



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:29 am BST

PDB ID : 4EMQ  
Title : Crystal structure of a single mutant of Dronpa, the green-on-state PDM1-4  
Authors : Ngan, N.B.; Van Hecke, K.; Van Meervelt, L.  
Deposited on : 2012-04-12  
Resolution : 1.95 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

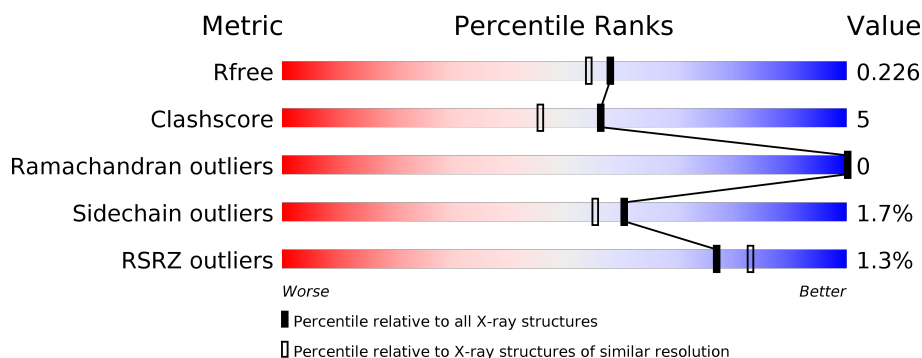
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	255	<div> <div></div> <div>76% 7% 16%</div> </div>
1	B	255	<div> <div>4%</div> <div>68% 15% 16%</div> </div>
1	C	255	<div> <div></div> <div>76% 7% 16%</div> </div>
1	D	255	<div> <div></div> <div>75% 9% 16%</div> </div>
1	E	255	<div> <div>%</div> <div>79% 16%</div> </div>
1	F	255	<div> <div>%</div> <div>76% 7% 16%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11412 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	4	0
			1744	1110	293	331	10			
1	B	214	Total	C	N	O	S	0	2	0
			1717	1095	289	323	10			
1	C	214	Total	C	N	O	S	0	4	0
			1739	1107	294	328	10			
1	D	215	Total	C	N	O	S	0	3	0
			1746	1111	293	332	10			
1	E	214	Total	C	N	O	S	0	3	0
			1729	1102	292	325	10			
1	F	214	Total	C	N	O	S	0	1	0
			1728	1102	291	325	10			

