



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 01:45 PM UTC

PDB ID : 4IZN / pdb_00004izn
Title : Structure of pcDronpa-A69T mutant
Authors : De Zitter, E.; Nguyen Bich, N.; Van Meervelt, L.; Moeyaert, B.
Deposited on : 2013-01-30
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	:	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

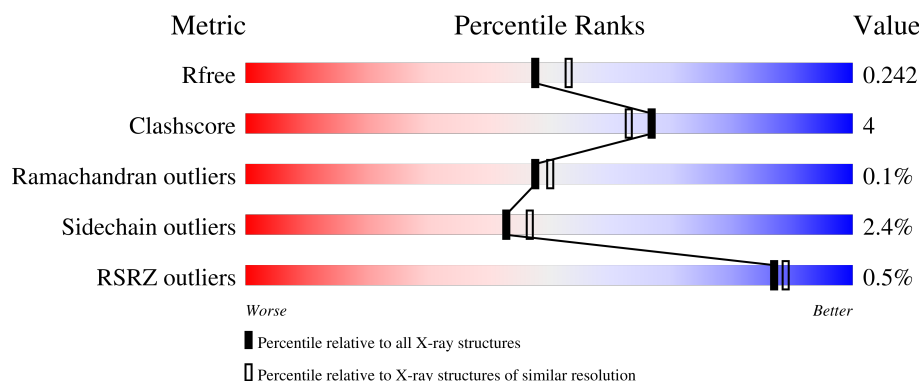
1 Overall quality at a glance

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	255	
1	B	255	
1	C	255	
1	D	255	
1	E	255	

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Mol	Chain	Length	Quality of chain
1	F	255	% 75%10%15%
1	G	255	76%9%15%
1	H	255	% 70%15%15%
1	I	255	78%7%15%
1	J	255	% 75%10%15%
1	K	255	77%7%15%
1	L	255	77%9%15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22725 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 Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	4	0
			1759	1126	296	328	9			
1	B	218	Total	C	N	O	S	0	4	0
			1781	1141	301	329	10			
1	C	217	Total	C	N	O	S	0	4	0
			1755	1124	297	325	9			
1	D	218	Total	C	N	O	S	0	2	0
			1758	1125	296	328	9			
1	E	218	Total	C	N	O	S	0	3	0
			1773	1136	300	328	9			
1	F	218	Total	C	N	O	S	0	3	0
			1771	1134	299	328	10			
1	G	218	Total	C	N	O	S	0	3	0
			1773	1136	300	328	9			
1	H	217	Total	C	N	O	S	0	4	0
			1760	1125	296	330	9			
1	I	217	Total	C	N	O	S	0	5	0
			1773	1136	298	330	9			
1	J	218	Total	C	N	O	S	0	3	0
			1770	1133	298	329	10			
1	K	218	Total	C	N	O	S	0	6	0
			1792	1147	303	333	9			
1	L	218	Total	C	N	O	S	0	2	0
			1767	1132	298	327	10			

