



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:26 AM GMT

PDB ID : 2GX2
Title : Crystal structural and functional analysis of GFP-like fluorescent protein Dronpa
Authors : Hwang, K.Y.; Nam, K.-H.; Park, S.-Y.; Sugiyama, K.
Deposited on : 2006-05-08
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

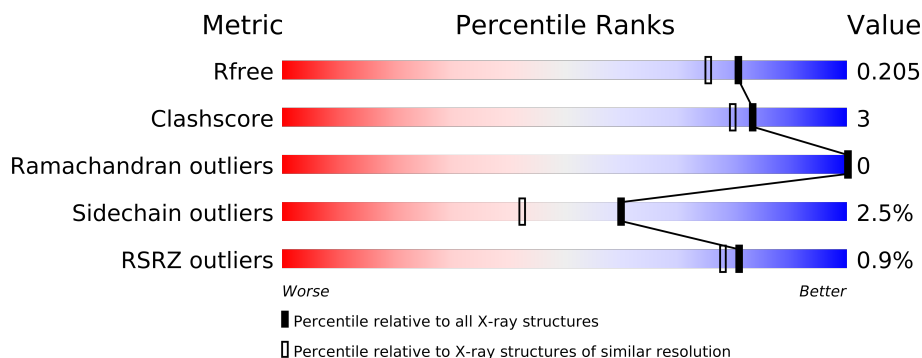
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	241	
1	B	241	
1	C	241	
1	D	241	
1	E	241	
1	F	241	
1	G	241	
1	H	241	
1	I	241	
1	J	241	
1	K	241	
1	L	241	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	3027	-	X
2	MG	A	3031	-	X
2	MG	A	3033	-	X
2	MG	B	3041	-	X
2	MG	B	3042	-	X
2	MG	B	3044	-	X
2	MG	C	3004	-	X
2	MG	C	3012	-	X
2	MG	C	3016	-	X
2	MG	C	3039	-	X
2	MG	D	3013	-	X
2	MG	D	3020	-	X
2	MG	E	3001	-	X
2	MG	E	3002	-	X
2	MG	E	3023	-	X
2	MG	F	3008	-	X
2	MG	F	3045	-	X
2	MG	G	3057	-	X
2	MG	H	3032	-	X
2	MG	H	3038	-	X
2	MG	H	3060	-	X
2	MG	I	3005	-	X
2	MG	I	3019	-	X
2	MG	J	3017	-	X
2	MG	K	3036	-	X
2	MG	K	3050	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23035 atoms, of which 0 are hydrogen and 0 are deuterium.

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	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	B	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	C	218	Total	C	N	O	S	0	0	0
			1762	1125	298	330	9			
1	D	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	E	218	Total	C	N	O	S	0	0	0
			1762	1125	298	330	9			
1	F	218	Total	C	N	O	S	0	0	0
			1762	1125	298	330	9			
1	G	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	H	218	Total	C	N	O	S	0	0	0
			1762	1125	298	330	9			
1	I	218	Total	C	N	O	S	0	0	0
			1762	1125	298	330	9			
1	J	217	Total	C	N	O	S	0	0	0
			1751	1119	294	329	9			
1	K	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	L	214	Total	C	N	O	S	0	0	0
			1730	1105	291	325	9			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
A	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
A	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
A	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
A	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
A	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
A	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
A	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
A	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
B	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
B	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
B	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
B	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
B	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
B	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
B	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
B	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
B	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
C	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
C	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
C	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
C	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
C	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
C	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
C	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
C	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
C	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
D	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
D	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
D	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
D	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
D	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
D	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
D	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
D	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
E	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
E	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
E	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
E	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
E	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
E	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
E	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
E	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
E	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
E	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
E	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
E	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
F	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
F	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
F	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
F	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
F	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
F	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
F	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
F	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
F	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
F	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
F	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
G	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
G	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
G	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
G	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
G	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
G	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
G	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
G	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
G	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
G	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
G	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
G	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
G	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
G	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
G	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
G	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
G	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
G	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
G	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
G	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
G	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
G	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
G	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
H	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
H	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
H	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
H	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
H	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
H	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
H	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
H	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
H	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
H	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
H	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
H	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
H	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
H	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
H	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
H	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
H	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
H	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
H	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
H	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
H	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
H	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
I	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
I	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
I	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
I	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
I	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
I	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
I	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
I	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
I	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
I	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
I	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
I	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
I	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
I	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
I	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
I	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
I	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
I	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
I	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
I	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
I	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
I	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
I	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
J	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
J	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
J	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
J	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
J	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
J	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
J	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
J	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
J	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
J	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
J	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
J	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
J	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
J	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
J	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
J	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
J	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
J	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
J	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
J	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
J	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
J	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
K	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
K	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
K	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
K	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6
K	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
K	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
K	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
K	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
K	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
K	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
K	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
K	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
K	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
K	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
K	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
K	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
K	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
K	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
K	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
K	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
K	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
K	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
K	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6
L	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
L	-17	ARG	-	EXPRESSION TAG	UNP Q5TLG6
L	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
L	-15	SER	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-14	HIS	-	EXPRESSION TAG	UNP Q5TLG6
L	-13	HIS	-	EXPRESSION TAG	UNP Q5TLG6
L	-12	HIS	-	EXPRESSION TAG	UNP Q5TLG6
L	-11	HIS	-	EXPRESSION TAG	UNP Q5TLG6
L	-10	HIS	-	EXPRESSION TAG	UNP Q5TLG6
L	-9	HIS	-	EXPRESSION TAG	UNP Q5TLG6
L	-8	GLY	-	EXPRESSION TAG	UNP Q5TLG6
L	-7	SER	-	EXPRESSION TAG	UNP Q5TLG6
L	-6	LEU	-	EXPRESSION TAG	UNP Q5TLG6
L	-5	VAL	-	EXPRESSION TAG	UNP Q5TLG6
L	-4	PRO	-	EXPRESSION TAG	UNP Q5TLG6
L	-3	ARG	-	EXPRESSION TAG	UNP Q5TLG6
L	-2	GLY	-	EXPRESSION TAG	UNP Q5TLG6
L	-1	SER	-	EXPRESSION TAG	UNP Q5TLG6
L	0	MET	-	EXPRESSION TAG	UNP Q5TLG6
L	1	VAL	-	EXPRESSION TAG	UNP Q5TLG6
L	62	GYS	CYS	CHROMOPHORE	UNP Q5TLG6
L	62	GYS	TYR	CHROMOPHORE	UNP Q5TLG6
L	62	GYS	GLY	CHROMOPHORE	UNP Q5TLG6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Mg 3 3	0	0
2	J	1	Total Mg 1 1	0	0
2	D	7	Total Mg 7 7	0	0
2	K	6	Total Mg 6 6	0	0
2	E	7	Total Mg 7 7	0	0
2	H	4	Total Mg 4 4	0	0
2	B	8	Total Mg 8 8	0	0
2	I	4	Total Mg 4 4	0	0
2	C	8	Total Mg 8 8	0	0
2	A	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	3	Total 3	Mg 3	0	0
2	F	5	Total 5	Mg 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total 135	O 135	0	0
3	B	196	Total 196	O 196	0	0
3	C	190	Total 190	O 190	0	0
3	D	158	Total 158	O 158	0	0
3	E	216	Total 216	O 216	0	0
3	F	172	Total 172	O 172	0	0
3	G	219	Total 219	O 219	0	0
3	H	186	Total 186	O 186	0	0
3	I	157	Total 157	O 157	0	0
3	J	134	Total 134	O 134	0	0
3	K	127	Total 127	O 127	0	0
3	L	142	Total 142	O 142	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

