



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:55 am BST

PDB ID : 4IZN  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

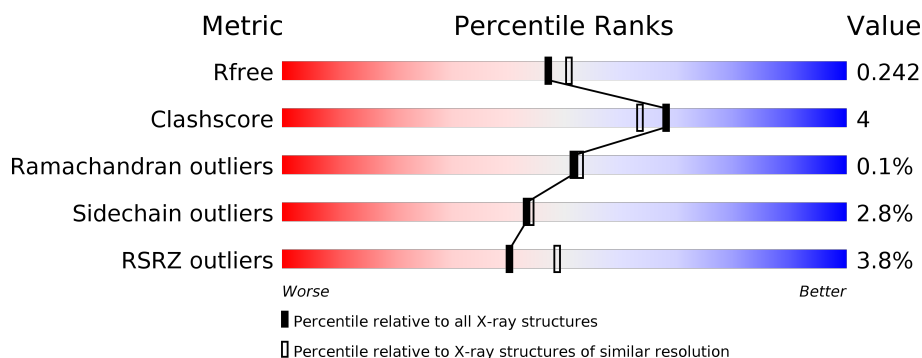
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>15%</div> </div> </div>
1	B	255	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>15%</div> </div> </div>
1	C	255	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>15%</div> </div> </div>
1	D	255	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>15%</div> </div> </div>
1	E	255	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>15%</div> </div> </div>
1	F	255	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	255	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>77%</div><div>8%</div><div>15%</div></div></div>
1	H	255	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>70%</div><div>15%</div><div>15%</div></div></div>
1	I	255	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>78%</div><div>6%</div><div>15%</div></div></div>
1	J	255	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>75%</div><div>10%</div><div>•</div><div>15%</div></div></div>
1	K	255	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>78%</div><div>7%</div><div>•</div><div>15%</div></div></div>
1	L	255	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>7%</div><div>•</div><div>15%</div></div></div>

## 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 (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	K	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	L	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

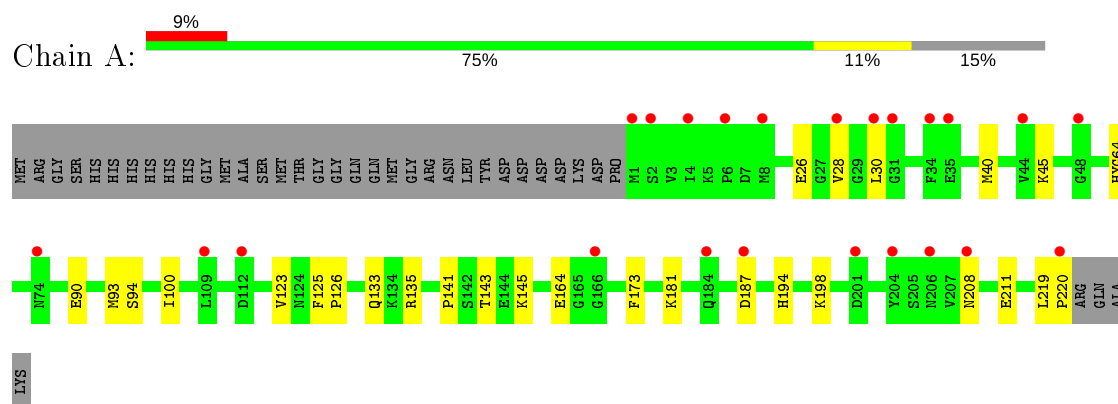
- Molecule 3 is water.

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

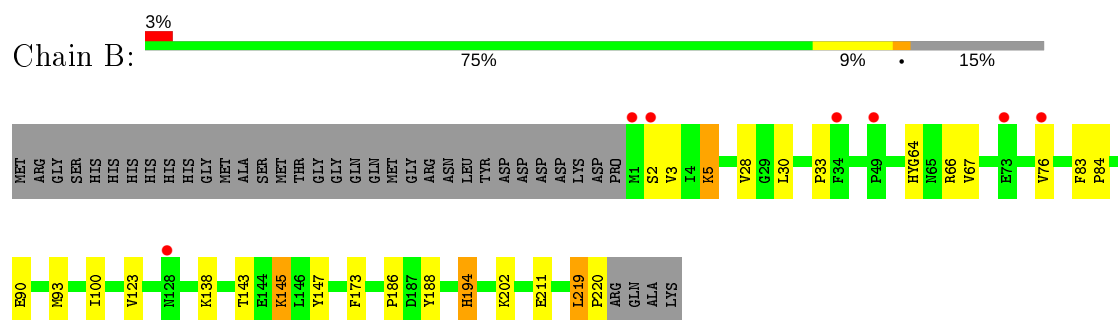
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

