



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 PM UTC

PDB ID : 8S33 / pdb_00008s33
Title : Malic semialdehyde dehydrogenase (MSA-DH) from *Acinetobacter baumannii*
Authors : Piskol, F.; Lukat, P.; Blankenfeldt, W.; Jahn, D.; Moser, J.
Deposited on : 2024-02-19
Resolution : 2.59 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

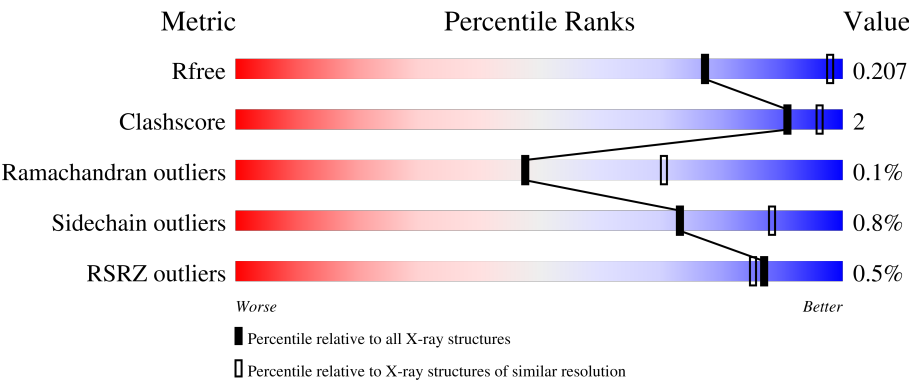
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	510	91%5%
1	B	510	% 90%5%
1	C	510	% 88%6%5%
1	D	510	92%5%
1	E	510	93%5%