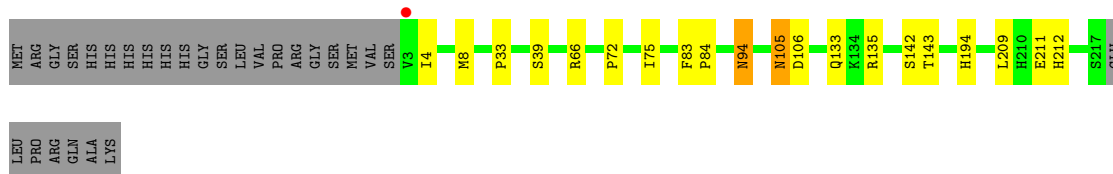
- Molecule 1: fluorescent protein Dronpa

Chain A: 



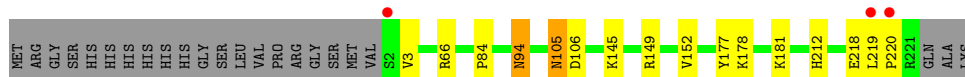
- Molecule 1: fluorescent protein Dronpa

Chain B: 



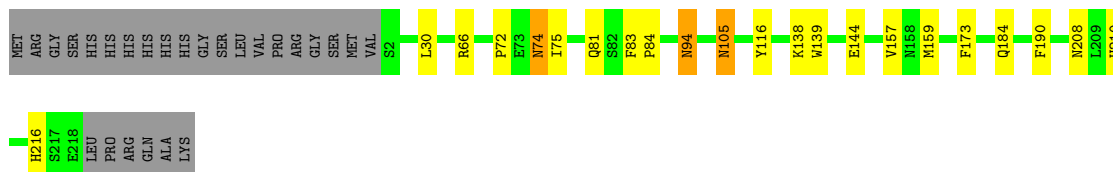
- Molecule 1: fluorescent protein Dronpa

Chain C: 



- Molecule 1: fluorescent protein Dronpa

Chain D: 



- Molecule 1: fluorescent protein Dronpa

Chain E: 



- Molecule 1: fluorescent protein Dronpa

Relative abundance of amino acids in the protein. The chart shows the relative abundance of various amino acids, with the y-axis representing the relative abundance from 0 to 100. The x-axis lists the amino acids. The bars are color-coded: MET (grey), ARG (grey), GLY (grey), SER (grey), HIS (grey), HIS (grey), HIS (grey), HIS (grey), GLY (grey), SER (grey), LEU (grey), VAL (grey), PRO (grey), ARG (grey), GLY (grey), SER (grey), MET (grey), VAL (grey), S2 (red), H21 (yellow), SY662 (yellow), K70 (yellow), Q81 (yellow), N94 (orange), N105 (orange), D106 (yellow), Q133 (yellow), R134 (green), R135 (yellow), W139 (yellow), V157 (yellow), L161 (yellow), F173 (yellow), V183 (yellow), I195 (yellow), N208 (yellow), L209 (yellow), H210 (yellow), E214 (yellow), A215 (green), H216 (green), S217 (green), and E218 (green). The bars for S2, H21, SY662, K70, Q81, N94, N105, D106, Q133, R134, R135, W139, V157, L161, F173, V183, I195, N208, L209, H210, E214, A215, H216, S217, and E218 are all at 100% relative abundance. The bars for MET, ARG, GLY, SER, HIS, HIS, HIS, HIS, GLY, SER, LEU, VAL, PRO, ARG, GLY, SER, MET, VAL, and S2 are at approximately 50% relative abundance. The bars for N94, N105, and D106 are at approximately 25% relative abundance. The bars for Q133, R134, R135, W139, V157, L161, F173, V183, I195, N208, L209, H210, E214, A215, H216, S217, and E218 are at approximately 10% relative abundance.

- Chain G: 

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	GLY	SER	LEU	VAL	PRO	ARG	GLY	SER	MET	VAL	S2	V3	P72	I75	Q81	N94	N105	Y116	E144	K145	V157	Q184	N208	L209	H210	E213	LEU	PRO	ARG	GLN	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

- Chain H: 

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	GLY	SER	LEU	VAL	PRO	ARG	GLY	SER	MET	VAL	S2	V3	S39	K45	Q81	F83	P84	N94	N105	Y116	Q184	N208	L209	H210	E211	H212	H216	S217	E218	L219	P220	R221	ALA	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

- Chain I:

Sequence logo for position 199. The y-axis represents information content in bits (0 to 0.4). The x-axis shows amino acids. The most conserved position is S2, with a high frequency of Serine (S) and a small peak for Valine (V). Other positions like K5, M8, K11, K32, P33, S39, S76, R66, V67, Y71, P72, Q81, S82, F83, N94, N105, K138, E144, V157, Q184, H194, and I195 show lower conservation. The logo is color-coded by amino acid type: yellow for hydrophobic, green for polar, orange for charged, and grey for basic.

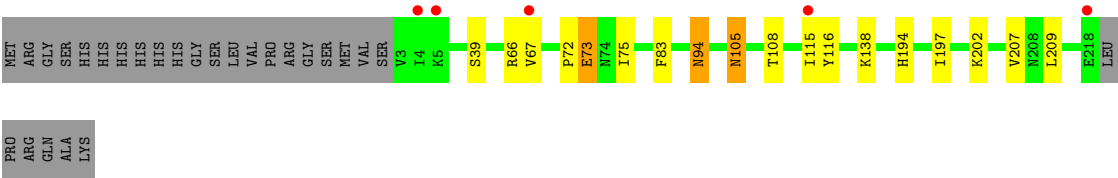
- Chain J:

Diagram illustrating the structure of the human PTPN22 protein, showing various domains and residues. The protein is represented as a grey cylinder with a red dot indicating a mutation site. The diagram includes labels for various residues and domains, such as MET, ARG, GLY, SER, HIS, P209, E218, L219, P220, ARG, GLN, ALA, LYS, K11, S39, SYG62, N65, R66, V67, P72, E73, N74, I75, Q81, S82, F83, P84, N84, N105, D106, C113, Y116, V137, K138, S162, C171, D172, F173, and S174.