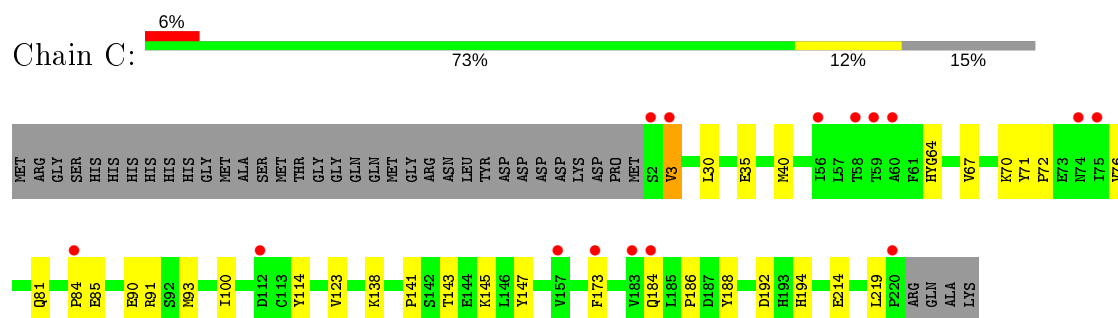
#### • Molecule 1: Fluorescent protein Dronpa



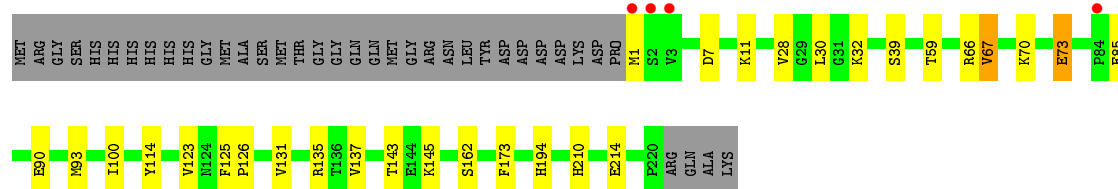
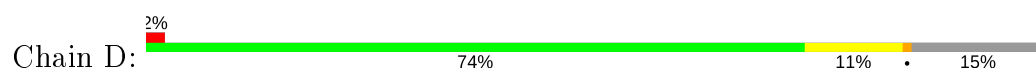
#### • Molecule 1: Fluorescent protein Dronpa



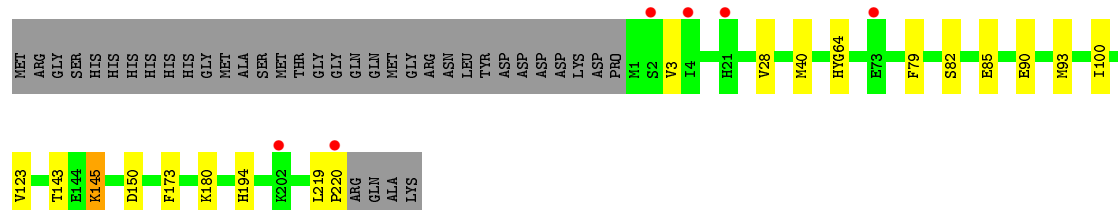
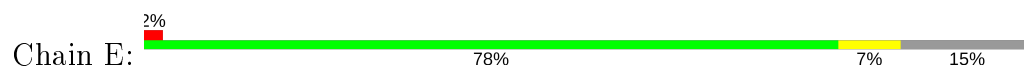
#### • Molecule 1: Fluorescent protein Dronpa



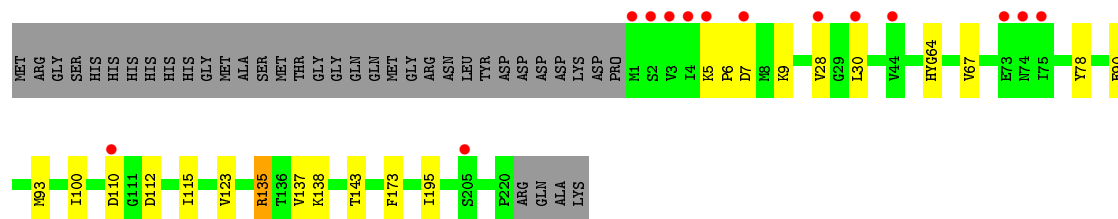
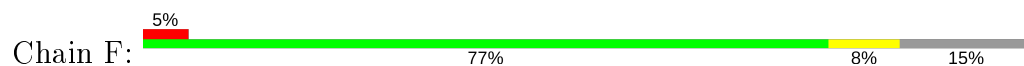
#### • Molecule 1: Fluorescent protein Dronpa



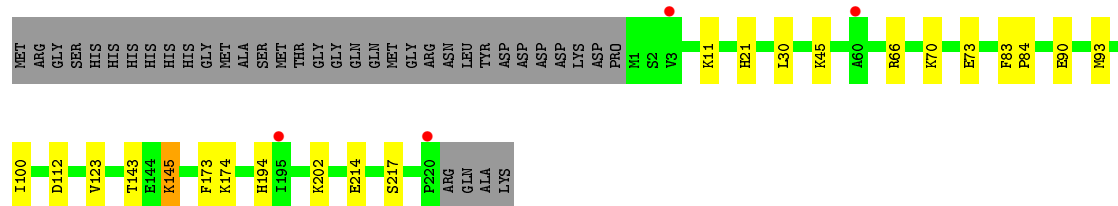
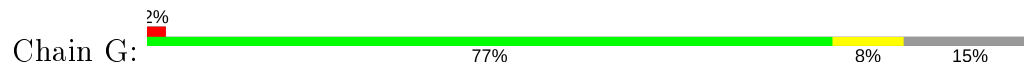
- Molecule 1: Fluorescent protein Dronpa