There are 492 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	expression tag	UNP Q5TLG6
A	-31	ARG	-	expression tag	UNP Q5TLG6
A	-30	GLY	-	expression tag	UNP Q5TLG6
A	-29	SER	-	expression tag	UNP Q5TLG6
A	-28	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	HIS	-	expression tag	UNP Q5TLG6
A	-26	HIS	-	expression tag	UNP Q5TLG6
A	-25	HIS	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	GLY	-	expression tag	UNP Q5TLG6
A	-21	MET	-	expression tag	UNP Q5TLG6
A	-20	ALA	-	expression tag	UNP Q5TLG6
A	-19	SER	-	expression tag	UNP Q5TLG6
A	-18	MET	-	expression tag	UNP Q5TLG6
A	-17	THR	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6
A	-15	GLY	-	expression tag	UNP Q5TLG6
A	-14	GLN	-	expression tag	UNP Q5TLG6
A	-13	GLN	-	expression tag	UNP Q5TLG6
A	-12	MET	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	ARG	-	expression tag	UNP Q5TLG6
A	-9	ASN	-	expression tag	UNP Q5TLG6
A	-8	LEU	-	expression tag	UNP Q5TLG6
A	-7	TYR	-	expression tag	UNP Q5TLG6
A	-6	ASP	-	expression tag	UNP Q5TLG6
A	-5	ASP	-	expression tag	UNP Q5TLG6
A	-4	ASP	-	expression tag	UNP Q5TLG6
A	-3	ASP	-	expression tag	UNP Q5TLG6
A	-2	LYS	-	expression tag	UNP Q5TLG6
A	-1	ASP	-	expression tag	UNP Q5TLG6
A	0	PRO	-	expression tag	UNP Q5TLG6
A	60	ALA	VAL	engineered mutation	UNP Q5TLG6
A	64	CR8	CYS	chromophore	UNP Q5TLG6
A	64	CR8	TYR	chromophore	UNP Q5TLG6
A	64	CR8	GLY	chromophore	UNP Q5TLG6
A	69	THR	ALA	engineered mutation	UNP Q5TLG6
A	94	SER	ASN	engineered mutation	UNP Q5TLG6
A	102	ILE	ASN	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	-32	MET	-	expression tag	UNP Q5TLG6
B	-31	ARG	-	expression tag	UNP Q5TLG6
B	-30	GLY	-	expression tag	UNP Q5TLG6
B	-29	SER	-	expression tag	UNP Q5TLG6
B	-28	HIS	-	expression tag	UNP Q5TLG6
B	-27	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-26	HIS	-	expression tag	UNP Q5TLG6
B	-25	HIS	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	GLY	-	expression tag	UNP Q5TLG6
B	-21	MET	-	expression tag	UNP Q5TLG6
B	-20	ALA	-	expression tag	UNP Q5TLG6
B	-19	SER	-	expression tag	UNP Q5TLG6
B	-18	MET	-	expression tag	UNP Q5TLG6
B	-17	THR	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	GLY	-	expression tag	UNP Q5TLG6
B	-14	GLN	-	expression tag	UNP Q5TLG6
B	-13	GLN	-	expression tag	UNP Q5TLG6
B	-12	MET	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	ARG	-	expression tag	UNP Q5TLG6
B	-9	ASN	-	expression tag	UNP Q5TLG6
B	-8	LEU	-	expression tag	UNP Q5TLG6
B	-7	TYR	-	expression tag	UNP Q5TLG6
B	-6	ASP	-	expression tag	UNP Q5TLG6
B	-5	ASP	-	expression tag	UNP Q5TLG6
B	-4	ASP	-	expression tag	UNP Q5TLG6
B	-3	ASP	-	expression tag	UNP Q5TLG6
B	-2	LYS	-	expression tag	UNP Q5TLG6
B	-1	ASP	-	expression tag	UNP Q5TLG6
B	0	PRO	-	expression tag	UNP Q5TLG6
B	60	ALA	VAL	engineered mutation	UNP Q5TLG6
B	64	CR8	CYS	chromophore	UNP Q5TLG6
B	64	CR8	TYR	chromophore	UNP Q5TLG6
B	64	CR8	GLY	chromophore	UNP Q5TLG6
B	69	THR	ALA	engineered mutation	UNP Q5TLG6
B	94	SER	ASN	engineered mutation	UNP Q5TLG6
B	102	ILE	ASN	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	-32	MET	-	expression tag	UNP Q5TLG6
C	-31	ARG	-	expression tag	UNP Q5TLG6
C	-30	GLY	-	expression tag	UNP Q5TLG6
C	-29	SER	-	expression tag	UNP Q5TLG6
C	-28	HIS	-	expression tag	UNP Q5TLG6
C	-27	HIS	-	expression tag	UNP Q5TLG6
C	-26	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	HIS	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	GLY	-	expression tag	UNP Q5TLG6
C	-21	MET	-	expression tag	UNP Q5TLG6
C	-20	ALA	-	expression tag	UNP Q5TLG6
C	-19	SER	-	expression tag	UNP Q5TLG6
C	-18	MET	-	expression tag	UNP Q5TLG6
C	-17	THR	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	GLY	-	expression tag	UNP Q5TLG6
C	-14	GLN	-	expression tag	UNP Q5TLG6
C	-13	GLN	-	expression tag	UNP Q5TLG6
C	-12	MET	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	ARG	-	expression tag	UNP Q5TLG6
C	-9	ASN	-	expression tag	UNP Q5TLG6
C	-8	LEU	-	expression tag	UNP Q5TLG6
C	-7	TYR	-	expression tag	UNP Q5TLG6
C	-6	ASP	-	expression tag	UNP Q5TLG6
C	-5	ASP	-	expression tag	UNP Q5TLG6
C	-4	ASP	-	expression tag	UNP Q5TLG6
C	-3	ASP	-	expression tag	UNP Q5TLG6
C	-2	LYS	-	expression tag	UNP Q5TLG6
C	-1	ASP	-	expression tag	UNP Q5TLG6
C	0	PRO	-	expression tag	UNP Q5TLG6
C	60	ALA	VAL	engineered mutation	UNP Q5TLG6
C	64	CR8	CYS	chromophore	UNP Q5TLG6
C	64	CR8	TYR	chromophore	UNP Q5TLG6
C	64	CR8	GLY	chromophore	UNP Q5TLG6
C	69	THR	ALA	engineered mutation	UNP Q5TLG6
C	94	SER	ASN	engineered mutation	UNP Q5TLG6
C	102	ILE	ASN	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	-32	MET	-	expression tag	UNP Q5TLG6
D	-31	ARG	-	expression tag	UNP Q5TLG6
D	-30	GLY	-	expression tag	UNP Q5TLG6
D	-29	SER	-	expression tag	UNP Q5TLG6
D	-28	HIS	-	expression tag	UNP Q5TLG6
D	-27	HIS	-	expression tag	UNP Q5TLG6
D	-26	HIS	-	expression tag	UNP Q5TLG6
D	-25	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	GLY	-	expression tag	UNP Q5TLG6
D	-21	MET	-	expression tag	UNP Q5TLG6
D	-20	ALA	-	expression tag	UNP Q5TLG6
D	-19	SER	-	expression tag	UNP Q5TLG6
D	-18	MET	-	expression tag	UNP Q5TLG6
D	-17	THR	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	GLY	-	expression tag	UNP Q5TLG6
D	-14	GLN	-	expression tag	UNP Q5TLG6
D	-13	GLN	-	expression tag	UNP Q5TLG6
D	-12	MET	-	expression tag	UNP Q5TLG6
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	ARG	-	expression tag	UNP Q5TLG6
D	-9	ASN	-	expression tag	UNP Q5TLG6
D	-8	LEU	-	expression tag	UNP Q5TLG6
D	-7	TYR	-	expression tag	UNP Q5TLG6
D	-6	ASP	-	expression tag	UNP Q5TLG6
D	-5	ASP	-	expression tag	UNP Q5TLG6
D	-4	ASP	-	expression tag	UNP Q5TLG6
D	-3	ASP	-	expression tag	UNP Q5TLG6
D	-2	LYS	-	expression tag	UNP Q5TLG6
D	-1	ASP	-	expression tag	UNP Q5TLG6
D	0	PRO	-	expression tag	UNP Q5TLG6
D	60	ALA	VAL	engineered mutation	UNP Q5TLG6
D	64	CR8	CYS	chromophore	UNP Q5TLG6
D	64	CR8	TYR	chromophore	UNP Q5TLG6
D	64	CR8	GLY	chromophore	UNP Q5TLG6
D	69	THR	ALA	engineered mutation	UNP Q5TLG6
D	94	SER	ASN	engineered mutation	UNP Q5TLG6
D	102	ILE	ASN	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
E	-32	MET	-	expression tag	UNP Q5TLG6
E	-31	ARG	-	expression tag	UNP Q5TLG6
E	-30	GLY	-	expression tag	UNP Q5TLG6
E	-29	SER	-	expression tag	UNP Q5TLG6
E	-28	HIS	-	expression tag	UNP Q5TLG6
E	-27	HIS	-	expression tag	UNP Q5TLG6
E	-26	HIS	-	expression tag	UNP Q5TLG6
E	-25	HIS	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	GLY	-	expression tag	UNP Q5TLG6
E	-21	MET	-	expression tag	UNP Q5TLG6
E	-20	ALA	-	expression tag	UNP Q5TLG6
E	-19	SER	-	expression tag	UNP Q5TLG6
E	-18	MET	-	expression tag	UNP Q5TLG6
E	-17	THR	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	GLY	-	expression tag	UNP Q5TLG6
E	-14	GLN	-	expression tag	UNP Q5TLG6
E	-13	GLN	-	expression tag	UNP Q5TLG6
E	-12	MET	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6
E	-10	ARG	-	expression tag	UNP Q5TLG6
E	-9	ASN	-	expression tag	UNP Q5TLG6
E	-8	LEU	-	expression tag	UNP Q5TLG6
E	-7	TYR	-	expression tag	UNP Q5TLG6
E	-6	ASP	-	expression tag	UNP Q5TLG6
E	-5	ASP	-	expression tag	UNP Q5TLG6
E	-4	ASP	-	expression tag	UNP Q5TLG6
E	-3	ASP	-	expression tag	UNP Q5TLG6
E	-2	LYS	-	expression tag	UNP Q5TLG6
E	-1	ASP	-	expression tag	UNP Q5TLG6
E	0	PRO	-	expression tag	UNP Q5TLG6
E	60	ALA	VAL	engineered mutation	UNP Q5TLG6
E	64	CR8	CYS	chromophore	UNP Q5TLG6
E	64	CR8	TYR	chromophore	UNP Q5TLG6
E	64	CR8	GLY	chromophore	UNP Q5TLG6
E	69	THR	ALA	engineered mutation	UNP Q5TLG6
E	94	SER	ASN	engineered mutation	UNP Q5TLG6
E	102	ILE	ASN	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	engineered mutation	UNP Q5TLG6
F	-32	MET	-	expression tag	UNP Q5TLG6
F	-31	ARG	-	expression tag	UNP Q5TLG6
F	-30	GLY	-	expression tag	UNP Q5TLG6
F	-29	SER	-	expression tag	UNP Q5TLG6
F	-28	HIS	-	expression tag	UNP Q5TLG6
F	-27	HIS	-	expression tag	UNP Q5TLG6
F	-26	HIS	-	expression tag	UNP Q5TLG6
F	-25	HIS	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	GLY	-	expression tag	UNP Q5TLG6
F	-21	MET	-	expression tag	UNP Q5TLG6
F	-20	ALA	-	expression tag	UNP Q5TLG6
F	-19	SER	-	expression tag	UNP Q5TLG6
F	-18	MET	-	expression tag	UNP Q5TLG6
F	-17	THR	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	GLY	-	expression tag	UNP Q5TLG6
F	-14	GLN	-	expression tag	UNP Q5TLG6
F	-13	GLN	-	expression tag	UNP Q5TLG6
F	-12	MET	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	ARG	-	expression tag	UNP Q5TLG6
F	-9	ASN	-	expression tag	UNP Q5TLG6
F	-8	LEU	-	expression tag	UNP Q5TLG6
F	-7	TYR	-	expression tag	UNP Q5TLG6
F	-6	ASP	-	expression tag	UNP Q5TLG6
F	-5	ASP	-	expression tag	UNP Q5TLG6
F	-4	ASP	-	expression tag	UNP Q5TLG6
F	-3	ASP	-	expression tag	UNP Q5TLG6
F	-2	LYS	-	expression tag	UNP Q5TLG6
F	-1	ASP	-	expression tag	UNP Q5TLG6
F	0	PRO	-	expression tag	UNP Q5TLG6
F	60	ALA	VAL	engineered mutation	UNP Q5TLG6
F	64	CR8	CYS	chromophore	UNP Q5TLG6
F	64	CR8	TYR	chromophore	UNP Q5TLG6
F	64	CR8	GLY	chromophore	UNP Q5TLG6
F	69	THR	ALA	engineered mutation	UNP Q5TLG6
F	94	SER	ASN	engineered mutation	UNP Q5TLG6
F	102	ILE	ASN	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	engineered mutation	UNP Q5TLG6
G	-32	MET	-	expression tag	UNP Q5TLG6
G	-31	ARG	-	expression tag	UNP Q5TLG6
G	-30	GLY	-	expression tag	UNP Q5TLG6
G	-29	SER	-	expression tag	UNP Q5TLG6
G	-28	HIS	-	expression tag	UNP Q5TLG6
G	-27	HIS	-	expression tag	UNP Q5TLG6
G	-26	HIS	-	expression tag	UNP Q5TLG6
G	-25	HIS	-	expression tag	UNP Q5TLG6