- Chain K:

Amino Acid	Percentage (%)
MET	0.5
ARG	0.5
GLY	0.5
SER	0.5
HIS	0.5
HIS	0.5
HIS	0.5
HIS	0.5
HIS	0.5
GLY	0.5
SER	0.5
LEU	0.5
VAL	0.5
PRO	0.5
ARG	0.5
GLY	0.5
MET	0.5
MET	0.5
VAL	0.5
SER	8.5
V3	8.5
I4	12.5
L30	10.5
S39	10.5
R66	10.5
V67	10.5
K70	10.5
E73	12.5
F83	10.5
N94	10.5
N105	10.5
Y116	10.5
K138	10.5
I195	10.5
L209	10.5
E214	10.5
S217	12.5
GLU	12.5
LEU	12.5
PRO	12.5
ARG	12.5
GLN	12.5
ALA	12.5

- Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.09Å 106.16Å 110.07Å 61.17° 70.85° 86.21°	Depositor
Resolution (Å)	19.99 – 1.80 37.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.99-1.80) 94.1 (37.49-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.209 0.178 , 0.205	Depositor DCC
R_{free} test set	11803 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.3	EDS
Estimated twinning fraction	0.005 for -h,-k,-h-k+l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 236555 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23035	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.32	0/1760	0.63	0/2375
1	B	0.35	0/1745	0.66	0/2355
1	C	0.35	0/1787	0.66	0/2412
1	D	0.34	0/1760	0.66	0/2375
1	E	0.34	0/1787	0.65	0/2412
1	F	0.34	0/1787	0.65	0/2412
1	G	0.35	0/1760	0.66	0/2375
1	H	0.34	0/1787	0.66	0/2412
1	I	0.33	0/1787	0.64	0/2412
1	J	0.32	0/1776	0.70	2/2398 (0.1%)
1	K	0.31	0/1745	0.61	0/2355
1	L	0.30	0/1754	0.62	0/2367
All	All	0.33	0/21235	0.65	2/28660 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	218	GLU	N-CA-C	12.00	143.41	111.00
1	J	218	GLU	CB-CA-C	-8.72	92.97	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1736	0	1661	10	0
1	B	1721	0	1650	13	0
1	C	1762	0	1692	9	0
1	D	1736	0	1661	12	0
1	E	1762	0	1692	9	0
1	F	1762	0	1692	14	0
1	G	1736	0	1661	7	0
1	H	1762	0	1692	9	0
1	I	1762	0	1692	14	0
1	J	1751	0	1679	16	0
1	K	1721	0	1650	7	0
1	L	1730	0	1656	10	0
2	A	6	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	7	0	0	0	0
2	E	7	0	0	0	0
2	F	5	0	0	0	0
2	G	3	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	1	0	0	0	0
2	K	6	0	0	0	0
2	L	3	0	0	0	0
3	A	135	0	0	0	0
3	B	196	0	0	0	0
3	C	190	0	0	0	0
3	D	158	0	0	1	0
3	E	216	0	0	0	0
3	F	172	0	0	1	0
3	G	219	0	0	0	0
3	H	186	0	0	0	0
3	I	157	0	0	0	0
3	J	134	0	0	0	0
3	K	127	0	0	0	0
3	L	142	0	0	1	0
All	All	23035	0	20078	123	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:GLN:HE21	1:B:135:ARG:HE	1.18	0.91
1:I:8:MET:HE3	1:I:33:PRO:HG2	1.65	0.78
1:F:133:GLN:HE21	1:F:135:ARG:HE	1.36	0.74
1:A:76:VAL:HG22	1:A:186:PRO:HB3	1.73	0.71
1:G:81:GLN:HE22	1:G:184:GLN:H	1.39	0.70
1:B:133:GLN:NE2	1:B:135:ARG:HE	1.90	0.69
1:D:74:ASN:H	1:D:74:ASN:HD22	1.44	0.64
1:I:81:GLN:HE22	1:I:184:GLN:H	1.47	0.62
1:F:133:GLN:NE2	1:F:135:ARG:HE	1.99	0.60
1:J:11:LYS:HG3	1:J:113:CYS:SG	2.42	0.60
1:I:221:ARG:NH2	1:J:219:LEU:HD22	2.18	0.59
1:C:152:VAL:HG22	1:C:177:TYR:O	2.04	0.58
1:H:216:HIS:CE1	1:H:219:LEU:HD21	2.40	0.57
1:H:3:VAL:HG21	1:H:84:PRO:HD3	1.87	0.56
1:L:108:THR:OG1	1:L:115:ILE:HG23	2.04	0.56
1:C:219:LEU:HA	1:C:220:PRO:C	2.26	0.55
1:C:152:VAL:HG21	1:C:178:LYS:HG2	1.88	0.55
1:K:67:VAL:HG21	1:K:83:PHE:HE1	1.72	0.55
1:J:67:VAL:HG11	1:J:83:PHE:CE1	2.40	0.55
1:B:8:MET:HE3	1:B:33:PRO:HG2	1.87	0.55
1:L:105:ASN:HD21	1:L:116:TYR:HB3	1.74	0.53
1:B:142:SER:O	1:C:219:LEU:HD21	2.08	0.53
1:F:21:HIS:HB3	3:F:3218:HOH:O	2.09	0.53
1:D:105:ASN:HD21	1:D:116:TYR:HB3	1.74	0.53
1:E:105:ASN:HD21	1:E:116:TYR:HB3	1.74	0.53
1:I:67:VAL:HG11	1:I:83:PHE:HE1	1.73	0.53
1:I:67:VAL:HG11	1:I:83:PHE:CE1	2.44	0.53
1:A:67:VAL:HG11	1:A:83:PHE:CE1	2.44	0.53
1:J:67:VAL:HG11	1:J:83:PHE:HE1	1.74	0.52
1:L:67:VAL:HG11	1:L:83:PHE:CE1	2.45	0.52
1:F:81:GLN:HE21	1:F:183:VAL:HG13	1.74	0.52
1:C:94:ASN:HD22	1:C:94:ASN:C	2.13	0.52
1:D:72:PRO:HD2	1:D:75:ILE:HD12	1.91	0.51
1:F:216:HIS:CE1	1:F:219:LEU:HD21	2.44	0.51
1:K:67:VAL:HG21	1:K:83:PHE:CE1	2.46	0.51
1:B:4:ILE:HG23	1:B:8:MET:HE1	1.93	0.51
1:A:133:GLN:HE21	1:E:48:GLY:H	1.58	0.50
1:I:221:ARG:HD3	1:J:192:ASP:OD2	2.12	0.50
1:F:94:ASN:HD22	1:F:94:ASN:C	2.16	0.49
1:G:94:ASN:C	1:G:94:ASN:HD22	2.16	0.49
1:D:94:ASN:HD22	1:D:94:ASN:C	2.16	0.49
1:L:202:LYS:HB3	3:L:3192:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:171:CYS:HG	1:J:173:PHE:HE1	1.59	0.48
1:H:208:ASN:OD1	1:H:210:HIS:HE1	1.96	0.48
1:B:94:ASN:C	1:B:94:ASN:HD22	2.16	0.48
1:H:94:ASN:C	1:H:94:ASN:HD22	2.17	0.48
1:L:67:VAL:HG11	1:L:83:PHE:HE1	1.77	0.47
1:I:144:GLU:HA	1:I:157:VAL:HB	1.95	0.47
1:I:94:ASN:C	1:I:94:ASN:HD22	2.18	0.47