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Mol	Chain	Length	Quality of chain
1	F	510	91% 5%
1	G	510	90% 5% 5%
1	H	510	90% 5% 5%
1	I	510	% 88% 6% 5%
1	J	510	% 90% 6%
1	K	510	91% 5%
1	L	510	% 89% 5% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 89169 atoms, of which 44306 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 Succinate-semialdehyde dehydrogenase [NAD(P)+].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	483	Total	C	H	N	O	S	0	0	0
			7350	2333	3689	618	694	16			
1	B	483	Total	C	H	N	O	S	0	0	0
			7348	2333	3687	617	695	16			
1	C	482	Total	C	H	N	O	S	0	0	0
			7324	2326	3674	616	692	16			
1	D	483	Total	C	H	N	O	S	0	0	0
			7351	2334	3688	618	695	16			
1	E	482	Total	C	H	N	O	S	0	0	0
			7320	2326	3668	616	694	16			
1	F	482	Total	C	H	N	O	S	0	0	0
			7331	2328	3677	616	694	16			
1	G	482	Total	C	H	N	O	S	0	0	0
			7341	2330	3683	617	695	16			
1	H	483	Total	C	H	N	O	S	0	0	0
			7351	2334	3688	618	695	16			
1	I	482	Total	C	H	N	O	S	0	0	0
			7332	2328	3678	616	694	16			
1	J	481	Total	C	H	N	O	S	0	1	0
			7331	2328	3678	616	692	17			
1	K	482	Total	C	H	N	O	S	0	0	0
			7317	2325	3669	616	691	16			
1	L	482	Total	C	H	N	O	S	0	0	0
			7326	2327	3674	617	692	16			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP D0C9N7
A	-25	LYS	-	expression tag	UNP D0C9N7
A	-24	HIS	-	expression tag	UNP D0C9N7
A	-23	HIS	-	expression tag	UNP D0C9N7
A	-22	HIS	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	HIS	-	expression tag	UNP D0C9N7
A	-20	HIS	-	expression tag	UNP D0C9N7
A	-19	HIS	-	expression tag	UNP D0C9N7
A	-18	PRO	-	expression tag	UNP D0C9N7
A	-17	MET	-	expression tag	UNP D0C9N7
A	-16	SER	-	expression tag	UNP D0C9N7
A	-15	ASP	-	expression tag	UNP D0C9N7
A	-14	TYR	-	expression tag	UNP D0C9N7
A	-13	ASP	-	expression tag	UNP D0C9N7
A	-12	ILE	-	expression tag	UNP D0C9N7
A	-11	PRO	-	expression tag	UNP D0C9N7
A	-10	THR	-	expression tag	UNP D0C9N7
A	-9	THR	-	expression tag	UNP D0C9N7
A	-8	GLU	-	expression tag	UNP D0C9N7
A	-7	ASN	-	expression tag	UNP D0C9N7
A	-6	LEU	-	expression tag	UNP D0C9N7
A	-5	TYR	-	expression tag	UNP D0C9N7
A	-4	PHE	-	expression tag	UNP D0C9N7
A	-3	GLN	-	expression tag	UNP D0C9N7
A	-2	GLY	-	expression tag	UNP D0C9N7
A	-1	ALA	-	expression tag	UNP D0C9N7
A	0	MET	-	expression tag	UNP D0C9N7
A	1	VAL	-	expression tag	UNP D0C9N7
B	-26	MET	-	initiating methionine	UNP D0C9N7
B	-25	LYS	-	expression tag	UNP D0C9N7
B	-24	HIS	-	expression tag	UNP D0C9N7
B	-23	HIS	-	expression tag	UNP D0C9N7
B	-22	HIS	-	expression tag	UNP D0C9N7
B	-21	HIS	-	expression tag	UNP D0C9N7
B	-20	HIS	-	expression tag	UNP D0C9N7
B	-19	HIS	-	expression tag	UNP D0C9N7
B	-18	PRO	-	expression tag	UNP D0C9N7
B	-17	MET	-	expression tag	UNP D0C9N7
B	-16	SER	-	expression tag	UNP D0C9N7
B	-15	ASP	-	expression tag	UNP D0C9N7
B	-14	TYR	-	expression tag	UNP D0C9N7
B	-13	ASP	-	expression tag	UNP D0C9N7
B	-12	ILE	-	expression tag	UNP D0C9N7
B	-11	PRO	-	expression tag	UNP D0C9N7
B	-10	THR	-	expression tag	UNP D0C9N7
B	-9	THR	-	expression tag	UNP D0C9N7
B	-8	GLU	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	ASN	-	expression tag	UNP D0C9N7
B	-6	LEU	-	expression tag	UNP D0C9N7
B	-5	TYR	-	expression tag	UNP D0C9N7
B	-4	PHE	-	expression tag	UNP D0C9N7
B	-3	GLN	-	expression tag	UNP D0C9N7
B	-2	GLY	-	expression tag	UNP D0C9N7
B	-1	ALA	-	expression tag	UNP D0C9N7
B	0	MET	-	expression tag	UNP D0C9N7
B	1	VAL	-	expression tag	UNP D0C9N7
C	-26	MET	-	initiating methionine	UNP D0C9N7
C	-25	LYS	-	expression tag	UNP D0C9N7
C	-24	HIS	-	expression tag	UNP D0C9N7
C	-23	HIS	-	expression tag	UNP D0C9N7
C	-22	HIS	-	expression tag	UNP D0C9N7
C	-21	HIS	-	expression tag	UNP D0C9N7
C	-20	HIS	-	expression tag	UNP D0C9N7
C	-19	HIS	-	expression tag	UNP D0C9N7
C	-18	PRO	-	expression tag	UNP D0C9N7
C	-17	MET	-	expression tag	UNP D0C9N7
C	-16	SER	-	expression tag	UNP D0C9N7
C	-15	ASP	-	expression tag	UNP D0C9N7
C	-14	TYR	-	expression tag	UNP D0C9N7
C	-13	ASP	-	expression tag	UNP D0C9N7
C	-12	ILE	-	expression tag	UNP D0C9N7
C	-11	PRO	-	expression tag	UNP D0C9N7
C	-10	THR	-	expression tag	UNP D0C9N7
C	-9	THR	-	expression tag	UNP D0C9N7
C	-8	GLU	-	expression tag	UNP D0C9N7
C	-7	ASN	-	expression tag	UNP D0C9N7
C	-6	LEU	-	expression tag	UNP D0C9N7
C	-5	TYR	-	expression tag	UNP D0C9N7
C	-4	PHE	-	expression tag	UNP D0C9N7
C	-3	GLN	-	expression tag	UNP D0C9N7
C	-2	GLY	-	expression tag	UNP D0C9N7
C	-1	ALA	-	expression tag	UNP D0C9N7
C	0	MET	-	expression tag	UNP D0C9N7
C	1	VAL	-	expression tag	UNP D0C9N7
D	-26	MET	-	initiating methionine	UNP D0C9N7
D	-25	LYS	-	expression tag	UNP D0C9N7
D	-24	HIS	-	expression tag	UNP D0C9N7
D	-23	HIS	-	expression tag	UNP D0C9N7
D	-22	HIS	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	HIS	-	expression tag	UNP D0C9N7
D	-20	HIS	-	expression tag	UNP D0C9N7
D	-19	HIS	-	expression tag	UNP D0C9N7
D	-18	PRO	-	expression tag	UNP D0C9N7
D	-17	MET	-	expression tag	UNP D0C9N7
D	-16	SER	-	expression tag	UNP D0C9N7
D	-15	ASP	-	expression tag	UNP D0C9N7
D	-14	TYR	-	expression tag	UNP D0C9N7
D	-13	ASP	-	expression tag	UNP D0C9N7
D	-12	ILE	-	expression tag	UNP D0C9N7
D	-11	PRO	-	expression tag	UNP D0C9N7
D	-10	THR	-	expression tag	UNP D0C9N7
D	-9	THR	-	expression tag	UNP D0C9N7
D	-8	GLU	-	expression tag	UNP D0C9N7
D	-7	ASN	-	expression tag	UNP D0C9N7
D	-6	LEU	-	expression tag	UNP D0C9N7
D	-5	TYR	-	expression tag	UNP D0C9N7
D	-4	PHE	-	expression tag	UNP D0C9N7
D	-3	GLN	-	expression tag	UNP D0C9N7
D	-2	GLY	-	expression tag	UNP D0C9N7
D	-1	ALA	-	expression tag	UNP D0C9N7
D	0	MET	-	expression tag	UNP D0C9N7
D	1	VAL	-	expression tag	UNP D0C9N7
E	-26	MET	-	initiating methionine	UNP D0C9N7
E	-25	LYS	-	expression tag	UNP D0C9N7
E	-24	HIS	-	expression tag	UNP D0C9N7
E	-23	HIS	-	expression tag	UNP D0C9N7
E	-22	HIS	-	expression tag	UNP D0C9N7
E	-21	HIS	-	expression tag	UNP D0C9N7
E	-20	HIS	-	expression tag	UNP D0C9N7
E	-19	HIS	-	expression tag	UNP D0C9N7
E	-18	PRO	-	expression tag	UNP D0C9N7
E	-17	MET	-	expression tag	UNP D0C9N7
E	-16	SER	-	expression tag	UNP D0C9N7
E	-15	ASP	-	expression tag	UNP D0C9N7
E	-14	TYR	-	expression tag	UNP D0C9N7
E	-13	ASP	-	expression tag	UNP D0C9N7
E	-12	ILE	-	expression tag	UNP D0C9N7
E	-11	PRO	-	expression tag	UNP D0C9N7
E	-10	THR	-	expression tag	UNP D0C9N7
E	-9	THR	-	expression tag	UNP D0C9N7
E	-8	GLU	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ASN	-	expression tag	UNP D0C9N7
E	-6	LEU	-	expression tag	UNP D0C9N7
E	-5	TYR	-	expression tag	UNP D0C9N7
E	-4	PHE	-	expression tag	UNP D0C9N7
E	-3	GLN	-	expression tag	UNP D0C9N7
E	-2	GLY	-	expression tag	UNP D0C9N7
E	-1	ALA	-	expression tag	UNP D0C9N7
E	0	MET	-	expression tag	UNP D0C9N7
E	1	VAL	-	expression tag	UNP D0C9N7
F	-26	MET	-	initiating methionine	UNP D0C9N7
F	-25	LYS	-	expression tag	UNP D0C9N7
F	-24	HIS	-	expression tag	UNP D0C9N7
F	-23	HIS	-	expression tag	UNP D0C9N7
F	-22	HIS	-	expression tag	UNP D0C9N7
F	-21	HIS	-	expression tag	UNP D0C9N7
F	-20	HIS	-	expression tag	UNP D0C9N7
F	-19	HIS	-	expression tag	UNP D0C9N7
F	-18	PRO	-	expression tag	UNP D0C9N7
F	-17	MET	-	expression tag	UNP D0C9N7
F	-16	SER	-	expression tag	UNP D0C9N7
F	-15	ASP	-	expression tag	UNP D0C9N7
F	-14	TYR	-	expression tag	UNP D0C9N7
F	-13	ASP	-	expression tag	UNP D0C9N7
F	-12	ILE	-	expression tag	UNP D0C9N7
F	-11	PRO	-	expression tag	UNP D0C9N7
F	-10	THR	-	expression tag	UNP D0C9N7
F	-9	THR	-	expression tag	UNP D0C9N7
F	-8	GLU	-	expression tag	UNP D0C9N7
F	-7	ASN	-	expression tag	UNP D0C9N7
F	-6	LEU	-	expression tag	UNP D0C9N7
F	-5	TYR	-	expression tag	UNP D0C9N7
F	-4	PHE	-	expression tag	UNP D0C9N7
F	-3	GLN	-	expression tag	UNP D0C9N7
F	-2	GLY	-	expression tag	UNP D0C9N7
F	-1	ALA	-	expression tag	UNP D0C9N7
F	0	MET	-	expression tag	UNP D0C9N7
F	1	VAL	-	expression tag	UNP D0C9N7
G	-26	MET	-	initiating methionine	UNP D0C9N7
G	-25	LYS	-	expression tag	UNP D0C9N7
G	-24	HIS	-	expression tag	UNP D0C9N7
G	-23	HIS	-	expression tag	UNP D0C9N7
G	-22	HIS	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	HIS	-	expression tag	UNP D0C9N7
G	-20	HIS	-	expression tag	UNP D0C9N7
G	-19	HIS	-	expression tag	UNP D0C9N7
G	-18	PRO	-	expression tag	UNP D0C9N7
G	-17	MET	-	expression tag	UNP D0C9N7
G	-16	SER	-	expression tag	UNP D0C9N7
G	-15	ASP	-	expression tag	UNP D0C9N7
G	-14	TYR	-	expression tag	UNP D0C9N7
G	-13	ASP	-	expression tag	UNP D0C9N7
G	-12	ILE	-	expression tag	UNP D0C9N7
G	-11	PRO	-	expression tag	UNP D0C9N7
G	-10	THR	-	expression tag	UNP D0C9N7
G	-9	THR	-	expression tag	UNP D0C9N7
G	-8	GLU	-	expression tag	UNP D0C9N7
G	-7	ASN	-	expression tag	UNP D0C9N7
G	-6	LEU	-	expression tag	UNP D0C9N7
G	-5	TYR	-	expression tag	UNP D0C9N7
G	-4	PHE	-	expression tag	UNP D0C9N7
G	-3	GLN	-	expression tag	UNP D0C9N7
G	-2	GLY	-	expression tag	UNP D0C9N7
G	-1	ALA	-	expression tag	UNP D0C9N7
G	0	MET	-	expression tag	UNP D0C9N7
G	1	VAL	-	expression tag	UNP D0C9N7
H	-26	MET	-	initiating methionine	UNP D0C9N7
H	-25	LYS	-	expression tag	UNP D0C9N7
H	-24	HIS	-	expression tag	UNP D0C9N7
H	-23	HIS	-	expression tag	UNP D0C9N7
H	-22	HIS	-	expression tag	UNP D0C9N7
H	-21	HIS	-	expression tag	UNP D0C9N7
H	-20	HIS	-	expression tag	UNP D0C9N7
H	-19	HIS	-	expression tag	UNP D0C9N7
H	-18	PRO	-	expression tag	UNP D0C9N7
H	-17	MET	-	expression tag	UNP D0C9N7
H	-16	SER	-	expression tag	UNP D0C9N7
H	-15	ASP	-	expression tag	UNP D0C9N7
H	-14	TYR	-	expression tag	UNP D0C9N7
H	-13	ASP	-	expression tag	UNP D0C9N7
H	-12	ILE	-	expression tag	UNP D0C9N7
H	-11	PRO	-	expression tag	UNP D0C9N7
H	-10	THR	-	expression tag	UNP D0C9N7
H	-9	THR	-	expression tag	UNP D0C9N7
H	-8	GLU	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	expression tag	UNP D0C9N7
H	-6	LEU	-	expression tag	UNP D0C9N7
H	-5	TYR	-	expression tag	UNP D0C9N7
H	-4	PHE	-	expression tag	UNP D0C9N7
H	-3	GLN	-	expression tag	UNP D0C9N7
H	-2	GLY	-	expression tag	UNP D0C9N7
H	-1	ALA	-	expression tag	UNP D0C9N7
H	0	MET	-	expression tag	UNP D0C9N7
H	1	VAL	-	expression tag	UNP D0C9N7
I	-26	MET	-	initiating methionine	UNP D0C9N7
I	-25	LYS	-	expression tag	UNP D0C9N7
I	-24	HIS	-	expression tag	UNP D0C9N7
I	-23	HIS	-	expression tag	UNP D0C9N7
I	-22	HIS	-	expression tag	UNP D0C9N7
I	-21	HIS	-	expression tag	UNP D0C9N7
I	-20	HIS	-	expression tag	UNP D0C9N7
I	-19	HIS	-	expression tag	UNP D0C9N7
I	-18	PRO	-	expression tag	UNP D0C9N7
I	-17	MET	-	expression tag	UNP D0C9N7
I	-16	SER	-	expression tag	UNP D0C9N7
I	-15	ASP	-	expression tag	UNP D0C9N7
I	-14	TYR	-	expression tag	UNP D0C9N7
I	-13	ASP	-	expression tag	UNP D0C9N7
I	-12	ILE	-	expression tag	UNP D0C9N7
I	-11	PRO	-	expression tag	UNP D0C9N7
I	-10	THR	-	expression tag	UNP D0C9N7
I	-9	THR	-	expression tag	UNP D0C9N7
I	-8	GLU	-	expression tag	UNP D0C9N7
I	-7	ASN	-	expression tag	UNP D0C9N7
I	-6	LEU	-	expression tag	UNP D0C9N7
I	-5	TYR	-	expression tag	UNP D0C9N7
I	-4	PHE	-	expression tag	UNP D0C9N7
I	-3	GLN	-	expression tag	UNP D0C9N7
I	-2	GLY	-	expression tag	UNP D0C9N7
I	-1	ALA	-	expression tag	UNP D0C9N7
I	0	MET	-	expression tag	UNP D0C9N7
I	1	VAL	-	expression tag	UNP D0C9N7
J	-26	MET	-	initiating methionine	UNP D0C9N7
J	-25	LYS	-	expression tag	UNP D0C9N7
J	-24	HIS	-	expression tag	UNP D0C9N7
J	-23	HIS	-	expression tag	UNP D0C9N7
J	-22	HIS	-	expression tag	UNP D0C9N7