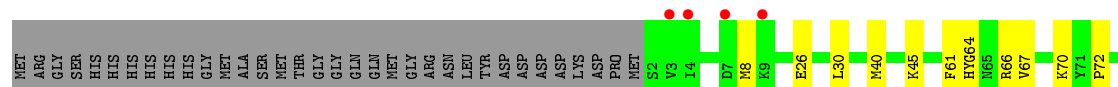
- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa

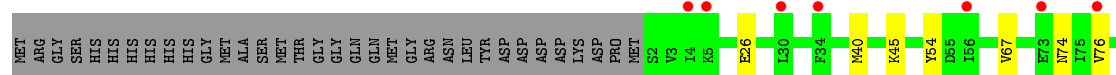
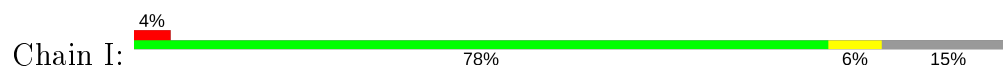


- Molecule 1: Fluorescent protein Dronpa

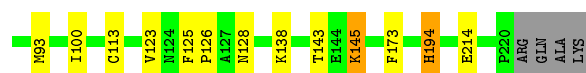
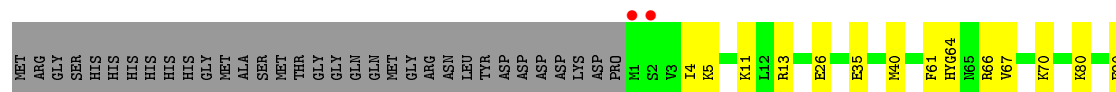




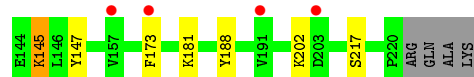
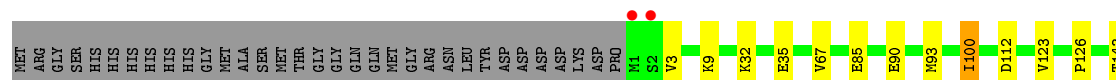
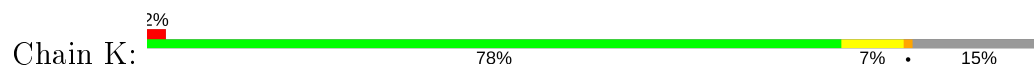
• Molecule 1: Fluorescent protein Dronpa



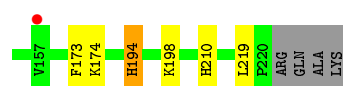
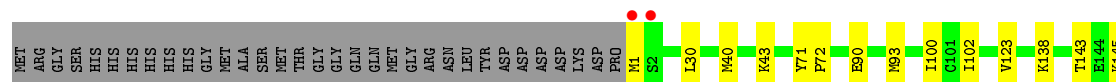
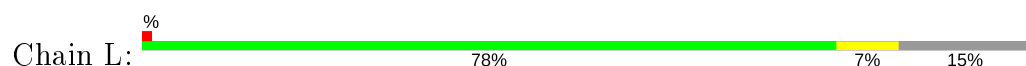
• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.70 Å 180.93 Å 113.16 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.16 Å)	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	8094 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.36	0/1794	0.55	0/2429
1	B	0.41	0/1816	0.58	0/2452
1	C	0.38	0/1787	0.55	0/2417
1	D	0.40	0/1786	0.59	0/2415
1	E	0.42	0/1805	0.59	0/2438
1	F	0.38	0/1803	0.55	0/2436
1	G	0.43	0/1805	0.58	0/2438
1	H	0.38	0/1792	0.56	0/2426
1	I	0.39	0/1811	0.56	0/2448
1	J	0.44	0/1801	0.59	0/2432
1	K	0.41	0/1830	0.57	0/2472
1	L	0.45	0/1795	0.60	0/2424
All	All	0.40	0/21625	0.57	0/29227