1:A:105:ASN:HD21	1:A:116:TYR:HB3	1.78	0.47
1:G:72:PRO:HD2	1:G:75:ILE:HD12	1.97	0.47
1:G:105:ASN:HD21	1:G:116:TYR:HB3	1.80	0.46
1:E:72:PRO:HD2	1:E:75:ILE:HD12	1.98	0.46
1:L:72:PRO:HD2	1:L:75:ILE:HD12	1.98	0.46
1:I:221:ARG:HH21	1:J:219:LEU:HD22	1.79	0.46
1:G:81:GLN:NE2	1:G:184:GLN:H	2.09	0.45
1:J:105:ASN:HD21	1:J:116:TYR:HB3	1.80	0.45
1:J:72:PRO:HD2	1:J:75:ILE:HD12	1.99	0.45
1:D:81:GLN:HE22	1:D:184:GLN:H	1.64	0.45
1:I:8:MET:CE	1:I:33:PRO:HG2	2.42	0.45
1:B:8:MET:CE	1:B:33:PRO:HG2	2.46	0.45
1:B:72:PRO:HD2	1:B:75:ILE:HD12	1.99	0.45
1:B:143:THR:H	1:C:145:LYS:NZ	2.15	0.45
1:F:219:LEU:HA	1:F:220:PRO:C	2.38	0.45
1:A:94:ASN:HD22	1:A:94:ASN:C	2.19	0.45
1:I:39:SER:HA	1:I:209:LEU:O	2.18	0.44
1:J:81:GLN:HE22	1:J:184:GLN:CB	2.30	0.44
3:D:3176:HOH:O	1:E:138:LYS:HE2	2.16	0.44
1:J:39:SER:HA	1:J:209:LEU:O	2.18	0.44
1:H:81:GLN:HE22	1:H:184:GLN:H	1.66	0.44
1:C:105:ASN:HD22	1:C:106:ASP:N	2.15	0.44
1:C:3:VAL:HG21	1:C:84:PRO:HD3	1.99	0.44
1:I:5:LYS:O	1:I:8:MET:HE2	2.17	0.44
1:E:147:TYR:HB3	1:E:188:TYR:CD1	2.52	0.44
1:F:70:LYS:HB3	1:F:214:GLU:HG2	1.99	0.44
1:I:62:GYS:HE1	1:I:195:ILE:HB	2.00	0.43
1:F:81:GLN:NE2	1:F:183:VAL:HG13	2.33	0.43
1:L:73:GLU:CD	1:L:73:GLU:H	2.21	0.43
1:E:157:VAL:HG13	1:E:173:PHE:HB2	2.00	0.43
1:L:197:ILE:HG23	1:L:207:VAL:HG13	1.99	0.43
1:B:105:ASN:HD22	1:B:106:ASP:N	2.16	0.43
1:C:149:ARG:O	1:C:152:VAL:HG12	2.18	0.43
1:A:115:ILE:HD12	1:A:115:ILE:N	2.34	0.42
1:A:67:VAL:HG11	1:A:83:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:157:VAL:HG13	1:D:173:PHE:HB2	2.01	0.42
1:F:157:VAL:HG12	1:F:173:PHE:HB2	2.02	0.42
1:K:105:ASN:HD21	1:K:116:TYR:HB3	1.84	0.42
1:J:83:PHE:HB3	1:J:84:PRO:HA	2.00	0.42
1:D:30:LEU:N	1:D:30:LEU:HD23	2.35	0.42
1:A:133:GLN:NE2	1:E:48:GLY:H	2.17	0.42
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.02	0.42
1:I:71:TYR:HA	1:I:72:PRO:HD3	1.95	0.42
1:B:39:SER:HA	1:B:209:LEU:O	2.20	0.42
1:E:71:TYR:HA	1:E:72:PRO:HD3	1.91	0.41
1:D:208:ASN:OD1	1:D:210:HIS:HE1	2.03	0.41
1:A:3:VAL:HG23	1:A:4:ILE:HG12	2.01	0.41
1:F:105:ASN:HD22	1:F:106:ASP:N	2.18	0.41
1:K:195:ILE:HD11	1:K:209:LEU:HD21	2.03	0.41
1:J:137:VAL:HB	1:J:162:SER:OG	2.19	0.41
1:J:94:ASN:HD22	1:J:94:ASN:C	2.22	0.41
1:L:39:SER:HA	1:L:209:LEU:O	2.20	0.41
1:H:39:SER:HA	1:H:209:LEU:O	2.21	0.41
1:K:39:SER:HA	1:K:209:LEU:O	2.20	0.41
1:G:144:GLU:HA	1:G:157:VAL:HB	2.02	0.41
1:D:190:PHE:HB2	1:D:216:HIS:CE1	2.55	0.41
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.03	0.41
1:F:62:GYS:HE1	1:F:195:ILE:HB	2.03	0.41
1:E:219:LEU:HA	1:E:220:PRO:C	2.41	0.41
1:J:105:ASN:HD22	1:J:106:ASP:N	2.19	0.40
1:A:11:LYS:HD3	1:A:28:VAL:HG12	2.02	0.40
1:D:139:TRP:CZ3	1:D:159:MET:HB3	2.56	0.40
1:K:30:LEU:HD23	1:K:30:LEU:N	2.36	0.40
1:B:211:GLU:HG2	1:B:212:HIS:N	2.36	0.40
1:F:208:ASN:OD1	1:F:210:HIS:HE1	2.04	0.40
1:D:144:GLU:HA	1:D:157:VAL:HB	2.04	0.40
1:G:208:ASN:OD1	1:G:210:HIS:HE1	2.04	0.40
1:H:105:ASN:HD21	1:H:116:TYR:HB3	1.85	0.40
1:H:83:PHE:HB3	1:H:84:PRO:HA	2.03	0.40
1:H:211:GLU:HG2	1:H:212:HIS:N	2.37	0.40
1:F:139:TRP:CZ3	1:F:161:LEU:HG	2.56	0.40
1:J:62:GYS:HB12	1:J:195:ILE:HD12	2.04	0.40
1:K:70:LYS:HB3	1:K:214:GLU:HG2	2.03	0.40
1:L:94:ASN:C	1:L:94:ASN:HD22	2.24	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	212/241 (88%)	208 (98%)	4 (2%)	0	100	100
1	B	210/241 (87%)	207 (99%)	3 (1%)	0	100	100
1	C	215/241 (89%)	209 (97%)	6 (3%)	0	100	100
1	D	212/241 (88%)	209 (99%)	3 (1%)	0	100	100
1	E	215/241 (89%)	212 (99%)	3 (1%)	0	100	100
1	F	215/241 (89%)	213 (99%)	2 (1%)	0	100	100
1	G	212/241 (88%)	210 (99%)	2 (1%)	0	100	100
1	H	215/241 (89%)	213 (99%)	2 (1%)	0	100	100
1	I	215/241 (89%)	212 (99%)	3 (1%)	0	100	100
1	J	214/241 (89%)	210 (98%)	4 (2%)	0	100	100
1	K	210/241 (87%)	208 (99%)	2 (1%)	0	100	100
1	L	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
All	All	2556/2892 (88%)	2516 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/207 (89%)	181 (98%)	4 (2%)	64	48
1	B	183/207 (88%)	179 (98%)	4 (2%)	64	48
1	C	188/207 (91%)	182 (97%)	6 (3%)	51	32
1	D	185/207 (89%)	180 (97%)	5 (3%)	57	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	188/207 (91%)	185 (98%)	3 (2%)	75	63
1	F	188/207 (91%)	185 (98%)	3 (2%)	75	63
1	G	185/207 (89%)	182 (98%)	3 (2%)	75	63
1	H	188/207 (91%)	184 (98%)	4 (2%)	66	51
1	I	188/207 (91%)	180 (96%)	8 (4%)	40	19
1	J	187/207 (90%)	182 (97%)	5 (3%)	57	39
1	K	183/207 (88%)	179 (98%)	4 (2%)	64	48
1	L	184/207 (89%)	178 (97%)	6 (3%)	50	30
All	All	2232/2484 (90%)	2177 (98%)	55 (2%)	60	42

