



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 04:24 pm BST

PDB ID : 9TSN / pdb_00009tsn
Title : ProteinMPNN mutated KREP domain of PF3D7_1343700 (PfK13-KREP, 59,4% sequence identity)
Authors : Amann, M.; Straesser, T.; Einsle, O.; Guenther, S.
Deposited on : 2025-12-30
Resolution : 2.15 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 : 1.8.4, CSD as541be (2020)
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

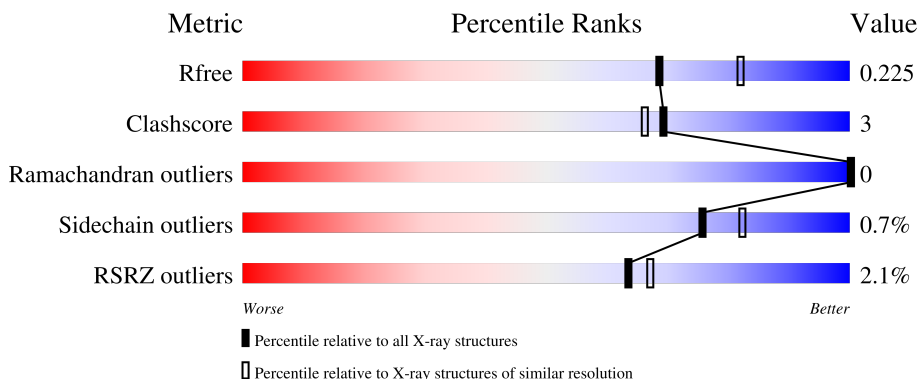
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	306	 3% 87% 6% 7%
1	B	306	 3% 84% 10% 6%
1	C	306	 3% 85% 8% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7129 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 Kelch protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2231	1439	367	422	3			
1	B	289	Total	C	N	O	S	0	1	0
			2255	1448	373	431	3			
1	C	287	Total	C	N	O	S	0	1	0
			2250	1445	372	430	3			

