Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 06:02 AM EST

PDB ID	:	6NQP
Title	:	Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2), Y63(2,3-F2Y)
Authors	:	Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.
Deposited on	:	2019-01-21
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

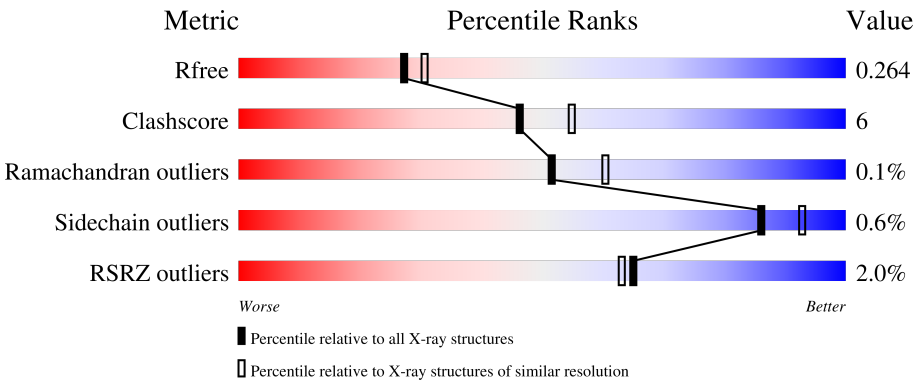
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	.% 75% 9% • 15%
1	B	255	2% 73% 12% 15%
1	C	255	2% 73% 11% 15%
1	D	255	2% 75% 9% 15%
1	E	255	2% 72% 13% 15%

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Mol	Chain	Length	Quality of chain
1	F	255	% 73% 12% 15%
1	G	255	2% 72% 12% • 15%
1	H	255	% 75% 9% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14646 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
			Total	C	F	N	O	S			
1	A	216	1731	1103	2	291	326	9	0	1	0
1	B	217	1755	1122	2	295	327	9	0	2	0
1	C	216	1731	1105	2	292	323	9	0	0	0
1	D	216	1735	1107	2	292	325	9	0	0	0
1	E	216	1735	1111	2	291	322	9	0	0	0
1	F	216	1752	1118	2	295	328	9	0	2	0
1	G	216	1724	1101	2	289	323	9	0	0	0
1	H	216	1723	1101	2	287	324	9	0	0	0