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	105	ASN
1	A	145	LYS
1	A	194	HIS
1	B	66	ARG
1	B	94	ASN
1	B	105	ASN
1	B	194	HIS
1	C	66	ARG
1	C	94	ASN
1	C	105	ASN
1	C	181	LYS
1	C	212	HIS
1	C	218	GLU
1	D	66	ARG
1	D	74	ASN
1	D	94	ASN
1	D	105	ASN
1	D	138	LYS
1	E	67	VAL
1	E	105	ASN
1	E	138	LYS
1	F	94	ASN
1	F	105	ASN
1	F	218	GLU
1	G	94	ASN

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Mol	Chain	Res	Type
1	G	105	ASN
1	G	145	LYS
1	H	45	LYS
1	H	94	ASN
1	H	105	ASN
1	H	218	GLU
1	I	11	LYS
1	I	32	LYS
1	I	66	ARG
1	I	94	ASN
1	I	105	ASN
1	I	138	LYS
1	I	194	HIS
1	I	221	ARG
1	J	66	ARG
1	J	94	ASN
1	J	105	ASN
1	J	138	LYS
1	J	194	HIS
1	K	66	ARG
1	K	94	ASN
1	K	105	ASN
1	K	138	LYS
1	L	66	ARG
1	L	73	GLU
1	L	94	ASN
1	L	105	ASN
1	L	138	LYS
1	L	194	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	94	ASN
1	A	105	ASN
1	A	124	ASN
1	A	133	GLN
1	A	158	ASN
1	A	184	GLN
1	A	194	HIS
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	210	HIS
1	B	38	GLN
1	B	94	ASN
1	B	105	ASN
1	B	133	GLN
1	B	194	HIS
1	B	210	HIS
1	C	38	GLN
1	C	94	ASN
1	C	105	ASN
1	C	210	HIS
1	D	38	GLN
1	D	74	ASN
1	D	81	GLN
1	D	94	ASN
1	D	105	ASN
1	D	133	GLN
1	D	184	GLN
1	D	194	HIS
1	D	210	HIS
1	E	38	GLN
1	E	105	ASN
1	E	210	HIS
1	F	38	GLN
1	F	81	GLN
1	F	94	ASN
1	F	105	ASN
1	F	133	GLN
1	F	210	HIS
1	G	81	GLN
1	G	94	ASN
1	G	105	ASN
1	G	158	ASN
1	G	194	HIS
1	G	210	HIS
1	H	38	GLN
1	H	81	GLN
1	H	94	ASN
1	H	105	ASN
1	H	194	HIS
1	H	210	HIS
1	I	38	GLN

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Mol	Chain	Res	Type
1	I	81	GLN
1	I	94	ASN
1	I	105	ASN
1	I	133	GLN
1	I	194	HIS
1	I	210	HIS
1	J	38	GLN
1	J	81	GLN
1	J	94	ASN
1	J	105	ASN
1	J	124	ASN
1	J	194	HIS
1	J	210	HIS
1	K	38	GLN
1	K	81	GLN
1	K	94	ASN
1	K	105	ASN
1	K	124	ASN
1	K	210	HIS
1	L	38	GLN
1	L	81	GLN
1	L	94	ASN
1	L	105	ASN
1	L	133	GLN
1	L	184	GLN
1	L	210	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	GYS	A	62	1	22,22,23	3.80	5 (22%)	28,30,32	2.02	7 (25%)
1	GYS	B	62	1	22,22,23	3.82	6 (27%)	28,30,32	1.86	6 (21%)
1	GYS	C	62	1	22,22,23	3.71	6 (27%)	28,30,32	1.84	5 (17%)
1	GYS	D	62	1	22,22,23	3.78	5 (22%)	28,30,32	1.97	6 (21%)
1	GYS	E	62	1	22,22,23	3.69	6 (27%)	28,30,32	1.81	5 (17%)
1	GYS	F	62	1	22,22,23	3.75	8 (36%)	28,30,32	2.05	5 (17%)
1	GYS	G	62	1	22,22,23	3.81	7 (31%)	28,30,32	2.04	6 (21%)
1	GYS	H	62	1	22,22,23	3.77	6 (27%)	28,30,32	1.99	7 (25%)
1	GYS	I	62	1	22,22,23	3.79	6 (27%)	28,30,32	1.87	5 (17%)
1	GYS	J	62	1	22,22,23	3.89	5 (22%)	28,30,32	1.90	4 (14%)
1	GYS	K	62	1	22,22,23	3.69	6 (27%)	28,30,32	1.95	5 (17%)
1	GYS	L	62	1	22,22,23	3.73	6 (27%)	28,30,32	1.98	6 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYS	A	62	1	-	0/10/29/30	0/2/2/2
1	GYS	B	62	1	-	0/10/29/30	0/2/2/2
1	GYS	C	62	1	-	0/10/29/30	0/2/2/2
1	GYS	D	62	1	-	0/10/29/30	0/2/2/2
1	GYS	E	62	1	-	0/10/29/30	0/2/2/2
1	GYS	F	62	1	-	0/10/29/30	0/2/2/2
1	GYS	G	62	1	-	0/10/29/30	0/2/2/2
1	GYS	H	62	1	-	0/10/29/30	0/2/2/2
1	GYS	I	62	1	-	0/10/29/30	0/2/2/2
1	GYS	J	62	1	-	0/10/29/30	0/2/2/2
1	GYS	K	62	1	-	0/10/29/30	0/2/2/2
1	GYS	L	62	1	-	0/10/29/30	0/2/2/2

