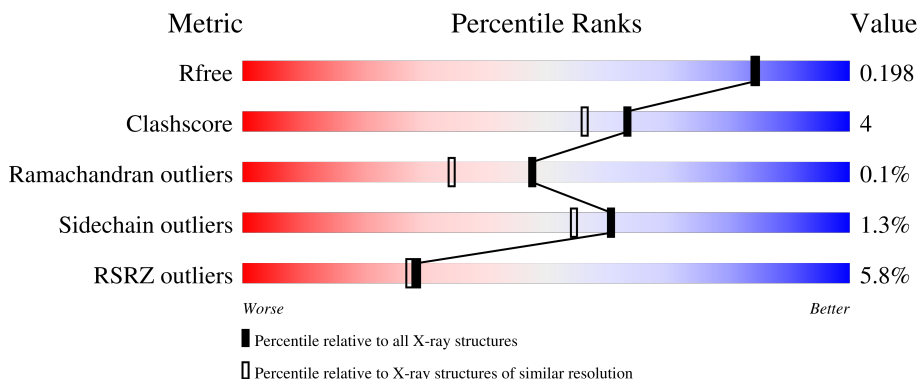
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	176	
1	B	176	
1	C	176	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	176	<p>6% 78% 5% • 16%</p>
1	E	176	<p>4% 82% • • 14%</p>
1	F	176	<p>5% 76% 5% •• 18%</p>
1	G	176	<p>12% 69% 12% • 18%</p>
1	H	176	<p>% 84% 5% 11%</p>
1	I	176	<p>2% 81% 8% 11%</p>
1	J	176	<p>10% 72% 8% • 19%</p>
1	K	176	<p>6% 70% 5% • 23%</p>
1	L	176	<p>4% 78% 6% • 14%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16207 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 oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	155	1248	790	224	229	1	4	0	5	0
1	B	150	1199	755	219	220	1	4	0	4	0
1	C	150	1232	778	230	221	1	2	0	8	0
1	D	147	1197	756	218	219	1	3	0	7	0
1	E	151	1196	752	220	221	1	2	0	1	0
1	F	145	1167	736	215	212	1	3	0	4	0
1	G	145	1171	741	214	212	1	3	0	5	0
1	H	156	1246	787	223	230	1	5	0	3	0
1	I	157	1286	814	231	235	1	5	0	8	0
1	J	143	1145	722	210	210	1	2	0	4	0
1	K	135	1082	685	198	195	1	3	0	3	0
1	L	151	1201	756	220	221	1	3	0	2	0