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1665	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1781	0	1720	16	0
1	C	1755	0	1674	21	0
1	D	1758	0	1678	18	0
1	E	1773	0	1707	11	0
1	F	1771	0	1701	13	0
1	G	1773	0	1707	15	0
1	H	1760	0	1661	20	0
1	I	1773	0	1696	11	0
1	J	1770	0	1702	17	0
1	K	1792	0	1724	12	0
1	L	1767	0	1702	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
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	2	0
3	D	96	0	0	3	0
3	E	138	0	0	2	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	20337	158	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 (158) 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:123:VAL:HB	1:L:90:GLU:HB3	1.86	0.57
1:K:90:GLU:HB3	1:L:123:VAL:HB	1.86	0.57
1:A:164:GLU:O	3:A:476:HOH:O	2.17	0.57
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:133[B]:GLN:NE2	3:I:510:HOH:O	2.39	0.55
1:I:90:GLU:HB3	1:J:123:VAL:HB	1.89	0.55
1:D:11:LYS:HG2	1:D:28:VAL:HG12	1.89	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: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: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:C:64:CR8:H8	3:C:456:HOH:O	2.11	0.50
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:H:64:CR8:H4	1:H:195:ILE:HB	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:7:ASP:OD1	1:D:32:LYS:NZ	2.30	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
1:F:9:LYS:NZ	1:F:112:ASP:OD2	2.37	0.48
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:E:64:CR8:H8	3:E:418: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:K:85:GLU:CD	1:K:181:LYS:HD3	2.35	0.46
1:B:138:LYS:NZ	1:B:194:HIS:HE1	2.14	0.46
1:E:93:MET:HG2	1:E:173:PHE:CE1	2.51	0.45
1:G:45:LYS:HD2	1:G:45:LYS:HA	1.81	0.45
1:B:66:ARG:CZ	1:B:66:ARG:HA	2.46	0.45
1:C:85:GLU:N	1:C:85:GLU:OE1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:PHE:O	1:H:64:CR8:H171	2.17	0.45
1:H:70:LYS:HB3	1:H:214:GLU:HG2	1.97	0.45
1:J:40:MET:HE2	1:J:40:MET:HB2	1.85	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: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
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:A:93:MET:HG2	1:A:173:PHE:CE1	2.52	0.44
1:G:66:ARG:NE	1:G:66:ARG:HA	2.32	0.43
1:H:40:MET:HE2	1:H:40:MET:HB2	1.81	0.43
1:J:66:ARG:CZ	1:J:66:ARG:HA	2.47	0.43
1:J:11:LYS:HG3	1:J:113:CYS:SG	2.57	0.43
1:C:40:MET:HB2	1:C:40:MET:HE2	1.80	0.43
1:L:40:MET:HB2	1:L:40:MET:HE2	1.81	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:B:76:VAL:HB	1:B:186:PRO:HB3	2.00	0.43
1:A:219:LEU:HG	1:C:192:ASP:HB3	2.01	0.43
1:D:67:VAL:HG11	1:D:114:TYR:CZ	2.54	0.43
1:A:40:MET:HE2	1:A:40:MET:HB2	1.88	0.42
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:A:187:ASP:OD2	1:A:187:ASP:N	2.52	0.42
1:C:67:VAL:HG11	1:C:114:TYR:CZ	2.54	0.42
1:C:35:GLU:HA	1:C:70:LYS:HE3	2.00	0.42
1:J:93:MET:HG2	1:J:173:PHE:CE1	2.54	0.42
1:E:40:MET:HB2	1:E:40:MET:HE2	1.79	0.42
1:G:83:PHE:HB3	1:G:84:PRO:HA	2.01	0.42
1:H:66:ARG:NE	1:H:66:ARG:HA	2.34	0.42
1:J:4:ILE:HD13	1:J:80:LYS:HG2	2.01	0.42
1:I:40:MET:HB2	1:I:40:MET:HE2	1.89	0.42
1:K:32:LYS:HD3	1:K:35:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:64:CR8:H4	1:F:195:ILE:HB	2.02	0.41
1:B:33:PRO:HB3	1:B:67:VAL:HG12	2.02	0.41
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.01	0.41
1:A:143:THR:H	1:C:145:LYS:NZ	2.18	0.41
1:C:71:TYR:HA	1:C:72:PRO:HD3	1.94	0.41
1:H:125:PHE:CE1	1:H:131:VAL:HG21	2.55	0.41
1:F:143:THR:H	1:H:145:LYS:NZ	2.18	0.41
1:D:73:GLU:HG2	1:D:73:GLU:H	1.60	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:147:TYR:HB3	1:C:188:TYR:CD1	2.56	0.41
1:C:91:ARG:HD2	3:C:433:HOH:O	2.21	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:N	1:G:112:ASP:OD1	2.54	0.41
1:J:61:PHE:O	1:J:64:CR8:H171	2.21	0.41
1:J:138:LYS:HZ1	1:J:194:HIS:HE1	1.69	0.41
1:J:61:PHE:C	1:J:64:CR8:H171	2.41	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: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:HA	1:L:219:LEU:HD23	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	219/255 (86%)	214 (98%)	5 (2%)	0	100	100
1	B	219/255 (86%)	217 (99%)	1 (0%)	1 (0%)	29	22
1	C	217/255 (85%)	213 (98%)	4 (2%)	0	100	100
1	D	217/255 (85%)	213 (98%)	4 (2%)	0	100	100
1	E	218/255 (86%)	215 (99%)	2 (1%)	1 (0%)	29	22
1	F	218/255 (86%)	212 (97%)	5 (2%)	1 (0%)	29	22
1	G	218/255 (86%)	216 (99%)	2 (1%)	0	100	100
1	H	218/255 (86%)	215 (99%)	3 (1%)	0	100	100
1	I	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
1	J	218/255 (86%)	217 (100%)	1 (0%)	0	100	100
1	K	221/255 (87%)	218 (99%)	3 (1%)	0	100	100
1	L	217/255 (85%)	213 (98%)	4 (2%)	0	100	100
All	All	2619/3060 (86%)	2580 (98%)	36 (1%)	3 (0%)	51	53