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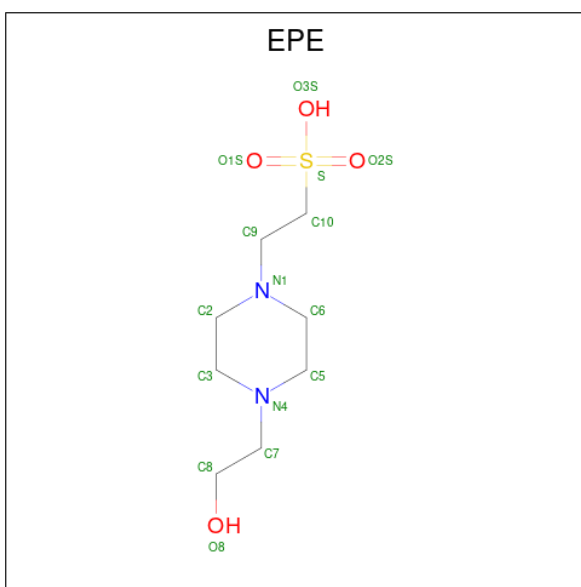
Chain	Residue	Modelled	Actual	Comment	Reference
J	-21	HIS	-	expression tag	UNP D0C9N7
J	-20	HIS	-	expression tag	UNP D0C9N7
J	-19	HIS	-	expression tag	UNP D0C9N7
J	-18	PRO	-	expression tag	UNP D0C9N7
J	-17	MET	-	expression tag	UNP D0C9N7
J	-16	SER	-	expression tag	UNP D0C9N7
J	-15	ASP	-	expression tag	UNP D0C9N7
J	-14	TYR	-	expression tag	UNP D0C9N7
J	-13	ASP	-	expression tag	UNP D0C9N7
J	-12	ILE	-	expression tag	UNP D0C9N7
J	-11	PRO	-	expression tag	UNP D0C9N7
J	-10	THR	-	expression tag	UNP D0C9N7
J	-9	THR	-	expression tag	UNP D0C9N7
J	-8	GLU	-	expression tag	UNP D0C9N7
J	-7	ASN	-	expression tag	UNP D0C9N7
J	-6	LEU	-	expression tag	UNP D0C9N7
J	-5	TYR	-	expression tag	UNP D0C9N7
J	-4	PHE	-	expression tag	UNP D0C9N7
J	-3	GLN	-	expression tag	UNP D0C9N7
J	-2	GLY	-	expression tag	UNP D0C9N7
J	-1	ALA	-	expression tag	UNP D0C9N7
J	0	MET	-	expression tag	UNP D0C9N7
J	1	VAL	-	expression tag	UNP D0C9N7
K	-26	MET	-	initiating methionine	UNP D0C9N7
K	-25	LYS	-	expression tag	UNP D0C9N7
K	-24	HIS	-	expression tag	UNP D0C9N7
K	-23	HIS	-	expression tag	UNP D0C9N7
K	-22	HIS	-	expression tag	UNP D0C9N7
K	-21	HIS	-	expression tag	UNP D0C9N7
K	-20	HIS	-	expression tag	UNP D0C9N7
K	-19	HIS	-	expression tag	UNP D0C9N7
K	-18	PRO	-	expression tag	UNP D0C9N7
K	-17	MET	-	expression tag	UNP D0C9N7
K	-16	SER	-	expression tag	UNP D0C9N7
K	-15	ASP	-	expression tag	UNP D0C9N7
K	-14	TYR	-	expression tag	UNP D0C9N7
K	-13	ASP	-	expression tag	UNP D0C9N7
K	-12	ILE	-	expression tag	UNP D0C9N7
K	-11	PRO	-	expression tag	UNP D0C9N7
K	-10	THR	-	expression tag	UNP D0C9N7
K	-9	THR	-	expression tag	UNP D0C9N7
K	-8	GLU	-	expression tag	UNP D0C9N7