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	expression tag	UNP Q92VL2
A	-21	HIS	-	expression tag	UNP Q92VL2
A	-20	HIS	-	expression tag	UNP Q92VL2
A	-19	HIS	-	expression tag	UNP Q92VL2
A	-18	HIS	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	HIS	-	expression tag	UNP Q92VL2
A	-16	HIS	-	expression tag	UNP Q92VL2
A	-15	SER	-	expression tag	UNP Q92VL2
A	-14	SER	-	expression tag	UNP Q92VL2
A	-13	GLY	-	expression tag	UNP Q92VL2
A	-12	VAL	-	expression tag	UNP Q92VL2
A	-11	ASP	-	expression tag	UNP Q92VL2
A	-10	LEU	-	expression tag	UNP Q92VL2
A	-9	GLY	-	expression tag	UNP Q92VL2
A	-8	THR	-	expression tag	UNP Q92VL2
A	-7	GLU	-	expression tag	UNP Q92VL2
A	-6	ASN	-	expression tag	UNP Q92VL2
A	-5	LEU	-	expression tag	UNP Q92VL2
A	-4	TYR	-	expression tag	UNP Q92VL2
A	-3	PHE	-	expression tag	UNP Q92VL2
A	-2	GLN	-	expression tag	UNP Q92VL2
A	-1	SER	-	expression tag	UNP Q92VL2
A	0	MSE	-	expression tag	UNP Q92VL2
B	-22	MSE	-	expression tag	UNP Q92VL2
B	-21	HIS	-	expression tag	UNP Q92VL2
B	-20	HIS	-	expression tag	UNP Q92VL2
B	-19	HIS	-	expression tag	UNP Q92VL2
B	-18	HIS	-	expression tag	UNP Q92VL2
B	-17	HIS	-	expression tag	UNP Q92VL2
B	-16	HIS	-	expression tag	UNP Q92VL2
B	-15	SER	-	expression tag	UNP Q92VL2
B	-14	SER	-	expression tag	UNP Q92VL2
B	-13	GLY	-	expression tag	UNP Q92VL2
B	-12	VAL	-	expression tag	UNP Q92VL2
B	-11	ASP	-	expression tag	UNP Q92VL2
B	-10	LEU	-	expression tag	UNP Q92VL2
B	-9	GLY	-	expression tag	UNP Q92VL2
B	-8	THR	-	expression tag	UNP Q92VL2
B	-7	GLU	-	expression tag	UNP Q92VL2
B	-6	ASN	-	expression tag	UNP Q92VL2
B	-5	LEU	-	expression tag	UNP Q92VL2
B	-4	TYR	-	expression tag	UNP Q92VL2
B	-3	PHE	-	expression tag	UNP Q92VL2
B	-2	GLN	-	expression tag	UNP Q92VL2
B	-1	SER	-	expression tag	UNP Q92VL2
B	0	MSE	-	expression tag	UNP Q92VL2
C	-22	MSE	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	HIS	-	expression tag	UNP Q92VL2
C	-20	HIS	-	expression tag	UNP Q92VL2
C	-19	HIS	-	expression tag	UNP Q92VL2
C	-18	HIS	-	expression tag	UNP Q92VL2
C	-17	HIS	-	expression tag	UNP Q92VL2
C	-16	HIS	-	expression tag	UNP Q92VL2
C	-15	SER	-	expression tag	UNP Q92VL2
C	-14	SER	-	expression tag	UNP Q92VL2
C	-13	GLY	-	expression tag	UNP Q92VL2
C	-12	VAL	-	expression tag	UNP Q92VL2
C	-11	ASP	-	expression tag	UNP Q92VL2
C	-10	LEU	-	expression tag	UNP Q92VL2
C	-9	GLY	-	expression tag	UNP Q92VL2
C	-8	THR	-	expression tag	UNP Q92VL2
C	-7	GLU	-	expression tag	UNP Q92VL2
C	-6	ASN	-	expression tag	UNP Q92VL2
C	-5	LEU	-	expression tag	UNP Q92VL2
C	-4	TYR	-	expression tag	UNP Q92VL2
C	-3	PHE	-	expression tag	UNP Q92VL2
C	-2	GLN	-	expression tag	UNP Q92VL2
C	-1	SER	-	expression tag	UNP Q92VL2
C	0	MSE	-	expression tag	UNP Q92VL2
D	-22	MSE	-	expression tag	UNP Q92VL2
D	-21	HIS	-	expression tag	UNP Q92VL2
D	-20	HIS	-	expression tag	UNP Q92VL2
D	-19	HIS	-	expression tag	UNP Q92VL2
D	-18	HIS	-	expression tag	UNP Q92VL2
D	-17	HIS	-	expression tag	UNP Q92VL2
D	-16	HIS	-	expression tag	UNP Q92VL2
D	-15	SER	-	expression tag	UNP Q92VL2
D	-14	SER	-	expression tag	UNP Q92VL2
D	-13	GLY	-	expression tag	UNP Q92VL2
D	-12	VAL	-	expression tag	UNP Q92VL2
D	-11	ASP	-	expression tag	UNP Q92VL2
D	-10	LEU	-	expression tag	UNP Q92VL2
D	-9	GLY	-	expression tag	UNP Q92VL2
D	-8	THR	-	expression tag	UNP Q92VL2
D	-7	GLU	-	expression tag	UNP Q92VL2
D	-6	ASN	-	expression tag	UNP Q92VL2
D	-5	LEU	-	expression tag	UNP Q92VL2
D	-4	TYR	-	expression tag	UNP Q92VL2
D	-3	PHE	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLN	-	expression tag	UNP Q92VL2
D	-1	SER	-	expression tag	UNP Q92VL2
D	0	MSE	-	expression tag	UNP Q92VL2
E	-22	MSE	-	expression tag	UNP Q92VL2
E	-21	HIS	-	expression tag	UNP Q92VL2
E	-20	HIS	-	expression tag	UNP Q92VL2
E	-19	HIS	-	expression tag	UNP Q92VL2
E	-18	HIS	-	expression tag	UNP Q92VL2
E	-17	HIS	-	expression tag	UNP Q92VL2
E	-16	HIS	-	expression tag	UNP Q92VL2
E	-15	SER	-	expression tag	UNP Q92VL2
E	-14	SER	-	expression tag	UNP Q92VL2
E	-13	GLY	-	expression tag	UNP Q92VL2
E	-12	VAL	-	expression tag	UNP Q92VL2
E	-11	ASP	-	expression tag	UNP Q92VL2
E	-10	LEU	-	expression tag	UNP Q92VL2
E	-9	GLY	-	expression tag	UNP Q92VL2
E	-8	THR	-	expression tag	UNP Q92VL2
E	-7	GLU	-	expression tag	UNP Q92VL2
E	-6	ASN	-	expression tag	UNP Q92VL2
E	-5	LEU	-	expression tag	UNP Q92VL2
E	-4	TYR	-	expression tag	UNP Q92VL2
E	-3	PHE	-	expression tag	UNP Q92VL2
E	-2	GLN	-	expression tag	UNP Q92VL2
E	-1	SER	-	expression tag	UNP Q92VL2
E	0	MSE	-	expression tag	UNP Q92VL2
F	-22	MSE	-	expression tag	UNP Q92VL2
F	-21	HIS	-	expression tag	UNP Q92VL2
F	-20	HIS	-	expression tag	UNP Q92VL2
F	-19	HIS	-	expression tag	UNP Q92VL2
F	-18	HIS	-	expression tag	UNP Q92VL2
F	-17	HIS	-	expression tag	UNP Q92VL2
F	-16	HIS	-	expression tag	UNP Q92VL2
F	-15	SER	-	expression tag	UNP Q92VL2
F	-14	SER	-	expression tag	UNP Q92VL2
F	-13	GLY	-	expression tag	UNP Q92VL2
F	-12	VAL	-	expression tag	UNP Q92VL2
F	-11	ASP	-	expression tag	UNP Q92VL2
F	-10	LEU	-	expression tag	UNP Q92VL2
F	-9	GLY	-	expression tag	UNP Q92VL2
F	-8	THR	-	expression tag	UNP Q92VL2
F	-7	GLU	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	ASN	-	expression tag	UNP Q92VL2
F	-5	LEU	-	expression tag	UNP Q92VL2
F	-4	TYR	-	expression tag	UNP Q92VL2
F	-3	PHE	-	expression tag	UNP Q92VL2
F	-2	GLN	-	expression tag	UNP Q92VL2
F	-1	SER	-	expression tag	UNP Q92VL2
F	0	MSE	-	expression tag	UNP Q92VL2
G	-22	MSE	-	expression tag	UNP Q92VL2
G	-21	HIS	-	expression tag	UNP Q92VL2
G	-20	HIS	-	expression tag	UNP Q92VL2