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%)	44	46
1	B	191/217 (88%)	183 (96%)	8 (4%)	30	28
1	C	186/217 (86%)	183 (98%)	3 (2%)	62	67
1	D	186/217 (86%)	180 (97%)	6 (3%)	39	38
1	E	189/217 (87%)	185 (98%)	4 (2%)	53	57
1	F	189/217 (87%)	184 (97%)	5 (3%)	46	47
1	G	189/217 (87%)	182 (96%)	7 (4%)	34	32
1	H	186/217 (86%)	179 (96%)	7 (4%)	33	31
1	I	189/217 (87%)	185 (98%)	4 (2%)	53	57
1	J	189/217 (87%)	184 (97%)	5 (3%)	46	47
1	K	192/217 (88%)	186 (97%)	6 (3%)	40	39
1	L	188/217 (87%)	184 (98%)	4 (2%)	53	57
All	All	2259/2604 (87%)	2195 (97%)	64 (3%)	43	44

All (64) 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	181	LYS
1	B	5	LYS
1	B	28	VAL
1	B	30	LEU
1	B	100	ILE
1	B	145	LYS
1	B	194	HIS
1	B	202	LYS
1	B	219	LEU
1	C	3	VAL
1	C	30	LEU
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	D	194	HIS

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Mol	Chain	Res	Type
1	E	28	VAL
1	E	100	ILE
1	E	145	LYS
1	E	194	HIS
1	F	28	VAL
1	F	30	LEU
1	F	67	VAL
1	F	100	ILE
1	F	135	ARG
1	G	21[A]	HIS
1	G	21[B]	HIS
1	G	30	LEU
1	G	100	ILE
1	G	145	LYS
1	G	194	HIS
1	G	217	SER
1	H	8	MET
1	H	30	LEU
1	H	67	VAL
1	H	100	ILE
1	H	135	ARG
1	H	187	ASP
1	H	194	HIS
1	I	67	VAL
1	I	100	ILE
1	I	145	LYS
1	I	181	LYS
1	J	5	LYS
1	J	67	VAL
1	J	100	ILE
1	J	145	LYS
1	J	194	HIS
1	K	3	VAL
1	K	67	VAL
1	K	100	ILE
1	K	145	LYS
1	K	202	LYS
1	K	217	SER
1	L	1	MET
1	L	30	LEU
1	L	100	ILE
1	L	194	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	ASN
1	B	194	HIS
1	C	194	HIS
1	D	194	HIS
1	D	210	HIS
1	E	194	HIS
1	F	194	HIS
1	G	194	HIS
1	H	158	ASN
1	I	194	HIS
1	J	194	HIS
1	L	194	HIS
1	L	210	HIS

### 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	B	64	1	20,27,28	2.46	6 (30%)	17,37,39	1.26	1 (5%)
1	CR8	H	64	1	20,27,28	2.52	8 (40%)	17,37,39	1.51	4 (23%)
1	CR8	K	64	1	20,27,28	2.38	5 (25%)	17,37,39	1.64	5 (29%)
1	CR8	I	64	1	20,27,28	2.44	8 (40%)	17,37,39	1.56	4 (23%)
1	CR8	D	64	1	20,27,28	2.43	7 (35%)	17,37,39	1.42	3 (17%)
1	CR8	G	64	1	20,27,28	2.40	6 (30%)	17,37,39	1.59	3 (17%)
1	CR8	E	64	1	20,27,28	2.32	5 (25%)	17,37,39	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CR8	C	64	1	20,27,28	2.38	6 (30%)	17,37,39	1.47	3 (17%)
1	CR8	F	64	1	20,27,28	2.46	6 (30%)	17,37,39	1.34	2 (11%)
1	CR8	A	64	1	20,27,28	2.39	6 (30%)	17,37,39	1.42	3 (17%)
1	CR8	J	64	1	20,27,28	2.47	8 (40%)	17,37,39	1.17	2 (11%)
1	CR8	L	64	1	20,27,28	2.47	5 (25%)	17,37,39	1.54	2 (11%)