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-7	ASN	-	expression tag	UNP D0C9N7
K	-6	LEU	-	expression tag	UNP D0C9N7
K	-5	TYR	-	expression tag	UNP D0C9N7
K	-4	PHE	-	expression tag	UNP D0C9N7
K	-3	GLN	-	expression tag	UNP D0C9N7
K	-2	GLY	-	expression tag	UNP D0C9N7
K	-1	ALA	-	expression tag	UNP D0C9N7
K	0	MET	-	expression tag	UNP D0C9N7
K	1	VAL	-	expression tag	UNP D0C9N7
L	-26	MET	-	initiating methionine	UNP D0C9N7
L	-25	LYS	-	expression tag	UNP D0C9N7
L	-24	HIS	-	expression tag	UNP D0C9N7
L	-23	HIS	-	expression tag	UNP D0C9N7
L	-22	HIS	-	expression tag	UNP D0C9N7
L	-21	HIS	-	expression tag	UNP D0C9N7
L	-20	HIS	-	expression tag	UNP D0C9N7
L	-19	HIS	-	expression tag	UNP D0C9N7
L	-18	PRO	-	expression tag	UNP D0C9N7
L	-17	MET	-	expression tag	UNP D0C9N7
L	-16	SER	-	expression tag	UNP D0C9N7
L	-15	ASP	-	expression tag	UNP D0C9N7
L	-14	TYR	-	expression tag	UNP D0C9N7
L	-13	ASP	-	expression tag	UNP D0C9N7
L	-12	ILE	-	expression tag	UNP D0C9N7
L	-11	PRO	-	expression tag	UNP D0C9N7
L	-10	THR	-	expression tag	UNP D0C9N7
L	-9	THR	-	expression tag	UNP D0C9N7
L	-8	GLU	-	expression tag	UNP D0C9N7
L	-7	ASN	-	expression tag	UNP D0C9N7
L	-6	LEU	-	expression tag	UNP D0C9N7
L	-5	TYR	-	expression tag	UNP D0C9N7
L	-4	PHE	-	expression tag	UNP D0C9N7
L	-3	GLN	-	expression tag	UNP D0C9N7
L	-2	GLY	-	expression tag	UNP D0C9N7
L	-1	ALA	-	expression tag	UNP D0C9N7
L	0	MET	-	expression tag	UNP D0C9N7
L	1	VAL	-	expression tag	UNP D0C9N7

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	B	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	C	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	D	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	E	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	H	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	J	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	K	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0
2	L	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	63	Total	O	0	0
			63	63		
3	C	79	Total	O	0	0
			79	79		

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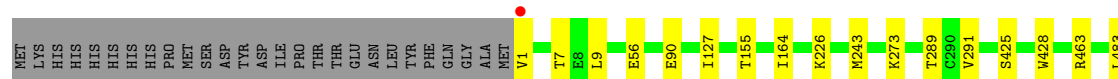
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	50	Total 50	O 50	0	0
3	E	102	Total 102	O 102	0	0
3	F	112	Total 112	O 112	0	0
3	G	98	Total 98	O 98	0	0
3	H	73	Total 73	O 73	0	0
3	I	55	Total 55	O 55	0	0
3	J	55	Total 55	O 55	0	0
3	K	51	Total 51	O 51	0	0
3	L	50	Total 50	O 50	0	0

3 Residue-property plots [i](#)

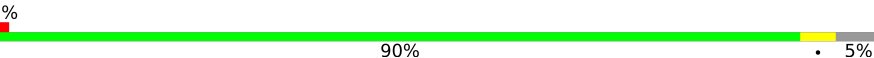
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

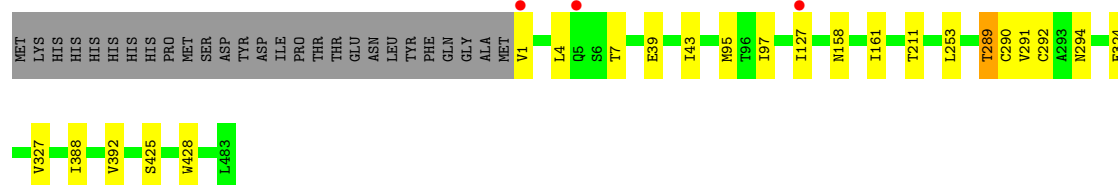
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain A:  91% 5%



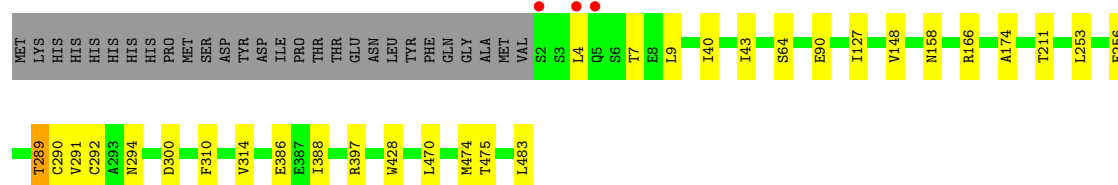
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain B:  90% 5%

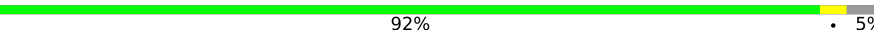


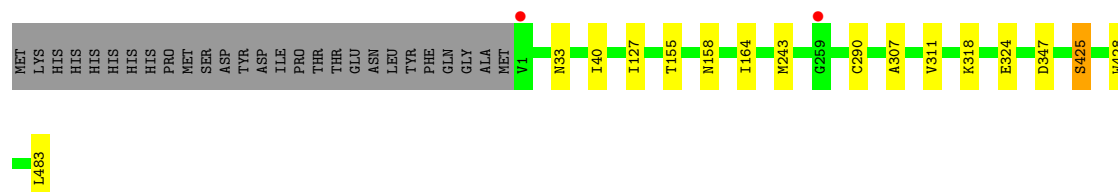
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain C:  88% 6% 5%



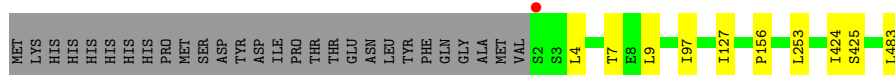
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain D:  92% 5%



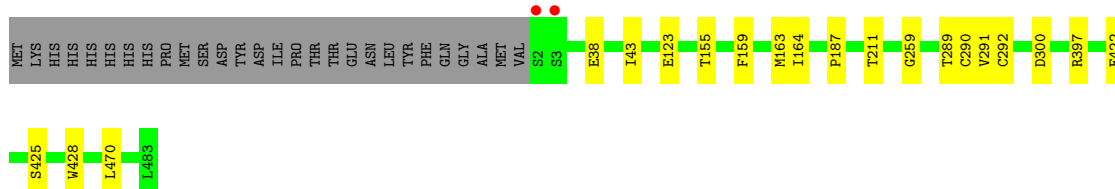
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain E:  93% 5%



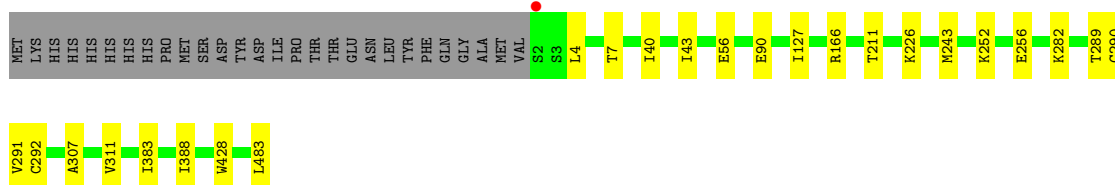
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain F:  91% 5%



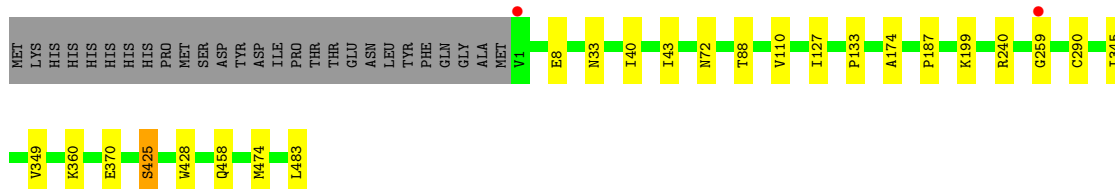
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain G:  90% 5% 5%



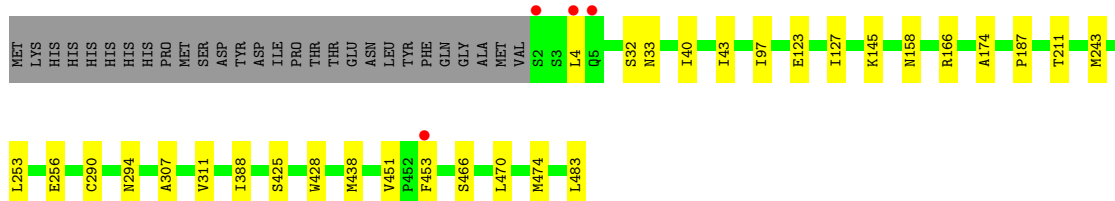
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain H:  90% 5% 5%