G	-24	HIS	-	expression tag	UNP Q5TLG6
G	-23	HIS	-	expression tag	UNP Q5TLG6
G	-22	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	MET	-	expression tag	UNP Q5TLG6
G	-20	ALA	-	expression tag	UNP Q5TLG6
G	-19	SER	-	expression tag	UNP Q5TLG6
G	-18	MET	-	expression tag	UNP Q5TLG6
G	-17	THR	-	expression tag	UNP Q5TLG6
G	-16	GLY	-	expression tag	UNP Q5TLG6
G	-15	GLY	-	expression tag	UNP Q5TLG6
G	-14	GLN	-	expression tag	UNP Q5TLG6
G	-13	GLN	-	expression tag	UNP Q5TLG6
G	-12	MET	-	expression tag	UNP Q5TLG6
G	-11	GLY	-	expression tag	UNP Q5TLG6
G	-10	ARG	-	expression tag	UNP Q5TLG6
G	-9	ASN	-	expression tag	UNP Q5TLG6
G	-8	LEU	-	expression tag	UNP Q5TLG6
G	-7	TYR	-	expression tag	UNP Q5TLG6
G	-6	ASP	-	expression tag	UNP Q5TLG6
G	-5	ASP	-	expression tag	UNP Q5TLG6
G	-4	ASP	-	expression tag	UNP Q5TLG6
G	-3	ASP	-	expression tag	UNP Q5TLG6
G	-2	LYS	-	expression tag	UNP Q5TLG6
G	-1	ASP	-	expression tag	UNP Q5TLG6
G	0	PRO	-	expression tag	UNP Q5TLG6
G	60	ALA	VAL	engineered mutation	UNP Q5TLG6
G	64	CR8	CYS	chromophore	UNP Q5TLG6
G	64	CR8	TYR	chromophore	UNP Q5TLG6
G	64	CR8	GLY	chromophore	UNP Q5TLG6
G	69	THR	ALA	engineered mutation	UNP Q5TLG6
G	94	SER	ASN	engineered mutation	UNP Q5TLG6
G	102	ILE	ASN	engineered mutation	UNP Q5TLG6
G	218	GLY	GLU	engineered mutation	UNP Q5TLG6
H	-32	MET	-	expression tag	UNP Q5TLG6
H	-31	ARG	-	expression tag	UNP Q5TLG6
H	-30	GLY	-	expression tag	UNP Q5TLG6
H	-29	SER	-	expression tag	UNP Q5TLG6
H	-28	HIS	-	expression tag	UNP Q5TLG6
H	-27	HIS	-	expression tag	UNP Q5TLG6
H	-26	HIS	-	expression tag	UNP Q5TLG6
H	-25	HIS	-	expression tag	UNP Q5TLG6
H	-24	HIS	-	expression tag	UNP Q5TLG6
H	-23	HIS	-	expression tag	UNP Q5TLG6
H	-22	GLY	-	expression tag	UNP Q5TLG6
H	-21	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	ALA	-	expression tag	UNP Q5TLG6
H	-19	SER	-	expression tag	UNP Q5TLG6
H	-18	MET	-	expression tag	UNP Q5TLG6
H	-17	THR	-	expression tag	UNP Q5TLG6
H	-16	GLY	-	expression tag	UNP Q5TLG6
H	-15	GLY	-	expression tag	UNP Q5TLG6
H	-14	GLN	-	expression tag	UNP Q5TLG6
H	-13	GLN	-	expression tag	UNP Q5TLG6
H	-12	MET	-	expression tag	UNP Q5TLG6
H	-11	GLY	-	expression tag	UNP Q5TLG6
H	-10	ARG	-	expression tag	UNP Q5TLG6
H	-9	ASN	-	expression tag	UNP Q5TLG6
H	-8	LEU	-	expression tag	UNP Q5TLG6
H	-7	TYR	-	expression tag	UNP Q5TLG6
H	-6	ASP	-	expression tag	UNP Q5TLG6
H	-5	ASP	-	expression tag	UNP Q5TLG6
H	-4	ASP	-	expression tag	UNP Q5TLG6
H	-3	ASP	-	expression tag	UNP Q5TLG6
H	-2	LYS	-	expression tag	UNP Q5TLG6
H	-1	ASP	-	expression tag	UNP Q5TLG6
H	0	PRO	-	expression tag	UNP Q5TLG6
H	60	ALA	VAL	engineered mutation	UNP Q5TLG6
H	64	CR8	CYS	chromophore	UNP Q5TLG6
H	64	CR8	TYR	chromophore	UNP Q5TLG6
H	64	CR8	GLY	chromophore	UNP Q5TLG6
H	69	THR	ALA	engineered mutation	UNP Q5TLG6
H	94	SER	ASN	engineered mutation	UNP Q5TLG6
H	102	ILE	ASN	engineered mutation	UNP Q5TLG6
H	218	GLY	GLU	engineered mutation	UNP Q5TLG6
I	-32	MET	-	expression tag	UNP Q5TLG6
I	-31	ARG	-	expression tag	UNP Q5TLG6
I	-30	GLY	-	expression tag	UNP Q5TLG6
I	-29	SER	-	expression tag	UNP Q5TLG6
I	-28	HIS	-	expression tag	UNP Q5TLG6
I	-27	HIS	-	expression tag	UNP Q5TLG6
I	-26	HIS	-	expression tag	UNP Q5TLG6
I	-25	HIS	-	expression tag	UNP Q5TLG6
I	-24	HIS	-	expression tag	UNP Q5TLG6
I	-23	HIS	-	expression tag	UNP Q5TLG6
I	-22	GLY	-	expression tag	UNP Q5TLG6
I	-21	MET	-	expression tag	UNP Q5TLG6
I	-20	ALA	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-19	SER	-	expression tag	UNP Q5TLG6
I	-18	MET	-	expression tag	UNP Q5TLG6
I	-17	THR	-	expression tag	UNP Q5TLG6
I	-16	GLY	-	expression tag	UNP Q5TLG6
I	-15	GLY	-	expression tag	UNP Q5TLG6
I	-14	GLN	-	expression tag	UNP Q5TLG6
I	-13	GLN	-	expression tag	UNP Q5TLG6
I	-12	MET	-	expression tag	UNP Q5TLG6
I	-11	GLY	-	expression tag	UNP Q5TLG6
I	-10	ARG	-	expression tag	UNP Q5TLG6
I	-9	ASN	-	expression tag	UNP Q5TLG6
I	-8	LEU	-	expression tag	UNP Q5TLG6
I	-7	TYR	-	expression tag	UNP Q5TLG6
I	-6	ASP	-	expression tag	UNP Q5TLG6
I	-5	ASP	-	expression tag	UNP Q5TLG6
I	-4	ASP	-	expression tag	UNP Q5TLG6
I	-3	ASP	-	expression tag	UNP Q5TLG6
I	-2	LYS	-	expression tag	UNP Q5TLG6
I	-1	ASP	-	expression tag	UNP Q5TLG6
I	0	PRO	-	expression tag	UNP Q5TLG6
I	60	ALA	VAL	engineered mutation	UNP Q5TLG6
I	64	CR8	CYS	chromophore	UNP Q5TLG6
I	64	CR8	TYR	chromophore	UNP Q5TLG6
I	64	CR8	GLY	chromophore	UNP Q5TLG6
I	69	THR	ALA	engineered mutation	UNP Q5TLG6
I	94	SER	ASN	engineered mutation	UNP Q5TLG6
I	102	ILE	ASN	engineered mutation	UNP Q5TLG6
I	218	GLY	GLU	engineered mutation	UNP Q5TLG6
J	-32	MET	-	expression tag	UNP Q5TLG6
J	-31	ARG	-	expression tag	UNP Q5TLG6
J	-30	GLY	-	expression tag	UNP Q5TLG6
J	-29	SER	-	expression tag	UNP Q5TLG6
J	-28	HIS	-	expression tag	UNP Q5TLG6
J	-27	HIS	-	expression tag	UNP Q5TLG6
J	-26	HIS	-	expression tag	UNP Q5TLG6
J	-25	HIS	-	expression tag	UNP Q5TLG6
J	-24	HIS	-	expression tag	UNP Q5TLG6
J	-23	HIS	-	expression tag	UNP Q5TLG6
J	-22	GLY	-	expression tag	UNP Q5TLG6
J	-21	MET	-	expression tag	UNP Q5TLG6
J	-20	ALA	-	expression tag	UNP Q5TLG6
J	-19	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-18	MET	-	expression tag	UNP Q5TLG6
J	-17	THR	-	expression tag	UNP Q5TLG6
J	-16	GLY	-	expression tag	UNP Q5TLG6
J	-15	GLY	-	expression tag	UNP Q5TLG6
J	-14	GLN	-	expression tag	UNP Q5TLG6
J	-13	GLN	-	expression tag	UNP Q5TLG6
J	-12	MET	-	expression tag	UNP Q5TLG6
J	-11	GLY	-	expression tag	UNP Q5TLG6
J	-10	ARG	-	expression tag	UNP Q5TLG6
J	-9	ASN	-	expression tag	UNP Q5TLG6
J	-8	LEU	-	expression tag	UNP Q5TLG6
J	-7	TYR	-	expression tag	UNP Q5TLG6
J	-6	ASP	-	expression tag	UNP Q5TLG6
J	-5	ASP	-	expression tag	UNP Q5TLG6
J	-4	ASP	-	expression tag	UNP Q5TLG6
J	-3	ASP	-	expression tag	UNP Q5TLG6
J	-2	LYS	-	expression tag	UNP Q5TLG6
J	-1	ASP	-	expression tag	UNP Q5TLG6
J	0	PRO	-	expression tag	UNP Q5TLG6
J	60	ALA	VAL	engineered mutation	UNP Q5TLG6
J	64	CR8	CYS	chromophore	UNP Q5TLG6
J	64	CR8	TYR	chromophore	UNP Q5TLG6
J	64	CR8	GLY	chromophore	UNP Q5TLG6
J	69	THR	ALA	engineered mutation	UNP Q5TLG6
J	94	SER	ASN	engineered mutation	UNP Q5TLG6
J	102	ILE	ASN	engineered mutation	UNP Q5TLG6
J	218	GLY	GLU	engineered mutation	UNP Q5TLG6
K	-32	MET	-	expression tag	UNP Q5TLG6
K	-31	ARG	-	expression tag	UNP Q5TLG6
K	-30	GLY	-	expression tag	UNP Q5TLG6
K	-29	SER	-	expression tag	UNP Q5TLG6
K	-28	HIS	-	expression tag	UNP Q5TLG6
K	-27	HIS	-	expression tag	UNP Q5TLG6
K	-26	HIS	-	expression tag	UNP Q5TLG6
K	-25	HIS	-	expression tag	UNP Q5TLG6
K	-24	HIS	-	expression tag	UNP Q5TLG6
K	-23	HIS	-	expression tag	UNP Q5TLG6
K	-22	GLY	-	expression tag	UNP Q5TLG6
K	-21	MET	-	expression tag	UNP Q5TLG6
K	-20	ALA	-	expression tag	UNP Q5TLG6
K	-19	SER	-	expression tag	UNP Q5TLG6
K	-18	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-17	THR	-	expression tag	UNP Q5TLG6
K	-16	GLY	-	expression tag	UNP Q5TLG6
K	-15	GLY	-	expression tag	UNP Q5TLG6
K	-14	GLN	-	expression tag	UNP Q5TLG6
K	-13	GLN	-	expression tag	UNP Q5TLG6
K	-12	MET	-	expression tag	UNP Q5TLG6
K	-11	GLY	-	expression tag	UNP Q5TLG6
K	-10	ARG	-	expression tag	UNP Q5TLG6
K	-9	ASN	-	expression tag	UNP Q5TLG6
K	-8	LEU	-	expression tag	UNP Q5TLG6
K	-7	TYR	-	expression tag	UNP Q5TLG6
K	-6	ASP	-	expression tag	UNP Q5TLG6
K	-5	ASP	-	expression tag	UNP Q5TLG6
K	-4	ASP	-	expression tag	UNP Q5TLG6
K	-3	ASP	-	expression tag	UNP Q5TLG6
K	-2	LYS	-	expression tag	UNP Q5TLG6
K	-1	ASP	-	expression tag	UNP Q5TLG6
K	0	PRO	-	expression tag	UNP Q5TLG6
K	60	ALA	VAL	engineered mutation	UNP Q5TLG6
K	64	CR8	CYS	chromophore	UNP Q5TLG6
K	64	CR8	TYR	chromophore	UNP Q5TLG6
K	64	CR8	GLY	chromophore	UNP Q5TLG6
K	69	THR	ALA	engineered mutation	UNP Q5TLG6
K	94	SER	ASN	engineered mutation	UNP Q5TLG6
K	102	ILE	ASN	engineered mutation	UNP Q5TLG6
K	218	GLY	GLU	engineered mutation	UNP Q5TLG6
L	-32	MET	-	expression tag	UNP Q5TLG6
L	-31	ARG	-	expression tag	UNP Q5TLG6
L	-30	GLY	-	expression tag	UNP Q5TLG6
L	-29	SER	-	expression tag	UNP Q5TLG6
L	-28	HIS	-	expression tag	UNP Q5TLG6
L	-27	HIS	-	expression tag	UNP Q5TLG6
L	-26	HIS	-	expression tag	UNP Q5TLG6
L	-25	HIS	-	expression tag	UNP Q5TLG6
L	-24	HIS	-	expression tag	UNP Q5TLG6
L	-23	HIS	-	expression tag	UNP Q5TLG6
L	-22	GLY	-	expression tag	UNP Q5TLG6
L	-21	MET	-	expression tag	UNP Q5TLG6
L	-20	ALA	-	expression tag	UNP Q5TLG6
L	-19	SER	-	expression tag	UNP Q5TLG6
L	-18	MET	-	expression tag	UNP Q5TLG6
L	-17	THR	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-16	GLY	-	expression tag	UNP Q5TLG6
L	-15	GLY	-	expression tag	UNP Q5TLG6
L	-14	GLN	-	expression tag	UNP Q5TLG6
L	-13	GLN	-	expression tag	UNP Q5TLG6
L	-12	MET	-	expression tag	UNP Q5TLG6
L	-11	GLY	-	expression tag	UNP Q5TLG6
L	-10	ARG	-	expression tag	UNP Q5TLG6
L	-9	ASN	-	expression tag	UNP Q5TLG6
L	-8	LEU	-	expression tag	UNP Q5TLG6
L	-7	TYR	-	expression tag	UNP Q5TLG6
L	-6	ASP	-	expression tag	UNP Q5TLG6
L	-5	ASP	-	expression tag	UNP Q5TLG6
L	-4	ASP	-	expression tag	UNP Q5TLG6
L	-3	ASP	-	expression tag	UNP Q5TLG6
L	-2	LYS	-	expression tag	UNP Q5TLG6
L	-1	ASP	-	expression tag	UNP Q5TLG6
L	0	PRO	-	expression tag	UNP Q5TLG6
L	60	ALA	VAL	engineered mutation	UNP Q5TLG6
L	64	CR8	CYS	chromophore	UNP Q5TLG6
L	64	CR8	TYR	chromophore	UNP Q5TLG6
L	64	CR8	GLY	chromophore	UNP Q5TLG6
L	69	THR	ALA	engineered mutation	UNP Q5TLG6
L	94	SER	ASN	engineered mutation	UNP Q5TLG6
L	102	ILE	ASN	engineered mutation	UNP Q5TLG6
L	218	GLY	GLU	engineered mutation	UNP Q5TLG6

