Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

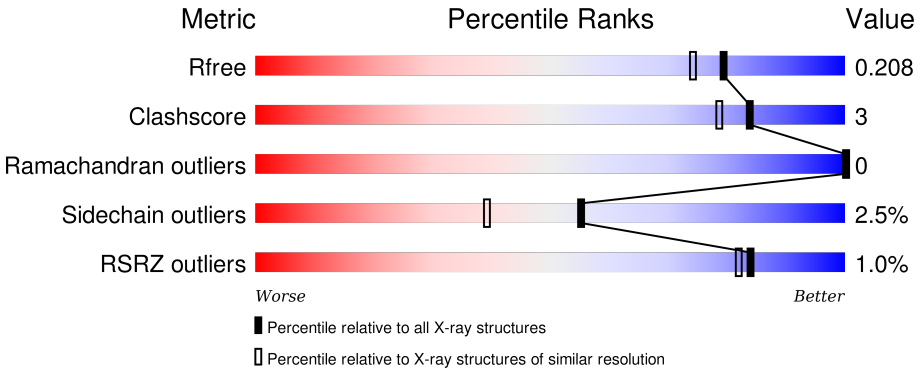
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. 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 <=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	241	83% 5% • 11%
1	B	241	80% 7% • 12%
1	C	241	% 84% 6% • 10%
1	D	241	80% 8% • 11%
1	E	241	85% 5% • 10%

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Mol	Chain	Length	Quality of chain
1	F	241	81% 8% • 10%
1	G	241	84% • • 11%
1	H	241	% 83% 7% • 10%
1	I	241	2% 81% 9% • 10%
1	J	241	% 79% 10% • 10%
1	K	241	% 83% 5% 12%
1	L	241	3% 81% 6% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	3026	-	-	-	X
2	MG	A	3031	-	-	-	X
2	MG	C	3016	-	-	-	X
2	MG	F	3045	-	-	-	X
2	MG	G	3040	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23035 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	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 Mg 3 3	0	0
2	F	5	Total Mg 5 5	0	0

- Molecule 3 is water.

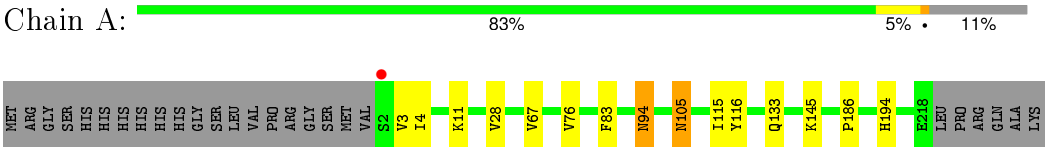
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	135	Total O 135 135	0	0
3	B	196	Total O 196 196	0	0
3	C	190	Total O 190 190	0	0
3	D	158	Total O 158 158	0	0
3	E	216	Total O 216 216	0	0
3	F	172	Total O 172 172	0	0
3	G	219	Total O 219 219	0	0
3	H	186	Total O 186 186	0	0
3	I	157	Total O 157 157	0	0
3	J	134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

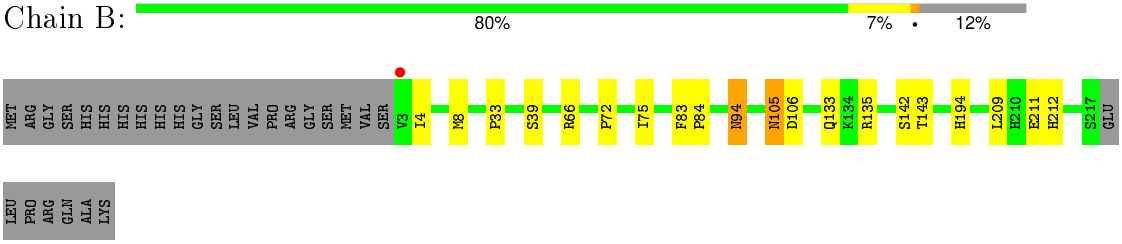
- Molecule 1: fluorescent protein Dronpa

Chain A:



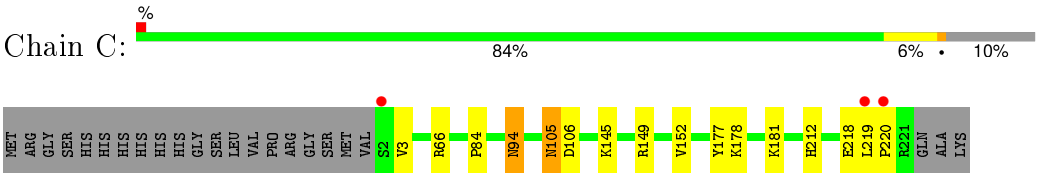
- Molecule 1: fluorescent protein Dronpa

Chain B:



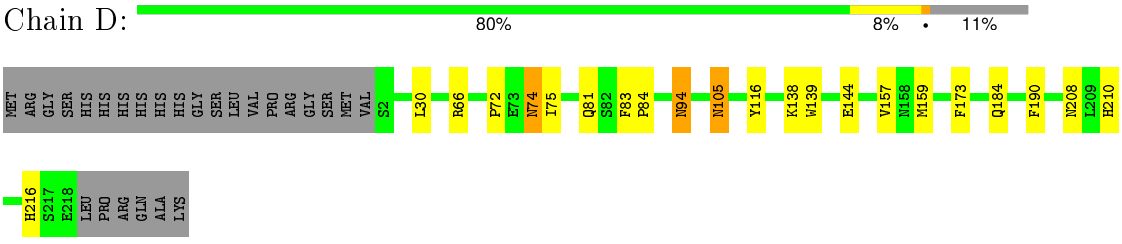
- Molecule 1: fluorescent protein Dronpa

Chain C:



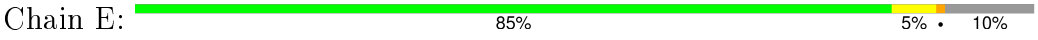
- Molecule 1: fluorescent protein Dronpa

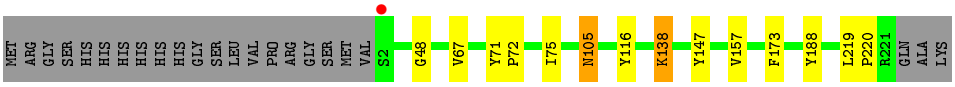
Chain D:



- Molecule 1: fluorescent protein Dronpa

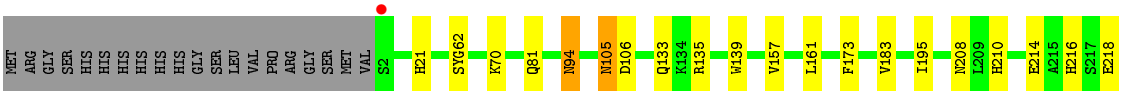
Chain E:





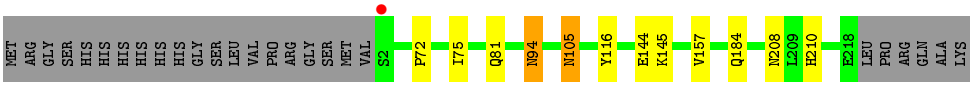
• Molecule 1: fluorescent protein Dronpa

Chain F:



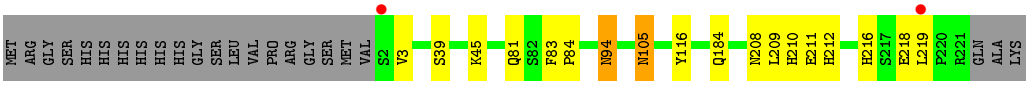
• Molecule 1: fluorescent protein Dronpa

Chain G:



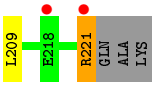
• Molecule 1: fluorescent protein Dronpa

Chain H:



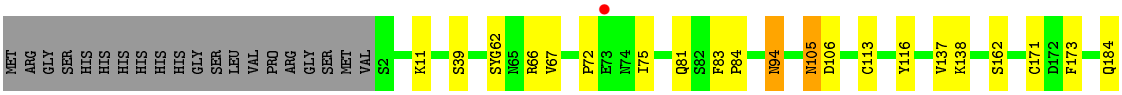
• Molecule 1: fluorescent protein Dronpa

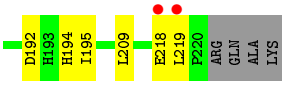
Chain I:



• Molecule 1: fluorescent protein Dronpa

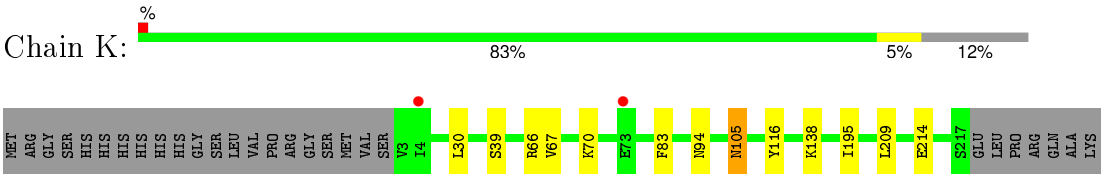
Chain J:





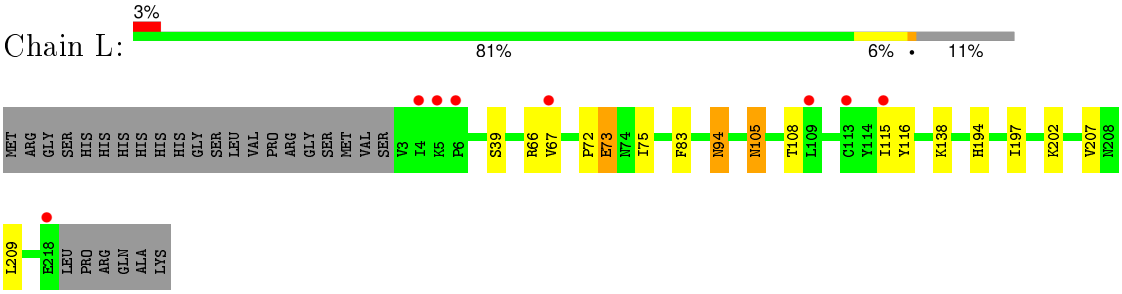
• Molecule 1: fluorescent protein Dronpa

Chain K:



- Molecule 1: fluorescent protein Dronpa

Chain L:



4 Data and refinement statistics (i)

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) 79.1 (37.49-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.209 0.182 , 0.208	Depositor DCC
R_{free} test set	11796 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
Estimated twinning fraction	0.005 for -h,-k,-h-k+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(^{o})	Ideal(^{o})
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 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	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

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

All (123) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:LYS:HB3	3:L:3192:HOH:O	2.12	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/207 (89%)	181 (98%)	4 (2%)	60	45
1	B	183/207 (88%)	179 (98%)	4 (2%)	60	45
1	C	188/207 (91%)	182 (97%)	6 (3%)	46	29
1	D	185/207 (89%)	180 (97%)	5 (3%)	52	36
1	E	188/207 (91%)	185 (98%)	3 (2%)	70	59
1	F	188/207 (91%)	185 (98%)	3 (2%)	70	59
1	G	185/207 (89%)	182 (98%)	3 (2%)	70	59
1	H	188/207 (91%)	184 (98%)	4 (2%)	61	47
1	I	188/207 (91%)	180 (96%)	8 (4%)	35	17
1	J	187/207 (90%)	182 (97%)	5 (3%)	52	36
1	K	183/207 (88%)	179 (98%)	4 (2%)	60	45
1	L	184/207 (89%)	178 (97%)	6 (3%)	45	27
All	All	2232/2484 (90%)	2177 (98%)	55 (2%)	55	39

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

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Mol	Chain	Res	Type
1	F	94	ASN
1	F	105	ASN
1	F	218	GLU
1	G	94	ASN
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

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Mol	Chain	Res	Type
1	A	158	ASN
1	A	184	GLN
1	A	194	HIS
1	A	206	ASN
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