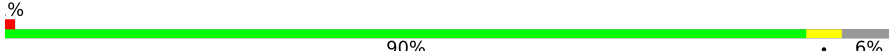


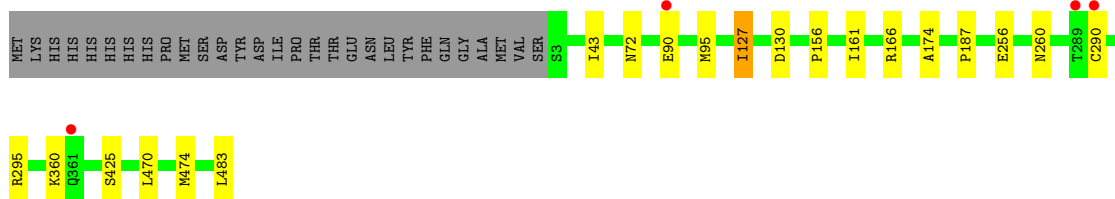
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain I:  88% 6% 5%

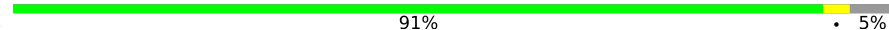


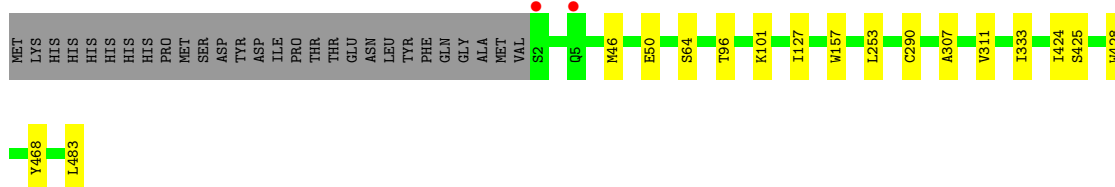
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain J:  90% 6%

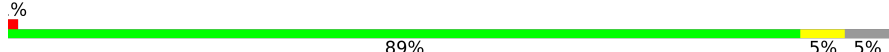


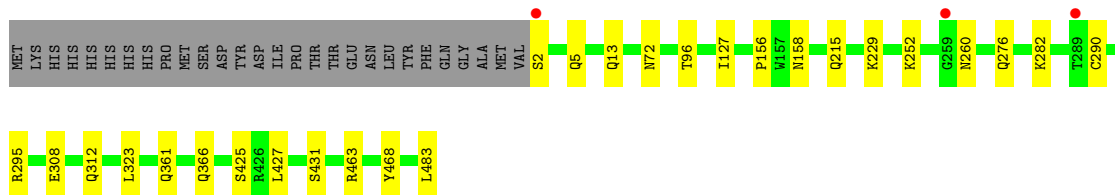
- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain K:  91% 5%



- Molecule 1: Succinate-semialdehyde dehydrogenase [NAD(P)+]

Chain L:  89% 5% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.97Å 194.29Å 454.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.59 19.80 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.80-2.59) 99.3 (19.80-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.59Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.180 , 0.207 0.180 , 0.207	Depositor DCC
R_{free} test set	15955 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtrriage
Anisotropy	0.526	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	89169	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 35.41 % 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 5.8576e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.10	0/3728	0.24	0/5060
1	B	0.10	0/3728	0.24	0/5060
1	C	0.10	0/3717	0.25	0/5045
1	D	0.11	0/3730	0.24	0/5062
1	E	0.10	0/3719	0.25	0/5048
1	F	0.10	0/3721	0.25	0/5050
1	G	0.10	0/3725	0.26	0/5055
1	H	0.10	0/3730	0.25	0/5062
1	I	0.10	0/3721	0.25	0/5050
1	J	0.11	0/3723	0.25	0/5052
1	K	0.10	0/3715	0.25	0/5042
1	L	0.10	0/3719	0.26	0/5047
All	All	0.10	0/44676	0.25	0/60633

There are no bond length outliers.

There are no bond angle outliers.

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	3661	3689	3691	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3661	3687	3689	14	0
1	C	3650	3674	3673	18	0
1	D	3663	3688	3690	9	0
1	E	3652	3668	3667	9	0
1	F	3654	3677	3677	12	0
1	G	3658	3683	3683	19	0
1	H	3663	3688	3690	14	0
1	I	3654	3678	3677	22	0
1	J	3653	3678	3678	12	0
1	K	3648	3669	3668	11	0
1	L	3652	3674	3674	16	0
2	A	15	17	17	0	0
2	B	15	17	17	0	0
2	C	15	17	17	0	0
2	D	15	17	17	0	0
2	E	15	17	17	0	0
2	H	15	17	17	0	0
2	J	15	17	17	0	0
2	K	15	17	17	0	0
2	L	15	17	17	0	0
3	A	71	0	0	2	0
3	B	63	0	0	0	0
3	C	79	0	0	0	0
3	D	50	0	0	0	0
3	E	102	0	0	0	0
3	F	112	0	0	1	0
3	G	98	0	0	1	0
3	H	73	0	0	2	0
3	I	55	0	0	0	0
3	J	55	0	0	0	0
3	K	51	0	0	0	0
3	L	50	0	0	1	0
All	All	44863	44306	44310	147	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 2.