There are 408 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A077LQB4
A	2	SER	-	expression tag	UNP A0A077LQB4
A	3	GLY	-	expression tag	UNP A0A077LQB4
A	5	SER	PRO	engineered mutation	UNP A0A077LQB4
A	6	HIS	PHE	engineered mutation	UNP A0A077LQB4
A	9	ILE	VAL	engineered mutation	UNP A0A077LQB4
A	10	TYR	PHE	engineered mutation	UNP A0A077LQB4
A	11	VAL	CYS	engineered mutation	UNP A0A077LQB4
A	16	ASN	ASP	engineered mutation	UNP A0A077LQB4
A	24	VAL	MET	engineered mutation	UNP A0A077LQB4
A	26	VAL	LEU	engineered mutation	UNP A0A077LQB4
A	27	TYR	LEU	engineered mutation	UNP A0A077LQB4
A	29	TRP	ILE	engineered mutation	UNP A0A077LQB4
A	30	GLU	SER	engineered mutation	UNP A0A077LQB4
A	31	ASN	GLN	engineered mutation	UNP A0A077LQB4
A	32	ASN	GLN	engineered mutation	UNP A0A077LQB4
A	33	LYS	CYS	engineered mutation	UNP A0A077LQB4
A	35	VAL	ARG	engineered mutation	UNP A0A077LQB4
A	36	LYS	MET	engineered mutation	UNP A0A077LQB4
A	37	GLY	CYS	engineered mutation	UNP A0A077LQB4
A	40	PHE	MET	engineered mutation	UNP A0A077LQB4
A	41	LYS	SER	engineered mutation	UNP A0A077LQB4
A	43	PRO	LYS	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ARG	LYS	engineered mutation	UNP A0A077LQB4
A	50	PHE	ALA	engineered mutation	UNP A0A077LQB4
A	55	LYS	PHE	engineered mutation	UNP A0A077LQB4
A	56	ILE	LEU	engineered mutation	UNP A0A077LQB4
A	58	ILE	VAL	engineered mutation	UNP A0A077LQB4
A	59	ALA	PHE	engineered mutation	UNP A0A077LQB4
A	70	ASP	PHE	engineered mutation	UNP A0A077LQB4
A	71	THR	GLU	engineered mutation	UNP A0A077LQB4
A	74	ILE	VAL	engineered mutation	UNP A0A077LQB4
A	77	PRO	ARG	engineered mutation	UNP A0A077LQB4
A	78	LYS	LEU	engineered mutation	UNP A0A077LQB4
A	79	GLU	ARG	engineered mutation	UNP A0A077LQB4
A	80	ASN	ASP	engineered mutation	UNP A0A077LQB4
A	81	LYS	VAL	engineered mutation	UNP A0A077LQB4
A	83	SER	TYR	engineered mutation	UNP A0A077LQB4
A	84	ASP	VAL	engineered mutation	UNP A0A077LQB4
A	85	GLY	SER	engineered mutation	UNP A0A077LQB4
A	86	PRO	SER	engineered mutation	UNP A0A077LQB4
A	87	LYS	ASN	engineered mutation	UNP A0A077LQB4
A	89	LEU	ASN	engineered mutation	UNP A0A077LQB4
A	90	VAL	ILE	engineered mutation	UNP A0A077LQB4
A	96	ALA	CYS	engineered mutation	UNP A0A077LQB4
A	99	TYR	THR	engineered mutation	UNP A0A077LQB4
A	100	LEU	SER	engineered mutation	UNP A0A077LQB4
A	103	LYS	ARG	engineered mutation	UNP A0A077LQB4
A	106	VAL	CYS	engineered mutation	UNP A0A077LQB4
A	117	ASN	PRO	engineered mutation	UNP A0A077LQB4
A	118	SER	ASN	engineered mutation	UNP A0A077LQB4
A	124	PRO	HIS	engineered mutation	UNP A0A077LQB4
A	125	GLU	ARG	engineered mutation	UNP A0A077LQB4
A	126	LYS	MET	engineered mutation	UNP A0A077LQB4
A	127	ASN	LYS	engineered mutation	UNP A0A077LQB4
A	128	GLU	ALA	engineered mutation	UNP A0A077LQB4
A	130	ILE	VAL	engineered mutation	UNP A0A077LQB4
A	131	PRO	GLU	engineered mutation	UNP A0A077LQB4
A	136	LYS	ASN	engineered mutation	UNP A0A077LQB4
A	138	ALA	PRO	engineered mutation	UNP A0A077LQB4
A	143	ALA	MET	engineered mutation	UNP A0A077LQB4
A	144	SER	CYS	engineered mutation	UNP A0A077LQB4
A	145	ALA	VAL	engineered mutation	UNP A0A077LQB4
A	148	ASN	ASP	engineered mutation	UNP A0A077LQB4
A	169	ASP	GLU	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	LYS	engineered mutation	UNP A0A077LQB4
A	172	THR	MET	engineered mutation	UNP A0A077LQB4
A	174	THR	LYS	engineered mutation	UNP A0A077LQB4
A	176	THR	GLU	engineered mutation	UNP A0A077LQB4
A	177	THR	GLN	engineered mutation	UNP A0A077LQB4
A	180	VAL	TYR	engineered mutation	UNP A0A077LQB4
A	181	PRO	ALA	engineered mutation	UNP A0A077LQB4
A	184	ILE	GLU	engineered mutation	UNP A0A077LQB4
A	185	PRO	ALA	engineered mutation	UNP A0A077LQB4
A	193	VAL	ASN	engineered mutation	UNP A0A077LQB4
A	194	SER	TYR	engineered mutation	UNP A0A077LQB4
A	195	GLY	LEU	engineered mutation	UNP A0A077LQB4
A	196	ASP	ASN	engineered mutation	UNP A0A077LQB4
A	197	LYS	GLN	engineered mutation	UNP A0A077LQB4
A	198	LEU	ILE	engineered mutation	UNP A0A077LQB4
A	201	ILE	VAL	engineered mutation	UNP A0A077LQB4
A	207	ASN	GLU	engineered mutation	UNP A0A077LQB4
A	212	ASN	ASP	engineered mutation	UNP A0A077LQB4
A	213	ASP	SER	engineered mutation	UNP A0A077LQB4
A	216	MET	GLN	engineered mutation	UNP A0A077LQB4
A	218	ASP	GLN	engineered mutation	UNP A0A077LQB4
A	220	GLU	PHE	engineered mutation	UNP A0A077LQB4
A	221	LYS	ASN	engineered mutation	UNP A0A077LQB4
A	223	GLU	ARG	engineered mutation	UNP A0A077LQB4
A	225	SER	GLN	engineered mutation	UNP A0A077LQB4
A	227	ILE	LEU	engineered mutation	UNP A0A077LQB4
A	229	PRO	GLY	engineered mutation	UNP A0A077LQB4
A	230	MET	VAL	engineered mutation	UNP A0A077LQB4
A	232	ILE	GLU	engineered mutation	UNP A0A077LQB4
A	233	PRO	LYS	engineered mutation	UNP A0A077LQB4
A	234	ARG	LYS	engineered mutation	UNP A0A077LQB4
A	239	SER	ALA	engineered mutation	UNP A0A077LQB4
A	241	SER	THR	engineered mutation	UNP A0A077LQB4
A	243	PRO	SER	engineered mutation	UNP A0A077LQB4
A	244	ASN	ASP	engineered mutation	UNP A0A077LQB4
A	246	PHE	TYR	engineered mutation	UNP A0A077LQB4
A	248	VAL	ILE	engineered mutation	UNP A0A077LQB4
A	259	GLU	SER	engineered mutation	UNP A0A077LQB4
A	260	THR	CYS	engineered mutation	UNP A0A077LQB4
A	261	TYR	HIS	engineered mutation	UNP A0A077LQB4
A	262	ARG	PHE	engineered mutation	UNP A0A077LQB4
A	263	TYR	PHE	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	264	ASP	SER	engineered mutation	UNP A0A077LQB4
A	266	ALA	ASP	engineered mutation	UNP A0A077LQB4
A	269	LYS	GLU	engineered mutation	UNP A0A077LQB4
A	271	THR	GLN	engineered mutation	UNP A0A077LQB4
A	272	LYS	LEU	engineered mutation	UNP A0A077LQB4
A	273	GLU	GLY	engineered mutation	UNP A0A077LQB4
A	274	ALA	PRO	engineered mutation	UNP A0A077LQB4
A	275	PRO	SER	engineered mutation	UNP A0A077LQB4
A	278	THR	VAL	engineered mutation	UNP A0A077LQB4
A	284	ALA	SER	engineered mutation	UNP A0A077LQB4
A	287	VAL	ILE	engineered mutation	UNP A0A077LQB4