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Mol	Chain	Res	Type
1	H	105	ASN
1	H	194	HIS
1	H	210	HIS
1	I	38	GLN
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 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	GYS	A	62	1	22,22,23	1.94	4 (18%)	27,30,32	2.20	5 (18%)
1	GYS	B	62	1	22,22,23	2.00	6 (27%)	27,30,32	2.12	5 (18%)
1	GYS	C	62	1	22,22,23	1.92	5 (22%)	27,30,32	2.12	4 (14%)
1	GYS	D	62	1	22,22,23	1.91	4 (18%)	27,30,32	2.14	6 (22%)
1	GYS	E	62	1	22,22,23	2.01	8 (36%)	27,30,32	2.08	4 (14%)
1	GYS	F	62	1	22,22,23	1.95	7 (31%)	27,30,32	2.28	4 (14%)
1	GYS	G	62	1	22,22,23	2.03	6 (27%)	27,30,32	2.25	4 (14%)
1	GYS	H	62	1	22,22,23	1.95	5 (22%)	27,30,32	2.21	5 (18%)
1	GYS	I	62	1	22,22,23	1.92	6 (27%)	27,30,32	2.18	4 (14%)
1	GYS	J	62	1	22,22,23	2.00	4 (18%)	27,30,32	2.17	5 (18%)
1	GYS	K	62	1	22,22,23	1.92	5 (22%)	27,30,32	2.23	5 (18%)
1	GYS	L	62	1	22,22,23	1.94	6 (27%)	27,30,32	2.24	5 (18%)