All (147) 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:G:4:LEU:H	1:G:4:LEU:HD23	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:90:GLU:N	1:J:90:GLU:OE1	2.26	0.67
1:H:259:GLY:O	3:H:601:HOH:O	2.12	0.67
1:I:33:ASN:N	1:I:40:ILE:HD11	2.10	0.66
1:H:240:ARG:NH1	1:H:458:GLN:OE1	2.30	0.64
1:G:4:LEU:HD11	1:G:40:ILE:CG2	2.26	0.64
1:E:424:ILE:HD12	1:E:424:ILE:H	1.63	0.63
1:I:307:ALA:O	1:I:311:VAL:HG23	2.00	0.62
1:C:294:ASN:OD1	1:C:388:ILE:HD12	2.00	0.61
1:G:7:THR:OG1	1:G:90:GLU:OE1	2.18	0.61
1:H:345:ILE:O	1:H:349:VAL:HG23	2.00	0.61
1:D:307:ALA:O	1:D:311:VAL:HG23	2.01	0.60
1:K:127:ILE:O	1:K:127:ILE:HG23	2.02	0.60
1:B:4:LEU:O	1:B:7:THR:HG22	2.02	0.59
1:H:8:GLU:OE2	1:H:199:LYS:NZ	2.34	0.59
1:C:388:ILE:HD12	1:C:388:ILE:H	1.68	0.58
1:A:56:GLU:OE1	1:A:226:LYS:NZ	2.37	0.58
1:B:388:ILE:HD13	1:B:392:VAL:HB	1.85	0.58
1:E:425:SER:OG	1:H:483:LEU:OXT	2.22	0.58
1:A:425:SER:OG	1:D:483:LEU:OXT	2.24	0.56
1:H:127:ILE:O	1:H:127:ILE:HG23	2.05	0.56
1:E:127:ILE:HG23	1:E:127:ILE:O	2.06	0.56
1:I:294:ASN:OD1	1:I:388:ILE:HD12	2.06	0.56
1:C:7:THR:HG23	1:C:90:GLU:OE1	2.07	0.55
1:D:127:ILE:O	1:D:127:ILE:HG23	2.05	0.55
1:K:425:SER:OG	1:L:483:LEU:OXT	2.24	0.55
1:B:127:ILE:HD12	1:B:127:ILE:O	2.07	0.55
1:F:425:SER:OG	1:G:483:LEU:OXT	2.26	0.54
1:B:127:ILE:O	1:B:127:ILE:CD1	2.56	0.53
1:L:127:ILE:O	1:L:127:ILE:HG23	2.09	0.53
1:C:166:ARG:NH2	1:C:256:GLU:OE1	2.42	0.52
1:I:388:ILE:HD12	1:I:388:ILE:H	1.74	0.52
1:A:483:LEU:OXT	1:D:425:SER:OG	2.27	0.52
1:I:166:ARG:NH2	1:I:256:GLU:OE1	2.43	0.52
1:A:127:ILE:O	1:A:127:ILE:HG23	2.10	0.51
1:E:424:ILE:HD11	1:F:422:GLU:O	2.10	0.51
1:J:43:ILE:HD13	1:J:187:PRO:HG3	1.92	0.51
1:C:4:LEU:H	1:C:4:LEU:HD23	1.75	0.50
1:A:463:ARG:NE	3:A:602:HOH:O	2.37	0.50
1:F:289:THR:HG22	1:F:291:VAL:H	1.75	0.50
1:L:463:ARG:NE	3:L:603:HOH:O	2.45	0.50
1:I:4:LEU:HD11	1:I:97:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:360:LYS:NZ	1:H:370:GLU:OE2	2.46	0.49
1:G:166:ARG:NH2	1:G:256:GLU:OE1	2.46	0.49
1:I:438:MET:HE1	1:I:453:PHE:CD2	2.48	0.49
1:L:361:GLN:NE2	1:L:366:GLN:O	2.46	0.49
1:I:174:ALA:HB1	1:I:474:MET:SD	2.53	0.49
1:I:4:LEU:HD12	1:I:40:ILE:HG23	1.95	0.49
1:I:145:LYS:NZ	1:K:468:TYR:OH	2.45	0.49
1:B:294:ASN:OD1	1:B:388:ILE:HG22	2.12	0.48
1:G:289:THR:HG22	1:G:291:VAL:H	1.78	0.48
1:L:96:THR:HG21	1:L:323:LEU:HD23	1.94	0.48
1:H:33:ASN:HB2	1:H:40:ILE:HD11	1.94	0.48
1:J:127:ILE:HD12	1:J:127:ILE:O	2.13	0.48
1:D:33:ASN:HB2	1:D:40:ILE:HD11	1.95	0.48
1:L:5:GLN:OE1	1:L:5:GLN:N	2.45	0.48
1:E:7:THR:HG22	1:E:9:LEU:H	1.79	0.48
1:L:427:LEU:O	1:L:431:SER:OG	2.19	0.48
1:G:383:ILE:CG1	1:G:388:ILE:HD11	2.44	0.48
1:G:4:LEU:HD11	1:G:40:ILE:HG22	1.94	0.47
1:E:424:ILE:HD12	1:E:424:ILE:N	2.29	0.47
1:L:260:ASN:O	1:L:295:ARG:NH1	2.46	0.47
1:K:96:THR:HG23	1:K:101:LYS:O	2.15	0.47
1:K:483:LEU:OXT	1:L:425:SER:OG	2.32	0.47
1:I:243:MET:HE3	1:K:253:LEU:HD11	1.96	0.47
1:B:289:THR:HG22	1:B:291:VAL:H	1.79	0.47
1:K:424:ILE:HD12	1:K:424:ILE:H	1.79	0.47
1:C:289:THR:HG22	1:C:291:VAL:H	1.79	0.47
1:F:38:GLU:HA	1:L:215:GLN:HE22	1.80	0.47
1:G:289:THR:HB	1:G:292:CYS:SG	2.55	0.47
1:J:174:ALA:HB1	1:J:474:MET:SD	2.56	0.46
1:F:43:ILE:HD12	1:F:211:THR:HB	1.97	0.46
1:I:32:SER:C	1:I:40:ILE:HD11	2.40	0.46
1:L:229:LYS:HG3	1:L:252:LYS:HB2	1.97	0.46
1:E:483:LEU:OXT	1:H:425:SER:OG	2.34	0.45
1:G:4:LEU:O	1:G:7:THR:HG22	2.17	0.45
1:G:127:ILE:HG13	1:H:133:PRO:HG3	1.97	0.45
1:A:7:THR:HG21	1:A:90:GLU:HB3	1.98	0.45
1:A:273:LYS:NZ	3:A:605:HOH:O	2.48	0.45
1:C:4:LEU:HD11	1:C:40:ILE:CG2	2.46	0.45
1:G:252:LYS:NZ	3:G:508:HOH:O	2.49	0.45
1:A:289:THR:HG22	1:A:291:VAL:H	1.82	0.45
1:H:72:ASN:OD1	3:H:602:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:260:ASN:O	1:J:295:ARG:NH1	2.50	0.45
1:B:425:SER:OG	1:C:483:LEU:OXT	2.34	0.45
1:I:127:ILE:CG2	1:I:470:LEU:HD23	2.47	0.45
1:I:43:ILE:HD12	1:I:211:THR:HB	2.00	0.44
1:J:130:ASP:OD2	1:L:468:TYR:OH	2.30	0.44
1:K:157:TRP:CZ2	1:K:333:ILE:HG21	2.52	0.44
1:L:308:GLU:O	1:L:312:GLN:HG3	2.17	0.44
1:B:1:VAL:HG11	1:B:97:ILE:HD13	1.98	0.44
1:E:253:LEU:HD11	1:G:243:MET:HE3	1.99	0.44
1:C:174:ALA:HB1	1:C:474:MET:SD	2.57	0.44
1:C:289:THR:HB	1:C:292:CYS:SG	2.58	0.44
1:E:4:LEU:HD11	1:E:97:ILE:HG21	1.99	0.44
1:J:166:ARG:NH2	1:J:256:GLU:OE1	2.51	0.43
1:I:483:LEU:OXT	1:J:425:SER:OG	2.36	0.43
1:J:127:ILE:CG2	1:J:470:LEU:HD23	2.47	0.43
1:A:7:THR:HG22	1:A:9:LEU:H	1.84	0.43
1:B:289:THR:HB	1:B:292:CYS:SG	2.59	0.43
1:F:123:GLU:HB3	1:F:470:LEU:HD22	2.01	0.43
1:I:243:MET:HG3	1:I:253:LEU:HD13	2.00	0.43
1:B:43:ILE:HD12	1:B:211:THR:HB	2.01	0.43
1:I:40:ILE:H	1:I:40:ILE:HD12	1.84	0.43
1:D:155:THR:HG21	1:D:164:ILE:HD13	2.01	0.42
1:I:123:GLU:HB3	1:I:470:LEU:HD22	2.01	0.42
1:G:43:ILE:HD12	1:G:211:THR:HB	2.02	0.42
1:B:324:GLU:HB2	1:B:327:VAL:HG21	2.01	0.42
1:F:43:ILE:HD13	1:F:187:PRO:HG3	2.02	0.42
1:F:259:GLY:O	3:F:501:HOH:O	2.22	0.42
1:D:318:LYS:NZ	1:D:324:GLU:OE2	2.51	0.42
1:G:56:GLU:OE1	1:G:226:LYS:NZ	2.49	0.42
1:A:155:THR:HG21	1:A:164:ILE:HD13	2.02	0.42
1:A:243:MET:HE3	1:C:253:LEU:HD11	2.02	0.42
1:H:174:ALA:HB1	1:H:474:MET:SD	2.60	0.42
1:L:276:GLN:HA	1:L:276:GLN:OE1	2.19	0.42
1:F:289:THR:HB	1:F:292:CYS:SG	2.60	0.42
1:G:282:LYS:HD3	1:G:282:LYS:C	2.45	0.42
1:G:383:ILE:HG12	1:G:388:ILE:HD11	2.02	0.42
1:G:307:ALA:O	1:G:311:VAL:HG23	2.20	0.41
1:B:253:LEU:HD11	1:D:243:MET:HE3	2.02	0.41
1:C:127:ILE:HG22	1:C:470:LEU:HD23	2.02	0.41
1:C:148:VAL:HG12	1:C:475:THR:HG23	2.02	0.41
1:L:323:LEU:HD23	1:L:323:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ASP:OD1	1:J:360:LYS:NZ	2.53	0.41
1:I:451:VAL:C	1:I:466:SER:HB3	2.45	0.41
1:B:95:MET:CE	1:B:161:ILE:HD12	2.50	0.41
1:F:155:THR:HG21	1:F:164:ILE:HD13	2.01	0.41
1:B:127:ILE:HD12	1:B:127:ILE:C	2.45	0.41
1:I:438:MET:HE1	1:I:453:PHE:CE2	2.55	0.41
1:K:307:ALA:O	1:K:311:VAL:HG23	2.20	0.41
1:C:7:THR:HG22	1:C:9:LEU:H	1.85	0.41
1:C:43:ILE:HD12	1:C:211:THR:HB	2.03	0.41
1:F:159:PHE:O	1:F:163:MET:HG2	2.21	0.41
1:C:310:PHE:O	1:C:314:VAL:HG23	2.21	0.41
1:F:300:ASP:OD1	1:F:397:ARG:NH1	2.46	0.41
1:G:282:LYS:HD3	1:G:282:LYS:O	2.21	0.41
1:H:43:ILE:HD13	1:H:187:PRO:HG3	2.02	0.40
1:H:88:THR:HA	1:H:110:VAL:HG11	2.03	0.40
1:I:425:SER:OG	1:J:483:LEU:OXT	2.39	0.40
1:C:300:ASP:OD1	1:C:397:ARG:NE	2.47	0.40
1:I:127:ILE:HD13	1:I:474:MET:CE	2.51	0.40
1:K:46:MET:HE2	1:K:50:GLU:HG2	2.02	0.40
1:K:127:ILE:O	1:K:127:ILE:CG2	2.68	0.40
1:C:127:ILE:O	1:C:127:ILE:HG13	2.22	0.40
1:J:95:MET:HE3	1:J:161:ILE:HD12	2.03	0.40
1:L:2:SER:O	1:L:2:SER:OG	2.37	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	481/510 (94%)	465 (97%)	16 (3%)	0	100	100
1	B	481/510 (94%)	459 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	480/510 (94%)	461 (96%)	19 (4%)	0	100	100
1	D	481/510 (94%)	462 (96%)	19 (4%)	0	100	100
1	E	480/510 (94%)	462 (96%)	17 (4%)	1 (0%)	43	66
1	F	480/510 (94%)	463 (96%)	17 (4%)	0	100	100
1	G	480/510 (94%)	464 (97%)	16 (3%)	0	100	100
1	H	481/510 (94%)	462 (96%)	19 (4%)	0	100	100
1	I	480/510 (94%)	461 (96%)	18 (4%)	1 (0%)	43	66
1	J	480/510 (94%)	459 (96%)	20 (4%)	1 (0%)	43	66
1	K	480/510 (94%)	465 (97%)	15 (3%)	0	100	100
1	L	480/510 (94%)	462 (96%)	17 (4%)	1 (0%)	43	66
All	All	5764/6120 (94%)	5545 (96%)	215 (4%)	4 (0%)	48	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	187	PRO
1	E	156	PRO
1	J	156	PRO
1	L	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/408 (94%)	380 (100%)	2 (0%)	81	92
1	B	382/408 (94%)	377 (99%)	5 (1%)	61	82
1	C	380/408 (93%)	374 (98%)	6 (2%)	55	79
1	D	382/408 (94%)	378 (99%)	4 (1%)	68	86
1	E	380/408 (93%)	380 (100%)	0	100	100
1	F	381/408 (93%)	379 (100%)	2 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	382/408 (94%)	380 (100%)	2 (0%)	81	92
1	H	382/408 (94%)	379 (99%)	3 (1%)	73	88
1	I	381/408 (93%)	378 (99%)	3 (1%)	73	88
1	J	381/408 (93%)	377 (99%)	4 (1%)	68	86
1	K	379/408 (93%)	376 (99%)	3 (1%)	73	88
1	L	380/408 (93%)	375 (99%)	5 (1%)	61	82
All	All	4572/4896 (93%)	4533 (99%)	39 (1%)	73	87