G	-19	HIS	-	expression tag	UNP Q92VL2
G	-18	HIS	-	expression tag	UNP Q92VL2
G	-17	HIS	-	expression tag	UNP Q92VL2
G	-16	HIS	-	expression tag	UNP Q92VL2
G	-15	SER	-	expression tag	UNP Q92VL2
G	-14	SER	-	expression tag	UNP Q92VL2
G	-13	GLY	-	expression tag	UNP Q92VL2
G	-12	VAL	-	expression tag	UNP Q92VL2
G	-11	ASP	-	expression tag	UNP Q92VL2
G	-10	LEU	-	expression tag	UNP Q92VL2
G	-9	GLY	-	expression tag	UNP Q92VL2
G	-8	THR	-	expression tag	UNP Q92VL2
G	-7	GLU	-	expression tag	UNP Q92VL2
G	-6	ASN	-	expression tag	UNP Q92VL2
G	-5	LEU	-	expression tag	UNP Q92VL2
G	-4	TYR	-	expression tag	UNP Q92VL2
G	-3	PHE	-	expression tag	UNP Q92VL2
G	-2	GLN	-	expression tag	UNP Q92VL2
G	-1	SER	-	expression tag	UNP Q92VL2
G	0	MSE	-	expression tag	UNP Q92VL2
H	-22	MSE	-	expression tag	UNP Q92VL2
H	-21	HIS	-	expression tag	UNP Q92VL2
H	-20	HIS	-	expression tag	UNP Q92VL2
H	-19	HIS	-	expression tag	UNP Q92VL2
H	-18	HIS	-	expression tag	UNP Q92VL2
H	-17	HIS	-	expression tag	UNP Q92VL2
H	-16	HIS	-	expression tag	UNP Q92VL2
H	-15	SER	-	expression tag	UNP Q92VL2
H	-14	SER	-	expression tag	UNP Q92VL2
H	-13	GLY	-	expression tag	UNP Q92VL2
H	-12	VAL	-	expression tag	UNP Q92VL2
H	-11	ASP	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	LEU	-	expression tag	UNP Q92VL2
H	-9	GLY	-	expression tag	UNP Q92VL2
H	-8	THR	-	expression tag	UNP Q92VL2
H	-7	GLU	-	expression tag	UNP Q92VL2
H	-6	ASN	-	expression tag	UNP Q92VL2
H	-5	LEU	-	expression tag	UNP Q92VL2
H	-4	TYR	-	expression tag	UNP Q92VL2
H	-3	PHE	-	expression tag	UNP Q92VL2
H	-2	GLN	-	expression tag	UNP Q92VL2
H	-1	SER	-	expression tag	UNP Q92VL2
H	0	MSE	-	expression tag	UNP Q92VL2
I	-22	MSE	-	expression tag	UNP Q92VL2
I	-21	HIS	-	expression tag	UNP Q92VL2
I	-20	HIS	-	expression tag	UNP Q92VL2
I	-19	HIS	-	expression tag	UNP Q92VL2
I	-18	HIS	-	expression tag	UNP Q92VL2
I	-17	HIS	-	expression tag	UNP Q92VL2
I	-16	HIS	-	expression tag	UNP Q92VL2
I	-15	SER	-	expression tag	UNP Q92VL2
I	-14	SER	-	expression tag	UNP Q92VL2
I	-13	GLY	-	expression tag	UNP Q92VL2
I	-12	VAL	-	expression tag	UNP Q92VL2
I	-11	ASP	-	expression tag	UNP Q92VL2
I	-10	LEU	-	expression tag	UNP Q92VL2
I	-9	GLY	-	expression tag	UNP Q92VL2
I	-8	THR	-	expression tag	UNP Q92VL2
I	-7	GLU	-	expression tag	UNP Q92VL2
I	-6	ASN	-	expression tag	UNP Q92VL2
I	-5	LEU	-	expression tag	UNP Q92VL2
I	-4	TYR	-	expression tag	UNP Q92VL2
I	-3	PHE	-	expression tag	UNP Q92VL2
I	-2	GLN	-	expression tag	UNP Q92VL2
I	-1	SER	-	expression tag	UNP Q92VL2
I	0	MSE	-	expression tag	UNP Q92VL2
J	-22	MSE	-	expression tag	UNP Q92VL2
J	-21	HIS	-	expression tag	UNP Q92VL2
J	-20	HIS	-	expression tag	UNP Q92VL2
J	-19	HIS	-	expression tag	UNP Q92VL2
J	-18	HIS	-	expression tag	UNP Q92VL2
J	-17	HIS	-	expression tag	UNP Q92VL2
J	-16	HIS	-	expression tag	UNP Q92VL2
J	-15	SER	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-14	SER	-	expression tag	UNP Q92VL2
J	-13	GLY	-	expression tag	UNP Q92VL2
J	-12	VAL	-	expression tag	UNP Q92VL2
J	-11	ASP	-	expression tag	UNP Q92VL2
J	-10	LEU	-	expression tag	UNP Q92VL2
J	-9	GLY	-	expression tag	UNP Q92VL2
J	-8	THR	-	expression tag	UNP Q92VL2
J	-7	GLU	-	expression tag	UNP Q92VL2
J	-6	ASN	-	expression tag	UNP Q92VL2
J	-5	LEU	-	expression tag	UNP Q92VL2
J	-4	TYR	-	expression tag	UNP Q92VL2
J	-3	PHE	-	expression tag	UNP Q92VL2
J	-2	GLN	-	expression tag	UNP Q92VL2
J	-1	SER	-	expression tag	UNP Q92VL2
J	0	MSE	-	expression tag	UNP Q92VL2
K	-22	MSE	-	expression tag	UNP Q92VL2
K	-21	HIS	-	expression tag	UNP Q92VL2
K	-20	HIS	-	expression tag	UNP Q92VL2
K	-19	HIS	-	expression tag	UNP Q92VL2
K	-18	HIS	-	expression tag	UNP Q92VL2
K	-17	HIS	-	expression tag	UNP Q92VL2
K	-16	HIS	-	expression tag	UNP Q92VL2
K	-15	SER	-	expression tag	UNP Q92VL2
K	-14	SER	-	expression tag	UNP Q92VL2
K	-13	GLY	-	expression tag	UNP Q92VL2
K	-12	VAL	-	expression tag	UNP Q92VL2
K	-11	ASP	-	expression tag	UNP Q92VL2
K	-10	LEU	-	expression tag	UNP Q92VL2
K	-9	GLY	-	expression tag	UNP Q92VL2
K	-8	THR	-	expression tag	UNP Q92VL2
K	-7	GLU	-	expression tag	UNP Q92VL2
K	-6	ASN	-	expression tag	UNP Q92VL2
K	-5	LEU	-	expression tag	UNP Q92VL2
K	-4	TYR	-	expression tag	UNP Q92VL2
K	-3	PHE	-	expression tag	UNP Q92VL2
K	-2	GLN	-	expression tag	UNP Q92VL2
K	-1	SER	-	expression tag	UNP Q92VL2
K	0	MSE	-	expression tag	UNP Q92VL2
L	-22	MSE	-	expression tag	UNP Q92VL2
L	-21	HIS	-	expression tag	UNP Q92VL2
L	-20	HIS	-	expression tag	UNP Q92VL2
L	-19	HIS	-	expression tag	UNP Q92VL2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	HIS	-	expression tag	UNP Q92VL2
L	-17	HIS	-	expression tag	UNP Q92VL2
L	-16	HIS	-	expression tag	UNP Q92VL2
L	-15	SER	-	expression tag	UNP Q92VL2
L	-14	SER	-	expression tag	UNP Q92VL2
L	-13	GLY	-	expression tag	UNP Q92VL2
L	-12	VAL	-	expression tag	UNP Q92VL2
L	-11	ASP	-	expression tag	UNP Q92VL2
L	-10	LEU	-	expression tag	UNP Q92VL2
L	-9	GLY	-	expression tag	UNP Q92VL2
L	-8	THR	-	expression tag	UNP Q92VL2
L	-7	GLU	-	expression tag	UNP Q92VL2
L	-6	ASN	-	expression tag	UNP Q92VL2
L	-5	LEU	-	expression tag	UNP Q92VL2
L	-4	TYR	-	expression tag	UNP Q92VL2
L	-3	PHE	-	expression tag	UNP Q92VL2
L	-2	GLN	-	expression tag	UNP Q92VL2
L	-1	SER	-	expression tag	UNP Q92VL2
L	0	MSE	-	expression tag	UNP Q92VL2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	203	Total O 203 203	0	0
3	B	195	Total O 195 195	0	0
3	C	147	Total O 149 149	0	2
3	D	165	Total O 165 165	0	0
3	E	146	Total O 147 147	0	1
3	F	124	Total O 124 124	0	0
3	G	105	Total O 106 106	0	1