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	-	0/8/29/30	0/2/2/2
1	GYS	B	62	1	-	0/8/29/30	0/2/2/2
1	GYS	C	62	1	-	0/8/29/30	0/2/2/2
1	GYS	D	62	1	-	0/8/29/30	0/2/2/2
1	GYS	E	62	1	-	0/8/29/30	0/2/2/2
1	GYS	F	62	1	-	0/8/29/30	0/2/2/2
1	GYS	G	62	1	-	0/8/29/30	0/2/2/2
1	GYS	H	62	1	-	0/8/29/30	0/2/2/2
1	GYS	I	62	1	-	0/8/29/30	0/2/2/2
1	GYS	J	62	1	-	0/8/29/30	0/2/2/2
1	GYS	K	62	1	-	0/8/29/30	0/2/2/2
1	GYS	L	62	1	-	0/8/29/30	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	GYS	CA2-C2	-4.10	1.44	1.48
1	B	62	GYS	CA2-C2	-3.97	1.44	1.48
1	J	62	GYS	CA2-C2	-3.88	1.44	1.48
1	C	62	GYS	CA2-C2	-3.81	1.44	1.48
1	D	62	GYS	CG2-CB2	-3.78	1.39	1.46
1	E	62	GYS	CA2-C2	-3.71	1.44	1.48
1	K	62	GYS	CG2-CB2	-3.63	1.39	1.46
1	A	62	GYS	CG2-CB2	-3.63	1.39	1.46
1	B	62	GYS	CG2-CB2	-3.59	1.39	1.46
1	J	62	GYS	CG2-CB2	-3.52	1.39	1.46
1	L	62	GYS	CG2-CB2	-3.52	1.39	1.46
1	F	62	GYS	CG2-CB2	-3.51	1.39	1.46
1	C	62	GYS	CG2-CB2	-3.50	1.39	1.46
1	G	62	GYS	CA2-C2	-3.48	1.44	1.48
1	L	62	GYS	CA2-C2	-3.47	1.44	1.48
1	K	62	GYS	CA2-C2	-3.47	1.44	1.48
1	H	62	GYS	CA2-C2	-3.46	1.44	1.48
1	A	62	GYS	CA2-C2	-3.45	1.44	1.48
1	E	62	GYS	CG2-CB2	-3.33	1.40	1.46
1	G	62	GYS	CG2-CB2	-3.30	1.40	1.46
1	H	62	GYS	CG2-CB2	-3.29	1.40	1.46
1	I	62	GYS	CA2-C2	-3.11	1.45	1.48
1	I	62	GYS	CG2-CB2	-2.98	1.40	1.46
1	F	62	GYS	CA2-C2	-2.84	1.45	1.48
1	E	62	GYS	C1-N2	-2.01	1.29	1.32
1	B	62	GYS	CD1-CG2	2.02	1.43	1.39
1	L	62	GYS	CE1-CD1	2.04	1.42	1.38
1	B	62	GYS	CE1-CD1	2.04	1.42	1.38
1	E	62	GYS	CE2-CD2	2.06	1.42	1.38
1	L	62	GYS	CD1-CG2	2.10	1.43	1.39
1	E	62	GYS	CE1-CD1	2.11	1.42	1.38
1	C	62	GYS	CE1-CZ	2.11	1.43	1.38
1	I	62	GYS	CE1-CD1	2.12	1.42	1.38
1	K	62	GYS	CD1-CG2	2.13	1.43	1.39
1	E	62	GYS	CD1-CG2	2.19	1.43	1.39
1	G	62	GYS	CD1-CG2	2.19	1.43	1.39
1	F	62	GYS	CD1-CG2	2.24	1.43	1.39
1	H	62	GYS	CE1-CD1	2.26	1.42	1.38
1	I	62	GYS	CD1-CG2	2.28	1.43	1.39
1	G	62	GYS	CE1-CD1	2.30	1.42	1.38
1	F	62	GYS	CE1-CZ	2.30	1.43	1.38
1	D	62	GYS	CD2-CG2	2.35	1.43	1.39
1	F	62	GYS	CE1-CD1	2.41	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	62	GYS	CD2-CG2	2.44	1.44	1.39
1	L	62	GYS	CD2-CG2	2.46	1.44	1.39
1	A	62	GYS	CD2-CG2	2.48	1.44	1.39
1	I	62	GYS	CD2-CG2	2.48	1.44	1.39
1	B	62	GYS	CD2-CG2	2.51	1.44	1.39
1	H	62	GYS	CD2-CG2	2.54	1.44	1.39
1	C	62	GYS	CD2-CG2	2.55	1.44	1.39
1	G	62	GYS	CD2-CG2	2.57	1.44	1.39
1	E	62	GYS	CD2-CG2	2.64	1.44	1.39
1	J	62	GYS	CD2-CG2	2.65	1.44	1.39
1	F	62	GYS	CD2-CG2	2.69	1.44	1.39
1	C	62	GYS	CB2-CA2	4.43	1.39	1.35
1	D	62	GYS	CB2-CA2	4.47	1.39	1.35