A	288	VAL	ALA	engineered mutation	UNP A0A077LQB4
A	290	ASN	-	expression tag	UNP A0A077LQB4
A	291	GLY	-	expression tag	UNP A0A077LQB4
A	292	SER	-	expression tag	UNP A0A077LQB4
A	293	GLY	-	expression tag	UNP A0A077LQB4
A	294	SER	-	expression tag	UNP A0A077LQB4
A	295	HIS	-	expression tag	UNP A0A077LQB4
A	296	HIS	-	expression tag	UNP A0A077LQB4
A	297	TRP	-	expression tag	UNP A0A077LQB4
A	298	GLY	-	expression tag	UNP A0A077LQB4
A	299	SER	-	expression tag	UNP A0A077LQB4
A	300	THR	-	expression tag	UNP A0A077LQB4
A	301	HIS	-	expression tag	UNP A0A077LQB4
A	302	HIS	-	expression tag	UNP A0A077LQB4
A	303	HIS	-	expression tag	UNP A0A077LQB4
A	304	HIS	-	expression tag	UNP A0A077LQB4
A	305	HIS	-	expression tag	UNP A0A077LQB4
A	306	HIS	-	expression tag	UNP A0A077LQB4
B	1	MET	-	initiating methionine	UNP A0A077LQB4
B	2	SER	-	expression tag	UNP A0A077LQB4
B	3	GLY	-	expression tag	UNP A0A077LQB4
B	5	SER	PRO	engineered mutation	UNP A0A077LQB4
B	6	HIS	PHE	engineered mutation	UNP A0A077LQB4
B	9	ILE	VAL	engineered mutation	UNP A0A077LQB4
B	10	TYR	PHE	engineered mutation	UNP A0A077LQB4
B	11	VAL	CYS	engineered mutation	UNP A0A077LQB4
B	16	ASN	ASP	engineered mutation	UNP A0A077LQB4
B	24	VAL	MET	engineered mutation	UNP A0A077LQB4
B	26	VAL	LEU	engineered mutation	UNP A0A077LQB4
B	27	TYR	LEU	engineered mutation	UNP A0A077LQB4
B	29	TRP	ILE	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	GLU	SER	engineered mutation	UNP A0A077LQB4
B	31	ASN	GLN	engineered mutation	UNP A0A077LQB4
B	32	ASN	GLN	engineered mutation	UNP A0A077LQB4
B	33	LYS	CYS	engineered mutation	UNP A0A077LQB4
B	35	VAL	ARG	engineered mutation	UNP A0A077LQB4
B	36	LYS	MET	engineered mutation	UNP A0A077LQB4
B	37	GLY	CYS	engineered mutation	UNP A0A077LQB4
B	40	PHE	MET	engineered mutation	UNP A0A077LQB4
B	41	LYS	SER	engineered mutation	UNP A0A077LQB4
B	43	PRO	LYS	engineered mutation	UNP A0A077LQB4
B	44	ARG	LYS	engineered mutation	UNP A0A077LQB4
B	50	PHE	ALA	engineered mutation	UNP A0A077LQB4
B	55	LYS	PHE	engineered mutation	UNP A0A077LQB4
B	56	ILE	LEU	engineered mutation	UNP A0A077LQB4
B	58	ILE	VAL	engineered mutation	UNP A0A077LQB4
B	59	ALA	PHE	engineered mutation	UNP A0A077LQB4
B	70	ASP	PHE	engineered mutation	UNP A0A077LQB4
B	71	THR	GLU	engineered mutation	UNP A0A077LQB4
B	74	ILE	VAL	engineered mutation	UNP A0A077LQB4
B	77	PRO	ARG	engineered mutation	UNP A0A077LQB4
B	78	LYS	LEU	engineered mutation	UNP A0A077LQB4
B	79	GLU	ARG	engineered mutation	UNP A0A077LQB4
B	80	ASN	ASP	engineered mutation	UNP A0A077LQB4
B	81	LYS	VAL	engineered mutation	UNP A0A077LQB4
B	83	SER	TYR	engineered mutation	UNP A0A077LQB4
B	84	ASP	VAL	engineered mutation	UNP A0A077LQB4
B	85	GLY	SER	engineered mutation	UNP A0A077LQB4
B	86	PRO	SER	engineered mutation	UNP A0A077LQB4
B	87	LYS	ASN	engineered mutation	UNP A0A077LQB4
B	89	LEU	ASN	engineered mutation	UNP A0A077LQB4
B	90	VAL	ILE	engineered mutation	UNP A0A077LQB4
B	96	ALA	CYS	engineered mutation	UNP A0A077LQB4
B	99	TYR	THR	engineered mutation	UNP A0A077LQB4
B	100	LEU	SER	engineered mutation	UNP A0A077LQB4
B	103	LYS	ARG	engineered mutation	UNP A0A077LQB4
B	106	VAL	CYS	engineered mutation	UNP A0A077LQB4
B	117	ASN	PRO	engineered mutation	UNP A0A077LQB4
B	118	SER	ASN	engineered mutation	UNP A0A077LQB4
B	124	PRO	HIS	engineered mutation	UNP A0A077LQB4
B	125	GLU	ARG	engineered mutation	UNP A0A077LQB4
B	126	LYS	MET	engineered mutation	UNP A0A077LQB4
B	127	ASN	LYS	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	128	GLU	ALA	engineered mutation	UNP A0A077LQB4
B	130	ILE	VAL	engineered mutation	UNP A0A077LQB4
B	131	PRO	GLU	engineered mutation	UNP A0A077LQB4
B	136	LYS	ASN	engineered mutation	UNP A0A077LQB4
B	138	ALA	PRO	engineered mutation	UNP A0A077LQB4
B	143	ALA	MET	engineered mutation	UNP A0A077LQB4
B	144	SER	CYS	engineered mutation	UNP A0A077LQB4
B	145	ALA	VAL	engineered mutation	UNP A0A077LQB4
B	148	ASN	ASP	engineered mutation	UNP A0A077LQB4
B	169	ASP	GLU	engineered mutation	UNP A0A077LQB4
B	171	ALA	LYS	engineered mutation	UNP A0A077LQB4
B	172	THR	MET	engineered mutation	UNP A0A077LQB4
B	174	THR	LYS	engineered mutation	UNP A0A077LQB4
B	176	THR	GLU	engineered mutation	UNP A0A077LQB4
B	177	THR	GLN	engineered mutation	UNP A0A077LQB4
B	180	VAL	TYR	engineered mutation	UNP A0A077LQB4
B	181	PRO	ALA	engineered mutation	UNP A0A077LQB4
B	184	ILE	GLU	engineered mutation	UNP A0A077LQB4
B	185	PRO	ALA	engineered mutation	UNP A0A077LQB4
B	193	VAL	ASN	engineered mutation	UNP A0A077LQB4
B	194	SER	TYR	engineered mutation	UNP A0A077LQB4
B	195	GLY	LEU	engineered mutation	UNP A0A077LQB4
B	196	ASP	ASN	engineered mutation	UNP A0A077LQB4
B	197	LYS	GLN	engineered mutation	UNP A0A077LQB4
B	198	LEU	ILE	engineered mutation	UNP A0A077LQB4
B	201	ILE	VAL	engineered mutation	UNP A0A077LQB4
B	207	ASN	GLU	engineered mutation	UNP A0A077LQB4
B	212	ASN	ASP	engineered mutation	UNP A0A077LQB4
B	213	ASP	SER	engineered mutation	UNP A0A077LQB4
B	216	MET	GLN	engineered mutation	UNP A0A077LQB4
B	218	ASP	GLN	engineered mutation	UNP A0A077LQB4
B	220	GLU	PHE	engineered mutation	UNP A0A077LQB4
B	221	LYS	ASN	engineered mutation	UNP A0A077LQB4
B	223	GLU	ARG	engineered mutation	UNP A0A077LQB4
B	225	SER	GLN	engineered mutation	UNP A0A077LQB4
B	227	ILE	LEU	engineered mutation	UNP A0A077LQB4
B	229	PRO	GLY	engineered mutation	UNP A0A077LQB4
B	230	MET	VAL	engineered mutation	UNP A0A077LQB4
B	232	ILE	GLU	engineered mutation	UNP A0A077LQB4
B	233	PRO	LYS	engineered mutation	UNP A0A077LQB4
B	234	ARG	LYS	engineered mutation	UNP A0A077LQB4
B	239	SER	ALA	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	SER	THR	engineered mutation	UNP A0A077LQB4
B	243	PRO	SER	engineered mutation	UNP A0A077LQB4
B	244	ASN	ASP	engineered mutation	UNP A0A077LQB4
B	246	PHE	TYR	engineered mutation	UNP A0A077LQB4
B	248	VAL	ILE	engineered mutation	UNP A0A077LQB4
B	259	GLU	SER	engineered mutation	UNP A0A077LQB4