There are 222 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	-31	ARG	-	EXPRESSION TAG	UNP Q5TLG6
A	-30	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-29	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-25	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-24	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-23	HIS	-	EXPRESSION TAG	UNP Q5TLG6
A	-22	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	-20	ALA	-	EXPRESSION TAG	UNP Q5TLG6
A	-19	SER	-	EXPRESSION TAG	UNP Q5TLG6
A	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	-17	THR	-	EXPRESSION TAG	UNP Q5TLG6
A	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-14	GLN	-	EXPRESSION TAG	UNP Q5TLG6
A	-13	GLN	-	EXPRESSION TAG	UNP Q5TLG6
A	-12	MET	-	EXPRESSION TAG	UNP Q5TLG6
A	-11	GLY	-	EXPRESSION TAG	UNP Q5TLG6
A	-10	ARG	-	EXPRESSION TAG	UNP Q5TLG6
A	-9	ASP	-	EXPRESSION TAG	UNP Q5TLG6
A	-8	LEU	-	EXPRESSION TAG	UNP Q5TLG6
A	-7	TYR	-	EXPRESSION TAG	UNP Q5TLG6
A	-6	ASP	-	EXPRESSION TAG	UNP Q5TLG6
A	-5	ASP	-	EXPRESSION TAG	UNP Q5TLG6
A	-4	ASP	-	EXPRESSION TAG	UNP Q5TLG6
A	-3	ASP	-	EXPRESSION TAG	UNP Q5TLG6
A	-2	LYS	-	EXPRESSION TAG	UNP Q5TLG6
A	-1	ASP	-	EXPRESSION TAG	UNP Q5TLG6
A	0	PRO	-	EXPRESSION TAG	UNP Q5TLG6
A	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
A	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
A	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
A	145	ASN	LYS	ENGINEERED MUTATION	UNP Q5TLG6
B	-32	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	-31	ARG	-	EXPRESSION TAG	UNP Q5TLG6
B	-30	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-29	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-25	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-24	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-23	HIS	-	EXPRESSION TAG	UNP Q5TLG6
B	-22	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	-20	ALA	-	EXPRESSION TAG	UNP Q5TLG6
B	-19	SER	-	EXPRESSION TAG	UNP Q5TLG6
B	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	-17	THR	-	EXPRESSION TAG	UNP Q5TLG6
B	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-15	GLY	-	EXPRESSION TAG	UNP Q5TLG6
B	-14	GLN	-	EXPRESSION TAG	UNP Q5TLG6
B	-13	GLN	-	EXPRESSION TAG	UNP Q5TLG6
B	-12	MET	-	EXPRESSION TAG	UNP Q5TLG6
B	-11	GLY	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	EXPRESSION TAG	UNP Q5TLG6
B	-9	ASP	-	EXPRESSION TAG	UNP Q5TLG6
B	-8	LEU	-	EXPRESSION TAG	UNP Q5TLG6
B	-7	TYR	-	EXPRESSION TAG	UNP Q5TLG6
B	-6	ASP	-	EXPRESSION TAG	UNP Q5TLG6
B	-5	ASP	-	EXPRESSION TAG	UNP Q5TLG6
B	-4	ASP	-	EXPRESSION TAG	UNP Q5TLG6
B	-3	ASP	-	EXPRESSION TAG	UNP Q5TLG6
B	-2	LYS	-	EXPRESSION TAG	UNP Q5TLG6
B	-1	ASP	-	EXPRESSION TAG	UNP Q5TLG6
B	0	PRO	-	EXPRESSION TAG	UNP Q5TLG6
B	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
B	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
B	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
B	145	ASN	LYS	ENGINEERED MUTATION	UNP Q5TLG6
C	-32	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	-31	ARG	-	EXPRESSION TAG	UNP Q5TLG6
C	-30	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-29	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-25	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-24	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-23	HIS	-	EXPRESSION TAG	UNP Q5TLG6
C	-22	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	-20	ALA	-	EXPRESSION TAG	UNP Q5TLG6
C	-19	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	-17	THR	-	EXPRESSION TAG	UNP Q5TLG6
C	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-15	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-14	GLN	-	EXPRESSION TAG	UNP Q5TLG6
C	-13	GLN	-	EXPRESSION TAG	UNP Q5TLG6
C	-12	MET	-	EXPRESSION TAG	UNP Q5TLG6
C	-11	GLY	-	EXPRESSION TAG	UNP Q5TLG6