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0
2	G	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total K 1 1	0	0
2	I	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	K	1	Total K 1 1	0	0
2	L	1	Total K 1 1	0	0

- Molecule 3 is water.

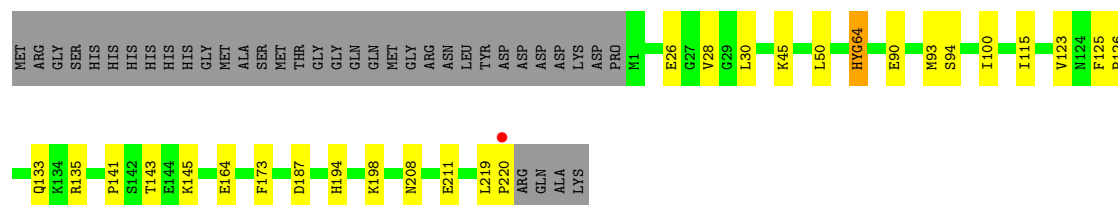
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	80	Total O 80 80	0	0
3	B	116	Total O 116 116	0	0
3	C	77	Total O 77 77	0	0
3	D	96	Total O 96 96	0	0
3	E	138	Total O 138 138	0	0
3	F	89	Total O 89 89	0	0
3	G	171	Total O 171 171	0	0
3	H	87	Total O 87 87	0	0
3	I	139	Total O 139 139	0	0
3	J	171	Total O 171 171	0	0
3	K	128	Total O 128 128	0	0
3	L	189	Total O 189 189	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.

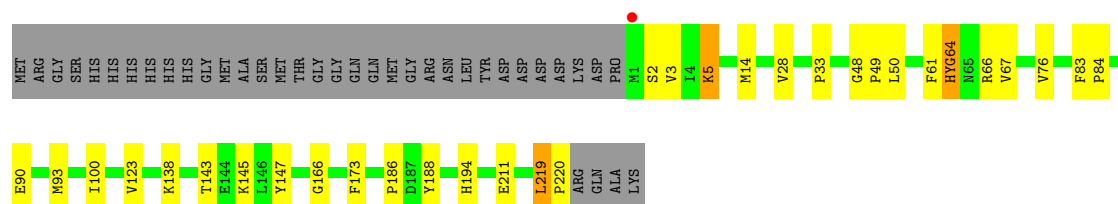
• Molecule 1: Fluorescent protein Dronpa

Chain A: 



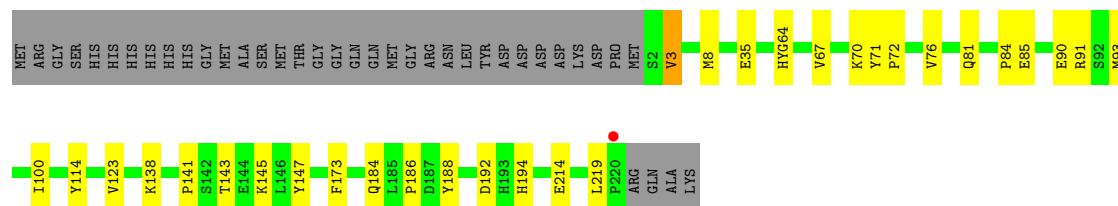
• Molecule 1: Fluorescent protein Dronpa

Chain B: 



• Molecule 1: Fluorescent protein Dronpa

Chain C: 



• Molecule 1: Fluorescent protein Dronpa

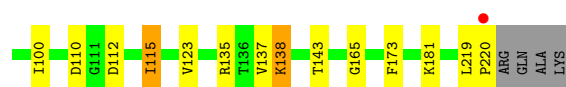
Chain D: 



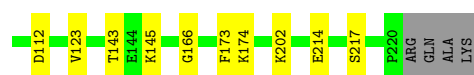
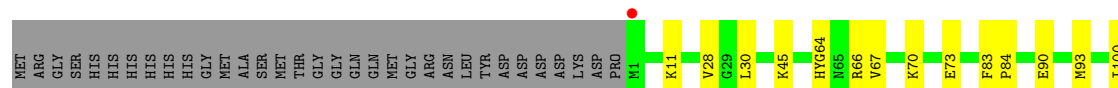
Chain E: 78% 7% 15%