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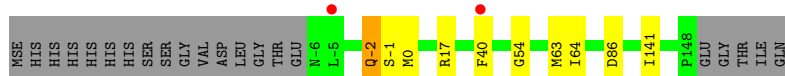
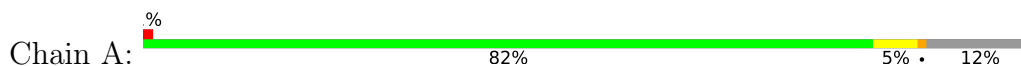
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	188	Total 188	O 188	0	0
3	I	166	Total 167	O 167	0	1
3	J	133	Total 134	O 134	0	1
3	K	117	Total 118	O 118	0	1
3	L	140	Total 140	O 140	0	0

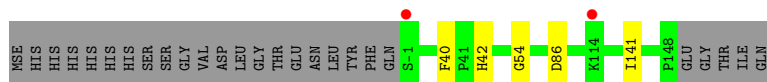
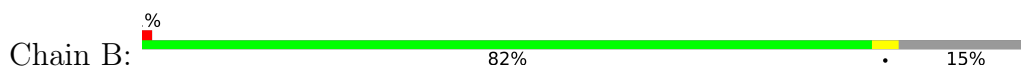
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

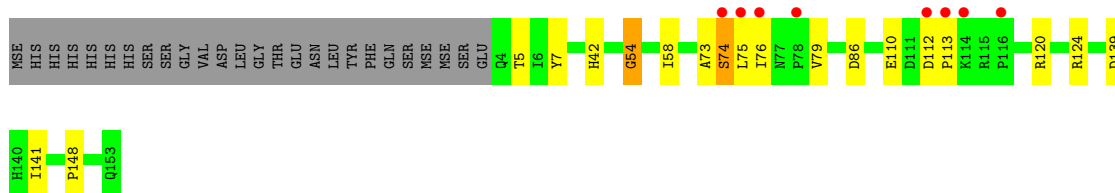
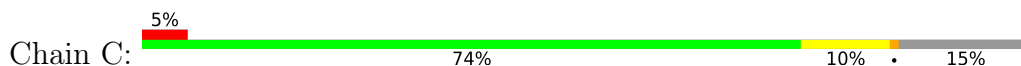
- Molecule 1: oxidase



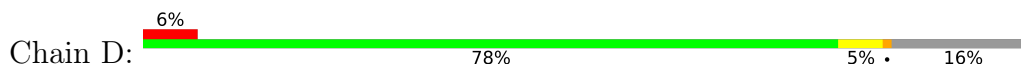
- Molecule 1: oxidase



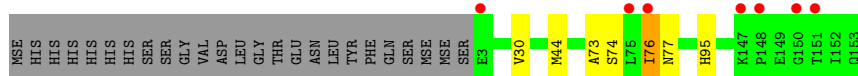
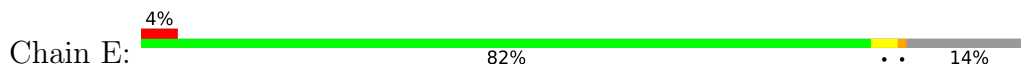
- Molecule 1: oxidase