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	B	64	1	-	3/8/25/26	0/3/3/3
1	CR8	H	64	1	-	2/8/25/26	0/3/3/3
1	CR8	K	64	1	-	2/8/25/26	0/3/3/3
1	CR8	I	64	1	-	2/8/25/26	0/3/3/3
1	CR8	D	64	1	-	2/8/25/26	0/3/3/3
1	CR8	G	64	1	-	2/8/25/26	0/3/3/3
1	CR8	E	64	1	-	4/8/25/26	0/3/3/3
1	CR8	C	64	1	-	4/8/25/26	0/3/3/3
1	CR8	F	64	1	-	2/8/25/26	0/3/3/3
1	CR8	A	64	1	-	5/8/25/26	0/3/3/3
1	CR8	J	64	1	-	2/8/25/26	0/3/3/3
1	CR8	L	64	1	-	2/8/25/26	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	64	CR8	C8-C7	6.93	1.52	1.36
1	J	64	CR8	C8-C7	6.79	1.52	1.36
1	B	64	CR8	C8-C7	6.68	1.52	1.36
1	F	64	CR8	C8-C7	6.66	1.52	1.36
1	D	64	CR8	C8-C7	6.39	1.51	1.36
1	I	64	CR8	C8-C7	6.35	1.51	1.36
1	L	64	CR8	C8-C7	6.32	1.51	1.36
1	A	64	CR8	C8-C7	6.28	1.51	1.36
1	C	64	CR8	C8-C7	6.24	1.51	1.36
1	G	64	CR8	C8-C7	6.21	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	64	CR8	C8-C7	6.17	1.51	1.36
1	K	64	CR8	C8-C7	5.99	1.50	1.36
1	L	64	CR8	O3-C1	5.08	1.40	1.24
1	G	64	CR8	O3-C1	4.82	1.39	1.24
1	D	64	CR8	O3-C1	4.75	1.39	1.24
1	B	64	CR8	O3-C1	4.73	1.39	1.24
1	J	64	CR8	O3-C1	4.60	1.38	1.24
1	K	64	CR8	O3-C1	4.59	1.38	1.24
1	E	64	CR8	O3-C1	4.52	1.38	1.24
1	A	64	CR8	O3-C1	4.52	1.38	1.24
1	F	64	CR8	O3-C1	4.47	1.38	1.24
1	H	64	CR8	O3-C1	4.47	1.38	1.24
1	C	64	CR8	O3-C1	4.43	1.38	1.24
1	I	64	CR8	O3-C1	4.30	1.37	1.24
1	L	64	CR8	O25-C12	-3.71	1.21	1.32
1	L	64	CR8	C2-C1	-3.68	1.37	1.45
1	G	64	CR8	O25-C12	-3.58	1.21	1.32
1	C	64	CR8	O25-C12	-3.55	1.22	1.32
1	D	64	CR8	O25-C12	-3.55	1.22	1.32
1	K	64	CR8	C2-C1	-3.53	1.37	1.45
1	G	64	CR8	C2-C1	-3.51	1.37	1.45
1	H	64	CR8	C2-C1	-3.49	1.37	1.45
1	B	64	CR8	O25-C12	-3.48	1.22	1.32
1	K	64	CR8	O25-C12	-3.46	1.22	1.32
1	D	64	CR8	C2-C1	-3.44	1.38	1.45
1	K	64	CR8	C4-C1	-3.40	1.38	1.45
1	C	64	CR8	C2-C1	-3.38	1.38	1.45
1	A	64	CR8	O25-C12	-3.37	1.22	1.32
1	B	64	CR8	C2-C1	-3.37	1.38	1.45
1	F	64	CR8	C2-C1	-3.34	1.38	1.45
1	F	64	CR8	O25-C12	-3.34	1.22	1.32
1	I	64	CR8	C2-C1	-3.25	1.38	1.45
1	I	64	CR8	O25-C12	-3.22	1.23	1.32
1	J	64	CR8	O25-C12	-3.22	1.23	1.32
1	C	64	CR8	C4-C1	-3.22	1.38	1.45
1	L	64	CR8	C4-C1	-3.22	1.38	1.45
1	A	64	CR8	C4-C1	-3.16	1.38	1.45
1	H	64	CR8	O25-C12	-3.14	1.23	1.32
1	E	64	CR8	C4-C1	-3.11	1.38	1.45
1	E	64	CR8	O25-C12	-3.10	1.23	1.32
1	A	64	CR8	C2-C1	-3.10	1.38	1.45
1	F	64	CR8	C4-C1	-3.05	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	64	CR8	C4-C1	-3.05	1.38	1.45
1	I	64	CR8	C4-C1	-3.04	1.39	1.45
1	B	64	CR8	C4-C1	-3.01	1.39	1.45
1	G	64	CR8	C4-C1	-2.96	1.39	1.45
1	H	64	CR8	C4-C1	-2.83	1.39	1.45
1	J	64	CR8	C2-C1	-2.82	1.39	1.45
1	D	64	CR8	C4-C1	-2.73	1.39	1.45
1	E	64	CR8	C2-C1	-2.66	1.39	1.45
1	J	64	CR8	C17-N13	-2.57	1.44	1.49
1	H	64	CR8	C14-N15	-2.51	1.31	1.34
1	I	64	CR8	C17-N13	-2.45	1.44	1.49
1	I	64	CR8	C14-N15	-2.38	1.31	1.34
1	D	64	CR8	C14-N15	-2.26	1.31	1.34