There are 328 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	expression tag	UNP Q5TLG6
A	-26	SER	-	expression tag	UNP Q5TLG6
A	-25	SER	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	HIS	-	expression tag	UNP Q5TLG6
A	-21	HIS	-	expression tag	UNP Q5TLG6
A	-20	HIS	-	expression tag	UNP Q5TLG6
A	-19	HIS	-	expression tag	UNP Q5TLG6
A	-18	SER	-	expression tag	UNP Q5TLG6
A	-17	SER	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6
A	-15	LEU	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	VAL	-	expression tag	UNP Q5TLG6
A	-13	PRO	-	expression tag	UNP Q5TLG6
A	-12	GLY	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	SER	-	expression tag	UNP Q5TLG6
A	-9	HIS	-	expression tag	UNP Q5TLG6
A	-8	MET	-	expression tag	UNP Q5TLG6
A	-7	VAL	-	expression tag	UNP Q5TLG6
A	-6	SER	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	GLY	-	expression tag	UNP Q5TLG6
A	-3	GLU	-	expression tag	UNP Q5TLG6
A	-2	GLU	-	expression tag	UNP Q5TLG6
A	-1	ASN	-	expression tag	UNP Q5TLG6
A	0	ASN	-	expression tag	UNP Q5TLG6
A	1	MET	-	expression tag	UNP Q5TLG6
A	2	ALA	-	expression tag	UNP Q5TLG6
A	63	KY4	CYS	chromophore	UNP Q5TLG6
A	63	KY4	TYR	chromophore	UNP Q5TLG6
A	63	KY4	GLY	chromophore	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
A	224	MET	-	expression tag	UNP Q5TLG6
A	225	ASP	-	expression tag	UNP Q5TLG6
A	226	GLU	-	expression tag	UNP Q5TLG6
A	227	LEU	-	expression tag	UNP Q5TLG6
A	228	TYR	-	expression tag	UNP Q5TLG6
A	229	LYS	-	expression tag	UNP Q5TLG6
B	-27	GLY	-	expression tag	UNP Q5TLG6
B	-26	SER	-	expression tag	UNP Q5TLG6
B	-25	SER	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	HIS	-	expression tag	UNP Q5TLG6
B	-21	HIS	-	expression tag	UNP Q5TLG6
B	-20	HIS	-	expression tag	UNP Q5TLG6
B	-19	HIS	-	expression tag	UNP Q5TLG6
B	-18	SER	-	expression tag	UNP Q5TLG6
B	-17	SER	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	LEU	-	expression tag	UNP Q5TLG6
B	-14	VAL	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	PRO	-	expression tag	UNP Q5TLG6
B	-12	GLY	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	SER	-	expression tag	UNP Q5TLG6
B	-9	HIS	-	expression tag	UNP Q5TLG6
B	-8	MET	-	expression tag	UNP Q5TLG6
B	-7	VAL	-	expression tag	UNP Q5TLG6
B	-6	SER	-	expression tag	UNP Q5TLG6
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	GLY	-	expression tag	UNP Q5TLG6
B	-3	GLU	-	expression tag	UNP Q5TLG6
B	-2	GLU	-	expression tag	UNP Q5TLG6
B	-1	ASN	-	expression tag	UNP Q5TLG6
B	0	ASN	-	expression tag	UNP Q5TLG6
B	1	MET	-	expression tag	UNP Q5TLG6
B	2	ALA	-	expression tag	UNP Q5TLG6
B	63	KY4	CYS	chromophore	UNP Q5TLG6
B	63	KY4	TYR	chromophore	UNP Q5TLG6
B	63	KY4	GLY	chromophore	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	224	MET	-	expression tag	UNP Q5TLG6
B	225	ASP	-	expression tag	UNP Q5TLG6
B	226	GLU	-	expression tag	UNP Q5TLG6
B	227	LEU	-	expression tag	UNP Q5TLG6
B	228	TYR	-	expression tag	UNP Q5TLG6
B	229	LYS	-	expression tag	UNP Q5TLG6
C	-27	GLY	-	expression tag	UNP Q5TLG6
C	-26	SER	-	expression tag	UNP Q5TLG6
C	-25	SER	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	HIS	-	expression tag	UNP Q5TLG6
C	-21	HIS	-	expression tag	UNP Q5TLG6
C	-20	HIS	-	expression tag	UNP Q5TLG6
C	-19	HIS	-	expression tag	UNP Q5TLG6
C	-18	SER	-	expression tag	UNP Q5TLG6
C	-17	SER	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	LEU	-	expression tag	UNP Q5TLG6
C	-14	VAL	-	expression tag	UNP Q5TLG6
C	-13	PRO	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	SER	-	expression tag	UNP Q5TLG6
C	-9	HIS	-	expression tag	UNP Q5TLG6
C	-8	MET	-	expression tag	UNP Q5TLG6
C	-7	VAL	-	expression tag	UNP Q5TLG6
C	-6	SER	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6
C	-4	GLY	-	expression tag	UNP Q5TLG6
C	-3	GLU	-	expression tag	UNP Q5TLG6
C	-2	GLU	-	expression tag	UNP Q5TLG6
C	-1	ASN	-	expression tag	UNP Q5TLG6
C	0	ASN	-	expression tag	UNP Q5TLG6
C	1	MET	-	expression tag	UNP Q5TLG6
C	2	ALA	-	expression tag	UNP Q5TLG6
C	63	KY4	CYS	chromophore	UNP Q5TLG6
C	63	KY4	TYR	chromophore	UNP Q5TLG6
C	63	KY4	GLY	chromophore	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	224	MET	-	expression tag	UNP Q5TLG6
C	225	ASP	-	expression tag	UNP Q5TLG6
C	226	GLU	-	expression tag	UNP Q5TLG6
C	227	LEU	-	expression tag	UNP Q5TLG6
C	228	TYR	-	expression tag	UNP Q5TLG6
C	229	LYS	-	expression tag	UNP Q5TLG6
D	-27	GLY	-	expression tag	UNP Q5TLG6
D	-26	SER	-	expression tag	UNP Q5TLG6
D	-25	SER	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	HIS	-	expression tag	UNP Q5TLG6
D	-21	HIS	-	expression tag	UNP Q5TLG6
D	-20	HIS	-	expression tag	UNP Q5TLG6
D	-19	HIS	-	expression tag	UNP Q5TLG6
D	-18	SER	-	expression tag	UNP Q5TLG6
D	-17	SER	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	LEU	-	expression tag	UNP Q5TLG6
D	-14	VAL	-	expression tag	UNP Q5TLG6
D	-13	PRO	-	expression tag	UNP Q5TLG6
D	-12	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6
D	-8	MET	-	expression tag	UNP Q5TLG6
D	-7	VAL	-	expression tag	UNP Q5TLG6
D	-6	SER	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	GLY	-	expression tag	UNP Q5TLG6
D	-3	GLU	-	expression tag	UNP Q5TLG6
D	-2	GLU	-	expression tag	UNP Q5TLG6
D	-1	ASN	-	expression tag	UNP Q5TLG6
D	0	ASN	-	expression tag	UNP Q5TLG6
D	1	MET	-	expression tag	UNP Q5TLG6
D	2	ALA	-	expression tag	UNP Q5TLG6
D	63	KY4	CYS	chromophore	UNP Q5TLG6
D	63	KY4	TYR	chromophore	UNP Q5TLG6
D	63	KY4	GLY	chromophore	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	224	MET	-	expression tag	UNP Q5TLG6
D	225	ASP	-	expression tag	UNP Q5TLG6
D	226	GLU	-	expression tag	UNP Q5TLG6
D	227	LEU	-	expression tag	UNP Q5TLG6
D	228	TYR	-	expression tag	UNP Q5TLG6
D	229	LYS	-	expression tag	UNP Q5TLG6
E	-27	GLY	-	expression tag	UNP Q5TLG6
E	-26	SER	-	expression tag	UNP Q5TLG6
E	-25	SER	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	HIS	-	expression tag	UNP Q5TLG6
E	-21	HIS	-	expression tag	UNP Q5TLG6
E	-20	HIS	-	expression tag	UNP Q5TLG6
E	-19	HIS	-	expression tag	UNP Q5TLG6
E	-18	SER	-	expression tag	UNP Q5TLG6
E	-17	SER	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	LEU	-	expression tag	UNP Q5TLG6
E	-14	VAL	-	expression tag	UNP Q5TLG6
E	-13	PRO	-	expression tag	UNP Q5TLG6
E	-12	GLY	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	SER	-	expression tag	UNP Q5TLG6
E	-9	HIS	-	expression tag	UNP Q5TLG6
E	-8	MET	-	expression tag	UNP Q5TLG6
E	-7	VAL	-	expression tag	UNP Q5TLG6
E	-6	SER	-	expression tag	UNP Q5TLG6
E	-5	LYS	-	expression tag	UNP Q5TLG6
E	-4	GLY	-	expression tag	UNP Q5TLG6
E	-3	GLU	-	expression tag	UNP Q5TLG6
E	-2	GLU	-	expression tag	UNP Q5TLG6
E	-1	ASN	-	expression tag	UNP Q5TLG6
E	0	ASN	-	expression tag	UNP Q5TLG6
E	1	MET	-	expression tag	UNP Q5TLG6
E	2	ALA	-	expression tag	UNP Q5TLG6
E	63	KY4	CYS	chromophore	UNP Q5TLG6
E	63	KY4	TYR	chromophore	UNP Q5TLG6
E	63	KY4	GLY	chromophore	UNP Q5TLG6
E	159	THR	MET	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	engineered mutation	UNP Q5TLG6
E	224	MET	-	expression tag	UNP Q5TLG6
E	225	ASP	-	expression tag	UNP Q5TLG6
E	226	GLU	-	expression tag	UNP Q5TLG6
E	227	LEU	-	expression tag	UNP Q5TLG6
E	228	TYR	-	expression tag	UNP Q5TLG6
E	229	LYS	-	expression tag	UNP Q5TLG6
F	-27	GLY	-	expression tag	UNP Q5TLG6
F	-26	SER	-	expression tag	UNP Q5TLG6
F	-25	SER	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6
F	-22	HIS	-	expression tag	UNP Q5TLG6
F	-21	HIS	-	expression tag	UNP Q5TLG6
F	-20	HIS	-	expression tag	UNP Q5TLG6
F	-19	HIS	-	expression tag	UNP Q5TLG6
F	-18	SER	-	expression tag	UNP Q5TLG6
F	-17	SER	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	LEU	-	expression tag	UNP Q5TLG6
F	-14	VAL	-	expression tag	UNP Q5TLG6
F	-13	PRO	-	expression tag	UNP Q5TLG6
F	-12	GLY	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP Q5TLG6
F	-8	MET	-	expression tag	UNP Q5TLG6
F	-7	VAL	-	expression tag	UNP Q5TLG6
F	-6	SER	-	expression tag	UNP Q5TLG6
F	-5	LYS	-	expression tag	UNP Q5TLG6
F	-4	GLY	-	expression tag	UNP Q5TLG6
F	-3	GLU	-	expression tag	UNP Q5TLG6
F	-2	GLU	-	expression tag	UNP Q5TLG6
F	-1	ASN	-	expression tag	UNP Q5TLG6
F	0	ASN	-	expression tag	UNP Q5TLG6
F	1	MET	-	expression tag	UNP Q5TLG6
F	2	ALA	-	expression tag	UNP Q5TLG6
F	63	KY4	CYS	chromophore	UNP Q5TLG6
F	63	KY4	TYR	chromophore	UNP Q5TLG6
F	63	KY4	GLY	chromophore	UNP Q5TLG6
F	159	THR	MET	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	engineered mutation	UNP Q5TLG6
F	224	MET	-	expression tag	UNP Q5TLG6
F	225	ASP	-	expression tag	UNP Q5TLG6
F	226	GLU	-	expression tag	UNP Q5TLG6
F	227	LEU	-	expression tag	UNP Q5TLG6
F	228	TYR	-	expression tag	UNP Q5TLG6
F	229	LYS	-	expression tag	UNP Q5TLG6
G	-27	GLY	-	expression tag	UNP Q5TLG6
G	-26	SER	-	expression tag	UNP Q5TLG6
G	-25	SER	-	expression tag	UNP Q5TLG6
G	-24	HIS	-	expression tag	UNP Q5TLG6
G	-23	HIS	-	expression tag	UNP Q5TLG6
G	-22	HIS	-	expression tag	UNP Q5TLG6
G	-21	HIS	-	expression tag	UNP Q5TLG6
G	-20	HIS	-	expression tag	UNP Q5TLG6
G	-19	HIS	-	expression tag	UNP Q5TLG6
G	-18	SER	-	expression tag	UNP Q5TLG6
G	-17	SER	-	expression tag	UNP Q5TLG6
G	-16	GLY	-	expression tag	UNP Q5TLG6
G	-15	LEU	-	expression tag	UNP Q5TLG6
G	-14	VAL	-	expression tag	UNP Q5TLG6
G	-13	PRO	-	expression tag	UNP Q5TLG6
G	-12	GLY	-	expression tag	UNP Q5TLG6
G	-11	GLY	-	expression tag	UNP Q5TLG6
G	-10	SER	-	expression tag	UNP Q5TLG6
G	-9	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	MET	-	expression tag	UNP Q5TLG6
G	-7	VAL	-	expression tag	UNP Q5TLG6
G	-6	SER	-	expression tag	UNP Q5TLG6
G	-5	LYS	-	expression tag	UNP Q5TLG6
G	-4	GLY	-	expression tag	UNP Q5TLG6
G	-3	GLU	-	expression tag	UNP Q5TLG6
G	-2	GLU	-	expression tag	UNP Q5TLG6
G	-1	ASN	-	expression tag	UNP Q5TLG6
G	0	ASN	-	expression tag	UNP Q5TLG6
G	1	MET	-	expression tag	UNP Q5TLG6
G	2	ALA	-	expression tag	UNP Q5TLG6
G	63	KY4	CYS	chromophore	UNP Q5TLG6
G	63	KY4	TYR	chromophore	UNP Q5TLG6
G	63	KY4	GLY	chromophore	UNP Q5TLG6
G	159	THR	MET	engineered mutation	UNP Q5TLG6
G	218	GLY	GLU	engineered mutation	UNP Q5TLG6
G	224	MET	-	expression tag	UNP Q5TLG6
G	225	ASP	-	expression tag	UNP Q5TLG6
G	226	GLU	-	expression tag	UNP Q5TLG6
G	227	LEU	-	expression tag	UNP Q5TLG6
G	228	TYR	-	expression tag	UNP Q5TLG6
G	229	LYS	-	expression tag	UNP Q5TLG6
H	-27	GLY	-	expression tag	UNP Q5TLG6
H	-26	SER	-	expression tag	UNP Q5TLG6
H	-25	SER	-	expression tag	UNP Q5TLG6
H	-24	HIS	-	expression tag	UNP Q5TLG6
H	-23	HIS	-	expression tag	UNP Q5TLG6
H	-22	HIS	-	expression tag	UNP Q5TLG6
H	-21	HIS	-	expression tag	UNP Q5TLG6
H	-20	HIS	-	expression tag	UNP Q5TLG6
H	-19	HIS	-	expression tag	UNP Q5TLG6
H	-18	SER	-	expression tag	UNP Q5TLG6
H	-17	SER	-	expression tag	UNP Q5TLG6
H	-16	GLY	-	expression tag	UNP Q5TLG6
H	-15	LEU	-	expression tag	UNP Q5TLG6
H	-14	VAL	-	expression tag	UNP Q5TLG6
H	-13	PRO	-	expression tag	UNP Q5TLG6
H	-12	GLY	-	expression tag	UNP Q5TLG6
H	-11	GLY	-	expression tag	UNP Q5TLG6
H	-10	SER	-	expression tag	UNP Q5TLG6
H	-9	HIS	-	expression tag	UNP Q5TLG6
H	-8	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	VAL	-	expression tag	UNP Q5TLG6
H	-6	SER	-	expression tag	UNP Q5TLG6
H	-5	LYS	-	expression tag	UNP Q5TLG6
H	-4	GLY	-	expression tag	UNP Q5TLG6
H	-3	GLU	-	expression tag	UNP Q5TLG6
H	-2	GLU	-	expression tag	UNP Q5TLG6
H	-1	ASN	-	expression tag	UNP Q5TLG6
H	0	ASN	-	expression tag	UNP Q5TLG6
H	1	MET	-	expression tag	UNP Q5TLG6
H	2	ALA	-	expression tag	UNP Q5TLG6
H	63	KY4	CYS	chromophore	UNP Q5TLG6
H	63	KY4	TYR	chromophore	UNP Q5TLG6
H	63	KY4	GLY	chromophore	UNP Q5TLG6
H	159	THR	MET	engineered mutation	UNP Q5TLG6
H	218	GLY	GLU	engineered mutation	UNP Q5TLG6
H	224	MET	-	expression tag	UNP Q5TLG6
H	225	ASP	-	expression tag	UNP Q5TLG6
H	226	GLU	-	expression tag	UNP Q5TLG6
H	227	LEU	-	expression tag	UNP Q5TLG6
H	228	TYR	-	expression tag	UNP Q5TLG6
H	229	LYS	-	expression tag	UNP Q5TLG6