C	-10	ARG	-	EXPRESSION TAG	UNP Q5TLG6
C	-9	ASP	-	EXPRESSION TAG	UNP Q5TLG6
C	-8	LEU	-	EXPRESSION TAG	UNP Q5TLG6
C	-7	TYR	-	EXPRESSION TAG	UNP Q5TLG6
C	-6	ASP	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASP	-	EXPRESSION TAG	UNP Q5TLG6
C	-4	ASP	-	EXPRESSION TAG	UNP Q5TLG6
C	-3	ASP	-	EXPRESSION TAG	UNP Q5TLG6
C	-2	LYS	-	EXPRESSION TAG	UNP Q5TLG6
C	-1	ASP	-	EXPRESSION TAG	UNP Q5TLG6
C	0	PRO	-	EXPRESSION TAG	UNP Q5TLG6
C	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
C	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
C	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
C	145	ASN	LYS	ENGINEERED MUTATION	UNP Q5TLG6
D	-32	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-31	ARG	-	EXPRESSION TAG	UNP Q5TLG6
D	-30	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-29	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-25	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-24	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-23	HIS	-	EXPRESSION TAG	UNP Q5TLG6
D	-22	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-20	ALA	-	EXPRESSION TAG	UNP Q5TLG6
D	-19	SER	-	EXPRESSION TAG	UNP Q5TLG6
D	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-17	THR	-	EXPRESSION TAG	UNP Q5TLG6
D	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-15	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-14	GLN	-	EXPRESSION TAG	UNP Q5TLG6
D	-13	GLN	-	EXPRESSION TAG	UNP Q5TLG6
D	-12	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-11	GLY	-	EXPRESSION TAG	UNP Q5TLG6
D	-10	ARG	-	EXPRESSION TAG	UNP Q5TLG6
D	-9	ASP	-	EXPRESSION TAG	UNP Q5TLG6
D	-8	LEU	-	EXPRESSION TAG	UNP Q5TLG6
D	-7	TYR	-	EXPRESSION TAG	UNP Q5TLG6
D	-6	ASP	-	EXPRESSION TAG	UNP Q5TLG6
D	-5	ASP	-	EXPRESSION TAG	UNP Q5TLG6
D	-4	ASP	-	EXPRESSION TAG	UNP Q5TLG6
D	-3	ASP	-	EXPRESSION TAG	UNP Q5TLG6
D	-2	LYS	-	EXPRESSION TAG	UNP Q5TLG6
D	-1	ASP	-	EXPRESSION TAG	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	EXPRESSION TAG	UNP Q5TLG6
D	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
D	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
D	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
D	145	ASN	LYS	ENGINEERED MUTATION	UNP Q5TLG6
E	-32	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	-31	ARG	-	EXPRESSION TAG	UNP Q5TLG6
E	-30	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-29	SER	-	EXPRESSION TAG	UNP Q5TLG6
E	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-25	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-24	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-23	HIS	-	EXPRESSION TAG	UNP Q5TLG6
E	-22	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	-20	ALA	-	EXPRESSION TAG	UNP Q5TLG6
E	-19	SER	-	EXPRESSION TAG	UNP Q5TLG6
E	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	-17	THR	-	EXPRESSION TAG	UNP Q5TLG6
E	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-15	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-14	GLN	-	EXPRESSION TAG	UNP Q5TLG6
E	-13	GLN	-	EXPRESSION TAG	UNP Q5TLG6
E	-12	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	-11	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-10	ARG	-	EXPRESSION TAG	UNP Q5TLG6
E	-9	ASP	-	EXPRESSION TAG	UNP Q5TLG6
E	-8	LEU	-	EXPRESSION TAG	UNP Q5TLG6
E	-7	TYR	-	EXPRESSION TAG	UNP Q5TLG6
E	-6	ASP	-	EXPRESSION TAG	UNP Q5TLG6
E	-5	ASP	-	EXPRESSION TAG	UNP Q5TLG6
E	-4	ASP	-	EXPRESSION TAG	UNP Q5TLG6
E	-3	ASP	-	EXPRESSION TAG	UNP Q5TLG6
E	-2	LYS	-	EXPRESSION TAG	UNP Q5TLG6
E	-1	ASP	-	EXPRESSION TAG	UNP Q5TLG6
E	0	PRO	-	EXPRESSION TAG	UNP Q5TLG6
E	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
E	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
E	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
E	145	ASN	LYS	ENGINEERED MUTATION	UNP Q5TLG6