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	428	TRP
1	B	39	GLU
1	B	158	ASN
1	B	289	THR
1	B	290	CYS
1	B	428	TRP
1	C	64	SER
1	C	158	ASN
1	C	289	THR
1	C	290	CYS
1	C	386	GLU
1	C	428	TRP
1	D	158	ASN
1	D	290	CYS
1	D	425	SER
1	D	428	TRP
1	F	290	CYS
1	F	428	TRP
1	G	290	CYS
1	G	428	TRP
1	H	290	CYS
1	H	425	SER
1	H	428	TRP
1	I	158	ASN
1	I	290	CYS
1	I	428	TRP
1	J	72	ASN
1	J	127	ILE

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Mol	Chain	Res	Type
1	J	290[A]	CYS
1	J	290[B]	CYS
1	K	64	SER
1	K	290	CYS
1	K	428	TRP
1	L	13	GLN
1	L	72	ASN
1	L	158	ASN
1	L	282	LYS
1	L	290	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	276	GLN
1	B	158	ASN
1	B	245	GLN
1	B	276	GLN
1	B	361	GLN
1	C	13	GLN
1	C	245	GLN
1	C	361	GLN
1	D	245	GLN
1	D	433	GLN
1	E	245	GLN
1	E	276	GLN
1	F	13	GLN
1	F	245	GLN
1	F	276	GLN
1	F	433	GLN
1	G	139	GLN
1	G	315	GLN
1	G	361	GLN
1	G	407	GLN
1	G	433	GLN
1	H	72	ASN
1	H	139	GLN
1	I	13	GLN
1	I	63	GLN
1	I	158	ASN
1	I	245	GLN

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Mol	Chain	Res	Type
1	I	276	GLN
1	I	376	ASN
1	J	245	GLN
1	J	276	GLN
1	K	158	ASN
1	K	245	GLN
1	L	53	GLN
1	L	139	GLN
1	L	215	GLN
1	L	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	EPE	K	501	-	15,15,15	0.79	1 (6%)	19,20,20	1.71	3 (15%)
2	EPE	E	501	-	15,15,15	0.84	1 (6%)	19,20,20	1.64	3 (15%)
2	EPE	D	501	-	15,15,15	0.82	1 (6%)	19,20,20	1.69	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	C	501	-	15,15,15	0.91	1 (6%)	19,20,20	1.58	4 (21%)
2	EPE	A	501	-	15,15,15	0.80	1 (6%)	19,20,20	1.69	3 (15%)
2	EPE	L	501	-	15,15,15	0.92	1 (6%)	19,20,20	1.71	5 (26%)
2	EPE	H	501	-	15,15,15	0.80	1 (6%)	19,20,20	1.84	5 (26%)
2	EPE	B	501	-	15,15,15	0.82	1 (6%)	19,20,20	1.78	4 (21%)
2	EPE	J	501	-	15,15,15	0.85	1 (6%)	19,20,20	1.60	4 (21%)

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	EPE	K	501	-	-	6/9/19/19	0/1/1/1
2	EPE	E	501	-	-	7/9/19/19	0/1/1/1
2	EPE	D	501	-	-	6/9/19/19	0/1/1/1
2	EPE	C	501	-	-	6/9/19/19	0/1/1/1
2	EPE	A	501	-	-	7/9/19/19	0/1/1/1
2	EPE	L	501	-	-	5/9/19/19	0/1/1/1
2	EPE	H	501	-	-	5/9/19/19	0/1/1/1
2	EPE	B	501	-	-	4/9/19/19	0/1/1/1
2	EPE	J	501	-	-	7/9/19/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	EPE	C10-S	3.14	1.82	1.77
2	L	501	EPE	C10-S	3.11	1.81	1.77
2	J	501	EPE	C10-S	2.90	1.81	1.77
2	E	501	EPE	C10-S	2.84	1.81	1.77
2	B	501	EPE	C10-S	2.83	1.81	1.77
2	D	501	EPE	C10-S	2.80	1.81	1.77
2	A	501	EPE	C10-S	2.68	1.81	1.77
2	H	501	EPE	C10-S	2.67	1.81	1.77
2	K	501	EPE	C10-S	2.65	1.81	1.77