- Molecule 2 is water.

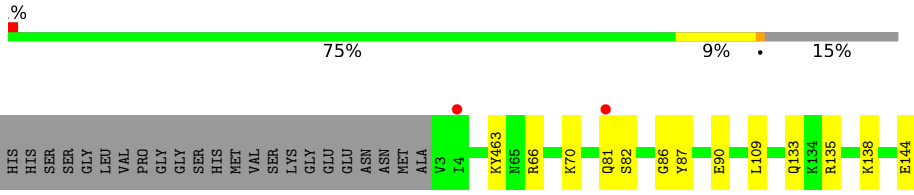
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	82	82	82	0	0
			Total	O		
2	B	122	122	122	0	0
			Total	O		
2	C	67	67	67	0	0
			Total	O		
2	D	108	108	108	0	0
			Total	O		
2	E	77	77	77	0	0
			Total	O		
2	F	105	105	105	0	0
			Total	O		
2	G	89	89	89	0	0
			Total	O		
2	H	110	110	110	0	0

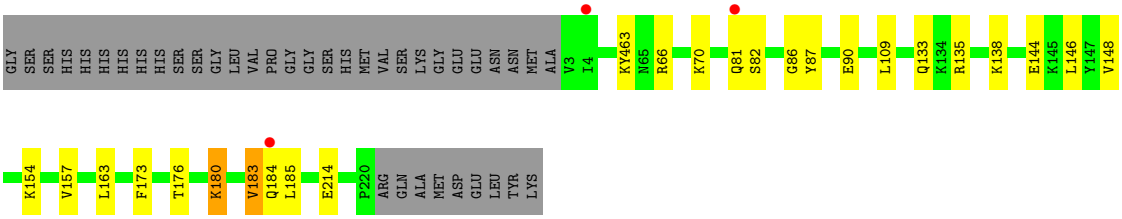
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fluorescent protein Dronpa

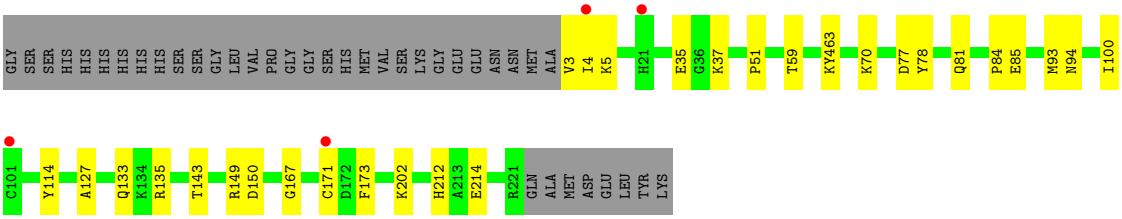
Chain A:





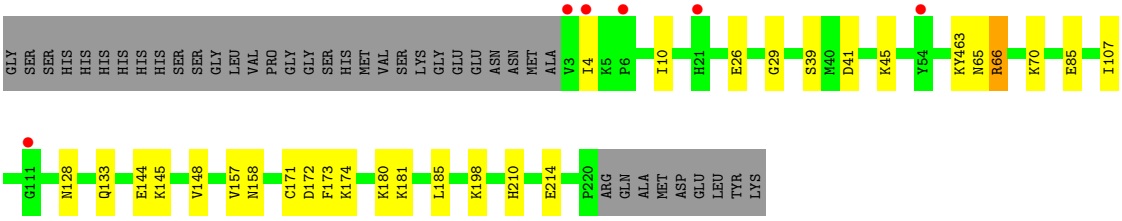
• Molecule 1: Fluorescent protein Dronpa

Chain B:



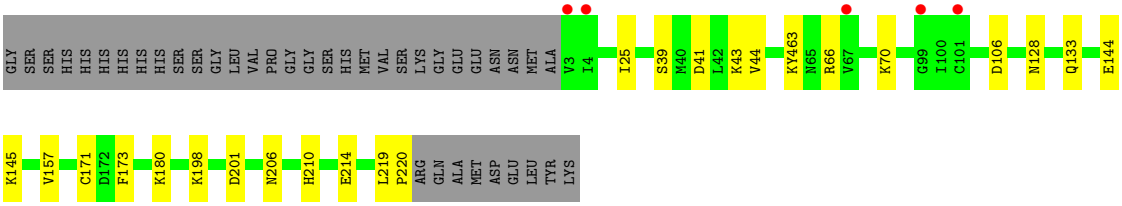
• Molecule 1: Fluorescent protein Dronpa

Chain C:



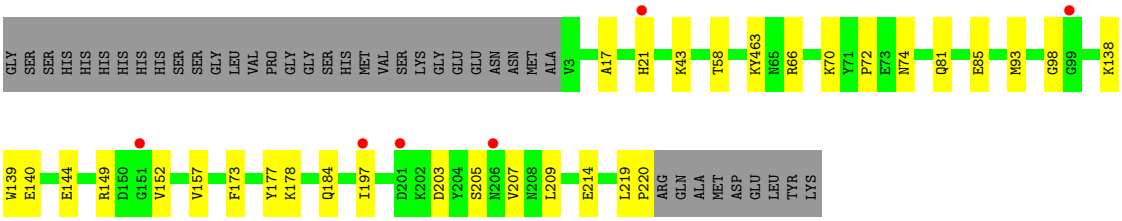
• Molecule 1: Fluorescent protein Dronpa

Chain D:



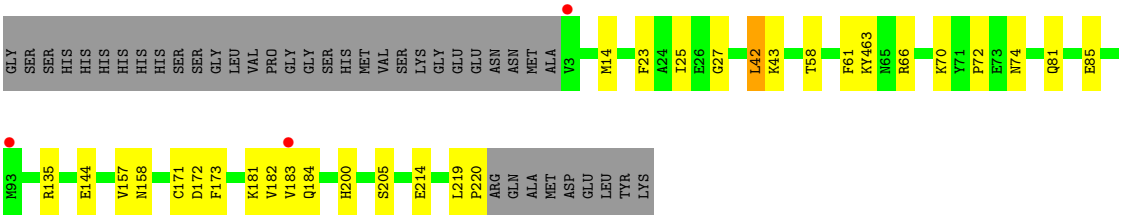
• Molecule 1: Fluorescent protein Dronpa

Chain E:



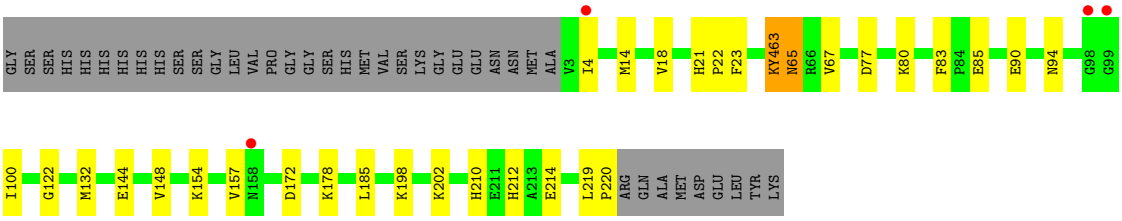
• Molecule 1: Fluorescent protein Dronpa

Chain F:



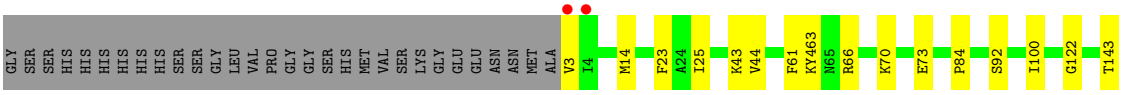
• Molecule 1: Fluorescent protein Dronpa

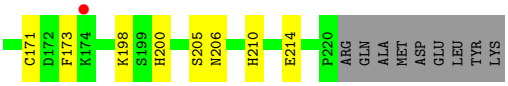
Chain G:



• Molecule 1: Fluorescent protein Dronpa

Chain H:




C171
D172
F173
K174
K198
S199
H200
S205
N206
H210
E214
P220
ARG
GLN
ALA
MET
ASP
GLU
LEU
TYR
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.30Å 85.97Å 143.02Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	39.25 – 2.20 39.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.25-2.20) 97.0 (39.50-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, R_{free}	0.225 , 0.260 0.228 , 0.264	Depositor DCC
R_{free} test set	4718 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14646	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2884e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KY4

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	0.34	1/1757 (0.1%)	0.56	0/2377
1	B	0.35	0/1784	0.60	0/2411
1	C	0.30	0/1754	0.55	0/2371
1	D	0.34	0/1758	0.56	0/2376
1	E	0.36	0/1758	0.58	0/2375
1	F	0.32	0/1778	0.55	0/2402
1	G	0.34	0/1747	0.55	1/2363 (0.0%)
1	H	0.33	0/1746	0.56	0/2364
All	All	0.34	1/14082 (0.0%)	0.56	1/19039 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	SER	C-N	-5.29	1.21	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	65	ASN	N-CA-C	-5.56	95.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1731	0	1618	21	0
1	B	1755	0	1674	27	0
1	C	1731	0	1635	18	0
1	D	1735	0	1639	14	0
1	E	1735	0	1648	24	0
1	F	1752	0	1667	23	0
1	G	1724	0	1618	28	0
1	H	1723	0	1608	15	0
2	A	82	0	0	4	0
2	B	122	0	0	12	0
2	C	67	0	0	5	0
2	D	108	0	0	3	0
2	E	77	0	0	5	0
2	F	105	0	0	3	0
2	G	89	0	0	4	0
2	H	110	0	0	1	0
All	All	14646	0	13107	169	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 6.