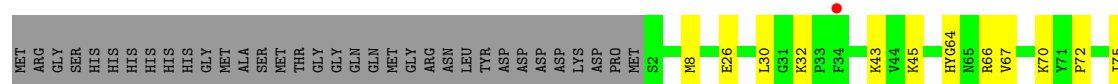
Chain F: 75% 10% 15%



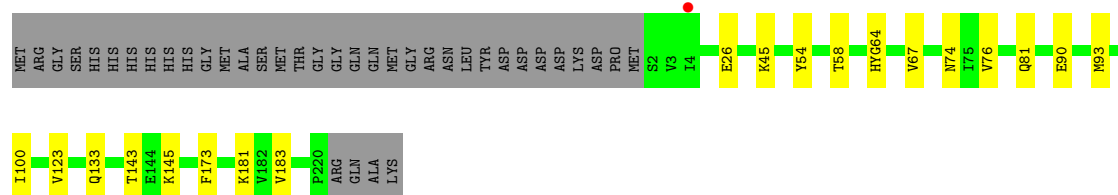
Chain G: 76% 9% 15%



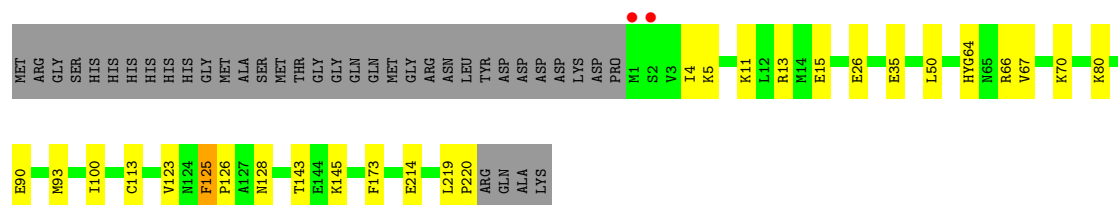
Chain H: %



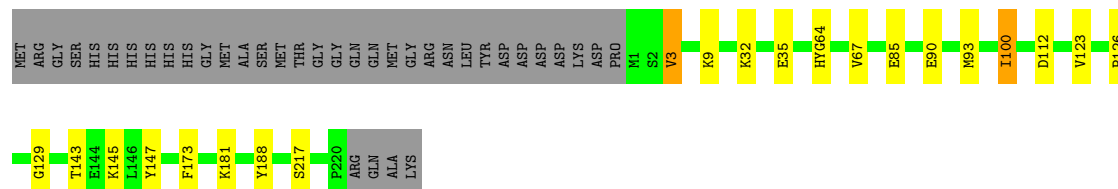
Chain I: 78% 7% 15%



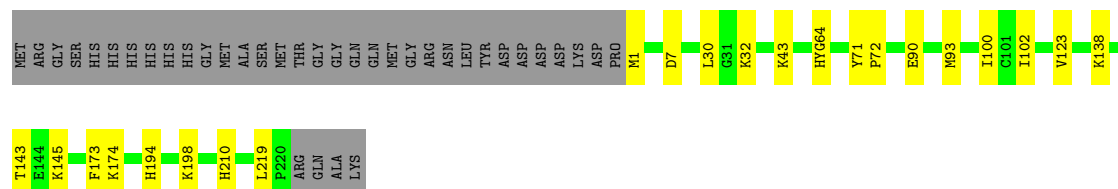
Chain J: %



Chain K: 77% 7% 15%



Chain L: 77% 9% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.70Å 180.93Å 113.16Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	34.80 – 2.15 34.80 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.80-2.15) 99.7 (34.80-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.192 , 0.245 0.192 , 0.242	Depositor DCC
R_{free} test set	8098 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22725	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CR8

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	0.43	0/1794	0.79	2/2429 (0.1%)
1	B	0.50	0/1816	0.80	3/2452 (0.1%)
1	C	0.44	0/1787	0.80	0/2417
1	D	0.48	0/1786	0.82	4/2415 (0.2%)
1	E	0.52	0/1805	0.81	0/2438
1	F	0.44	0/1803	0.82	3/2436 (0.1%)
1	G	0.51	0/1805	0.80	1/2438 (0.0%)
1	H	0.47	0/1792	0.82	6/2426 (0.2%)
1	I	0.47	0/1811	0.78	1/2448 (0.0%)
1	J	0.53	0/1801	0.83	4/2432 (0.2%)
1	K	0.49	0/1830	0.81	3/2472 (0.1%)
1	L	0.53	0/1795	0.78	0/2424
All	All	0.49	0/21625	0.81	27/29227 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	GLY	N-CA-C	6.40	120.23	112.48
1	F	58	THR	N-CA-C	6.40	118.26	111.28
1	J	125	PHE	CA-C-N	6.29	126.24	119.76
1	J	125	PHE	C-N-CA	6.29	126.24	119.76
1	K	3	VAL	N-CA-C	-6.25	105.27	111.77
1	I	58	THR	N-CA-C	5.72	117.52	111.28
1	H	165	GLY	N-CA-C	-5.71	107.23	115.27
1	D	125	PHE	CA-C-N	5.51	125.44	119.76
1	D	125	PHE	C-N-CA	5.51	125.44	119.76
1	F	165	GLY	N-CA-C	-5.45	107.15	115.00
1	J	50	LEU	CA-C-N	5.43	126.47	120.45
1	J	50	LEU	C-N-CA	5.43	126.47	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	LEU	CA-C-N	5.26	126.20	120.83
1	A	50	LEU	C-N-CA	5.26	126.20	120.83
1	G	166	GLY	N-CA-C	5.20	119.42	112.65
1	H	129	GLY	CA-C-N	5.20	124.87	119.56
1	H	129	GLY	C-N-CA	5.20	124.87	119.56
1	H	99	GLY	N-CA-C	-5.18	105.98	111.93
1	K	129	GLY	CA-C-N	5.17	124.84	119.56
1	K	129	GLY	C-N-CA	5.17	124.84	119.56
1	F	3	VAL	N-CA-C	-5.17	107.94	112.90
1	H	32	LYS	CA-C-N	5.09	126.20	119.84
1	H	32	LYS	C-N-CA	5.09	126.20	119.84
1	B	50	LEU	CA-C-N	5.07	126.00	120.83
1	B	50	LEU	C-N-CA	5.07	126.00	120.83
1	D	50	LEU	CA-C-N	5.02	126.02	120.45
1	D	50	LEU	C-N-CA	5.02	126.02	120.45