B	260	THR	CYS	engineered mutation	UNP A0A077LQB4
B	261	TYR	HIS	engineered mutation	UNP A0A077LQB4
B	262	ARG	PHE	engineered mutation	UNP A0A077LQB4
B	263	TYR	PHE	engineered mutation	UNP A0A077LQB4
B	264	ASP	SER	engineered mutation	UNP A0A077LQB4
B	266	ALA	ASP	engineered mutation	UNP A0A077LQB4
B	269	LYS	GLU	engineered mutation	UNP A0A077LQB4
B	271	THR	GLN	engineered mutation	UNP A0A077LQB4
B	272	LYS	LEU	engineered mutation	UNP A0A077LQB4
B	273	GLU	GLY	engineered mutation	UNP A0A077LQB4
B	274	ALA	PRO	engineered mutation	UNP A0A077LQB4
B	275	PRO	SER	engineered mutation	UNP A0A077LQB4
B	278	THR	VAL	engineered mutation	UNP A0A077LQB4
B	284	ALA	SER	engineered mutation	UNP A0A077LQB4
B	287	VAL	ILE	engineered mutation	UNP A0A077LQB4
B	288	VAL	ALA	engineered mutation	UNP A0A077LQB4
B	290	ASN	-	expression tag	UNP A0A077LQB4
B	291	GLY	-	expression tag	UNP A0A077LQB4
B	292	SER	-	expression tag	UNP A0A077LQB4
B	293	GLY	-	expression tag	UNP A0A077LQB4
B	294	SER	-	expression tag	UNP A0A077LQB4
B	295	HIS	-	expression tag	UNP A0A077LQB4
B	296	HIS	-	expression tag	UNP A0A077LQB4
B	297	TRP	-	expression tag	UNP A0A077LQB4
B	298	GLY	-	expression tag	UNP A0A077LQB4
B	299	SER	-	expression tag	UNP A0A077LQB4
B	300	THR	-	expression tag	UNP A0A077LQB4
B	301	HIS	-	expression tag	UNP A0A077LQB4
B	302	HIS	-	expression tag	UNP A0A077LQB4
B	303	HIS	-	expression tag	UNP A0A077LQB4
B	304	HIS	-	expression tag	UNP A0A077LQB4
B	305	HIS	-	expression tag	UNP A0A077LQB4
B	306	HIS	-	expression tag	UNP A0A077LQB4
C	1	MET	-	initiating methionine	UNP A0A077LQB4
C	2	SER	-	expression tag	UNP A0A077LQB4
C	3	GLY	-	expression tag	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	SER	PRO	engineered mutation	UNP A0A077LQB4
C	6	HIS	PHE	engineered mutation	UNP A0A077LQB4
C	9	ILE	VAL	engineered mutation	UNP A0A077LQB4
C	10	TYR	PHE	engineered mutation	UNP A0A077LQB4
C	11	VAL	CYS	engineered mutation	UNP A0A077LQB4
C	16	ASN	ASP	engineered mutation	UNP A0A077LQB4
C	24	VAL	MET	engineered mutation	UNP A0A077LQB4
C	26	VAL	LEU	engineered mutation	UNP A0A077LQB4
C	27	TYR	LEU	engineered mutation	UNP A0A077LQB4
C	29	TRP	ILE	engineered mutation	UNP A0A077LQB4
C	30	GLU	SER	engineered mutation	UNP A0A077LQB4
C	31	ASN	GLN	engineered mutation	UNP A0A077LQB4
C	32	ASN	GLN	engineered mutation	UNP A0A077LQB4
C	33	LYS	CYS	engineered mutation	UNP A0A077LQB4
C	35	VAL	ARG	engineered mutation	UNP A0A077LQB4
C	36	LYS	MET	engineered mutation	UNP A0A077LQB4
C	37	GLY	CYS	engineered mutation	UNP A0A077LQB4
C	40	PHE	MET	engineered mutation	UNP A0A077LQB4
C	41	LYS	SER	engineered mutation	UNP A0A077LQB4
C	43	PRO	LYS	engineered mutation	UNP A0A077LQB4
C	44	ARG	LYS	engineered mutation	UNP A0A077LQB4
C	50	PHE	ALA	engineered mutation	UNP A0A077LQB4
C	55	LYS	PHE	engineered mutation	UNP A0A077LQB4
C	56	ILE	LEU	engineered mutation	UNP A0A077LQB4
C	58	ILE	VAL	engineered mutation	UNP A0A077LQB4
C	59	ALA	PHE	engineered mutation	UNP A0A077LQB4
C	70	ASP	PHE	engineered mutation	UNP A0A077LQB4
C	71	THR	GLU	engineered mutation	UNP A0A077LQB4
C	74	ILE	VAL	engineered mutation	UNP A0A077LQB4
C	77	PRO	ARG	engineered mutation	UNP A0A077LQB4
C	78	LYS	LEU	engineered mutation	UNP A0A077LQB4
C	79	GLU	ARG	engineered mutation	UNP A0A077LQB4
C	80	ASN	ASP	engineered mutation	UNP A0A077LQB4
C	81	LYS	VAL	engineered mutation	UNP A0A077LQB4
C	83	SER	TYR	engineered mutation	UNP A0A077LQB4
C	84	ASP	VAL	engineered mutation	UNP A0A077LQB4
C	85	GLY	SER	engineered mutation	UNP A0A077LQB4
C	86	PRO	SER	engineered mutation	UNP A0A077LQB4
C	87	LYS	ASN	engineered mutation	UNP A0A077LQB4
C	89	LEU	ASN	engineered mutation	UNP A0A077LQB4
C	90	VAL	ILE	engineered mutation	UNP A0A077LQB4
C	96	ALA	CYS	engineered mutation	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	99	TYR	THR	engineered mutation	UNP A0A077LQB4
C	100	LEU	SER	engineered mutation	UNP A0A077LQB4
C	103	LYS	ARG	engineered mutation	UNP A0A077LQB4
C	106	VAL	CYS	engineered mutation	UNP A0A077LQB4
C	117	ASN	PRO	engineered mutation	UNP A0A077LQB4
C	118	SER	ASN	engineered mutation	UNP A0A077LQB4
C	124	PRO	HIS	engineered mutation	UNP A0A077LQB4
C	125	GLU	ARG	engineered mutation	UNP A0A077LQB4
C	126	LYS	MET	engineered mutation	UNP A0A077LQB4
C	127	ASN	LYS	engineered mutation	UNP A0A077LQB4
C	128	GLU	ALA	engineered mutation	UNP A0A077LQB4
C	130	ILE	VAL	engineered mutation	UNP A0A077LQB4
C	131	PRO	GLU	engineered mutation	UNP A0A077LQB4
C	136	LYS	ASN	engineered mutation	UNP A0A077LQB4
C	138	ALA	PRO	engineered mutation	UNP A0A077LQB4
C	143	ALA	MET	engineered mutation	UNP A0A077LQB4
C	144	SER	CYS	engineered mutation	UNP A0A077LQB4
C	145	ALA	VAL	engineered mutation	UNP A0A077LQB4
C	148	ASN	ASP	engineered mutation	UNP A0A077LQB4
C	169	ASP	GLU	engineered mutation	UNP A0A077LQB4
C	171	ALA	LYS	engineered mutation	UNP A0A077LQB4
C	172	THR	MET	engineered mutation	UNP A0A077LQB4
C	174	THR	LYS	engineered mutation	UNP A0A077LQB4
C	176	THR	GLU	engineered mutation	UNP A0A077LQB4
C	177	THR	GLN	engineered mutation	UNP A0A077LQB4
C	180	VAL	TYR	engineered mutation	UNP A0A077LQB4
C	181	PRO	ALA	engineered mutation	UNP A0A077LQB4
C	184	ILE	GLU	engineered mutation	UNP A0A077LQB4
C	185	PRO	ALA	engineered mutation	UNP A0A077LQB4
C	193	VAL	ASN	engineered mutation	UNP A0A077LQB4
C	194	SER	TYR	engineered mutation	UNP A0A077LQB4
C	195	GLY	LEU	engineered mutation	UNP A0A077LQB4
C	196	ASP	ASN	engineered mutation	UNP A0A077LQB4
C	197	LYS	GLN	engineered mutation	UNP A0A077LQB4
C	198	LEU	ILE	engineered mutation	UNP A0A077LQB4
C	201	ILE	VAL	engineered mutation	UNP A0A077LQB4
C	207	ASN	GLU	engineered mutation	UNP A0A077LQB4
C	212	ASN	ASP	engineered mutation	UNP A0A077LQB4
C	213	ASP	SER	engineered mutation	UNP A0A077LQB4
C	216	MET	GLN	engineered mutation	UNP A0A077LQB4
C	218	ASP	GLN	engineered mutation	UNP A0A077LQB4
C	220	GLU	PHE	engineered mutation	UNP A0A077LQB4