All (169) 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:G:63:KY4:N1	1:G:63:KY4:CA1	1.69	1.53
1:E:58:THR:HG21	1:E:197:ILE:HD11	1.32	1.06
1:F:27:GLY:HA3	1:F:42:LEU:HD12	1.48	0.95
1:E:58:THR:CG2	1:E:197:ILE:HD11	2.04	0.87
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.64	0.78
1:H:14:MET:HE3	1:H:23:PHE:HE2	1.49	0.78
1:D:106:ASP:OD1	1:D:180:LYS:NZ	2.17	0.76
1:G:4:ILE:HD11	1:G:83:PHE:HB2	1.69	0.75
1:A:81:GLN:OE1	1:A:184:GLN:HB2	1.89	0.72
1:A:81:GLN:O	1:A:183:VAL:CG1	2.37	0.71
1:A:86:GLY:O	1:A:180:LYS:HG3	1.91	0.71
1:A:81:GLN:O	1:A:183:VAL:HG11	1.91	0.70
1:A:135:ARG:NH1	2:A:301:HOH:O	2.25	0.70
1:F:200:HIS:NE2	2:F:302:HOH:O	2.24	0.70
1:F:70:LYS:HB3	1:F:214:GLU:HG2	1.75	0.69
1:D:201:ASP:OD2	2:D:301:HOH:O	2.09	0.69
1:B:94:ASN:HA	1:B:100:ILE:HD12	1.75	0.68
1:B:51:PRO:O	2:B:301:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:GLY:HA3	1:F:42:LEU:CD1	2.22	0.68
1:A:70:LYS:HB3	1:A:214:GLU:HG2	1.74	0.68
1:C:85:GLU:OE1	1:C:181:LYS:NZ	2.27	0.67
1:B:37:LYS:NZ	2:B:305:HOH:O	2.27	0.67
1:H:14:MET:HE3	1:H:23:PHE:CE2	2.30	0.67
1:C:26:GLU:OE2	1:C:45:LYS:HD2	1.95	0.66
1:F:27:GLY:CA	1:F:42:LEU:HD12	2.25	0.65
1:G:65:ASN:ND2	1:G:67:VAL:HG12	2.12	0.65
1:E:58:THR:HG21	1:E:197:ILE:CD1	2.21	0.64
1:F:14:MET:HE3	1:F:23:PHE:HE2	1.63	0.63
1:G:22:PRO:HD2	2:G:306:HOH:O	2.00	0.62
1:E:197:ILE:HG13	2:E:326:HOH:O	1.99	0.62
1:A:86:GLY:O	1:A:180:LYS:CG	2.48	0.61
1:B:70:LYS:HB3	1:B:214:GLU:HG2	1.82	0.61
1:G:63:KY4:N1	1:G:63:KY4:CB1	2.58	0.61
1:A:163:LEU:HB3	2:A:322:HOH:O	2.02	0.60
1:D:39:SER:HB2	1:D:210:HIS:CE1	2.36	0.59
1:B:5:LYS:HA	1:B:5:LYS:HE2	1.85	0.59
1:B:35:GLU:OE1	2:B:302:HOH:O	2.16	0.59
1:H:70:LYS:HB3	1:H:214:GLU:HG2	1.85	0.58
1:E:197:ILE:O	1:E:197:ILE:HG22	2.01	0.58
1:A:148:VAL:HG11	1:A:185:LEU:HD13	1.85	0.58
1:H:3:VAL:HG21	1:H:84:PRO:HD3	1.86	0.58
1:D:219:LEU:HD12	1:D:220:PRO:HD2	1.84	0.57
1:B:202:LYS:NZ	2:B:313:HOH:O	2.37	0.57
1:B:85:GLU:OE1	1:B:85:GLU:N	2.37	0.57
1:G:4:ILE:HD11	1:G:83:PHE:CB	2.33	0.57
1:D:70:LYS:HB3	1:D:214:GLU:HG2	1.88	0.55
1:E:219:LEU:HD23	1:E:220:PRO:HD2	1.86	0.55
1:E:197:ILE:HG12	1:E:209:LEU:HD13	1.89	0.55
1:C:128:ASN:HA	1:C:133:GLN:HE21	1.72	0.55
1:E:152:VAL:HG21	1:E:178:LYS:HG2	1.89	0.55
1:G:14:MET:HE3	1:G:23:PHE:HE2	1.71	0.55
1:A:81:GLN:O	1:A:183:VAL:HG12	2.06	0.54
1:B:143:THR:HG22	2:B:407:HOH:O	2.06	0.54
1:H:171:CYS:HG	1:H:173:PHE:HE1	1.55	0.54
1:H:44:VAL:HG12	1:H:205:SER:HA	1.89	0.54
1:B:133:GLN:HG3	1:B:135:ARG:NH2	2.22	0.54
1:F:135:ARG:NH1	2:F:310:HOH:O	2.41	0.54
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.89	0.53
1:C:145:LYS:NZ	2:C:302:HOH:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:GLU:HA	1:F:157:VAL:HB	1.90	0.53
1:D:25:ILE:HG12	1:D:44:VAL:HG22	1.91	0.53
1:B:167:GLY:CA	2:B:314:HOH:O	2.56	0.53
1:C:65:ASN:N	2:C:309:HOH:O	2.42	0.53
1:H:73:GLU:H	1:H:73:GLU:CD	2.12	0.52
1:G:148:VAL:HG21	1:G:185:LEU:HB3	1.89	0.52
1:B:94:ASN:CA	1:B:100:ILE:HD12	2.38	0.52
1:C:107:ILE:O	1:C:180:LYS:NZ	2.40	0.52
1:C:171:CYS:HG	1:C:173:PHE:HE1	1.55	0.52
1:H:198:LYS:HG3	1:H:210:HIS:CD2	2.44	0.52
1:B:100:ILE:HG21	1:H:92:SER:OG	2.10	0.52
1:E:43:LYS:HA	1:E:205:SER:O	2.10	0.51
1:E:138:LYS:HE2	1:E:139:TRP:O	2.10	0.51
1:E:144:GLU:HA	1:E:157:VAL:HB	1.91	0.51
1:G:144:GLU:HB2	1:G:157:VAL:HB	1.92	0.51
1:E:85:GLU:OE1	1:E:85:GLU:N	2.38	0.51
1:B:171:CYS:HG	1:B:173:PHE:HE2	1.55	0.51
1:G:77:ASP:OD2	1:G:80:LYS:N	2.36	0.51
1:F:182:VAL:HG12	1:F:182:VAL:O	2.09	0.51
1:B:59:THR:OG1	1:B:93:MET:HE1	2.11	0.50
1:G:65:ASN:CG	1:G:67:VAL:HG12	2.32	0.50
1:B:212:HIS:ND1	2:B:312:HOH:O	2.35	0.50
1:G:132:MET:HG2	2:G:303:HOH:O	2.11	0.50
1:E:152:VAL:HG22	1:E:177:TYR:O	2.11	0.50
1:F:183:VAL:HG12	1:F:184:GLN:N	2.27	0.50
1:G:21:HIS:HB3	2:G:372:HOH:O	2.12	0.49
1:A:81:GLN:O	1:A:81:GLN:HG2	2.12	0.49
1:B:149:ARG:HA	2:B:306:HOH:O	2.12	0.49
1:D:171:CYS:HG	1:D:173:PHE:HE1	1.58	0.49
1:G:154:LYS:NZ	2:G:301:HOH:O	2.26	0.49
1:H:25:ILE:HG12	1:H:44:VAL:HA	1.94	0.49
1:G:198:LYS:HD2	1:G:210:HIS:CG	2.48	0.48
1:D:41:ASP:OD2	2:D:302:HOH:O	2.20	0.48
1:E:140:GLU:O	2:E:301:HOH:O	2.20	0.48
1:H:143:THR:HG22	2:H:390:HOH:O	2.14	0.48
1:B:171:CYS:SG	1:B:173:PHE:HE2	2.37	0.48
1:F:14:MET:HE2	1:F:61:PHE:CZ	2.49	0.47
1:G:100:ILE:O	1:G:122:GLY:HA2	2.13	0.47
1:B:150:ASP:OD1	2:B:303:HOH:O	2.20	0.47
1:A:154:LYS:NZ	2:A:320:HOH:O	2.46	0.47
1:D:206:ASN:ND2	2:D:301:HOH:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:ASP:O	2:E:302:HOH:O	2.20	0.47
1:B:77:ASP:O	1:B:81:GLN:HG3	2.15	0.47
1:A:138:LYS:HB2	1:A:138:LYS:HE2	1.74	0.47
1:G:65:ASN:HD21	1:G:67:VAL:CG1	2.28	0.47
1:B:4:ILE:HD12	1:B:114:TYR:OH	2.15	0.47
1:G:63:KY4:N1	1:G:63:KY4:C1	2.64	0.46
1:C:66:ARG:HD3	2:C:306:HOH:O	2.14	0.46
1:C:39:SER:HB2	1:C:210:HIS:CE1	2.50	0.46
1:G:94:ASN:HB3	1:G:172:ASP:HB2	1.97	0.46
1:C:144:GLU:HA	1:C:157:VAL:HB	1.98	0.46
1:D:128:ASN:HA	1:D:133:GLN:NE2	2.31	0.46
1:E:93:MET:HG2	1:E:173:PHE:CD1	2.50	0.46
1:E:98:GLY:HA3	2:E:334:HOH:O	2.15	0.46
1:G:202:LYS:HB3	1:G:202:LYS:HE3	1.77	0.46
1:E:197:ILE:HG23	1:E:207:VAL:HG13	1.97	0.46
1:G:219:LEU:HD23	1:G:220:PRO:HA	1.98	0.45
1:A:90:GLU:HG3	1:A:176:THR:HB	1.98	0.45
1:C:41:ASP:OD2	2:C:301:HOH:O	2.20	0.45
1:H:200:HIS:HA	1:H:206:ASN:O	2.17	0.45
1:G:14:MET:HE3	1:G:23:PHE:CE2	2.51	0.45
1:F:72:PRO:HB2	1:F:74:ASN:OD1	2.16	0.45
1:A:133:GLN:HG3	1:A:135:ARG:HH21	1.82	0.45
1:B:150:ASP:HB2	2:B:372:HOH:O	2.17	0.45
1:E:58:THR:HG21	2:E:326:HOH:O	2.17	0.45
1:B:77:ASP:O	1:B:81:GLN:NE2	2.48	0.45
1:D:43:LYS:HZ2	1:D:43:LYS:HB3	1.81	0.45
1:H:100:ILE:O	1:H:122:GLY:HA2	2.17	0.44
1:F:171:CYS:HG	1:F:173:PHE:HE1	1.63	0.44
1:A:144:GLU:HA	1:A:157:VAL:HB	1.98	0.44
1:B:3:VAL:HG11	1:B:84:PRO:HB3	1.98	0.44
1:G:85:GLU:OE1	1:G:85:GLU:N	2.44	0.43
1:A:87:TYR:HA	1:A:180:LYS:HG2	2.00	0.43
1:C:158:ASN:OD1	1:C:172:ASP:HA	2.18	0.43
1:G:65:ASN:HD21	1:G:67:VAL:HG12	1.80	0.43
1:F:81:GLN:O	1:F:181:LYS:HE3	2.19	0.43
1:A:157:VAL:HG13	1:A:173:PHE:HB2	2.00	0.43
1:F:43:LYS:HA	1:F:205:SER:O	2.18	0.43
1:C:198:LYS:HA	1:C:198:LYS:HD2	1.67	0.43
1:G:144:GLU:CB	1:G:157:VAL:HB	2.47	0.43
1:C:148:VAL:HG21	1:C:185:LEU:HB3	2.00	0.43
1:F:14:MET:CE	1:F:23:PHE:HE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:LEU:HD23	1:F:220:PRO:HD2	2.00	0.43
1:E:72:PRO:HB2	1:E:74:ASN:OD1	2.20	0.42
1:D:144:GLU:HA	1:D:157:VAL:HB	2.00	0.42
1:F:58:THR:HG21	2:F:340:HOH:O	2.19	0.42
1:A:109:LEU:N	2:A:313:HOH:O	2.38	0.42
1:D:145:LYS:HE2	1:D:145:LYS:HB2	1.94	0.42
1:H:14:MET:HE1	1:H:61:PHE:CZ	2.54	0.42
1:E:149:ARG:O	1:E:152:VAL:HG12	2.20	0.42
1:G:18:VAL:HA	1:G:122:GLY:O	2.20	0.42
1:A:146:LEU:HA	1:A:154:LYS:O	2.20	0.42
1:F:219:LEU:HD23	1:F:219:LEU:HA	1.91	0.42
1:E:81:GLN:HE22	1:E:184:GLN:HB3	1.85	0.42
1:F:158[B]:ASN:ND2	1:F:172:ASP:OD1	2.53	0.42
1:B:78:TYR:HA	1:B:81:GLN:HE21	1.84	0.41
1:B:127:ALA:N	2:B:322:HOH:O	2.54	0.41
1:D:198:LYS:HA	1:D:198:LYS:HD2	1.72	0.41
1:C:10:ILE:N	1:C:29:GLY:O	2.48	0.41
1:G:90:GLU:OE2	1:G:178:LYS:NZ	2.41	0.41
1:A:133:GLN:HG3	1:A:135:ARG:NH2	2.35	0.41
1:F:85:GLU:OE1	1:F:85:GLU:N	2.44	0.41
1:F:14:MET:HE3	1:F:23:PHE:CE2	2.49	0.41
1:F:14:MET:CE	1:F:25:ILE:HD12	2.51	0.41
1:B:143:THR:CG2	2:B:407:HOH:O	2.66	0.41
1:C:85:GLU:OE1	1:C:85:GLU:N	2.49	0.41
1:E:17:ALA:HA	1:E:21:HIS:O	2.21	0.40
1:G:212:HIS:NE2	1:G:214:GLU:OE2	2.53	0.40
1:H:43:LYS:HA	1:H:205:SER:O	2.22	0.40
1:C:174:LYS:NZ	2:C:316:HOH:O	2.54	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	212/255 (83%)	207 (98%)	4 (2%)	1 (0%)	29	31
1	B	214/255 (84%)	210 (98%)	4 (2%)	0	100	100
1	C	211/255 (83%)	208 (99%)	3 (1%)	0	100	100
1	D	211/255 (83%)	208 (99%)	3 (1%)	0	100	100
1	E	211/255 (83%)	207 (98%)	4 (2%)	0	100	100
1	F	213/255 (84%)	210 (99%)	3 (1%)	0	100	100
1	G	211/255 (83%)	207 (98%)	4 (2%)	0	100	100
1	H	211/255 (83%)	208 (99%)	3 (1%)	0	100	100
All	All	1694/2040 (83%)	1665 (98%)	28 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	VAL