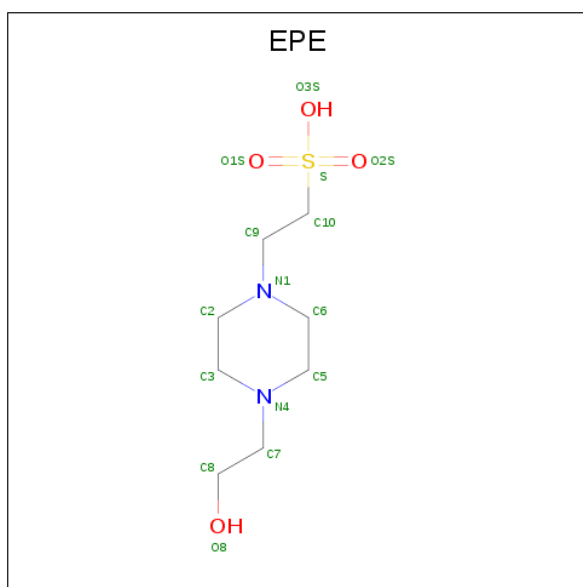
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-32	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-31	ARG	-	EXPRESSION TAG	UNP Q5TLG6
F	-30	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-29	SER	-	EXPRESSION TAG	UNP Q5TLG6
F	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-25	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-24	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-23	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-22	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-20	ALA	-	EXPRESSION TAG	UNP Q5TLG6
F	-19	SER	-	EXPRESSION TAG	UNP Q5TLG6
F	-18	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-17	THR	-	EXPRESSION TAG	UNP Q5TLG6
F	-16	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-15	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-14	GLN	-	EXPRESSION TAG	UNP Q5TLG6
F	-13	GLN	-	EXPRESSION TAG	UNP Q5TLG6
F	-12	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-11	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-10	ARG	-	EXPRESSION TAG	UNP Q5TLG6
F	-9	ASP	-	EXPRESSION TAG	UNP Q5TLG6
F	-8	LEU	-	EXPRESSION TAG	UNP Q5TLG6
F	-7	TYR	-	EXPRESSION TAG	UNP Q5TLG6
F	-6	ASP	-	EXPRESSION TAG	UNP Q5TLG6
F	-5	ASP	-	EXPRESSION TAG	UNP Q5TLG6
F	-4	ASP	-	EXPRESSION TAG	UNP Q5TLG6
F	-3	ASP	-	EXPRESSION TAG	UNP Q5TLG6
F	-2	LYS	-	EXPRESSION TAG	UNP Q5TLG6
F	-1	ASP	-	EXPRESSION TAG	UNP Q5TLG6
F	0	PRO	-	EXPRESSION TAG	UNP Q5TLG6
F	63	GYC	CYS	CHROMOPHORE	UNP Q5TLG6
F	63	GYC	TYR	CHROMOPHORE	UNP Q5TLG6
F	63	GYC	GLY	CHROMOPHORE	UNP Q5TLG6
F	145	ASN	LYS	ENGINEERED MUTATION	UNP Q5TLG6