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	1759	0	1655	15	0
1	B	1781	0	1710	18	0
1	C	1755	0	1664	20	0
1	D	1758	0	1668	18	0
1	E	1773	0	1697	10	0
1	F	1771	0	1691	16	0
1	G	1773	0	1697	15	0
1	H	1760	0	1651	17	0
1	I	1773	0	1686	10	0
1	J	1770	0	1692	14	0
1	K	1792	0	1714	12	0
1	L	1767	0	1692	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	80	0	0	1	0
3	B	116	0	0	0	0
3	C	77	0	0	1	0
3	D	96	0	0	3	0
3	E	138	0	0	1	0
3	F	89	0	0	3	0
3	G	171	0	0	4	0
3	H	87	0	0	0	0
3	I	139	0	0	3	0
3	J	171	0	0	1	0
3	K	128	0	0	0	0
3	L	189	0	0	2	0
All	All	22725	0	20217	154	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 (154) 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:110:ASP:HB2	1:F:115:ILE:HD11	1.67	0.75
1:I:74:ASN:ND2	3:I:527:HOH:O	2.24	0.69
1:D:59:THR:O	3:D:496:HOH:O	2.08	0.69
1:H:81:GLN:HE22	1:H:184:GLN:HB3	1.62	0.63
1:B:64:CR8:H23	1:B:211:GLU:HB2	1.84	0.60
1:G:11:LYS:NZ	3:G:564:HOH:O	2.29	0.59
1:F:5:LYS:O	1:F:7:ASP:N	2.36	0.59
1:H:26:GLU:HG3	1:H:45:LYS:HG3	1.84	0.58
1:K:90:GLU:HB3	1:L:123:VAL:HB	1.86	0.57
1:K:123:VAL:HB	1:L:90:GLU:HB3	1.86	0.57
1:A:164:GLU:O	3:A:476:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:VAL:HB	1:J:90:GLU:HB3	1.87	0.57
1:H:135:ARG:NH1	1:H:164:GLU:HB2	2.20	0.57
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.88	0.56
1:F:137:VAL:HG12	1:F:138:LYS:HG2	1.88	0.56
1:J:128[B]:ASN:ND2	3:J:506:HOH:O	2.39	0.55
1:F:78:TYR:OH	3:F:486:HOH:O	2.17	0.55
1:G:202:LYS:O	3:G:474:HOH:O	2.17	0.55
1:H:137:VAL:HG12	1:H:138:LYS:HG2	1.89	0.55
1:I:90:GLU:HB3	1:J:123:VAL:HB	1.89	0.55
1:I:133[B]:GLN:NE2	3:I:510:HOH:O	2.39	0.55
1:D:11:LYS:HG2	1:D:28:VAL:HG12	1.89	0.55
1:F:9:LYS:NZ	1:F:112:ASP:OD2	2.37	0.55
1:B:3:VAL:HG11	1:B:84:PRO:HB3	1.89	0.54
1:D:39:SER:HB2	1:D:210:HIS:CD2	2.42	0.54
1:E:90:GLU:HB3	1:F:123:VAL:HB	1.88	0.54
1:D:66:ARG:O	3:D:477:HOH:O	2.18	0.54
1:E:123:VAL:HB	1:F:90:GLU:HB3	1.90	0.53
1:H:135:ARG:HH12	1:H:164:GLU:HB2	1.73	0.53
1:D:7:ASP:OD1	1:D:32:LYS:NZ	2.30	0.52
1:J:70:LYS:HB3	1:J:214:GLU:HG2	1.91	0.52
1:A:123:VAL:HB	1:B:90:GLU:HB3	1.92	0.51
1:G:73:GLU:O	3:G:523:HOH:O	2.19	0.51
1:C:123:VAL:HB	1:D:90:GLU:HB3	1.92	0.51
1:K:100:ILE:CG1	1:L:102:ILE:HD11	2.41	0.51
1:D:125:PHE:CE1	1:D:131:VAL:HG21	2.46	0.51
1:K:85:GLU:CD	1:K:181:LYS:HD3	2.35	0.51
1:A:90:GLU:HB3	1:B:123:VAL:HB	1.93	0.51
1:A:26:GLU:HG3	1:A:45:LYS:HG3	1.93	0.51
1:K:100:ILE:HG13	1:L:102:ILE:HD11	1.94	0.50
1:G:123:VAL:HB	1:H:90:GLU:HB3	1.93	0.50
1:B:143:THR:H	1:D:145:LYS:NZ	2.10	0.49
1:C:76:VAL:HB	1:C:186:PRO:HB3	1.94	0.49
1:H:85:GLU:OE2	1:H:181:LYS:HD3	2.12	0.49
1:K:9:LYS:NZ	1:K:112:ASP:OD2	2.40	0.49
1:F:135:ARG:NH1	3:F:485:HOH:O	2.45	0.49
1:G:66:ARG:CZ	1:G:66:ARG:HA	2.43	0.49
1:H:76:VAL:HB	1:H:186:PRO:HB3	1.95	0.49
1:A:64:CR8:H23	1:A:211:GLU:HB2	1.95	0.49
1:K:93:MET:HG2	1:K:173:PHE:CE1	2.48	0.49
1:H:72:PRO:HD2	1:H:75:ILE:HD12	1.94	0.48
1:E:79:PHE:O	1:E:82:SER:OG	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:MET:HG2	1:F:173:PHE:CE1	2.48	0.48
1:G:90:GLU:HB3	1:H:123:VAL:HB	1.94	0.48
1:J:143:THR:H	1:L:145:LYS:NZ	2.12	0.48
1:C:93:MET:HG2	1:C:173:PHE:CE1	2.48	0.48
1:G:174:LYS:NZ	3:G:479:HOH:O	2.39	0.48
1:C:90:GLU:HB3	1:D:123:VAL:HB	1.96	0.48
1:D:70:LYS:HB3	1:D:214:GLU:HG2	1.95	0.48
1:H:93:MET:HG2	1:H:173:PHE:CE1	2.49	0.48
1:B:219:LEU:HD12	1:B:220:PRO:HA	1.96	0.48
1:C:141:PRO:HG3	1:C:194:HIS:CD2	2.49	0.47
1:G:70:LYS:HB3	1:G:214:GLU:HG2	1.94	0.47
1:B:5:LYS:N	1:B:5:LYS:HD2	2.30	0.47
1:E:143:THR:H	1:G:145:LYS:NZ	2.11	0.47
1:L:138:LYS:NZ	1:L:194:HIS:HE1	2.12	0.47
1:B:93:MET:HG2	1:B:173:PHE:CE1	2.50	0.47
1:D:85:GLU:OE1	1:D:85:GLU:N	2.38	0.47
1:F:135:ARG:HG2	3:F:485:HOH:O	2.14	0.47
1:I:143:THR:H	1:K:145:LYS:NZ	2.13	0.47
1:L:198:LYS:HG3	1:L:210:HIS:CD2	2.49	0.47
1:H:203[A]:ASP:OD1	1:H:205:SER:OG	2.24	0.47
1:I:93:MET:HG2	1:I:173:PHE:CE1	2.50	0.46
1:C:81:GLN:HE22	1:C:184:GLN:HB3	1.80	0.46
1:J:13:ARG:NH1	1:J:26:GLU:OE2	2.49	0.46
1:B:138:LYS:NZ	1:B:194:HIS:HE1	2.14	0.46
1:L:138:LYS:HZ3	1:L:194:HIS:HE1	1.63	0.46
1:E:93:MET:HG2	1:E:173:PHE:CE1	2.51	0.45
1:G:45:LYS:HA	1:G:45:LYS:HD2	1.81	0.45
1:B:66:ARG:CZ	1:B:66:ARG:HA	2.46	0.45
1:C:85:GLU:OE1	1:C:85:GLU:N	2.42	0.45
1:G:93:MET:HG2	1:G:173:PHE:CE1	2.52	0.45
1:A:198:LYS:HB2	1:A:208:ASN:OD1	2.17	0.45
1:H:70:LYS:HB3	1:H:214:GLU:HG2	1.97	0.45
1:F:5:LYS:C	1:F:7:ASP:H	2.23	0.45
1:L:93:MET:HG2	1:L:173:PHE:CE1	2.52	0.45
1:D:1:MET:O	3:D:489:HOH:O	2.21	0.45
1:A:145:LYS:NZ	1:C:143:THR:H	2.15	0.44
1:E:145:LYS:NZ	1:G:143:THR:H	2.15	0.44
1:L:174:LYS:HE2	3:L:466:HOH:O	2.18	0.44
1:C:8:MET:HE2	1:C:114:TYR:CZ	2.52	0.44
1:B:64:CR8:C23	1:B:211:GLU:HB2	2.47	0.44
1:I:26:GLU:HG3	1:I:45:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:LEU:HA	1:J:220:PRO:C	2.42	0.44
1:C:3:VAL:HG11	1:C:84:PRO:HB3	2.00	0.44
1:D:93:MET:HG2	1:D:173:PHE:CE1	2.53	0.44
1:L:7:ASP:OD1	1:L:32:LYS:NZ	2.48	0.44
1:A:93:MET:HG2	1:A:173:PHE:CE1	2.52	0.44
1:G:66:ARG:HA	1:G:66:ARG:NE	2.32	0.43
1:J:66:ARG:CZ	1:J:66:ARG:HA	2.47	0.43
1:E:2:SER:C	1:E:4:ILE:H	2.26	0.43
1:J:11:LYS:HG3	1:J:113:CYS:SG	2.57	0.43
1:F:138:LYS:HE2	1:F:138:LYS:HB2	1.83	0.43
1:D:125:PHE:HA	1:D:126:PRO:HD3	1.85	0.43
1:A:141:PRO:HG3	1:A:194:HIS:CE1	2.54	0.43
1:A:219:LEU:HG	1:C:192:ASP:HB3	2.01	0.43
1:B:76:VAL:HB	1:B:186:PRO:HB3	2.00	0.43
1:D:67:VAL:HG11	1:D:114:TYR:CZ	2.54	0.43
1:D:137:VAL:HB	1:D:162:SER:OG	2.19	0.42
1:E:85:GLU:O	1:E:180:LYS:HD2	2.19	0.42
1:J:35:GLU:HA	1:J:70:LYS:HE2	2.01	0.42
1:C:35:GLU:HA	1:C:70:LYS:HE3	2.00	0.42
1:C:67:VAL:HG11	1:C:114:TYR:CZ	2.54	0.42
1:J:93:MET:HG2	1:J:173:PHE:CE1	2.54	0.42
1:G:83:PHE:HB3	1:G:84:PRO:HA	2.01	0.42
1:H:66:ARG:HA	1:H:66:ARG:NE	2.34	0.42
1:J:4:ILE:HD13	1:J:80:LYS:HG2	2.01	0.42
1:K:32:LYS:HD3	1:K:35:GLU:OE2	2.19	0.42
1:E:219:LEU:HA	1:E:220:PRO:HD3	1.89	0.42
1:I:145:LYS:NZ	1:K:143:THR:H	2.16	0.42
1:B:145:LYS:NZ	1:D:143:THR:H	2.18	0.41
1:F:85:GLU:CD	1:F:181:LYS:HD3	2.44	0.41
1:I:76:VAL:HG13	1:I:81:GLN:HE22	1.84	0.41
1:L:71:TYR:HA	1:L:72:PRO:HD2	1.89	0.41
1:B:14:MET:HE3	1:B:61:PHE:CE2	2.55	0.41
1:F:85:GLU:CD	1:F:85:GLU:H	2.26	0.41
1:A:187:ASP:OD2	1:A:187:ASP:N	2.52	0.41
1:B:33:PRO:HB3	1:B:67:VAL:HG12	2.02	0.41
1:A:143:THR:H	1:C:145:LYS:NZ	2.18	0.41
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.01	0.41
1:C:71:TYR:HA	1:C:72:PRO:HD3	1.94	0.41
1:F:143:THR:H	1:H:145:LYS:NZ	2.18	0.41
1:H:125:PHE:CE1	1:H:131:VAL:HG21	2.55	0.41
1:D:73:GLU:H	1:D:73:GLU:HG2	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:LEU:HA	1:F:220:PRO:C	2.46	0.41
1:J:125:PHE:HA	1:J:126:PRO:HD3	1.84	0.41
1:A:133[B]:GLN:OE1	1:A:135:ARG:NE	2.35	0.41
1:C:91:ARG:HD2	3:C:433:HOH:O	2.21	0.41
1:C:147:TYR:HB3	1:C:188:TYR:CD1	2.56	0.41
1:A:125:PHE:HA	1:A:126:PRO:HD3	1.94	0.41
1:C:138:LYS:NZ	1:C:194:HIS:HE1	2.19	0.41
1:G:112:ASP:OD1	1:G:112:ASP:N	2.54	0.41
1:J:145:LYS:NZ	1:L:143:THR:H	2.19	0.41
1:K:147:TYR:HB3	1:K:188:TYR:CD1	2.56	0.40
1:B:147:TYR:HB3	1:B:188:TYR:CD1	2.56	0.40
1:E:150:ASP:O	3:E:454:HOH:O	2.22	0.40
1:K:126:PRO:HB3	3:L:531:HOH:O	2.21	0.40
1:L:43:LYS:HB3	1:L:43:LYS:HE3	1.94	0.40
1:A:219:LEU:HA	1:A:220:PRO:HD3	1.90	0.40
1:B:48:GLY:HA2	1:B:49:PRO:C	2.46	0.40
1:C:219:LEU:HD23	1:C:219:LEU:HA	1.86	0.40
1:H:219:LEU:HA	1:H:220:PRO:HD3	1.87	0.40
1:I:54:TYR:N	3:I:439:HOH:O	2.54	0.40
1:L:219:LEU:HD23	1:L:219:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/255 (85%)	213 (98%)	4 (2%)	0	100	100
1	B	217/255 (85%)	215 (99%)	1 (0%)	1 (0%)	24	20
1	C	215/255 (84%)	212 (99%)	3 (1%)	0	100	100
1	D	215/255 (84%)	211 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	216/255 (85%)	214 (99%)	1 (0%)	1 (0%)	24	20
1	F	216/255 (85%)	211 (98%)	4 (2%)	1 (0%)	24	20
1	G	216/255 (85%)	215 (100%)	1 (0%)	0	100	100
1	H	216/255 (85%)	214 (99%)	2 (1%)	0	100	100
1	I	217/255 (85%)	216 (100%)	1 (0%)	0	100	100
1	J	216/255 (85%)	216 (100%)	0	0	100	100
1	K	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
1	L	215/255 (84%)	212 (99%)	3 (1%)	0	100	100
All	All	2595/3060 (85%)	2566 (99%)	26 (1%)	3 (0%)	48	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	6	PRO
1	B	2	SER
1	E	3	VAL