1	F	62	GYS	CB2-CA2	4.64	1.39	1.35
1	K	62	GYS	CB2-CA2	4.65	1.39	1.35
1	L	62	GYS	CB2-CA2	4.83	1.39	1.35
1	B	62	GYS	CB2-CA2	4.88	1.39	1.35
1	A	62	GYS	CB2-CA2	4.91	1.39	1.35
1	E	62	GYS	CB2-CA2	4.97	1.39	1.35
1	I	62	GYS	CB2-CA2	5.08	1.39	1.35
1	H	62	GYS	CB2-CA2	5.12	1.39	1.35
1	J	62	GYS	CB2-CA2	5.26	1.39	1.35
1	G	62	GYS	CB2-CA2	5.45	1.39	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	62	GYS	CA2-C2-N3	-2.86	101.96	103.40
1	H	62	GYS	CA2-C2-N3	-2.78	102.01	103.40
1	C	62	GYS	CA2-C2-N3	-2.77	102.01	103.40
1	I	62	GYS	CA2-C2-N3	-2.76	102.01	103.40
1	B	62	GYS	CA2-C2-N3	-2.60	102.09	103.40
1	L	62	GYS	CA2-C2-N3	-2.60	102.10	103.40
1	G	62	GYS	CA2-C2-N3	-2.56	102.12	103.40
1	K	62	GYS	CA2-C2-N3	-2.44	102.17	103.40
1	E	62	GYS	CA2-C2-N3	-2.39	102.20	103.40
1	A	62	GYS	CA2-C2-N3	-2.34	102.22	103.40
1	J	62	GYS	N3-C1-N2	-2.17	109.88	111.56
1	D	62	GYS	N3-C1-N2	-2.12	109.92	111.56
1	J	62	GYS	CA2-C2-N3	-2.11	102.34	103.40
1	A	62	GYS	N3-C1-N2	-2.11	109.93	111.56
1	B	62	GYS	N3-C1-N2	-2.09	109.94	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	62	GYS	CA2-C2-N3	-2.09	102.35	103.40
1	K	62	GYS	N3-C1-N2	-2.05	109.97	111.56
1	L	62	GYS	CA1-C1-N2	2.10	127.93	123.38
1	H	62	GYS	CA1-C1-N2	2.16	128.06	123.38
1	D	62	GYS	CA1-C1-N2	2.22	128.20	123.38
1	D	62	GYS	CA2-N2-C1	2.68	108.14	105.71
1	A	62	GYS	CA2-N2-C1	3.04	108.47	105.71
1	H	62	GYS	CA2-N2-C1	3.08	108.50	105.71
1	L	62	GYS	CA2-N2-C1	3.10	108.53	105.71
1	E	62	GYS	CA2-N2-C1	3.19	108.60	105.71
1	C	62	GYS	CA2-N2-C1	3.19	108.61	105.71
1	G	62	GYS	CA2-N2-C1	3.22	108.63	105.71
1	F	62	GYS	CA2-N2-C1	3.25	108.66	105.71
1	B	62	GYS	CA2-N2-C1	3.31	108.71	105.71
1	I	62	GYS	CA2-N2-C1	3.33	108.73	105.71
1	K	62	GYS	CA2-N2-C1	3.38	108.78	105.71
1	J	62	GYS	CA2-N2-C1	3.50	108.88	105.71
1	A	62	GYS	C-CA3-N3	5.40	124.81	113.00
1	H	62	GYS	C-CA3-N3	5.41	124.85	113.00
1	D	62	GYS	C-CA3-N3	5.44	124.90	113.00
1	F	62	GYS	C-CA3-N3	5.50	125.04	113.00
1	G	62	GYS	C-CA3-N3	5.51	125.07	113.00
1	B	62	GYS	C-CA3-N3	5.63	125.34	113.00
1	E	62	GYS	C-CA3-N3	5.67	125.42	113.00
1	C	62	GYS	C-CA3-N3	5.69	125.46	113.00
1	J	62	GYS	C-CA3-N3	5.80	125.70	113.00
1	K	62	GYS	C-CA3-N3	5.81	125.71	113.00
1	L	62	GYS	C-CA3-N3	5.87	125.85	113.00
1	I	62	GYS	C-CA3-N3	5.99	126.13	113.00
1	E	62	GYS	O2-C2-CA2	7.34	134.91	130.95
1	B	62	GYS	O2-C2-CA2	7.39	134.94	130.95
1	C	62	GYS	O2-C2-CA2	7.41	134.95	130.95
1	J	62	GYS	O2-C2-CA2	7.58	135.04	130.95
1	I	62	GYS	O2-C2-CA2	7.69	135.10	130.95
1	D	62	GYS	O2-C2-CA2	7.84	135.18	130.95