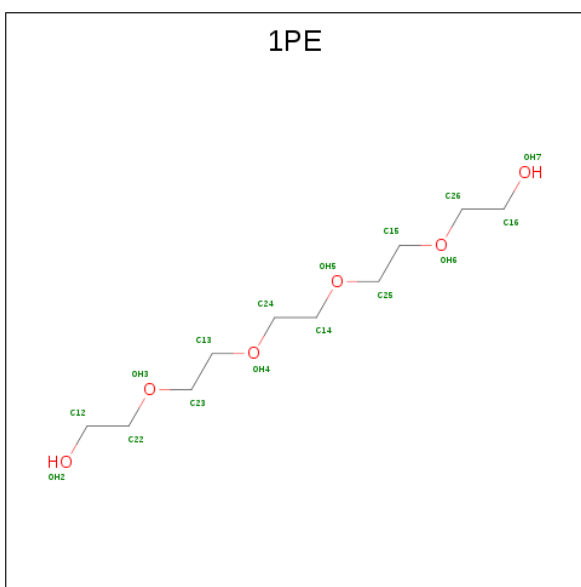
- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).





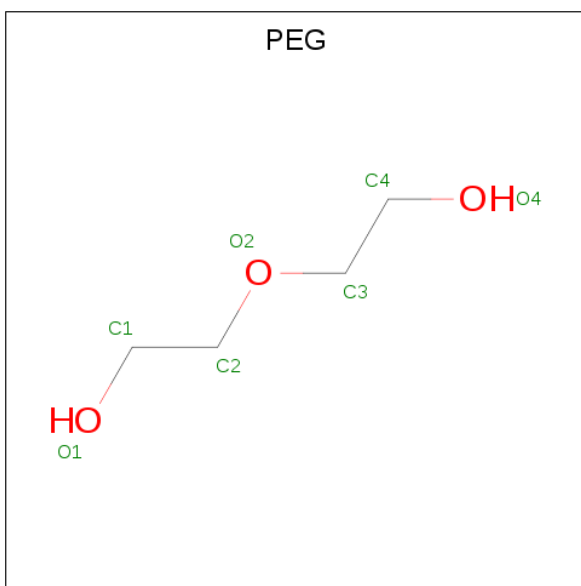
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	O	S		0	0
			5	1	3	1			
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	O	S		0	0
			5	1	3	1			
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	O	S		0	0
			5	1	3	1			

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		

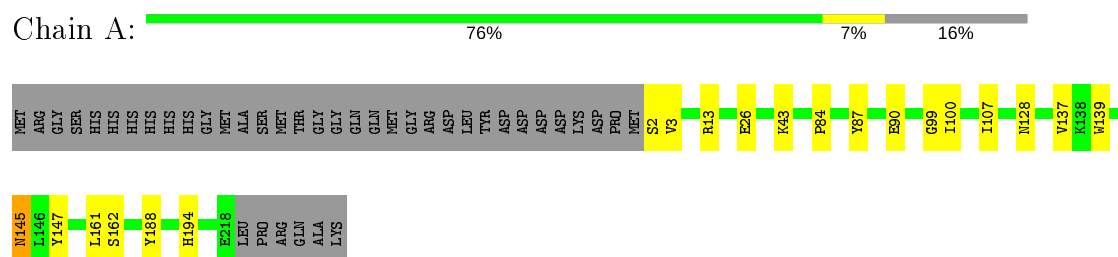
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	155	Total	O	0	0
			155	155		
5	B	99	Total	O	0	0
			99	99		
5	C	153	Total	O	0	0
			153	153		
5	D	170	Total	O	0	0
			170	170		
5	E	155	Total	O	0	0
			155	155		
5	F	152	Total	O	0	0
			152	152		

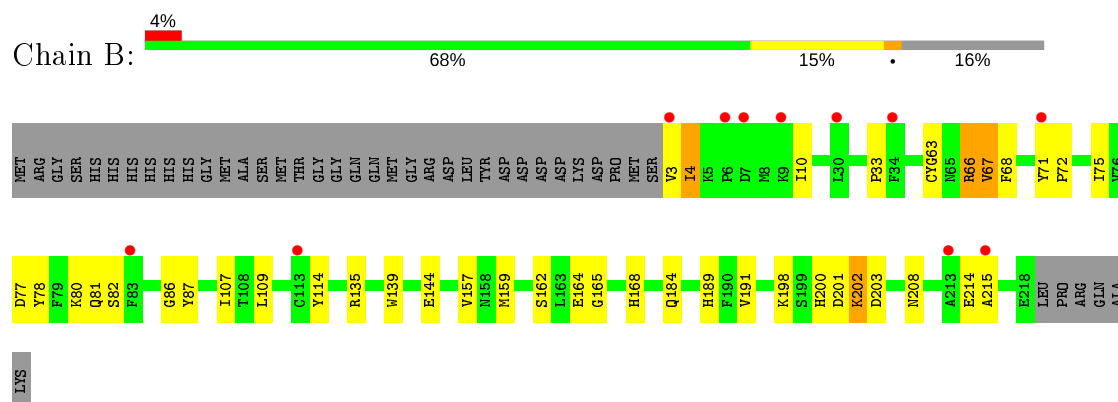
### 3 Residue-property plots [i](#)