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	185/217 (85%)	180 (97%)	5 (3%)	39	41
1	B	191/217 (88%)	187 (98%)	4 (2%)	47	52
1	C	186/217 (86%)	184 (99%)	2 (1%)	65	72
1	D	186/217 (86%)	181 (97%)	5 (3%)	39	41
1	E	189/217 (87%)	185 (98%)	4 (2%)	47	52
1	F	189/217 (87%)	183 (97%)	6 (3%)	34	36
1	G	189/217 (87%)	184 (97%)	5 (3%)	40	43
1	H	186/217 (86%)	178 (96%)	8 (4%)	26	24
1	I	189/217 (87%)	185 (98%)	4 (2%)	47	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	189/217 (87%)	185 (98%)	4 (2%)	47	52
1	K	192/217 (88%)	188 (98%)	4 (2%)	47	52
1	L	188/217 (87%)	185 (98%)	3 (2%)	55	61
All	All	2259/2604 (87%)	2205 (98%)	54 (2%)	43	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	30	LEU
1	A	94	SER
1	A	100	ILE
1	A	115	ILE
1	B	5	LYS
1	B	28	VAL
1	B	100	ILE
1	B	219	LEU
1	C	3	VAL
1	C	100	ILE
1	D	30	LEU
1	D	67	VAL
1	D	73	GLU
1	D	100	ILE
1	D	135	ARG
1	E	4	ILE
1	E	28	VAL
1	E	30	LEU
1	E	100	ILE
1	F	28	VAL
1	F	30	LEU
1	F	67	VAL
1	F	100	ILE
1	F	115	ILE
1	F	138	LYS
1	G	28	VAL
1	G	30	LEU
1	G	67	VAL
1	G	100	ILE
1	G	217	SER
1	H	8	MET
1	H	30	LEU

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Mol	Chain	Res	Type
1	H	43	LYS
1	H	67	VAL
1	H	81	GLN
1	H	100	ILE
1	H	135	ARG
1	H	187	ASP
1	I	67	VAL
1	I	100	ILE
1	I	181	LYS
1	I	183	VAL
1	J	5	LYS
1	J	15	GLU
1	J	67	VAL
1	J	100	ILE
1	K	3	VAL
1	K	67	VAL
1	K	100	ILE
1	K	217	SER
1	L	1	MET
1	L	30	LEU
1	L	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	HIS
1	B	212	HIS
1	C	194	HIS
1	D	194	HIS
1	E	194	HIS
1	F	65	ASN
1	F	194	HIS
1	F	212	HIS
1	G	194	HIS
1	H	38	GLN
1	I	38	GLN
1	I	194	HIS
1	J	21	HIS
1	J	38	GLN
1	J	194	HIS
1	L	194	HIS
1	L	208	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
1	CR8	D	64	1	25,27,28	1.96	6 (24%)	24,37,39	1.35	2 (8%)
1	CR8	H	64	1	25,27,28	1.96	6 (24%)	24,37,39	1.44	4 (16%)
1	CR8	J	64	1	25,27,28	1.96	6 (24%)	24,37,39	1.19	1 (4%)
1	CR8	G	64	1	25,27,28	1.94	5 (20%)	24,37,39	1.51	4 (16%)
1	CR8	I	64	1	25,27,28	1.86	5 (20%)	24,37,39	1.48	4 (16%)
1	CR8	B	64	1	25,27,28	2.00	6 (24%)	24,37,39	1.28	1 (4%)
1	CR8	C	64	1	25,27,28	1.95	7 (28%)	24,37,39	1.74	5 (20%)
1	CR8	L	64	1	25,27,28	2.03	5 (20%)	24,37,39	1.41	2 (8%)
1	CR8	F	64	1	25,27,28	1.95	5 (20%)	24,37,39	1.38	3 (12%)
1	CR8	K	64	1	25,27,28	1.92	6 (24%)	24,37,39	1.70	3 (12%)
1	CR8	A	64	1	25,27,28	1.92	5 (20%)	24,37,39	1.51	4 (16%)
1	CR8	E	64	1	25,27,28	1.88	5 (20%)	24,37,39	1.49	4 (16%)

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
1	CR8	D	64	1	-	3/12/25/26	0/3/3/3
1	CR8	H	64	1	-	3/12/25/26	0/3/3/3
1	CR8	J	64	1	-	3/12/25/26	0/3/3/3
1	CR8	G	64	1	-	2/12/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR8	I	64	1	-	3/12/25/26	0/3/3/3
1	CR8	B	64	1	-	3/12/25/26	0/3/3/3
1	CR8	C	64	1	-	3/12/25/26	0/3/3/3
1	CR8	L	64	1	-	2/12/25/26	0/3/3/3
1	CR8	F	64	1	-	2/12/25/26	0/3/3/3
1	CR8	K	64	1	-	2/12/25/26	0/3/3/3
1	CR8	A	64	1	-	6/12/25/26	0/3/3/3
1	CR8	E	64	1	-	4/12/25/26	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	64	CR8	C8-C7	5.61	1.52	1.39
1	J	64	CR8	C8-C7	5.48	1.52	1.39
1	B	64	CR8	C8-C7	5.37	1.52	1.39
1	F	64	CR8	C8-C7	5.36	1.52	1.39
1	D	64	CR8	C8-C7	5.10	1.51	1.39
1	L	64	CR8	O13-C11	5.08	1.40	1.24
1	I	64	CR8	C8-C7	5.06	1.51	1.39
1	L	64	CR8	C8-C7	5.03	1.51	1.39
1	A	64	CR8	C8-C7	4.99	1.51	1.39
1	C	64	CR8	C8-C7	4.95	1.51	1.39
1	G	64	CR8	C8-C7	4.93	1.51	1.39
1	E	64	CR8	C8-C7	4.89	1.51	1.39
1	G	64	CR8	O13-C11	4.82	1.39	1.24
1	D	64	CR8	O13-C11	4.75	1.39	1.24
1	B	64	CR8	O13-C11	4.72	1.39	1.24
1	K	64	CR8	C8-C7	4.71	1.50	1.39
1	J	64	CR8	O13-C11	4.60	1.38	1.24
1	K	64	CR8	O13-C11	4.59	1.38	1.24
1	E	64	CR8	O13-C11	4.52	1.38	1.24
1	A	64	CR8	O13-C11	4.52	1.38	1.24
1	F	64	CR8	O13-C11	4.47	1.38	1.24
1	H	64	CR8	O13-C11	4.46	1.38	1.24
1	C	64	CR8	O13-C11	4.43	1.38	1.24
1	I	64	CR8	O13-C11	4.30	1.37	1.24
1	L	64	CR8	C12-C11	-3.40	1.37	1.46
1	K	64	CR8	C12-C11	-3.26	1.37	1.46
1	G	64	CR8	C12-C11	-3.24	1.37	1.46
1	H	64	CR8	C12-C11	-3.23	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	CR8	C12-C11	-3.17	1.38	1.46
1	K	64	CR8	C4-C11	-3.14	1.38	1.46
1	C	64	CR8	C12-C11	-3.12	1.38	1.46
1	L	64	CR8	O2-C2	-3.12	1.21	1.31
1	B	64	CR8	C12-C11	-3.11	1.38	1.46
1	F	64	CR8	C12-C11	-3.09	1.38	1.46
1	I	64	CR8	C12-C11	-3.00	1.38	1.46
1	G	64	CR8	O2-C2	-2.99	1.21	1.31
1	C	64	CR8	C4-C11	-2.97	1.38	1.46
1	L	64	CR8	C4-C11	-2.97	1.38	1.46
1	C	64	CR8	O2-C2	-2.96	1.22	1.31
1	D	64	CR8	O2-C2	-2.96	1.22	1.31
1	A	64	CR8	C4-C11	-2.92	1.38	1.46
1	B	64	CR8	O2-C2	-2.90	1.22	1.31
1	K	64	CR8	O2-C2	-2.88	1.22	1.31
1	E	64	CR8	C4-C11	-2.87	1.38	1.46
1	A	64	CR8	C12-C11	-2.87	1.38	1.46
1	F	64	CR8	C4-C11	-2.82	1.38	1.46
1	J	64	CR8	C4-C11	-2.82	1.38	1.46
1	I	64	CR8	C4-C11	-2.81	1.39	1.46
1	A	64	CR8	O2-C2	-2.79	1.22	1.31
1	B	64	CR8	C4-C11	-2.78	1.39	1.46
1	F	64	CR8	O2-C2	-2.76	1.22	1.31
1	G	64	CR8	C4-C11	-2.74	1.39	1.46
1	I	64	CR8	O2-C2	-2.65	1.23	1.31
1	J	64	CR8	O2-C2	-2.64	1.23	1.31
1	H	64	CR8	C4-C11	-2.61	1.39	1.46
1	J	64	CR8	C12-C11	-2.60	1.39	1.46
1	H	64	CR8	O2-C2	-2.57	1.23	1.31
1	E	64	CR8	O2-C2	-2.53	1.23	1.31
1	D	64	CR8	C4-C11	-2.52	1.39	1.46
1	C	64	CR8	C8-CA2	-2.46	1.34	1.40
1	E	64	CR8	C12-C11	-2.46	1.39	1.46
1	K	64	CR8	C8-CA2	-2.41	1.34	1.40
1	C	64	CR8	C1-N3	2.16	1.40	1.37
1	D	64	CR8	C5-C4	2.14	1.40	1.35
1	H	64	CR8	C5-C4	2.10	1.40	1.35
1	B	64	CR8	C1-N3	2.05	1.40	1.37
1	J	64	CR8	C6-C12	2.03	1.40	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	CR8	C8-CA2-C2	-4.11	120.95	129.19
1	K	64	CR8	C8-CA2-C2	-4.10	120.98	129.19
1	L	64	CR8	C8-CA2-C2	-3.96	121.25	129.19
1	A	64	CR8	C8-CA2-C2	-3.93	121.31	129.19
1	I	64	CR8	C8-CA2-C2	-3.93	121.32	129.19
1	C	64	CR8	N3-C1-N2	3.81	114.49	111.48
1	D	64	CR8	C8-CA2-C2	-3.79	121.59	129.19
1	B	64	CR8	C8-CA2-C2	-3.70	121.78	129.19
1	E	64	CR8	C8-CA2-C2	-3.59	121.99	129.19
1	G	64	CR8	C8-CA2-C2	-3.38	122.42	129.19
1	K	64	CR8	N3-C1-N2	3.23	114.03	111.48
1	F	64	CR8	C8-CA2-C2	-3.15	122.87	129.19
1	J	64	CR8	C8-CA2-C2	-3.15	122.88	129.19
1	F	64	CR8	N3-C1-N2	3.09	113.92	111.48
1	H	64	CR8	N3-C1-N2	2.90	113.77	111.48
1	C	64	CR8	C4-C5-C7	-2.90	119.36	122.10
1	H	64	CR8	C8-CA2-C2	-2.78	123.62	129.19
1	G	64	CR8	C4-C5-C7	-2.71	119.54	122.10
1	I	64	CR8	N3-C1-N2	2.66	113.58	111.48
1	G	64	CR8	N3-C1-N2	2.64	113.57	111.48
1	C	64	CR8	CA2-N2-C1	-2.51	103.84	105.80
1	K	64	CR8	C4-C5-C7	-2.40	119.83	122.10
1	A	64	CR8	N3-C1-N2	2.40	113.38	111.48
1	D	64	CR8	C4-C5-C7	-2.33	119.90	122.10
1	G	64	CR8	C3-CA3-N3	2.32	117.70	112.43
1	H	64	CR8	O13-C11-C12	-2.31	117.84	121.56
1	A	64	CR8	C4-C5-C7	-2.27	119.95	122.10
1	L	64	CR8	C12-C6-C7	-2.21	120.01	122.10
1	E	64	CR8	N3-C1-N2	2.21	113.22	111.48
1	E	64	CR8	C12-C6-C7	-2.16	120.06	122.10
1	E	64	CR8	C4-C11-C12	2.13	120.62	116.67
1	A	64	CR8	C4-C11-C12	2.11	120.59	116.67
1	H	64	CR8	CA1-C20-C21	-2.09	109.76	113.23
1	I	64	CR8	C4-C5-C7	-2.07	120.14	122.10
1	F	64	CR8	C4-C5-C7	-2.07	120.14	122.10
1	I	64	CR8	C4-C11-C12	2.07	120.51	116.67
1	C	64	CR8	C4-C11-C12	2.07	120.51	116.67