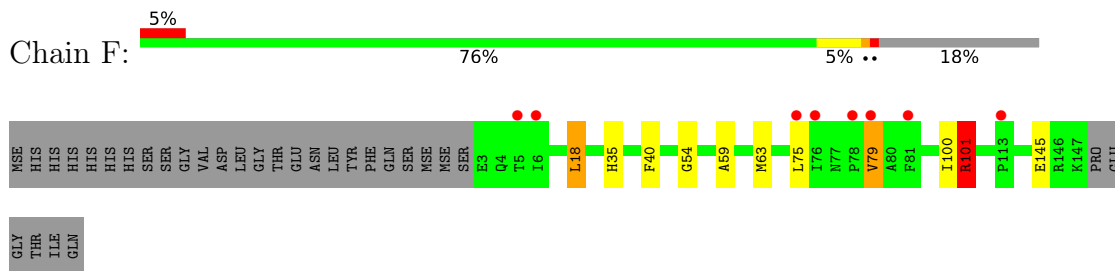
- Molecule 1: oxidase



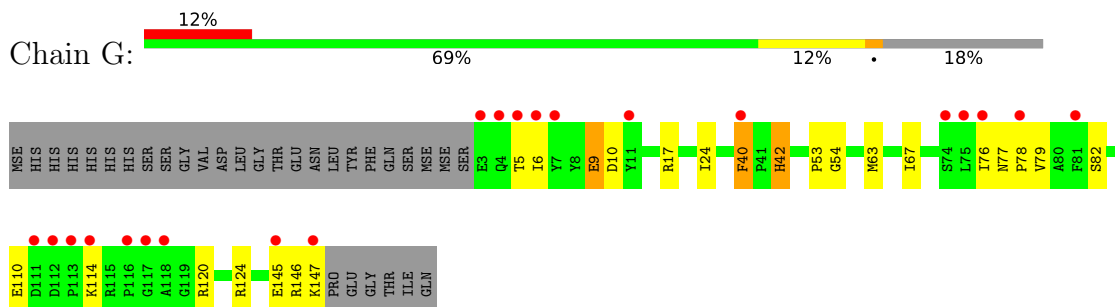
- Molecule 1: oxidase



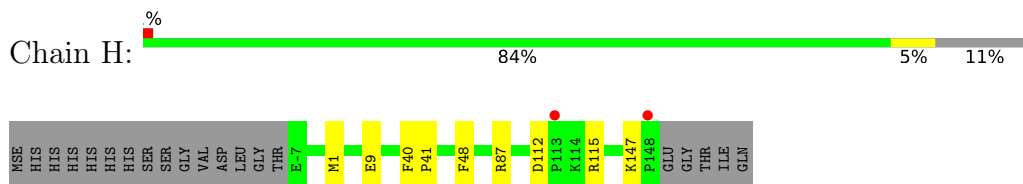
- Molecule 1: oxidase



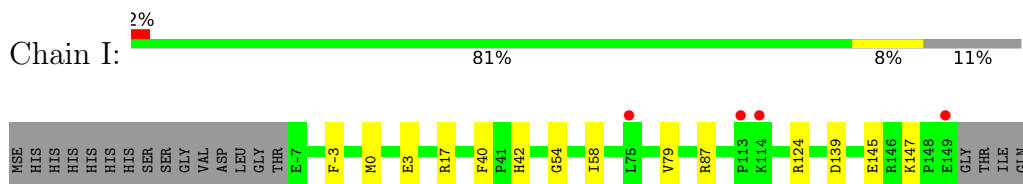
- Molecule 1: oxidase



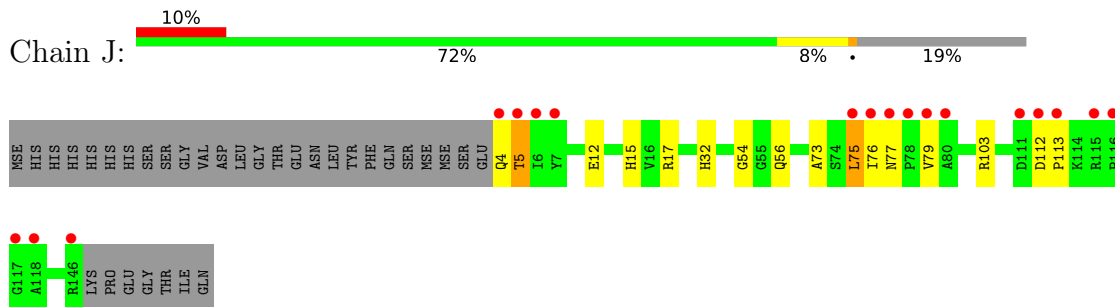
- Molecule 1: oxidase



- Molecule 1: oxidase

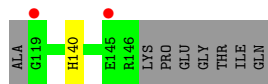
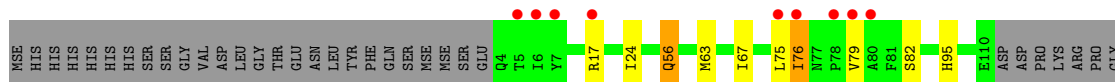


- Molecule 1: oxidase

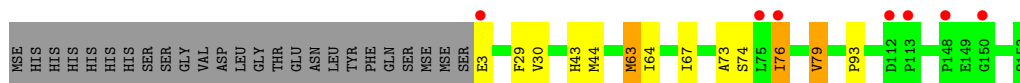
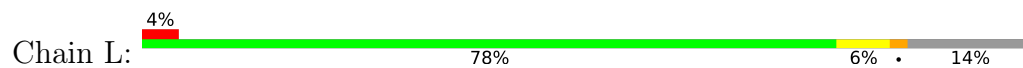


- Molecule 1: oxidase





- Molecule 1: oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.49Å 122.94Å 147.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.80) 99.7 (20.00-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 1.81Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.167 , 0.197 0.169 , 0.198	Depositor DCC
$R_{free}$ test set	9820 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.62 % 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 1.0947e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: CL

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	0.75	1/1282 (0.1%)	0.86	0/1729
1	B	0.83	2/1229 (0.2%)	0.97	4/1657 (0.2%)
1	C	0.87	5/1276 (0.4%)	0.86	3/1722 (0.2%)
1	D	0.92	4/1238 (0.3%)	0.86	2/1673 (0.1%)
1	E	0.65	0/1223	0.86	2/1652 (0.1%)
1	F	0.80	3/1197 (0.3%)	0.86	5/1616 (0.3%)
1	G	0.74	2/1205 (0.2%)	0.96	7/1628 (0.4%)
1	H	0.70	0/1279	0.85	0/1724
1	I	0.68	0/1329	0.82	0/1789
1	J	0.88	3/1175 (0.3%)	0.83	0/1589
1	K	0.70	1/1111 (0.1%)	0.78	0/1500
1	L	0.63	0/1231	0.84	1/1662 (0.1%)
All	All	0.77	21/14775 (0.1%)	0.86	24/19941 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	I	0	1
1	J	0	1
All	All	0	8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	56[A]	GLN	CA-C	12.48	1.68	1.52
1	D	56[B]	GLN	CA-C	12.48	1.68	1.52
1	J	56[A]	GLN	CA-C	10.38	1.65	1.52
1	J	56[B]	GLN	CA-C	10.38	1.65	1.52
1	B	42[A]	HIS	CA-C	9.04	1.65	1.52
1	B	42[B]	HIS	CA-C	9.04	1.65	1.52
1	F	101[A]	ARG	CA-C	8.33	1.62	1.52
1	F	101[B]	ARG	CA-C	8.33	1.62	1.52
1	G	42[A]	HIS	CA-C	7.63	1.63	1.52
1	G	42[B]	HIS	CA-C	7.63	1.63	1.52
1	J	103	ARG	C-O	-6.30	1.16	1.24
1	C	54[A]	GLY	C-O	-5.71	1.16	1.24
1	C	54[B]	GLY	C-O	-5.71	1.16	1.24
1	C	112	ASP	C-N	5.65	1.41	1.34
1	A	-2	GLN	C-O	-5.63	1.17	1.24
1	C	110	GLU	C-O	-5.56	1.17	1.23
1	D	54[A]	GLY	C-O	-5.34	1.16	1.24
1	D	54[B]	GLY	C-O	-5.34	1.16	1.24
1	K	56	GLN	C-O	-5.04	1.17	1.23
1	F	100	ILE	C-N	-5.02	1.26	1.33
1	C	113	PRO	N-CD	5.00	1.54	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42[A]	HIS	CA-C-O	10.36	131.80	120.20
1	B	42[B]	HIS	CA-C-O	10.36	131.80	120.20
1	G	42[A]	HIS	CA-C-O	10.31	131.96	119.49
1	G	42[B]	HIS	CA-C-O	10.31	131.96	119.49
1	L	63	MSE	CG-SE-CE	-8.11	81.08	98.92
1	G	42[A]	HIS	N-CA-C	8.02	120.93	111.71
1	G	42[B]	HIS	N-CA-C	8.02	120.93	111.71
1	C	74	SER	N-CA-C	5.91	123.39	110.80
1	B	42[A]	HIS	N-CA-C	5.79	119.16	111.75
1	B	42[B]	HIS	N-CA-C	5.79	119.16	111.75
1	F	40	PHE	CB-CA-C	5.63	118.26	109.42
1	E	77	ASN	CA-C-N	5.63	125.24	119.56
1	E	77	ASN	C-N-CA	5.63	125.24	119.56
1	F	101[A]	ARG	CA-C-N	-5.43	115.50	123.00
1	F	101[A]	ARG	C-N-CA	-5.43	115.50	123.00
1	F	101[B]	ARG	CA-C-N	-5.43	115.50	123.00
1	F	101[B]	ARG	C-N-CA	-5.43	115.50	123.00
1	D	77	ASN	CA-C-N	5.36	125.07	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	ASN	C-N-CA	5.36	125.07	119.82
1	G	40	PHE	CB-CA-C	5.30	117.90	109.52
1	C	112	ASP	CA-C-N	-5.18	113.70	119.19
1	C	112	ASP	C-N-CA	-5.18	113.70	119.19
1	G	77	ASN	CA-C-N	5.00	124.60	119.05
1	G	77	ASN	C-N-CA	5.00	124.60	119.05