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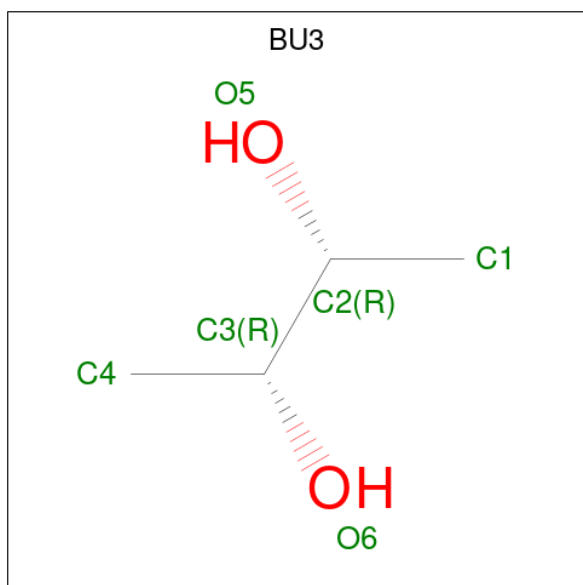
Chain	Residue	Modelled	Actual	Comment	Reference
C	221	LYS	ASN	engineered mutation	UNP A0A077LQB4
C	223	GLU	ARG	engineered mutation	UNP A0A077LQB4
C	225	SER	GLN	engineered mutation	UNP A0A077LQB4
C	227	ILE	LEU	engineered mutation	UNP A0A077LQB4
C	229	PRO	GLY	engineered mutation	UNP A0A077LQB4
C	230	MET	VAL	engineered mutation	UNP A0A077LQB4
C	232	ILE	GLU	engineered mutation	UNP A0A077LQB4
C	233	PRO	LYS	engineered mutation	UNP A0A077LQB4
C	234	ARG	LYS	engineered mutation	UNP A0A077LQB4
C	239	SER	ALA	engineered mutation	UNP A0A077LQB4
C	241	SER	THR	engineered mutation	UNP A0A077LQB4
C	243	PRO	SER	engineered mutation	UNP A0A077LQB4
C	244	ASN	ASP	engineered mutation	UNP A0A077LQB4
C	246	PHE	TYR	engineered mutation	UNP A0A077LQB4
C	248	VAL	ILE	engineered mutation	UNP A0A077LQB4
C	259	GLU	SER	engineered mutation	UNP A0A077LQB4
C	260	THR	CYS	engineered mutation	UNP A0A077LQB4
C	261	TYR	HIS	engineered mutation	UNP A0A077LQB4
C	262	ARG	PHE	engineered mutation	UNP A0A077LQB4
C	263	TYR	PHE	engineered mutation	UNP A0A077LQB4
C	264	ASP	SER	engineered mutation	UNP A0A077LQB4
C	266	ALA	ASP	engineered mutation	UNP A0A077LQB4
C	269	LYS	GLU	engineered mutation	UNP A0A077LQB4
C	271	THR	GLN	engineered mutation	UNP A0A077LQB4
C	272	LYS	LEU	engineered mutation	UNP A0A077LQB4
C	273	GLU	GLY	engineered mutation	UNP A0A077LQB4
C	274	ALA	PRO	engineered mutation	UNP A0A077LQB4
C	275	PRO	SER	engineered mutation	UNP A0A077LQB4
C	278	THR	VAL	engineered mutation	UNP A0A077LQB4
C	284	ALA	SER	engineered mutation	UNP A0A077LQB4
C	287	VAL	ILE	engineered mutation	UNP A0A077LQB4
C	288	VAL	ALA	engineered mutation	UNP A0A077LQB4
C	290	ASN	-	expression tag	UNP A0A077LQB4
C	291	GLY	-	expression tag	UNP A0A077LQB4
C	292	SER	-	expression tag	UNP A0A077LQB4
C	293	GLY	-	expression tag	UNP A0A077LQB4
C	294	SER	-	expression tag	UNP A0A077LQB4
C	295	HIS	-	expression tag	UNP A0A077LQB4
C	296	HIS	-	expression tag	UNP A0A077LQB4
C	297	TRP	-	expression tag	UNP A0A077LQB4
C	298	GLY	-	expression tag	UNP A0A077LQB4
C	299	SER	-	expression tag	UNP A0A077LQB4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	300	THR	-	expression tag	UNP A0A077LQB4
C	301	HIS	-	expression tag	UNP A0A077LQB4
C	302	HIS	-	expression tag	UNP A0A077LQB4
C	303	HIS	-	expression tag	UNP A0A077LQB4
C	304	HIS	-	expression tag	UNP A0A077LQB4
C	305	HIS	-	expression tag	UNP A0A077LQB4
C	306	HIS	-	expression tag	UNP A0A077LQB4