1	L	62	GYS	O2-C2-CA2	8.02	135.28	130.95
1	K	62	GYS	O2-C2-CA2	8.05	135.29	130.95
1	A	62	GYS	O2-C2-CA2	8.17	135.35	130.95
1	H	62	GYS	O2-C2-CA2	8.19	135.37	130.95
1	G	62	GYS	O2-C2-CA2	8.39	135.47	130.95
1	F	62	GYS	O2-C2-CA2	8.55	135.56	130.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	62	GYS	1	0
1	I	62	GYS	1	0
1	J	62	GYS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	214/241 (88%)	-0.11	1 (0%)	91	90	13, 23, 43, 63	0
1	B	212/241 (87%)	-0.30	1 (0%)	91	90	10, 17, 33, 51	0
1	C	217/241 (90%)	-0.32	3 (1%)	78	74	11, 17, 36, 68	0
1	D	214/241 (88%)	-0.28	0	100	100	10, 18, 38, 53	0
1	E	217/241 (90%)	-0.31	1 (0%)	91	90	11, 17, 33, 48	0
1	F	217/241 (90%)	-0.30	1 (0%)	91	90	10, 17, 36, 64	0
1	G	214/241 (88%)	-0.27	1 (0%)	91	90	10, 16, 33, 62	0
1	H	217/241 (90%)	-0.30	2 (0%)	85	83	11, 17, 32, 56	0
1	I	217/241 (90%)	-0.13	4 (1%)	71	67	11, 21, 45, 67	0
1	J	216/241 (89%)	-0.01	3 (1%)	78	74	12, 25, 46, 66	0
1	K	212/241 (87%)	0.12	2 (0%)	85	83	13, 27, 50, 62	0
1	L	213/241 (88%)	0.20	8 (3%)	44	38	15, 27, 49, 78	0
All	All	2580/2892 (89%)	-0.17	27 (1%)	84	82	10, 20, 43, 78	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	SER	4.6
1	J	219	LEU	4.4
1	C	2	SER	4.3
1	A	2	SER	4.0
1	C	219	LEU	3.6
1	J	218	GLU	3.5
1	G	2	SER	3.4
1	I	221	ARG	3.3
1	C	220	PRO	3.2
1	L	5	LYS	2.9
1	L	115	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	73	GLU	2.9
1	I	2	SER	2.8
1	L	4	ILE	2.7
1	B	3	VAL	2.6
1	E	2	SER	2.4
1	L	113	CYS	2.4
1	I	5	LYS	2.4
1	I	218	GLU	2.3
1	H	219	LEU	2.3
1	H	2	SER	2.2
1	L	218	GLU	2.2
1	K	4	ILE	2.1
1	L	6	PRO	2.1
1	L	109	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	GYS	L	62	21/22	0.92	0.10	-	23,25,28,36	0
1	GYS	H	62	21/22	0.96	0.10	-	11,14,15,22	0
1	GYS	B	62	21/22	0.96	0.09	-	11,13,16,29	0
1	GYS	D	62	21/22	0.95	0.09	-	13,15,16,24	0
1	GYS	F	62	21/22	0.95	0.09	-	11,13,17,31	0
1	GYS	I	62	21/22	0.95	0.09	-	15,19,22,30	0
1	GYS	K	62	21/22	0.94	0.09	-	21,24,29,37	0
1	GYS	E	62	21/22	0.95	0.10	-	12,13,15,22	0
1	GYS	G	62	21/22	0.95	0.09	-	13,14,17,30	0
1	GYS	A	62	21/22	0.94	0.09	-	15,19,23,34	0
1	GYS	C	62	21/22	0.95	0.09	-	12,14,17,28	0
1	GYS	J	62	21/22	0.94	0.11	-	20,21,26,38	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	C	3016	1/1	0.89	0.11	4.47	44,44,44,44	0
2	MG	G	3040	1/1	0.96	0.12	3.24	34,34,34,34	0
2	MG	F	3045	1/1	0.94	0.10	2.85	42,42,42,42	0
2	MG	A	3026	1/1	0.87	0.12	2.12	51,51,51,51	0
2	MG	A	3031	1/1	0.92	0.13	2.09	46,46,46,46	0
2	MG	B	3042	1/1	0.92	0.11	1.90	37,37,37,37	0