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54[B]	GLY	Mainchain
1	B	54[A]	GLY	Mainchain
1	C	54[B]	GLY	Mainchain
1	D	54[B]	GLY	Mainchain
1	F	54[B]	GLY	Mainchain
1	G	54[B]	GLY	Mainchain
1	I	54[A]	GLY	Mainchain
1	J	54[B]	GLY	Mainchain

## 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	1248	0	1236	16	0
1	B	1199	0	1184	6	0
1	C	1232	0	1235	10	0
1	D	1197	0	1184	7	0
1	E	1196	0	1180	10	0
1	F	1167	0	1156	12	0
1	G	1171	0	1161	16	0
1	H	1246	0	1231	7	0
1	I	1286	0	1277	8	0
1	J	1145	0	1128	17	0
1	K	1082	0	1076	9	0
1	L	1201	0	1189	15	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	203	0	0	1	0
3	B	195	0	0	0	0
3	C	149	0	0	4	0
3	D	165	0	0	1	0
3	E	147	0	0	1	0
3	F	124	0	0	2	0
3	G	106	0	0	3	0
3	H	188	0	0	0	0
3	I	167	0	0	3	0
3	J	134	0	0	4	0
3	K	118	0	0	0	0
3	L	140	0	0	1	0
All	All	16207	0	14237	115	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 4.