- Molecule 2 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: C₄H₁₀O₂).



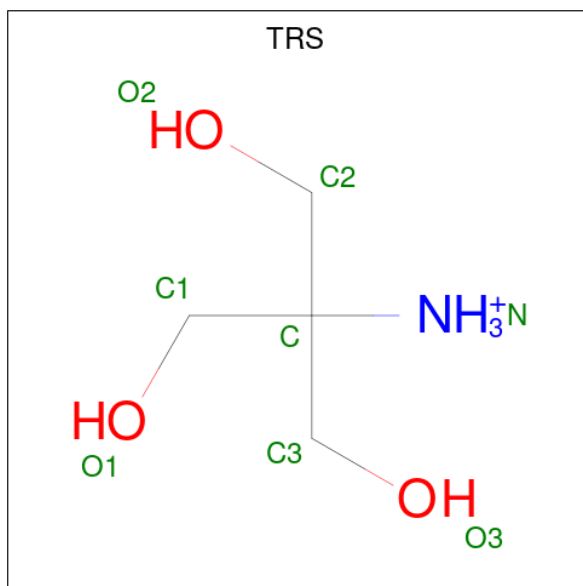
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

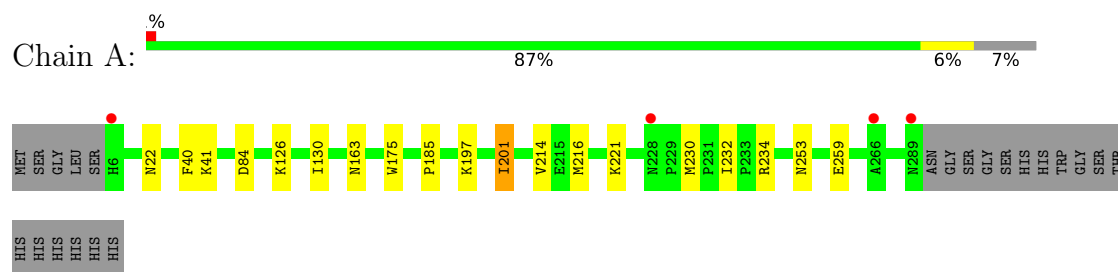
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total 140	O 140	0	0
5	B	138	Total 138	O 138	0	0
5	C	97	Total 97	O 97	0	0