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	181/217 (83%)	179 (99%)	2 (1%)	73	85
1	B	187/217 (86%)	187 (100%)	0	100	100
1	C	182/217 (84%)	180 (99%)	2 (1%)	73	85
1	D	183/217 (84%)	182 (100%)	1 (0%)	88	94
1	E	182/217 (84%)	181 (100%)	1 (0%)	88	94
1	F	187/217 (86%)	185 (99%)	2 (1%)	73	85
1	G	180/217 (83%)	180 (100%)	0	100	100
1	H	179/217 (82%)	178 (99%)	1 (1%)	86	93
All	All	1461/1736 (84%)	1452 (99%)	9 (1%)	86	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	180	LYS
1	C	4	ILE
1	C	66	ARG
1	D	66	ARG
1	E	66	ARG
1	F	42	LEU
1	F	66	ARG
1	H	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	KY4	C	63	1	24,24,25	2.93	6 (25%)	30,34,36	3.01	9 (30%)
1	KY4	B	63	1	24,24,25	3.06	8 (33%)	30,34,36	3.30	9 (30%)
1	KY4	D	63	1	24,24,25	2.94	5 (20%)	30,34,36	2.91	9 (30%)
1	KY4	H	63	1	24,24,25	3.03	6 (25%)	30,34,36	3.06	8 (26%)
1	KY4	G	63	1	24,24,25	2.30	8 (33%)	30,34,36	3.42	10 (33%)
1	KY4	E	63	1	24,24,25	3.03	7 (29%)	30,34,36	3.14	7 (23%)
1	KY4	A	63	1	24,24,25	2.98	7 (29%)	30,34,36	3.17	7 (23%)
1	KY4	F	63	1	24,24,25	3.09	7 (29%)	30,34,36	3.16	9 (30%)