All (115) 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:F:101[A]:ARG:HG2	1:F:101[A]:ARG:HH11	1.28	0.98
1:A:40:PHE:CZ	1:E:73:ALA:O	2.27	0.87
1:G:6:ILE:HG23	1:G:10:ASP:HB2	1.57	0.84
1:B:40:PHE:CZ	1:L:73:ALA:O	2.32	0.83
1:C:73:ALA:O	1:H:40:PHE:HZ	1.65	0.80
1:L:63:MSE:HE3	1:L:67:ILE:HD12	1.62	0.79
1:A:63:MSE:HE2	1:A:64:ILE:HD13	1.63	0.78
1:A:0:MSE:HE3	3:J:292:HOH:O	1.83	0.78
1:A:63:MSE:CE	1:A:64:ILE:HD13	2.17	0.75
1:J:77:ASN:HD21	1:J:79:VAL:HG22	1.51	0.75
1:A:40:PHE:CE1	1:E:76:ILE:HB	2.22	0.74
1:B:40:PHE:CE1	1:L:76:ILE:HG12	2.24	0.73
1:K:63[A]:MSE:HE3	1:K:67:ILE:HD12	1.68	0.73
3:C:317:HOH:O	1:E:95:HIS:HE1	1.73	0.71
1:F:101[A]:ARG:HG2	1:F:101[A]:ARG:NH1	1.96	0.71
1:B:40:PHE:CE1	1:L:73:ALA:O	2.46	0.69
1:G:147:LYS:HB3	3:G:304:HOH:O	1.92	0.69
1:G:40:PHE:HB3	1:G:42[B]:HIS:CE1	2.29	0.67
1:A:-2:GLN:OE1	1:J:15:HIS:HE1	1.78	0.66
1:G:79:VAL:HB	1:G:145:GLU:HB3	1.79	0.64
1:L:29:PHE:HB3	1:L:44[B]:MSE:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:HIS:HE1	1:J:32:HIS:ND1	1.96	0.63
1:A:40:PHE:HZ	1:E:73:ALA:O	1.79	0.63
1:K:17:ARG:HD3	1:K:75:LEU:HD13	1.81	0.63
1:F:101[A]:ARG:NH1	3:F:212:HOH:O	2.32	0.62
1:D:79:VAL:CG2	1:D:145:GLU:HB3	2.30	0.61
1:J:12:GLU:HG3	1:J:15:HIS:HB2	1.82	0.61
1:G:110:GLU:HG3	1:G:120:ARG:HB3	1.83	0.61
1:C:73:ALA:O	1:H:40:PHE:CZ	2.51	0.61
1:H:112:ASP:OD2	1:H:115:ARG:HD2	2.01	0.61
1:G:17:ARG:HB3	1:H:1[A]:MSE:HE3	1.83	0.60
1:F:79:VAL:HG13	1:F:145:GLU:HB2	1.83	0.60
1:F:101[A]:ARG:CZ	3:F:212:HOH:O	2.50	0.59
1:K:82:SER:OG	1:K:140:HIS:HE1	1.86	0.59
1:G:24:ILE:HG23	1:G:63[A]:MSE:HE1	1.84	0.59
1:C:42[B]:HIS:HD2	1:C:58:ILE:HD11	1.67	0.59
1:B:40:PHE:HE1	1:L:76:ILE:HG12	1.67	0.59
1:D:79:VAL:HG22	1:D:145:GLU:HB3	1.84	0.58
1:B:40:PHE:HZ	1:L:73:ALA:O	1.84	0.58
1:L:74:SER:O	1:L:76:ILE:HG13	2.04	0.58
1:J:17:ARG:HD2	1:J:75:LEU:HD13	1.86	0.58
1:L:30:VAL:HG22	1:L:44[A]:MSE:HE1	1.86	0.58
1:J:17:ARG:CD	1:J:75:LEU:HD13	2.34	0.58
1:K:17:ARG:CD	1:K:75:LEU:HD13	2.34	0.57
1:A:86:ASP:OD2	1:A:141:ILE:HD11	2.05	0.56
1:G:40:PHE:HB3	1:G:42[B]:HIS:HE1	1.69	0.56
1:F:59:ALA:HB1	1:F:63[A]:MSE:HE2	1.87	0.56
1:A:63:MSE:HE2	1:A:64:ILE:CD1	2.34	0.55
1:G:63[A]:MSE:HE3	1:G:67:ILE:HD12	1.88	0.55
1:F:101[A]:ARG:HH11	1:F:101[A]:ARG:CG	2.12	0.54
1:A:-2:GLN:OE1	1:J:15:HIS:CE1	2.60	0.54
1:D:79:VAL:HG22	1:D:145:GLU:CB	2.38	0.54
1:J:73:ALA:HA	1:J:76:ILE:HG23	1.89	0.54
1:G:5:THR:HG22	1:G:78:PRO:HG2	1.89	0.53
1:L:93:PRO:HG2	3:L:289:HOH:O	2.08	0.53
1:F:35:HIS:HD2	3:J:204:HOH:O	1.91	0.52
1:I:87:ARG:NH2	3:I:349:HOH:O	2.40	0.52
1:J:4:GLN:HA	3:J:294:HOH:O	2.08	0.52
1:F:18:LEU:HD13	1:F:101[B]:ARG:CZ	2.41	0.51
1:I:58:ILE:HD12	3:I:365:HOH:O	2.10	0.51
1:H:9:GLU:OE1	1:H:147:LYS:HG3	2.10	0.51
1:K:24:ILE:CG2	1:K:63[A]:MSE:HE1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:ARG:HD2	3:I:334:HOH:O	2.10	0.50
1:K:17:ARG:HD3	1:K:75:LEU:HD22	1.92	0.50
1:G:124:ARG:NH1	3:G:297:HOH:O	2.38	0.50
1:K:24:ILE:HG23	1:K:63[A]:MSE:HE1	1.94	0.50
1:A:86:ASP:CG	1:A:141:ILE:HD11	2.36	0.50
1:G:24:ILE:CG2	1:G:63[A]:MSE:HE1	2.41	0.49
1:B:86:ASP:CG	1:B:141:ILE:HD11	2.37	0.49
1:L:63:MSE:HE2	1:L:64:ILE:HD13	1.95	0.48
1:A:63:MSE:CE	1:A:64:ILE:CD1	2.90	0.48
1:J:5:THR:HG23	1:J:79:VAL:HG21	1.96	0.47
1:J:4:GLN:HG2	1:J:5:THR:H	1.80	0.47
1:L:43:HIS:O	1:L:44[B]:MSE:HE2	2.15	0.46
1:G:82:SER:HB2	3:G:282:HOH:O	2.15	0.46
1:A:40:PHE:CZ	1:E:76:ILE:HB	2.51	0.46
1:F:101[A]:ARG:NH1	1:F:101[A]:ARG:CG	2.74	0.46
3:C:264:HOH:O	1:L:76:ILE:HD13	2.16	0.45
1:F:35:HIS:CE1	1:J:32:HIS:ND1	2.82	0.45
1:J:17:ARG:HD3	1:J:75:LEU:HD22	1.98	0.45
1:H:41:PRO:HB2	1:H:48:PHE:CD2	2.52	0.45
1:C:124[A]:ARG:HD2	1:C:139:ASP:OD1	2.17	0.45
1:C:86:ASP:OD2	1:C:141:ILE:HD11	2.17	0.45
1:D:42[B]:HIS:H	1:D:42[B]:HIS:CD2	2.35	0.45
1:C:120[B]:ARG:NH1	3:C:274:HOH:O	2.44	0.44
1:I:40:PHE:HB3	1:I:42[B]:HIS:CD2	2.53	0.44
1:A:17:ARG:NH2	3:A:394:HOH:O	2.48	0.43
1:C:5:THR:HG23	1:C:79:VAL:HG22	2.01	0.43
3:C:317:HOH:O	1:E:95:HIS:CE1	2.57	0.43
1:E:74:SER:HB3	3:E:276:HOH:O	2.19	0.43
1:I:147:LYS:HB3	1:I:147:LYS:HE2	1.90	0.43
1:I:124:ARG:HD2	1:I:139:ASP:OD1	2.19	0.43
1:G:9:GLU:HG3	1:G:147:LYS:HE3	2.01	0.42
1:J:77:ASN:ND2	1:J:79:VAL:HG22	2.25	0.42
1:K:56:GLN:HG3	1:K:95:HIS:CD2	2.55	0.42
1:G:146:ARG:O	1:G:147:LYS:C	2.62	0.42
1:L:3:GLU:N	1:L:76:ILE:HD12	2.35	0.42
1:J:112:ASP:HA	1:J:113:PRO:HD3	1.92	0.42
1:G:40:PHE:CE1	1:K:76:ILE:HG12	2.54	0.42
1:I:79:VAL:HB	1:I:145:GLU:HB2	2.02	0.41
1:E:30:VAL:HG22	1:E:44:MSE:HE1	2.02	0.41
1:I:-3:PHE:HA	1:I:0[B]:MSE:HE3	2.01	0.41
1:C:5:THR:HG21	1:C:7:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.89	0.41
1:A:40:PHE:HD1	1:A:40:PHE:HA	1.76	0.41
1:A:40:PHE:CE1	1:E:73:ALA:O	2.71	0.41
1:D:13[B]:GLN:NE2	3:D:336:HOH:O	2.54	0.41
1:L:79:VAL:HG13	1:L:79:VAL:O	2.21	0.41
1:E:44:MSE:HB2	3:J:272:HOH:O	2.21	0.40
1:J:73:ALA:C	1:J:75:LEU:H	2.28	0.40
1:H:1[B]:MSE:HE3	1:H:1[B]:MSE:HB3	1.81	0.40
1:J:17:ARG:HD3	1:J:75:LEU:HD13	2.02	0.40
1:C:7:TYR:CE1	1:C:148:PRO:HD3	2.56	0.40
1:D:112:ASP:HA	1:D:113:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/176 (90%)	158 (100%)	0	0	100	100
1	B	152/176 (86%)	151 (99%)	1 (1%)	0	100	100
1	C	156/176 (89%)	155 (99%)	0	1 (1%)	21	11
1	D	152/176 (86%)	151 (99%)	1 (1%)	0	100	100
1	E	150/176 (85%)	148 (99%)	2 (1%)	0	100	100
1	F	147/176 (84%)	147 (100%)	0	0	100	100
1	G	148/176 (84%)	146 (99%)	2 (1%)	0	100	100
1	H	157/176 (89%)	155 (99%)	2 (1%)	0	100	100
1	I	163/176 (93%)	163 (100%)	0	0	100	100
1	J	145/176 (82%)	141 (97%)	4 (3%)	0	100	100
1	K	134/176 (76%)	132 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	151/176 (86%)	150 (99%)	1 (1%)	0	100	100
All	All	1813/2112 (86%)	1797 (99%)	15 (1%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	74	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	134/143 (94%)	133 (99%)	1 (1%)	76	73
1	B	128/143 (90%)	128 (100%)	0	100	100
1	C	131/143 (92%)	130 (99%)	1 (1%)	73	70
1	D	128/143 (90%)	126 (98%)	2 (2%)	55	47
1	E	126/143 (88%)	125 (99%)	1 (1%)	73	70
1	F	123/143 (86%)	118 (96%)	5 (4%)	27	15
1	G	124/143 (87%)	119 (96%)	5 (4%)	28	15
1	H	134/143 (94%)	133 (99%)	1 (1%)	76	73
1	I	139/143 (97%)	138 (99%)	1 (1%)	76	73
1	J	121/143 (85%)	119 (98%)	2 (2%)	53	45
1	K	115/143 (80%)	113 (98%)	2 (2%)	53	45
1	L	127/143 (89%)	125 (98%)	2 (2%)	55	47
All	All	1530/1716 (89%)	1507 (98%)	23 (2%)	61	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	C	76	ILE