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	62	GYS	O-C	15.08	1.21	1.11
1	D	62	GYS	O-C	14.89	1.21	1.11
1	I	62	GYS	O-C	14.83	1.21	1.11
1	A	62	GYS	O-C	14.83	1.21	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	GYS	O-C	14.81	1.21	1.11
1	F	62	GYS	O-C	14.64	1.21	1.11
1	H	62	GYS	O-C	14.60	1.21	1.11
1	G	62	GYS	O-C	14.53	1.21	1.11
1	C	62	GYS	O-C	14.49	1.21	1.11
1	L	62	GYS	O-C	14.48	1.21	1.11
1	K	62	GYS	O-C	14.37	1.21	1.11
1	E	62	GYS	O-C	14.03	1.21	1.11
1	G	62	GYS	CB2-CA2	7.02	1.39	1.35
1	J	62	GYS	CB2-CA2	6.76	1.39	1.35
1	H	62	GYS	CB2-CA2	6.59	1.39	1.35
1	I	62	GYS	CB2-CA2	6.54	1.39	1.35
1	E	62	GYS	CB2-CA2	6.40	1.39	1.35
1	A	62	GYS	CB2-CA2	6.32	1.39	1.35
1	B	62	GYS	CB2-CA2	6.28	1.39	1.35
1	L	62	GYS	CB2-CA2	6.21	1.39	1.35
1	K	62	GYS	CB2-CA2	5.98	1.39	1.35
1	F	62	GYS	CB2-CA2	5.97	1.39	1.35
1	D	62	GYS	CB2-CA2	5.75	1.39	1.35
1	C	62	GYS	CB2-CA2	5.70	1.39	1.35
1	D	62	GYS	CA2-C2	-4.04	1.44	1.48
1	B	62	GYS	CA2-C2	-3.91	1.44	1.48
1	D	62	GYS	CG2-CB2	-3.87	1.39	1.46
1	J	62	GYS	CA2-C2	-3.83	1.44	1.48
1	C	62	GYS	CA2-C2	-3.75	1.44	1.48
1	K	62	GYS	CG2-CB2	-3.71	1.39	1.46
1	A	62	GYS	CG2-CB2	-3.71	1.39	1.46
1	B	62	GYS	CG2-CB2	-3.66	1.39	1.46
1	E	62	GYS	CA2-C2	-3.66	1.44	1.48
1	L	62	GYS	CG2-CB2	-3.60	1.39	1.46
1	J	62	GYS	CG2-CB2	-3.60	1.39	1.46
1	F	62	GYS	CG2-CB2	-3.59	1.39	1.46
1	C	62	GYS	CG2-CB2	-3.57	1.39	1.46
1	G	62	GYS	CA2-C2	-3.42	1.44	1.48
1	L	62	GYS	CA2-C2	-3.42	1.44	1.48
1	K	62	GYS	CA2-C2	-3.41	1.44	1.48
1	H	62	GYS	CA2-C2	-3.40	1.44	1.48
1	E	62	GYS	CG2-CB2	-3.40	1.40	1.46
1	A	62	GYS	CA2-C2	-3.39	1.44	1.48
1	G	62	GYS	CG2-CB2	-3.37	1.40	1.46
1	H	62	GYS	CG2-CB2	-3.36	1.40	1.46
1	I	62	GYS	CA2-C2	-3.06	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	62	GYS	CG2-CB2	-3.05	1.40	1.46
1	F	62	GYS	CA2-C2	-2.78	1.45	1.48
1	F	62	GYS	CD2-CG2	2.67	1.44	1.39
1	J	62	GYS	CD2-CG2	2.62	1.44	1.39
1	E	62	GYS	CD2-CG2	2.62	1.44	1.39
1	G	62	GYS	CD2-CG2	2.55	1.44	1.39
1	C	62	GYS	CD2-CG2	2.53	1.44	1.39
1	H	62	GYS	CD2-CG2	2.52	1.44	1.39
1	B	62	GYS	CD2-CG2	2.49	1.44	1.39
1	I	62	GYS	CD2-CG2	2.46	1.44	1.39
1	A	62	GYS	CD2-CG2	2.46	1.44	1.39
1	L	62	GYS	CD2-CG2	2.44	1.44	1.39
1	K	62	GYS	CD2-CG2	2.42	1.44	1.39
1	D	62	GYS	CD2-CG2	2.33	1.43	1.39
1	I	62	GYS	CD1-CG2	2.26	1.43	1.39
1	F	62	GYS	CE1-CD1	2.26	1.43	1.38
1	F	62	GYS	CD1-CG2	2.22	1.43	1.39
1	F	62	GYS	CE1-CZ	2.21	1.43	1.38
1	G	62	GYS	CD1-CG2	2.17	1.43	1.39
1	E	62	GYS	CD1-CG2	2.17	1.43	1.39
1	G	62	GYS	CE1-CD1	2.16	1.42	1.38
1	H	62	GYS	CE1-CD1	2.12	1.42	1.38
1	K	62	GYS	CD1-CG2	2.11	1.43	1.39
1	L	62	GYS	CD1-CG2	2.08	1.43	1.39
1	C	62	GYS	CE1-CZ	2.03	1.43	1.38
1	B	62	GYS	CD1-CG2	2.00	1.43	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	GYS	O2-C2-CA2	7.97	135.56	130.96
1	G	62	GYS	O2-C2-CA2	7.81	135.47	130.96
1	H	62	GYS	O2-C2-CA2	7.62	135.37	130.96
1	A	62	GYS	O2-C2-CA2	7.61	135.35	130.96