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	KY4	C	63	1	-	3/9/29/30	0/2/2/2
1	KY4	B	63	1	-	3/9/29/30	0/2/2/2
1	KY4	D	63	1	-	2/9/29/30	0/2/2/2
1	KY4	H	63	1	-	2/9/29/30	0/2/2/2
1	KY4	G	63	1	-	4/9/29/30	0/2/2/2
1	KY4	E	63	1	-	3/9/29/30	0/2/2/2
1	KY4	A	63	1	-	3/9/29/30	0/2/2/2
1	KY4	F	63	1	-	3/9/29/30	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	KY4	CA2-C2	-12.40	1.36	1.48
1	B	63	KY4	CA2-C2	-12.34	1.36	1.48
1	H	63	KY4	CA2-C2	-12.15	1.36	1.48
1	E	63	KY4	CA2-C2	-12.03	1.36	1.48
1	A	63	KY4	CA2-C2	-11.91	1.36	1.48
1	C	63	KY4	CA2-C2	-11.62	1.37	1.48
1	D	63	KY4	CA2-C2	-11.56	1.37	1.48
1	G	63	KY4	CA3-C3	6.41	1.71	1.49
1	E	63	KY4	CG2-CB2	5.05	1.54	1.46
1	F	63	KY4	CG2-CB2	4.86	1.54	1.46
1	D	63	KY4	CG2-CB2	4.81	1.54	1.46
1	A	63	KY4	CG2-CB2	4.81	1.54	1.46
1	H	63	KY4	CG2-CB2	4.69	1.54	1.46
1	C	63	KY4	CG2-CB2	4.66	1.54	1.46
1	B	63	KY4	CG2-CB2	4.56	1.53	1.46
1	G	63	KY4	CA1-N1	4.02	1.69	1.48
1	G	63	KY4	C1-N2	-3.72	1.26	1.32
1	F	63	KY4	C2-N3	-3.57	1.31	1.39
1	B	63	KY4	C2-N3	-3.54	1.31	1.39
1	H	63	KY4	C2-N3	-3.46	1.31	1.39
1	D	63	KY4	C2-N3	-3.41	1.31	1.39
1	A	63	KY4	C2-N3	-3.40	1.31	1.39
1	G	63	KY4	C2-N3	-3.39	1.31	1.39
1	C	63	KY4	C2-N3	-3.38	1.31	1.39
1	E	63	KY4	C2-N3	-3.32	1.32	1.39
1	H	63	KY4	CB2-CA2	-3.05	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	KY4	CA2-N2	-3.01	1.32	1.38
1	F	63	KY4	CA2-N2	-2.99	1.32	1.38
1	D	63	KY4	CB2-CA2	-2.99	1.32	1.35
1	D	63	KY4	CA2-N2	-2.98	1.32	1.38
1	H	63	KY4	CA2-N2	-2.97	1.32	1.38
1	F	63	KY4	CB2-CA2	-2.90	1.32	1.35
1	B	63	KY4	CA2-N2	-2.85	1.32	1.38
1	A	63	KY4	CA2-N2	-2.79	1.32	1.38
1	B	63	KY4	CB2-CA2	-2.75	1.32	1.35
1	E	63	KY4	CA2-N2	-2.70	1.32	1.38
1	G	63	KY4	CZ-CE1	-2.68	1.36	1.39
1	G	63	KY4	CB2-CA2	2.64	1.37	1.35
1	C	63	KY4	CB2-CA2	-2.63	1.32	1.35
1	A	63	KY4	C1-N2	2.40	1.35	1.32
1	E	63	KY4	CB2-CA2	-2.36	1.33	1.35
1	G	63	KY4	CG2-CD1	2.32	1.40	1.39
1	H	63	KY4	OH-CZ	2.26	1.41	1.36
1	G	63	KY4	F2-CD1	-2.22	1.31	1.35
1	E	63	KY4	C1-N2	2.14	1.35	1.32
1	A	63	KY4	OH-CZ	2.11	1.40	1.36
1	B	63	KY4	C1-N2	2.09	1.35	1.32
1	A	63	KY4	CB2-CA2	-2.09	1.33	1.35
1	B	63	KY4	OH-CZ	2.09	1.40	1.36
1	F	63	KY4	O2-C2	-2.06	1.18	1.23
1	C	63	KY4	OH-CZ	2.06	1.40	1.36
1	F	63	KY4	C1-N2	2.05	1.35	1.32
1	B	63	KY4	O2-C2	-2.04	1.18	1.23
1	E	63	KY4	OH-CZ	2.03	1.40	1.36