1	B	64	CR8	C14-N15	-2.26	1.31	1.34
1	A	64	CR8	C14-N15	-2.24	1.31	1.34
1	F	64	CR8	C14-N15	-2.24	1.31	1.34
1	D	64	CR8	C5-C4	2.23	1.40	1.35
1	H	64	CR8	C5-C4	2.20	1.40	1.35
1	C	64	CR8	C14-N15	-2.20	1.31	1.34
1	G	64	CR8	C17-N13	-2.15	1.45	1.49
1	J	64	CR8	C6-C2	2.12	1.40	1.35
1	H	64	CR8	C17-N13	-2.12	1.45	1.49
1	J	64	CR8	C14-N15	-2.09	1.31	1.34
1	I	64	CR8	C5-C4	2.02	1.40	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	64	CR8	C-C17-N13	3.81	117.70	111.92
1	L	64	CR8	C-C17-N13	3.32	116.96	111.92
1	K	64	CR8	C-C17-N13	3.29	116.92	111.92
1	D	64	CR8	C-C17-N13	3.24	116.83	111.92
1	C	64	CR8	C4-C5-C7	-3.05	119.36	121.95
1	I	64	CR8	C20-C16-C14	-2.96	105.84	110.62
1	G	64	CR8	C4-C5-C7	-2.84	119.54	121.95
1	J	64	CR8	O19-C-C17	-2.59	118.96	126.32
1	I	64	CR8	O19-C-C17	-2.55	119.07	126.32
1	K	64	CR8	C4-C5-C7	-2.50	119.83	121.95
1	G	64	CR8	O19-C-C17	-2.46	119.33	126.32
1	D	64	CR8	C4-C5-C7	-2.42	119.90	121.95
1	K	64	CR8	O19-C-C17	-2.39	119.53	126.32
1	H	64	CR8	O19-C-C17	-2.37	119.59	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CR8	C4-C5-C7	-2.35	119.95	121.95
1	H	64	CR8	O3-C1-C2	-2.32	117.84	121.56
1	L	64	CR8	C2-C6-C7	-2.29	120.01	121.95
1	E	64	CR8	C4-C1-C2	2.27	120.62	116.62
1	A	64	CR8	C4-C1-C2	2.25	120.59	116.62
1	J	64	CR8	C-C17-N13	2.24	115.32	111.92
1	E	64	CR8	C2-C6-C7	-2.23	120.06	121.95
1	I	64	CR8	C4-C1-C2	2.21	120.51	116.62
1	C	64	CR8	C4-C1-C2	2.21	120.51	116.62
1	D	64	CR8	O19-C-C17	-2.20	120.06	126.32
1	F	64	CR8	O19-C-C17	-2.19	120.10	126.32
1	A	64	CR8	O19-C-C17	-2.15	120.22	126.32
1	I	64	CR8	C4-C5-C7	-2.13	120.14	121.95
1	F	64	CR8	C4-C5-C7	-2.13	120.14	121.95
1	K	64	CR8	C6-C7-C8	-2.10	115.98	121.90
1	C	64	CR8	O19-C-C17	-2.09	120.37	126.32
1	K	64	CR8	C4-C1-C2	2.07	120.26	116.62
1	H	64	CR8	C20-C16-C14	-2.05	107.30	110.62
1	B	64	CR8	O19-C-C17	-2.05	120.49	126.32
1	H	64	CR8	C6-C7-C8	-2.02	116.20	121.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	64	CR8	C16-C20-C21-N22
1	B	64	CR8	C16-C20-C21-C23
1	H	64	CR8	C16-C20-C21-N22
1	K	64	CR8	C16-C20-C21-N22
1	K	64	CR8	C16-C20-C21-C23
1	I	64	CR8	C16-C20-C21-N22
1	I	64	CR8	C16-C20-C21-C23
1	D	64	CR8	C16-C20-C21-N22
1	D	64	CR8	C16-C20-C21-C23
1	G	64	CR8	C16-C20-C21-N22
1	G	64	CR8	C16-C20-C21-C23
1	E	64	CR8	C16-C20-C21-N22
1	E	64	CR8	C16-C20-C21-C23
1	C	64	CR8	C16-C20-C21-N22
1	C	64	CR8	C16-C20-C21-C23
1	F	64	CR8	C16-C20-C21-N22
1	A	64	CR8	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
1	A	64	CR8	C16-C20-C21-N22
1	A	64	CR8	C16-C20-C21-C23
1	J	64	CR8	C16-C20-C21-N22
1	J	64	CR8	C16-C20-C21-C23
1	L	64	CR8	C16-C20-C21-N22
1	L	64	CR8	C16-C20-C21-C23
1	A	64	CR8	N-C16-C20-C21
1	B	64	CR8	N-C16-C20-C21
1	E	64	CR8	C5-C7-C8-C9
1	E	64	CR8	C6-C7-C8-C9
1	C	64	CR8	C5-C7-C8-C9
1	C	64	CR8	C6-C7-C8-C9
1	A	64	CR8	C5-C7-C8-C9
1	H	64	CR8	C16-C20-C21-C23
1	F	64	CR8	C16-C20-C21-C23