1	K	62	GYS	O2-C2-CA2	7.50	135.29	130.96
1	L	62	GYS	O2-C2-CA2	7.47	135.28	130.96
1	D	62	GYS	O2-C2-CA2	7.30	135.18	130.96
1	I	62	GYS	O2-C2-CA2	7.16	135.10	130.96
1	J	62	GYS	O2-C2-CA2	7.06	135.04	130.96
1	C	62	GYS	O2-C2-CA2	6.90	134.95	130.96
1	B	62	GYS	O2-C2-CA2	6.88	134.94	130.96
1	E	62	GYS	O2-C2-CA2	6.83	134.91	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GYS	CA3-N3-C2	-4.14	120.89	123.46
1	D	62	GYS	CA3-N3-C2	-3.95	121.01	123.46
1	J	62	GYS	CA2-N2-C1	3.85	108.88	105.79
1	K	62	GYS	CA2-N2-C1	3.73	108.78	105.79
1	I	62	GYS	CA2-N2-C1	3.66	108.73	105.79
1	B	62	GYS	CA2-N2-C1	3.64	108.71	105.79
1	F	62	GYS	CA2-N2-C1	3.57	108.66	105.79
1	G	62	GYS	CA2-N2-C1	3.54	108.63	105.79
1	C	62	GYS	CA2-N2-C1	3.51	108.61	105.79
1	E	62	GYS	CA2-N2-C1	3.50	108.60	105.79
1	G	62	GYS	CA3-N3-C2	-3.43	121.33	123.46
1	L	62	GYS	CA2-N2-C1	3.41	108.53	105.79
1	H	62	GYS	CA2-N2-C1	3.38	108.50	105.79
1	A	62	GYS	CA2-N2-C1	3.34	108.47	105.79
1	F	62	GYS	CA3-N3-C2	-3.29	121.42	123.46
1	H	62	GYS	CA3-N3-C2	-3.18	121.49	123.46
1	J	62	GYS	CA3-N3-C2	-3.14	121.51	123.46
1	L	62	GYS	CA3-N3-C2	-3.14	121.51	123.46
1	K	62	GYS	CA3-N3-C2	-3.08	121.55	123.46
1	B	62	GYS	CA3-N3-C2	-2.94	121.63	123.46
1	D	62	GYS	CA2-N2-C1	2.93	108.14	105.79
1	E	62	GYS	CA3-N3-C2	-2.82	121.71	123.46
1	D	62	GYS	CA1-C1-N3	-2.60	121.88	124.54
1	F	62	GYS	CA2-C2-N3	-2.59	101.96	103.44
1	H	62	GYS	CA1-C1-N3	-2.56	121.92	124.54
1	C	62	GYS	CA3-N3-C2	-2.56	121.88	123.46
1	H	62	GYS	CA2-C2-N3	-2.51	102.01	103.44
1	C	62	GYS	CA2-C2-N3	-2.50	102.01	103.44
1	I	62	GYS	CA2-C2-N3	-2.50	102.01	103.44
1	L	62	GYS	CA1-C1-N3	-2.43	122.05	124.54
1	I	62	GYS	CA1-C1-N3	-2.37	122.11	124.54
1	B	62	GYS	CA2-C2-N3	-2.35	102.09	103.44
1	L	62	GYS	CA2-C2-N3	-2.35	102.10	103.44
1	G	62	GYS	CA2-C2-N3	-2.31	102.12	103.44
1	J	62	GYS	N3-C1-N2	-2.22	109.88	111.51
1	K	62	GYS	CA2-C2-N3	-2.22	102.17	103.44
1	G	62	GYS	CA1-C1-N3	-2.20	122.29	124.54
1	E	62	GYS	CA2-C2-N3	-2.17	102.20	103.44
1	D	62	GYS	N3-C1-N2	-2.17	109.92	111.51
1	I	62	GYS	CA3-N3-C2	-2.15	122.12	123.46
1	A	62	GYS	N3-C1-N2	-2.16	109.93	111.51
1	B	62	GYS	N3-C1-N2	-2.14	109.94	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GYS	CA2-C2-N3	-2.13	102.22	103.44
1	C	62	GYS	CA1-C1-N3	-2.12	122.37	124.54
1	D	62	GYS	CA1-C1-N2	2.11	128.20	123.62
1	G	62	GYS	CG2-CB2-CA2	2.10	132.52	130.10
1	K	62	GYS	N3-C1-N2	-2.10	109.97	111.51
1	B	62	GYS	CA1-C1-N3	-2.05	122.44	124.54
1	H	62	GYS	CA1-C1-N2	2.05	128.06	123.62
1	H	62	GYS	N3-C1-N2	-2.04	110.01	111.51
1	F	62	GYS	CA1-C1-N3	-2.04	122.45	124.54
1	L	62	GYS	N3-C1-N2	-2.03	110.02	111.51
1	E	62	GYS	CA1-C1-N3	-2.03	122.46	124.54
1	A	62	GYS	CA3-N3-C1	2.02	128.92	124.64
1	A	62	GYS	CA1-C1-N3	-2.01	122.48	124.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 62 ligands modelled in this entry, 62 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.