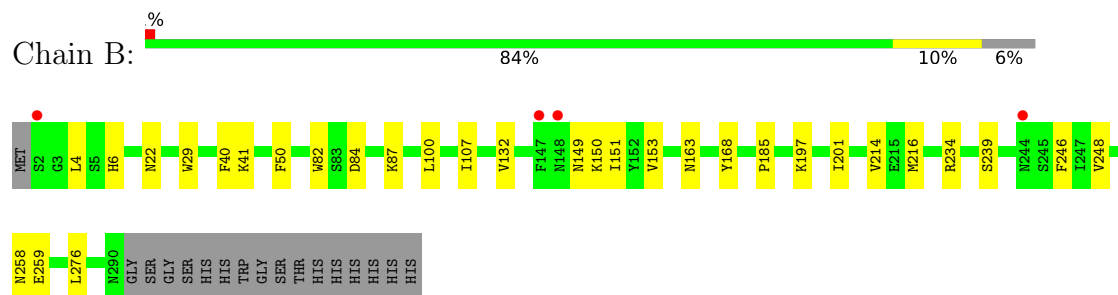
3 Residue-property plots [i](#)

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.

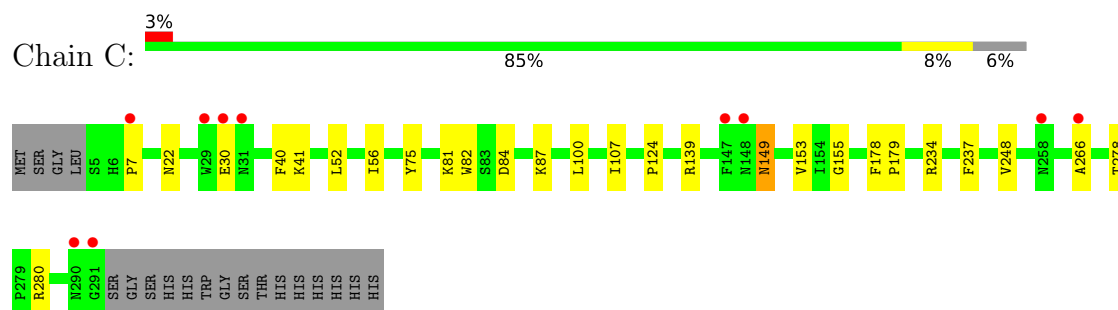
• Molecule 1: Kelch protein



• Molecule 1: Kelch protein



• Molecule 1: Kelch protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	92.43Å 92.43Å 90.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.04 – 2.15 80.04 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.04-2.15) 100.0 (80.04-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.187 , 0.223 0.190 , 0.225	Depositor DCC
R_{free} test set	2329 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.019 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7129	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, BU3, EDO

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	0.12	0/2299	0.37	0/3142
1	B	0.12	0/2322	0.37	0/3174
1	C	0.13	0/2318	0.38	0/3169
All	All	0.12	0/6939	0.37	0/9485