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	KY4	CA2-C2-N3	11.65	108.88	103.37
1	E	63	KY4	CA2-C2-N3	11.53	108.82	103.37
1	F	63	KY4	CA2-C2-N3	11.48	108.80	103.37
1	A	63	KY4	CA2-C2-N3	11.41	108.77	103.37
1	C	63	KY4	CA2-C2-N3	10.79	108.47	103.37
1	H	63	KY4	CA2-C2-N3	10.69	108.43	103.37
1	G	63	KY4	O3-C3-CA3	-10.61	94.35	126.39
1	D	63	KY4	CA2-C2-N3	10.34	108.26	103.37
1	B	63	KY4	O2-C2-CA2	-10.11	125.28	130.96
1	F	63	KY4	O2-C2-CA2	-9.65	125.54	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	63	KY4	O2-C2-CA2	-9.35	125.71	130.96
1	A	63	KY4	O2-C2-CA2	-9.28	125.75	130.96
1	E	63	KY4	O2-C2-CA2	-9.27	125.75	130.96
1	C	63	KY4	O2-C2-CA2	-8.63	126.11	130.96
1	D	63	KY4	O2-C2-CA2	-8.22	126.34	130.96
1	G	63	KY4	CA2-N2-C1	7.50	111.30	105.77
1	G	63	KY4	C2-CA2-N2	-7.25	103.85	108.93
1	A	63	KY4	N3-C1-N2	-5.68	107.52	111.45
1	B	63	KY4	N3-C1-N2	-5.17	107.87	111.45
1	G	63	KY4	CA2-C2-N3	5.07	105.77	103.37
1	E	63	KY4	N3-C1-N2	-5.02	107.98	111.45
1	G	63	KY4	CB2-CA2-C2	4.91	128.13	122.28
1	F	63	KY4	N3-C1-N2	-4.84	108.10	111.45
1	C	63	KY4	N3-C1-N2	-4.67	108.22	111.45
1	H	63	KY4	N3-C1-N2	-4.60	108.27	111.45
1	D	63	KY4	N3-C1-N2	-4.56	108.30	111.45
1	G	63	KY4	CA3-N3-C1	4.10	132.08	127.16
1	G	63	KY4	CA1-CB1-SG1	-3.84	106.16	114.44
1	A	63	KY4	CA2-N2-C1	3.68	108.49	105.77
1	H	63	KY4	CA1-CB1-SG1	-3.63	106.62	114.44
1	G	63	KY4	CZ-CE1-CD1	-3.56	118.75	121.60
1	B	63	KY4	CA1-CB1-SG1	-3.47	106.97	114.44
1	E	63	KY4	CA2-N2-C1	3.41	108.28	105.77
1	F	63	KY4	CA1-CB1-SG1	-3.32	107.29	114.44
1	C	63	KY4	CA2-N2-C1	3.28	108.19	105.77
1	B	63	KY4	CA2-N2-C1	3.17	108.11	105.77
1	D	63	KY4	CA2-N2-C1	3.06	108.03	105.77
1	F	63	KY4	CA2-N2-C1	2.95	107.95	105.77
1	B	63	KY4	O3-C3-CA3	-2.78	117.98	126.39
1	H	63	KY4	CA2-N2-C1	2.78	107.82	105.77
1	B	63	KY4	CD2-CG2-CD1	2.69	119.58	116.71
1	D	63	KY4	O3-C3-CA3	-2.66	118.35	126.39
1	E	63	KY4	C2-CA2-N2	-2.58	107.13	108.93
1	A	63	KY4	C2-CA2-N2	-2.51	107.17	108.93
1	C	63	KY4	CD2-CG2-CD1	2.50	119.39	116.71
1	C	63	KY4	O3-C3-CA3	-2.48	118.90	126.39
1	H	63	KY4	CD2-CG2-CD1	2.47	119.36	116.71
1	A	63	KY4	O3-C3-CA3	-2.43	119.05	126.39
1	F	63	KY4	O3-C3-CA3	-2.43	119.06	126.39
1	E	63	KY4	CA1-CB1-SG1	-2.42	109.23	114.44
1	C	63	KY4	CA1-CB1-SG1	-2.39	109.28	114.44
1	D	63	KY4	CG2-CB2-CA2	-2.37	126.12	130.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	KY4	CD2-CG2-CD1	2.31	119.18	116.71
1	H	63	KY4	CZ-CE1-CD1	-2.29	119.77	121.60
1	H	63	KY4	O3-C3-CA3	-2.26	119.57	126.39
1	C	63	KY4	CG2-CB2-CA2	-2.25	126.36	130.86
1	C	63	KY4	C2-CA2-N2	-2.20	107.39	108.93
1	D	63	KY4	CB2-CA2-C2	2.19	124.89	122.28
1	E	63	KY4	F2-CD1-CG2	2.15	121.64	119.68
1	G	63	KY4	F2-CD1-CG2	-2.14	117.74	119.68
1	D	63	KY4	CA1-CB1-SG1	-2.10	109.91	114.44
1	B	63	KY4	C2-CA2-N2	-2.09	107.47	108.93
1	F	63	KY4	CD2-CG2-CD1	2.09	118.95	116.71
1	G	63	KY4	CA3-N3-C2	-2.08	119.03	123.80
1	D	63	KY4	CD2-CG2-CD1	2.08	118.93	116.71
1	F	63	KY4	C2-CA2-N2	-2.06	107.49	108.93
1	B	63	KY4	CZ-CE1-CD1	-2.06	119.95	121.60
1	F	63	KY4	CG2-CB2-CA2	-2.02	126.82	130.86

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	KY4	C3-CA3-N3-C2
1	A	63	KY4	C2-CA2-CB2-CG2
1	B	63	KY4	C3-CA3-N3-C2
1	B	63	KY4	C2-CA2-CB2-CG2
1	C	63	KY4	C3-CA3-N3-C2
1	D	63	KY4	C3-CA3-N3-C2
1	E	63	KY4	C3-CA3-N3-C2
1	F	63	KY4	C3-CA3-N3-C2
1	G	63	KY4	N2-CA2-CB2-CG2
1	G	63	KY4	C2-CA2-CB2-CG2
1	H	63	KY4	C3-CA3-N3-C2
1	A	63	KY4	N2-CA2-CB2-CG2
1	B	63	KY4	N2-CA2-CB2-CG2
1	C	63	KY4	N2-CA2-CB2-CG2
1	E	63	KY4	N2-CA2-CB2-CG2
1	F	63	KY4	N2-CA2-CB2-CG2
1	H	63	KY4	N2-CA2-CB2-CG2
1	E	63	KY4	C2-CA2-CB2-CG2
1	D	63	KY4	N2-CA2-CB2-CG2
1	C	63	KY4	C2-CA2-CB2-CG2
1	F	63	KY4	C2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	G	63	KY4	C1-CA1-CB1-SG1
1	G	63	KY4	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	63	KY4	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	215/255 (84%)	0.15	3 (1%)	75	73	45, 57, 73, 103	0
1	B	216/255 (84%)	-0.02	4 (1%)	66	65	31, 43, 66, 82	0
1	C	215/255 (84%)	0.38	6 (2%)	53	51	50, 63, 79, 107	0
1	D	215/255 (84%)	-0.02	5 (2%)	60	58	32, 45, 65, 83	0
1	E	215/255 (84%)	0.32	6 (2%)	53	51	49, 60, 76, 88	0
1	F	215/255 (84%)	-0.01	3 (1%)	75	73	28, 42, 61, 74	0
1	G	215/255 (84%)	0.20	4 (1%)	66	65	50, 61, 77, 107	0
1	H	215/255 (84%)	-0.04	3 (1%)	75	73	29, 45, 65, 95	0
All	All	1721/2040 (84%)	0.12	34 (1%)	65	63	28, 54, 73, 107	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	CYS	5.5
1	D	4	ILE	4.2
1	G	158	ASN	4.1
1	E	21	HIS	4.1
1	E	151	GLY	4.0
1	H	4	ILE	4.0
1	D	3	VAL	3.9
1	H	3	VAL	3.7
1	C	4	ILE	3.5
1	A	184	GLN	3.5
1	G	4	ILE	3.4
1	A	4	ILE	3.2
1	A	81	GLN	3.1
1	C	3	VAL	3.1
1	D	101	CYS	2.9
1	C	21	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	171	CYS	2.7
1	G	99	GLY	2.7
1	D	67	VAL	2.7
1	B	4	ILE	2.6
1	E	206	ASN	2.6
1	C	54	TYR	2.5
1	D	99	GLY	2.4
1	G	98	GLY	2.4
1	E	197	ILE	2.3
1	C	6	PRO	2.3
1	F	3	VAL	2.2
1	C	111	GLY	2.2
1	E	201	ASP	2.2
1	F	93	MET	2.2
1	E	99	GLY	2.1
1	F	183	VAL	2.1
1	H	174	LYS	2.1
1	B	21	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KY4	G	63	23/24	0.88	0.15	52,55,62,64	0
1	KY4	A	63	23/24	0.92	0.13	48,51,57,59	0
1	KY4	B	63	23/24	0.93	0.12	29,38,47,49	0
1	KY4	E	63	23/24	0.94	0.13	51,54,58,59	0
1	KY4	C	63	23/24	0.94	0.11	54,59,67,68	0
1	KY4	F	63	23/24	0.95	0.12	23,30,40,49	0
1	KY4	D	63	23/24	0.95	0.11	26,35,41,48	0
1	KY4	H	63	23/24	0.96	0.12	32,40,43,50	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.