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, 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	215/241 (89%)	-0.13	1 (0%) 88 87	13, 22, 43, 63	0
1	B	213/241 (88%)	-0.34	1 (0%) 88 87	10, 17, 33, 51	0
1	C	218/241 (90%)	-0.35	3 (1%) 72 68	11, 17, 36, 68	0
1	D	215/241 (89%)	-0.31	0 100 100	10, 18, 38, 53	0
1	E	218/241 (90%)	-0.33	1 (0%) 88 87	11, 17, 33, 48	0
1	F	218/241 (90%)	-0.33	1 (0%) 88 87	10, 17, 36, 64	0
1	G	215/241 (89%)	-0.32	2 (0%) 81 78	10, 16, 33, 62	0
1	H	218/241 (90%)	-0.33	1 (0%) 88 87	11, 17, 32, 56	0
1	I	218/241 (90%)	-0.15	4 (1%) 65 60	11, 21, 45, 67	0
1	J	217/241 (90%)	-0.05	3 (1%) 72 68	12, 25, 46, 66	0
1	K	213/241 (88%)	0.07	2 (0%) 81 78	13, 27, 50, 62	0
1	L	214/241 (88%)	0.18	5 (2%) 57 51	15, 27, 49, 78	0
All	All	2592/2892 (89%)	-0.20	24 (0%) 81 78	10, 20, 43, 78	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	219	LEU	3.8
1	J	218	GLU	3.6
1	A	2	SER	3.6
1	F	2	SER	3.5
1	C	2	SER	3.4
1	C	219	LEU	3.3
1	I	221	ARG	2.9
1	I	2	SER	2.8
1	L	4	ILE	2.7
1	C	220	PRO	2.7
1	G	2	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	5	LYS	2.6
1	I	218	GLU	2.5
1	L	115	ILE	2.5
1	J	73	GLU	2.3
1	K	4	ILE	2.3
1	B	3	VAL	2.2
1	G	3	VAL	2.2
1	I	5	LYS	2.2
1	E	2	SER	2.2
1	L	218	GLU	2.2
1	H	219	LEU	2.1
1	L	67	VAL	2.1
1	K	73	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	GYS	H	62	21/22	0.10	0.72	11,14,15,22	0
1	GYS	J	62	21/22	0.11	0.65	20,21,26,38	0
1	GYS	E	62	21/22	0.10	0.64	12,13,15,22	0
1	GYS	C	62	21/22	0.09	0.54	12,14,17,28	0
1	GYS	F	62	21/22	0.09	0.38	11,13,17,31	0
1	GYS	B	62	21/22	0.09	0.19	11,13,16,29	0
1	GYS	I	62	21/22	0.09	0.09	15,19,22,30	0
1	GYS	D	62	21/22	0.09	0.06	13,15,16,24	0
1	GYS	G	62	21/22	0.09	0.06	13,14,17,30	0
1	GYS	A	62	21/22	0.09	-0.09	15,19,23,34	0
1	GYS	L	62	21/22	0.11	-0.16	23,25,28,36	0
1	GYS	K	62	21/22	0.10	-0.50	21,24,29,37	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	J	3017	1/1	0.22	14.76	62,62,62,62	0
2	MG	C	3039	1/1	0.36	10.21	54,54,54,54	0
2	MG	A	3027	1/1	0.14	8.38	42,42,42,42	0
2	MG	F	3045	1/1	0.12	6.22	42,42,42,42	0
2	MG	D	3020	1/1	0.16	4.77	57,57,57,57	0
2	MG	C	3016	1/1	0.11	4.47	44,44,44,44	0
2	MG	E	3023	1/1	0.10	3.85	41,41,41,41	0
2	MG	K	3036	1/1	0.17	3.75	52,52,52,52	0
2	MG	H	3038	1/1	0.22	3.63	52,52,52,52	0
2	MG	I	3019	1/1	0.21	3.60	46,46,46,46	0
2	MG	E	3002	1/1	0.16	3.45	51,51,51,51	0
2	MG	A	3033	1/1	0.10	3.17	45,45,45,45	0
2	MG	F	3008	1/1	0.18	3.14	39,39,39,39	0
2	MG	H	3060	1/1	0.15	2.95	49,49,49,49	0
2	MG	E	3001	1/1	0.10	2.79	40,40,40,40	0
2	MG	A	3031	1/1	0.14	2.71	46,46,46,46	0
2	MG	K	3050	1/1	0.10	2.67	38,38,38,38	0
2	MG	C	3004	1/1	0.10	2.65	47,47,47,47	0
2	MG	G	3057	1/1	0.11	2.64	43,43,43,43	0
2	MG	B	3042	1/1	0.12	2.51	37,37,37,37	0
2	MG	C	3012	1/1	0.17	2.44	43,43,43,43	0
2	MG	H	3032	1/1	0.11	2.40	44,44,44,44	0
2	MG	B	3044	1/1	0.15	2.31	46,46,46,46	0
2	MG	I	3005	1/1	0.12	2.26	40,40,40,40	0
2	MG	D	3013	1/1	0.12	2.20	51,51,51,51	0
2	MG	B	3041	1/1	0.10	2.19	52,52,52,52	0
2	MG	I	3022	1/1	0.09	1.96	40,40,40,40	0
2	MG	B	3043	1/1	0.11	1.90	47,47,47,47	0
2	MG	E	3030	1/1	0.12	1.50	58,58,58,58	0
2	MG	G	3040	1/1	0.09	1.34	34,34,34,34	0
2	MG	K	3035	1/1	0.12	1.29	50,50,50,50	0
2	MG	B	3046	1/1	0.09	1.10	41,41,41,41	0
2	MG	C	3014	1/1	0.15	1.03	49,49,49,49	0
2	MG	B	3029	1/1	0.11	0.93	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	3047	1/1	0.10	0.78	34,34,34,34	0
2	MG	C	3003	1/1	0.10	0.74	42,42,42,42	0
2	MG	A	3026	1/1	0.10	0.69	51,51,51,51	0
2	MG	D	3021	1/1	0.15	0.55	52,52,52,52	0
2	MG	D	3009	1/1	0.10	0.24	37,37,37,37	0
2	MG	A	3052	1/1	0.12	0.12	44,44,44,44	0
2	MG	L	3055	1/1	0.14	0.08	54,54,54,54	0
2	MG	E	3061	1/1	0.10	0.07	56,56,56,56	0
2	MG	F	3056	1/1	0.09	0.02	42,42,42,42	0
2	MG	D	3007	1/1	0.08	0.01	41,41,41,41	0
2	MG	I	3015	1/1	0.08	-0.11	26,26,26,26	0
2	MG	E	3059	1/1	0.10	-0.11	53,53,53,53	0
2	MG	L	3034	1/1	0.08	-0.33	31,31,31,31	0
2	MG	K	3051	1/1	0.10	-0.34	63,63,63,63	0
2	MG	A	3025	1/1	0.12	-0.47	51,51,51,51	0
2	MG	K	3053	1/1	0.10	-0.61	56,56,56,56	0
2	MG	C	3048	1/1	0.08	-0.69	38,38,38,38	0
2	MG	G	3058	1/1	0.07	-0.69	49,49,49,49	0
2	MG	H	3054	1/1	0.07	-0.77	21,21,21,21	0
2	MG	C	3010	1/1	0.06	-0.80	33,33,33,33	0
2	MG	B	3037	1/1	0.05	-0.80	36,36,36,36	0
2	MG	F	3006	1/1	0.06	-0.82	34,34,34,34	0
2	MG	E	3024	1/1	0.08	-0.90	46,46,46,46	0
2	MG	F	3063	1/1	0.08	-1.12	46,46,46,46	0
2	MG	D	3011	1/1	0.06	-1.31	40,40,40,40	0
2	MG	D	3018	1/1	0.08	-1.34	36,36,36,36	0
2	MG	L	3028	1/1	0.10	-2.22	39,39,39,39	0
2	MG	K	3049	1/1	0.04	-4.19	37,37,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.