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Mol	Chain	Res	Type
1	D	13[A]	GLN
1	D	13[B]	GLN
1	E	76	ILE
1	F	18	LEU
1	F	75	LEU
1	F	79	VAL
1	F	101[A]	ARG
1	F	101[B]	ARG
1	G	9	GLU
1	G	53[A]	PRO
1	G	53[B]	PRO
1	G	76	ILE
1	G	114	LYS
1	H	87	ARG
1	I	3	GLU
1	J	5	THR
1	J	75	LEU
1	K	76	ILE
1	K	79	VAL
1	L	76	ILE
1	L	79	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	HIS
1	A	56	GLN
1	E	56	GLN
1	E	95	HIS
1	F	35	HIS
1	G	15	HIS
1	J	15	HIS
1	J	77	ASN
1	K	95	HIS
1	K	140	HIS
1	L	153	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	151/176 (85%)	-0.34	2 (1%) 75 75	8, 17, 36, 56	5 (3%)
1	B	146/176 (82%)	-0.38	2 (1%) 73 73	8, 18, 30, 65	4 (2%)
1	C	148/176 (84%)	-0.17	8 (5%) 31 30	7, 15, 51, 76	8 (5%)
1	D	145/176 (82%)	-0.18	11 (7%) 20 18	9, 14, 55, 85	6 (4%)
1	E	149/176 (84%)	-0.08	7 (4%) 36 35	10, 20, 49, 69	1 (0%)
1	F	143/176 (81%)	0.12	8 (5%) 30 29	9, 20, 57, 77	3 (2%)
1	G	143/176 (81%)	0.37	21 (14%) 6 4	10, 22, 73, 93	4 (2%)
1	H	152/176 (86%)	-0.25	2 (1%) 75 75	6, 17, 46, 57	2 (1%)
1	I	153/176 (86%)	-0.12	4 (2%) 57 57	7, 18, 48, 74	7 (4%)
1	J	141/176 (80%)	0.18	18 (12%) 7 6	8, 19, 72, 114	4 (2%)
1	K	133/176 (75%)	0.09	11 (8%) 17 15	9, 21, 64, 71	2 (1%)
1	L	149/176 (84%)	0.03	7 (4%) 36 35	11, 21, 56, 88	1 (0%)
All	All	1753/2112 (83%)	-0.06	101 (5%) 29 27	6, 18, 57, 114	47 (2%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	76	ILE	7.2
1	E	76	ILE	7.0
1	A	-5	LEU	5.5
1	J	117	GLY	5.4
1	F	75	LEU	5.2
1	J	118	ALA	4.8
1	J	116	PRO	4.6
1	C	76	ILE	4.5
1	K	76	ILE	4.5
1	G	113	PRO	4.4
1	E	75	LEU	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	116	PRO	4.1
1	I	113	PRO	3.9
1	G	75	LEU	3.8
1	L	75	LEU	3.8
1	D	76	ILE	3.7
1	E	150	GLY	3.7
1	J	7	TYR	3.7
1	J	113	PRO	3.5
1	G	40	PHE	3.4
1	D	74	SER	3.4
1	C	75	LEU	3.4
1	G	74	SER	3.3
1	F	113	PRO	3.2
1	G	6	ILE	3.2
1	J	80	ALA	3.1
1	G	7	TYR	3.1
1	K	7	TYR	3.1
1	J	75	LEU	3.1
1	K	78	PRO	3.1
1	I	75	LEU	3.1
1	G	78	PRO	3.0
1	J	76	ILE	2.9
1	J	111	ASP	2.8
1	J	6	ILE	2.8
1	J	112	ASP	2.8
1	C	113	PRO	2.8
1	G	112	ASP	2.8
1	J	4	GLN	2.8
1	F	5	THR	2.8
1	G	76	ILE	2.8
1	D	114	LYS	2.7
1	K	80	ALA	2.7
1	C	78	PRO	2.7
1	D	113	PRO	2.7
1	L	148	PRO	2.7
1	G	114	LYS	2.7
1	K	79	VAL	2.7
1	G	117	GLY	2.7
1	K	145	GLU	2.6
1	E	3	GLU	2.6
1	D	4	GLN	2.5
1	D	75	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	75	LEU	2.5
1	K	5	THR	2.5
1	E	148	PRO	2.5
1	G	147	LYS	2.5
1	K	6	ILE	2.4
1	G	145	GLU	2.4
1	F	81	PHE	2.4
1	F	6	ILE	2.4
1	J	78	PRO	2.4
1	D	111	ASP	2.4
1	B	-1	SER	2.3
1	K	17	ARG	2.3
1	A	40	PHE	2.3
1	F	76	ILE	2.3
1	C	116	PRO	2.3
1	F	79	VAL	2.3
1	E	147	LYS	2.3
1	J	79	VAL	2.3
1	D	149	GLU	2.2
1	J	115	ARG	2.2
1	G	3	GLU	2.2
1	B	114	LYS	2.2
1	G	5	THR	2.2
1	G	11	TYR	2.2
1	D	115	ARG	2.2
1	J	5	THR	2.2
1	C	74	SER	2.2
1	F	78	PRO	2.2
1	L	113	PRO	2.2
1	G	111	ASP	2.1
1	L	150	GLY	2.1
1	C	114	LYS	2.1
1	G	81	PHE	2.1
1	D	79	VAL	2.1
1	I	149	GLU	2.1
1	J	77	ASN	2.1
1	C	112	ASP	2.1
1	I	114	LYS	2.1
1	L	3	GLU	2.1
1	G	4	GLN	2.1
1	G	118	ALA	2.1
1	K	119	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	113	PRO	2.0
1	D	118	ALA	2.0
1	J	146	ARG	2.0
1	L	112	ASP	2.0
1	E	151	THR	2.0
1	H	148	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	H	201	1/1	0.97	0.04	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.