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	EPE	C5-N4-C3	5.25	120.15	108.84
2	K	501	EPE	C5-N4-C3	4.89	119.37	108.84
2	D	501	EPE	C5-N4-C3	4.72	119.02	108.84
2	E	501	EPE	C5-N4-C3	4.70	118.97	108.84
2	H	501	EPE	C5-N4-C3	4.69	118.95	108.84
2	A	501	EPE	C5-N4-C3	4.62	118.79	108.84
2	L	501	EPE	C5-N4-C3	4.44	118.41	108.84
2	J	501	EPE	C5-N4-C3	3.97	117.40	108.84
2	C	501	EPE	C5-N4-C3	3.90	117.25	108.84
2	A	501	EPE	C7-N4-C5	3.54	120.67	111.24
2	H	501	EPE	C7-N4-C3	3.37	120.22	111.24
2	L	501	EPE	C7-N4-C3	3.03	119.31	111.24
2	H	501	EPE	C7-N4-C5	2.98	119.19	111.24
2	K	501	EPE	C7-N4-C3	2.98	119.18	111.24
2	J	501	EPE	C7-N4-C3	2.85	118.83	111.24
2	D	501	EPE	C7-N4-C3	2.84	118.81	111.24
2	J	501	EPE	O2S-S-C10	2.73	110.86	106.73
2	C	501	EPE	C7-N4-C5	2.71	118.47	111.24
2	E	501	EPE	C7-N4-C5	2.70	118.42	111.24
2	H	501	EPE	O1S-S-C10	2.66	110.74	106.73
2	L	501	EPE	C7-N4-C5	2.62	118.23	111.24
2	B	501	EPE	O2S-S-C10	2.62	110.69	106.73
2	J	501	EPE	C7-N4-C5	2.60	118.16	111.24
2	E	501	EPE	C7-N4-C3	2.56	118.06	111.24
2	C	501	EPE	C7-N4-C3	2.50	117.90	111.24
2	K	501	EPE	C7-N4-C5	2.39	117.61	111.24
2	L	501	EPE	O3S-S-C10	2.32	110.54	106.00
2	B	501	EPE	C7-N4-C5	2.29	117.34	111.24
2	A	501	EPE	C7-N4-C3	2.29	117.33	111.24
2	H	501	EPE	O2S-S-C10	2.27	110.16	106.73
2	B	501	EPE	O1S-S-C10	2.24	110.12	106.73
2	D	501	EPE	C7-N4-C5	2.19	117.09	111.24
2	L	501	EPE	O1S-S-C10	2.17	110.00	106.73
2	C	501	EPE	O3S-S-C10	2.12	110.16	106.00

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EPE	C8-C7-N4-C5
2	A	501	EPE	C9-C10-S-O1S
2	A	501	EPE	C9-C10-S-O3S
2	D	501	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
2	D	501	EPE	C9-C10-S-O3S
2	E	501	EPE	C9-C10-S-O1S
2	E	501	EPE	C9-C10-S-O2S
2	J	501	EPE	C9-C10-S-O1S
2	K	501	EPE	C9-C10-S-O1S
2	K	501	EPE	C9-C10-S-O3S
2	L	501	EPE	C9-C10-S-O1S
2	L	501	EPE	C9-C10-S-O2S
2	L	501	EPE	C9-C10-S-O3S
2	J	501	EPE	N4-C7-C8-O8
2	C	501	EPE	C9-C10-S-O3S
2	H	501	EPE	C9-C10-S-O3S
2	J	501	EPE	C9-C10-S-O3S
2	E	501	EPE	C9-C10-S-O3S
2	K	501	EPE	C8-C7-N4-C5
2	E	501	EPE	N4-C7-C8-O8
2	D	501	EPE	C8-C7-N4-C5
2	L	501	EPE	C8-C7-N4-C5
2	A	501	EPE	C10-C9-N1-C2
2	C	501	EPE	C10-C9-N1-C2
2	D	501	EPE	C10-C9-N1-C2
2	E	501	EPE	C10-C9-N1-C2
2	J	501	EPE	C10-C9-N1-C6
2	K	501	EPE	C10-C9-N1-C2
2	K	501	EPE	C10-C9-N1-C6
2	E	501	EPE	C8-C7-N4-C5
2	C	501	EPE	C8-C7-N4-C3
2	A	501	EPE	C9-C10-S-O2S
2	C	501	EPE	C9-C10-S-O1S
2	C	501	EPE	C9-C10-S-O2S
2	D	501	EPE	C9-C10-S-O2S
2	H	501	EPE	C9-C10-S-O1S
2	H	501	EPE	C9-C10-S-O2S
2	J	501	EPE	C9-C10-S-O2S
2	K	501	EPE	C9-C10-S-O2S
2	B	501	EPE	C10-C9-N1-C2
2	B	501	EPE	C10-C9-N1-C6
2	C	501	EPE	C10-C9-N1-C6
2	D	501	EPE	C10-C9-N1-C6
2	E	501	EPE	C10-C9-N1-C6
2	H	501	EPE	C10-C9-N1-C6
2	J	501	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
2	B	501	EPE	C8-C7-N4-C3
2	L	501	EPE	N4-C7-C8-O8
2	B	501	EPE	N4-C7-C8-O8
2	A	501	EPE	C10-C9-N1-C6
2	H	501	EPE	C10-C9-N1-C2
2	A	501	EPE	C8-C7-N4-C3
2	J	501	EPE	C8-C7-N4-C5

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 ⓘ

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	483/510 (94%)	-0.40	1 (0%) 91 90	48, 64, 85, 136	0
1	B	483/510 (94%)	-0.34	3 (0%) 85 83	51, 66, 90, 134	0
1	C	482/510 (94%)	-0.41	3 (0%) 85 83	49, 62, 81, 134	0
1	D	483/510 (94%)	-0.36	2 (0%) 88 86	50, 68, 87, 133	0
1	E	482/510 (94%)	-0.51	1 (0%) 91 90	46, 57, 75, 120	0
1	F	482/510 (94%)	-0.49	2 (0%) 88 86	47, 58, 75, 131	0
1	G	482/510 (94%)	-0.48	1 (0%) 91 90	46, 59, 78, 117	0
1	H	483/510 (94%)	-0.40	2 (0%) 88 86	45, 64, 90, 130	0
1	I	482/510 (94%)	-0.26	4 (0%) 82 80	49, 70, 95, 123	0
1	J	481/510 (94%)	-0.35	4 (0%) 82 80	51, 64, 80, 135	1 (0%)
1	K	482/510 (94%)	-0.31	2 (0%) 88 86	50, 65, 83, 127	0
1	L	482/510 (94%)	-0.37	3 (0%) 85 83	49, 65, 83, 144	0
All	All	5787/6120 (94%)	-0.39	28 (0%) 87 85	45, 63, 86, 144	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	5.0
1	H	1	VAL	4.9
1	J	290[A]	CYS	4.0
1	D	1	VAL	3.9
1	F	2	SER	3.7
1	D	259	GLY	3.3
1	I	2	SER	3.2
1	G	2	SER	3.2
1	I	4	LEU	3.2
1	B	5	GLN	3.0
1	E	2	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	2.9
1	C	2	SER	2.9
1	L	2	SER	2.7
1	I	5	GLN	2.7
1	F	3	SER	2.6
1	H	259	GLY	2.4
1	C	5	GLN	2.4
1	J	289	THR	2.3
1	L	289	THR	2.3
1	K	2	SER	2.3
1	K	5	GLN	2.2
1	C	4	LEU	2.1
1	I	453	PHE	2.1
1	J	361	GLN	2.0
1	J	90	GLU	2.0
1	L	259	GLY	2.0
1	B	127	ILE	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, 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	B-factors(Å ²)	Q<0.9
2	EPE	B	501	15/15	0.82	0.20	69,88,97,102	32
2	EPE	L	501	15/15	0.85	0.16	65,82,89,90	32
2	EPE	J	501	15/15	0.89	0.15	58,70,76,77	32
2	EPE	H	501	15/15	0.89	0.15	60,78,85,86	32
2	EPE	K	501	15/15	0.90	0.13	56,73,82,85	32
2	EPE	C	501	15/15	0.91	0.16	55,75,83,85	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EPE	E	501	15/15	0.91	0.13	51,69,82,85	32
2	EPE	A	501	15/15	0.91	0.13	58,77,92,97	32
2	EPE	D	501	15/15	0.92	0.12	56,74,82,82	32

6.5 Other polymers [i](#)

There are no such residues in this entry.