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 [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	2231	0	2148	14	0
1	B	2255	0	2159	18	0
1	C	2250	0	2145	16	0
2	A	6	0	10	2	0
3	C	4	0	6	0	0
4	C	8	0	12	0	0
5	A	140	0	0	0	0
5	B	138	0	0	1	0
5	C	97	0	0	1	0
All	All	7129	0	6480	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (46) 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:A:232:ILE:HD11	1:A:234:ARG:HH21	1.49	0.77
1:A:126:LYS:HD2	1:A:130:ILE:HD11	1.73	0.70
1:A:175:TRP:H	2:A:401:BU3:H11	1.60	0.66
1:B:258[B]:ASN:ND2	1:B:276:LEU:O	2.33	0.62
1:C:52:LEU:HD21	1:C:124:PRO:HG3	1.82	0.62
1:C:100:LEU:HD11	1:C:149:ASN:HA	1.82	0.61
1:B:41:LYS:NZ	1:B:84:ASP:OD2	2.35	0.60
1:C:278:THR:OG1	1:C:280[A]:ARG:NH2	2.37	0.56
1:B:107:ILE:HG21	1:B:153:VAL:HG21	1.87	0.55
1:B:87:LYS:NZ	5:B:402:HOH:O	2.39	0.55
1:A:175:TRP:H	2:A:401:BU3:C1	2.20	0.54
1:C:7:PRO:HD2	1:C:30:GLU:OE2	2.08	0.53
1:C:22:ASN:HA	1:C:40:PHE:CZ	2.45	0.52
1:C:237:PHE:CD1	1:C:248:VAL:HG13	2.46	0.51
1:A:22:ASN:HA	1:A:40:PHE:CZ	2.46	0.50
1:A:201[A]:ILE:HD11	1:A:230:MET:SD	2.52	0.49
1:A:41:LYS:NZ	1:A:84:ASP:OD2	2.44	0.49
1:B:258[B]:ASN:OD1	1:B:276:LEU:HB2	2.12	0.49
1:B:22:ASN:HA	1:B:40:PHE:CZ	2.48	0.49
1:A:197:LYS:HD3	1:A:216:MET:SD	2.53	0.48
1:C:107:ILE:HG21	1:C:153:VAL:HG21	1.96	0.48
1:A:201[B]:ILE:HG12	1:A:214:VAL:HG13	1.95	0.47
1:B:163:ASN:HB3	1:B:185:PRO:HG3	1.96	0.47
1:B:201:ILE:HG13	1:B:214:VAL:HG13	1.97	0.46
1:A:253:ASN:HB2	1:B:4:LEU:HD13	1.97	0.46
1:A:232:ILE:HD11	1:A:234:ARG:NH2	2.26	0.46
1:B:234:ARG:HD2	1:B:248:VAL:HG11	1.98	0.46
1:C:56:ILE:HB	1:C:75:TYR:HB3	1.98	0.46
1:A:221:LYS:HD3	1:C:266:ALA:HA	1.97	0.45
1:B:197:LYS:HD2	1:B:216:MET:SD	2.56	0.45
1:C:234:ARG:HD2	1:C:248:VAL:HG11	1.98	0.45
1:B:100:LEU:HD11	1:B:149:ASN:HA	2.00	0.44
1:A:163:ASN:HB3	1:A:185:PRO:HG3	1.99	0.43
1:B:234:ARG:HH22	1:B:259:GLU:HB2	1.84	0.43
1:C:87:LYS:NZ	5:C:502:HOH:O	2.40	0.43
1:C:41:LYS:NZ	1:C:84:ASP:OD2	2.51	0.43
1:B:40:PHE:HB3	1:B:82:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:HIS:HB3	1:B:29:TRP:CE2	2.54	0.42
1:C:234:ARG:HD2	1:C:248:VAL:CG1	2.49	0.42
1:A:259:GLU:OE1	1:A:259:GLU:N	2.52	0.42
1:B:151:ILE:HB	1:B:168:TYR:HB3	2.01	0.42
1:C:40:PHE:HB3	1:C:82:TRP:CD2	2.56	0.41
1:C:178:PHE:HA	1:C:179:PRO:HD3	1.93	0.41
1:B:239:SER:HB2	1:B:246:PHE:CZ	2.56	0.40
1:C:139:ARG:HD3	1:C:155:GLY:O	2.21	0.40
1:B:150:LYS:HD2	1:B:168:TYR:O	2.22	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	283/306 (92%)	276 (98%)	7 (2%)	0	100	100
1	B	288/306 (94%)	282 (98%)	6 (2%)	0	100	100
1	C	286/306 (94%)	279 (98%)	7 (2%)	0	100	100
All	All	857/918 (93%)	837 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	237/259 (92%)	235 (99%)	2 (1%)	73	79
1	B	239/259 (92%)	237 (99%)	2 (1%)	73	79
1	C	238/259 (92%)	236 (99%)	2 (1%)	73	79
All	All	714/777 (92%)	708 (99%)	6 (1%)	76	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201[A]	ILE
1	A	201[B]	ILE
1	B	50	PHE
1	B	132	VAL
1	C	81	LYS
1	C	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	53	ASN
1	B	54	ASN
1	B	62	ASN
1	C	6	HIS
1	C	208	HIS
1	C	209	ASN

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

3 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	$\# Z > 2$
4	TRS	C	402	-	7,7,7	0.34	0	9,9,9	0.60	0
3	EDO	C	401	-	3,3,3	0.27	0	2,2,2	0.33	0
2	BU3	A	401	-	4,5,5	0.30	0	6,6,6	0.48	0

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
4	TRS	C	402	-	-	3/9/9/9	-
3	EDO	C	401	-	-	0/1/1/1	-
2	BU3	A	401	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	BU3	C1-C2-C3-O6
2	A	401	BU3	O5-C2-C3-C4
2	A	401	BU3	C1-C2-C3-C4
2	A	401	BU3	O5-C2-C3-O6
4	C	402	TRS	N-C-C3-O3
4	C	402	TRS	C1-C-C3-O3
4	C	402	TRS	C2-C-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	BU3	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/306 (92%)	0.02	4 (1%) 73 77	19, 33, 50, 63	1 (0%)
1	B	289/306 (94%)	0.14	4 (1%) 73 77	25, 35, 52, 67	1 (0%)
1	C	287/306 (93%)	0.26	10 (3%) 47 51	19, 36, 59, 85	1 (0%)
All	All	860/918 (93%)	0.14	18 (2%) 63 67	19, 35, 55, 85	3 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	PHE	3.9
1	C	30	GLU	3.5
1	B	147	PHE	3.0
1	A	289	ASN	2.9
1	C	7	PRO	2.8
1	B	2	SER	2.7
1	C	148	ASN	2.6
1	B	148	ASN	2.6
1	B	244	ASN	2.5
1	C	290	ASN	2.4
1	A	6	HIS	2.4
1	C	291	GLY	2.4
1	C	31	ASN	2.3
1	A	266	ALA	2.3
1	C	266	ALA	2.1
1	C	29	TRP	2.1
1	C	258	ASN	2.1
1	A	228	ASN	2.0

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

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(\AA^2)	Q<0.9
4	TRS	C	402	8/8	0.71	0.16	52,57,59,59	0
3	EDO	C	401	4/4	0.86	0.14	45,46,49,50	0
2	BU3	A	401	6/6	0.87	0.13	28,35,36,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.