2	MG	I	3005	1/1	0.97	0.10	0.57	40,40,40,40	0
2	MG	D	3007	1/1	0.96	0.09	0.29	41,41,41,41	0
2	MG	A	3025	1/1	0.93	0.14	0.17	51,51,51,51	0
2	MG	C	3010	1/1	0.96	0.07	-0.20	33,33,33,33	0
2	MG	K	3053	1/1	0.95	0.09	-0.81	56,56,56,56	0
2	MG	K	3049	1/1	0.98	0.06	-3.86	37,37,37,37	0
2	MG	C	3003	1/1	0.97	0.13	-	42,42,42,42	0
2	MG	K	3035	1/1	0.94	0.12	-	50,50,50,50	0
2	MG	A	3027	1/1	0.91	0.12	-	42,42,42,42	0
2	MG	H	3054	1/1	0.99	0.07	-	21,21,21,21	0
2	MG	G	3057	1/1	0.97	0.14	-	43,43,43,43	0
2	MG	B	3047	1/1	0.98	0.11	-	34,34,34,34	0
2	MG	I	3015	1/1	0.98	0.08	-	26,26,26,26	0
2	MG	B	3041	1/1	0.93	0.13	-	52,52,52,52	0
2	MG	K	3036	1/1	0.54	0.19	-	52,52,52,52	0
2	MG	L	3034	1/1	0.94	0.08	-	31,31,31,31	0
2	MG	I	3022	1/1	0.93	0.09	-	40,40,40,40	0
2	MG	C	3039	1/1	0.72	0.41	-	54,54,54,54	0
2	MG	A	3052	1/1	0.95	0.13	-	44,44,44,44	0
2	MG	I	3019	1/1	0.88	0.25	-	46,46,46,46	0
2	MG	L	3028	1/1	0.97	0.14	-	39,39,39,39	0
2	MG	H	3032	1/1	0.86	0.13	-	44,44,44,44	0
2	MG	E	3059	1/1	0.79	0.11	-	53,53,53,53	0
2	MG	B	3043	1/1	0.87	0.10	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	B	3044	1/1	0.85	0.11	-	46,46,46,46	0
2	MG	E	3023	1/1	0.98	0.08	-	41,41,41,41	0
2	MG	E	3002	1/1	0.94	0.16	-	51,51,51,51	0
2	MG	G	3058	1/1	0.99	0.06	-	49,49,49,49	0
2	MG	D	3013	1/1	0.83	0.10	-	51,51,51,51	0
2	MG	K	3050	1/1	0.94	0.10	-	38,38,38,38	0
2	MG	H	3038	1/1	0.80	0.25	-	52,52,52,52	0
2	MG	H	3060	1/1	0.96	0.15	-	49,49,49,49	0
2	MG	F	3008	1/1	0.94	0.20	-	39,39,39,39	0
2	MG	B	3046	1/1	0.97	0.09	-	41,41,41,41	0
2	MG	J	3017	1/1	0.59	0.23	-	62,62,62,62	0
2	MG	D	3018	1/1	0.95	0.07	-	36,36,36,36	0
2	MG	L	3055	1/1	0.88	0.14	-	54,54,54,54	0
2	MG	B	3037	1/1	0.97	0.05	-	36,36,36,36	0
2	MG	F	3063	1/1	0.97	0.07	-	46,46,46,46	0
2	MG	B	3029	1/1	0.81	0.14	-	56,56,56,56	0
2	MG	C	3012	1/1	0.92	0.18	-	43,43,43,43	0
2	MG	E	3001	1/1	0.97	0.09	-	40,40,40,40	0
2	MG	A	3033	1/1	0.96	0.08	-	45,45,45,45	0
2	MG	E	3024	1/1	0.96	0.08	-	46,46,46,46	0
2	MG	D	3021	1/1	0.90	0.13	-	52,52,52,52	0
2	MG	D	3011	1/1	0.98	0.06	-	40,40,40,40	0
2	MG	K	3051	1/1	0.79	0.10	-	63,63,63,63	0
2	MG	F	3056	1/1	0.98	0.13	-	42,42,42,42	0
2	MG	C	3014	1/1	0.94	0.22	-	49,49,49,49	0
2	MG	D	3009	1/1	0.95	0.13	-	37,37,37,37	0
2	MG	C	3004	1/1	0.93	0.09	-	47,47,47,47	0
2	MG	D	3020	1/1	0.85	0.17	-	57,57,57,57	0
2	MG	F	3006	1/1	0.96	0.07	-	34,34,34,34	0
2	MG	E	3061	1/1	0.90	0.07	-	56,56,56,56	0
2	MG	C	3048	1/1	0.94	0.07	-	38,38,38,38	0
2	MG	E	3030	1/1	0.96	0.11	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.