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	CR8	CA1-C20-C21-N22

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Mol	Chain	Res	Type	Atoms
1	A	64	CR8	CA1-C20-C21-C23
1	B	64	CR8	CA1-C20-C21-N22
1	B	64	CR8	CA1-C20-C21-C23
1	C	64	CR8	CA1-C20-C21-N22
1	C	64	CR8	CA1-C20-C21-C23
1	D	64	CR8	CA1-C20-C21-N22
1	D	64	CR8	CA1-C20-C21-C23
1	E	64	CR8	CA1-C20-C21-N22
1	E	64	CR8	CA1-C20-C21-C23
1	F	64	CR8	CA1-C20-C21-N22
1	G	64	CR8	CA1-C20-C21-N22
1	G	64	CR8	CA1-C20-C21-C23
1	H	64	CR8	CA1-C20-C21-N22
1	I	64	CR8	CA1-C20-C21-N22
1	I	64	CR8	CA1-C20-C21-C23
1	J	64	CR8	CA1-C20-C21-N22
1	J	64	CR8	CA1-C20-C21-C23
1	K	64	CR8	CA1-C20-C21-N22
1	K	64	CR8	CA1-C20-C21-C23
1	L	64	CR8	CA1-C20-C21-N22
1	L	64	CR8	CA1-C20-C21-C23
1	F	64	CR8	CA1-C20-C21-C23
1	H	64	CR8	CA1-C20-C21-C23
1	A	64	CR8	C21-C20-CA1-N1
1	A	64	CR8	C3-CA3-N3-C2
1	D	64	CR8	C3-CA3-N3-C2
1	B	64	CR8	C21-C20-CA1-N1
1	A	64	CR8	C5-C7-C8-CA2
1	A	64	CR8	C6-C7-C8-CA2
1	C	64	CR8	C5-C7-C8-CA2
1	E	64	CR8	C5-C7-C8-CA2
1	E	64	CR8	C3-CA3-N3-C2
1	H	64	CR8	C3-CA3-N3-C2
1	I	64	CR8	C3-CA3-N3-C2
1	J	64	CR8	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	64	CR8	2	0
1	A	64	CR8	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are 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 ⓘ

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	217/255 (85%)	0.09	1 (0%) 87 89	18, 36, 60, 92	4 (1%)
1	B	217/255 (85%)	-0.09	1 (0%) 87 89	16, 29, 53, 78	4 (1%)
1	C	216/255 (84%)	-0.15	1 (0%) 87 89	17, 33, 56, 81	3 (1%)
1	D	217/255 (85%)	-0.22	0 100 100	16, 30, 53, 80	2 (0%)
1	E	217/255 (85%)	-0.29	2 (0%) 81 83	14, 26, 52, 80	3 (1%)
1	F	217/255 (85%)	0.01	2 (0%) 81 83	16, 34, 64, 97	3 (1%)
1	G	217/255 (85%)	-0.41	1 (0%) 87 89	11, 24, 46, 69	3 (1%)
1	H	216/255 (84%)	-0.07	2 (0%) 81 83	14, 32, 61, 77	4 (1%)
1	I	216/255 (84%)	-0.32	1 (0%) 87 89	14, 28, 51, 72	5 (2%)
1	J	217/255 (85%)	-0.37	2 (0%) 81 83	12, 24, 43, 83	3 (1%)
1	K	217/255 (85%)	-0.34	0 100 100	13, 25, 45, 81	6 (2%)
1	L	217/255 (85%)	-0.47	0 100 100	10, 22, 40, 62	2 (0%)
All	All	2601/3060 (85%)	-0.22	13 (0%) 87 89	10, 29, 55, 97	42 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	220	PRO	2.6
1	E	2	SER	2.6
1	F	220	PRO	2.5
1	G	1	MET	2.5
1	H	34	PHE	2.5
1	F	4	ILE	2.5
1	J	1	MET	2.4
1	A	220	PRO	2.3
1	I	4	ILE	2.2
1	C	220	PRO	2.2
1	B	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	2	SER	2.1
1	E	21[A]	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CR8	A	64	25/26	0.88	0.09	29,41,51,55	0
1	CR8	B	64	25/26	0.92	0.08	18,28,41,47	0
1	CR8	F	64	25/26	0.92	0.08	29,38,53,61	0
1	CR8	H	64	25/26	0.94	0.07	25,31,44,46	0
1	CR8	C	64	25/26	0.95	0.07	25,34,41,47	0
1	CR8	I	64	25/26	0.95	0.07	20,28,43,46	0
1	CR8	E	64	25/26	0.96	0.06	12,20,31,38	0
1	CR8	D	64	25/26	0.96	0.06	18,29,36,40	0
1	CR8	J	64	25/26	0.96	0.06	12,17,30,35	0
1	CR8	K	64	25/26	0.96	0.06	13,20,30,31	0
1	CR8	G	64	25/26	0.97	0.05	13,19,22,27	0
1	CR8	L	64	25/26	0.97	0.05	10,12,21,27	0

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	K	A	301	1/1	0.71	0.12	76,76,76,76	0
2	K	B	301	1/1	0.86	0.11	55,55,55,55	0
2	K	G	301	1/1	0.86	0.11	47,47,47,47	0
2	K	C	301	1/1	0.88	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	I	301	1/1	0.90	0.10	60,60,60,60	0
2	K	D	301	1/1	0.93	0.07	44,44,44,44	0
2	K	J	301	1/1	0.93	0.07	51,51,51,51	0
2	K	K	301	1/1	0.93	0.06	47,47,47,47	0
2	K	H	301	1/1	0.94	0.09	48,48,48,48	0
2	K	F	301	1/1	0.94	0.12	43,43,43,43	0
2	K	E	301	1/1	0.95	0.14	45,45,45,45	0
2	K	L	301	1/1	0.99	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.