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	64	CR8	2	0
1	H	64	CR8	2	0
1	E	64	CR8	1	0
1	C	64	CR8	1	0
1	F	64	CR8	1	0
1	A	64	CR8	1	0
1	J	64	CR8	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	217/255 (85%)	0.67	23 (10%) 6 9	18, 37, 60, 92	0
1	B	217/255 (85%)	0.19	7 (3%) 47 56	16, 30, 53, 78	0
1	C	216/255 (84%)	0.43	15 (6%) 16 23	17, 33, 56, 81	0
1	D	217/255 (85%)	0.02	4 (1%) 68 75	16, 30, 53, 80	0
1	E	217/255 (85%)	0.08	6 (2%) 53 62	14, 27, 52, 80	0
1	F	217/255 (85%)	0.34	14 (6%) 18 25	16, 34, 64, 97	0
1	G	217/255 (85%)	0.17	4 (1%) 68 75	12, 24, 46, 69	0
1	H	216/255 (84%)	0.14	4 (1%) 66 74	14, 32, 61, 77	0
1	I	216/255 (84%)	0.22	11 (5%) 28 36	14, 29, 51, 72	0
1	J	217/255 (85%)	0.04	2 (0%) 84 88	12, 24, 43, 83	0
1	K	217/255 (85%)	0.30	6 (2%) 53 62	13, 26, 45, 81	0
1	L	217/255 (85%)	0.09	3 (1%) 75 80	12, 22, 40, 62	0
All	All	2601/3060 (85%)	0.22	99 (3%) 40 49	12, 29, 55, 97	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.2
1	F	1	MET	5.3
1	B	1	MET	4.9
1	F	3	VAL	4.8
1	I	4	ILE	4.5
1	A	2	SER	4.1
1	D	1	MET	4.1
1	A	34	PHE	3.9
1	H	3	VAL	3.9
1	A	220	PRO	3.8
1	G	220	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	2	SER	3.8
1	C	2	SER	3.7
1	A	166	GLY	3.7
1	K	1	MET	3.6
1	A	112	ASP	3.4
1	A	4	ILE	3.3
1	D	3	VAL	3.3
1	K	2	SER	3.2
1	H	4	ILE	3.2
1	E	2	SER	3.2
1	B	73	GLU	3.1
1	A	30	LEU	3.1
1	F	4	ILE	3.1
1	F	73	GLU	3.0
1	A	184	GLN	2.9
1	H	9	LYS	2.9
1	K	157	VAL	2.8
1	A	31	GLY	2.8
1	L	157	VAL	2.8
1	F	205	SER	2.8
1	C	74	ASN	2.8
1	C	112	ASP	2.7
1	I	102	ILE	2.7
1	C	220	PRO	2.7
1	H	7	ASP	2.7
1	A	109	LEU	2.7
1	K	173	PHE	2.7
1	A	74	ASN	2.7
1	A	44	VAL	2.7
1	F	30	LEU	2.6
1	I	73	GLU	2.6
1	A	204	TYR	2.6
1	F	5	LYS	2.6
1	B	34	PHE	2.6
1	E	202	LYS	2.5
1	E	73	GLU	2.5
1	A	28	VAL	2.5
1	F	44	VAL	2.5
1	K	203[A]	ASP	2.5
1	C	75	ILE	2.5
1	A	6	PRO	2.5
1	D	2	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	173	PHE	2.4
1	L	2	SER	2.4
1	C	84	PRO	2.4
1	C	184	GLN	2.4
1	E	21[A]	HIS	2.4
1	K	191	VAL	2.3
1	I	184	GLN	2.3
1	C	183	VAL	2.3
1	A	206	ASN	2.3
1	I	34	PHE	2.3
1	D	84	PRO	2.3
1	I	220	PRO	2.3
1	A	208	ASN	2.3
1	B	76	VAL	2.2
1	C	157	VAL	2.2
1	B	2	SER	2.2
1	B	49	PRO	2.2
1	E	220	PRO	2.2
1	A	201	ASP	2.2
1	G	60	ALA	2.2
1	J	1	MET	2.2
1	I	30	LEU	2.2
1	C	3	VAL	2.2
1	F	75	ILE	2.2
1	I	56	ILE	2.2
1	I	112	ASP	2.2
1	A	187	ASP	2.1
1	L	1	MET	2.1
1	G	195	ILE	2.1
1	B	128[A]	ASN	2.1
1	C	58	THR	2.1
1	F	7	ASP	2.1
1	F	110	ASP	2.1
1	C	59	THR	2.1
1	C	60	ALA	2.1
1	E	4	ILE	2.0
1	F	74	ASN	2.0
1	F	28	VAL	2.0
1	J	2	SER	2.0
1	C	56	ILE	2.0
1	G	3	VAL	2.0
1	I	76	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	5	LYS	2.0
1	A	8	MET	2.0
1	A	35	GLU	2.0
1	A	48	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CR8	A	64	25/26	0.93	0.14	29,41,51,55	0
1	CR8	F	64	25/26	0.94	0.14	29,38,53,61	0
1	CR8	B	64	25/26	0.94	0.15	18,28,41,47	0
1	CR8	C	64	25/26	0.95	0.20	25,34,41,47	0
1	CR8	H	64	25/26	0.95	0.13	25,31,44,46	0
1	CR8	I	64	25/26	0.95	0.15	20,28,43,46	0
1	CR8	J	64	25/26	0.96	0.16	12,17,30,35	0
1	CR8	D	64	25/26	0.97	0.14	18,29,36,40	0
1	CR8	E	64	25/26	0.97	0.16	12,20,31,38	0
1	CR8	K	64	25/26	0.97	0.20	13,20,30,31	0
1	CR8	L	64	25/26	0.97	0.17	10,12,21,27	0
1	CR8	G	64	25/26	0.98	0.23	13,19,22,27	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	A	301	1/1	0.71	0.15	76,76,76,76	0
2	K	B	301	1/1	0.88	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	G	301	1/1	0.89	0.11	47,47,47,47	0
2	K	I	301	1/1	0.89	0.17	60,60,60,60	0
2	K	D	301	1/1	0.92	0.06	44,44,44,44	0
2	K	C	301	1/1	0.94	0.08	67,67,67,67	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	J	301	1/1	0.94	0.16	51,51,51,51	0
2	K	E	301	1/1	0.96	0.18	45,45,45,45	0
2	K	K	301	1/1	0.96	0.05	47,47,47,47	0
2	K	L	301	1/1	0.99	0.03	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.