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

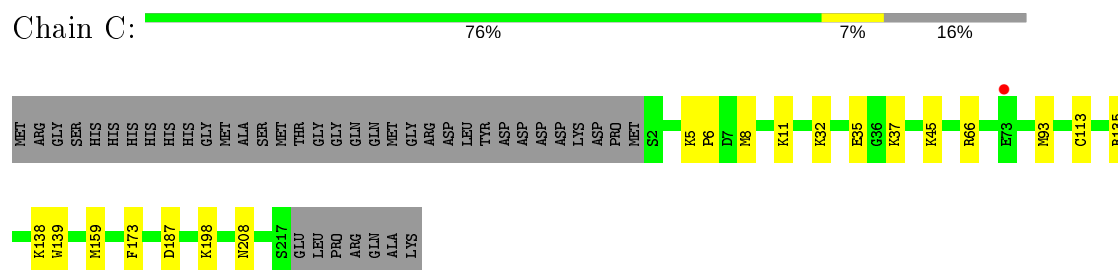
#### • Molecule 1: Fluorescent protein Dronpa



#### • Molecule 1: Fluorescent protein Dronpa

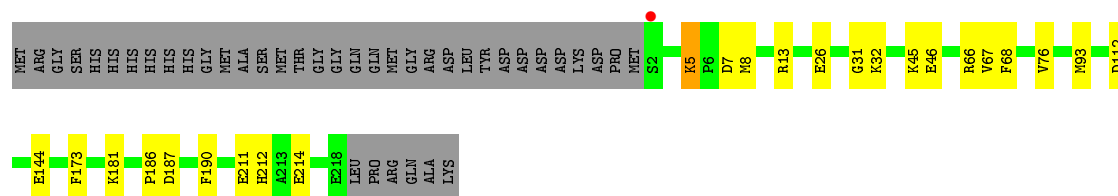


#### • Molecule 1: Fluorescent protein Dronpa

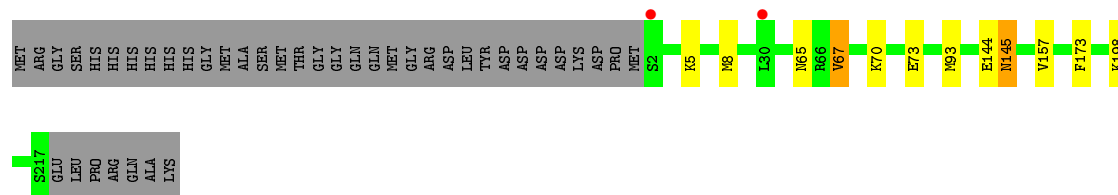
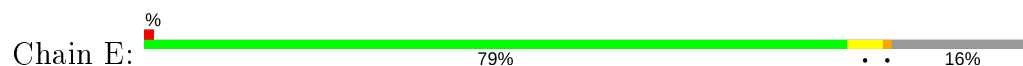


#### • Molecule 1: Fluorescent protein Dronpa

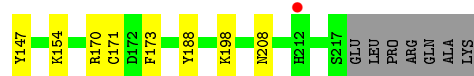
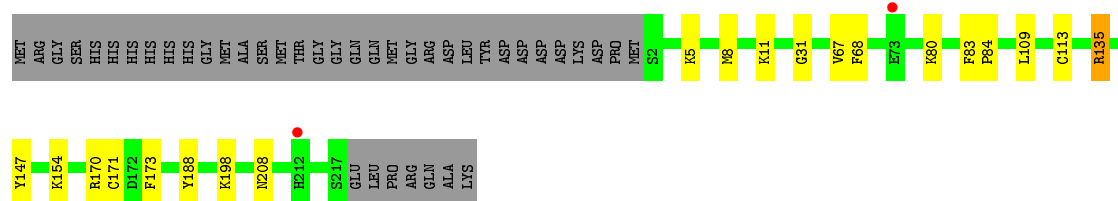
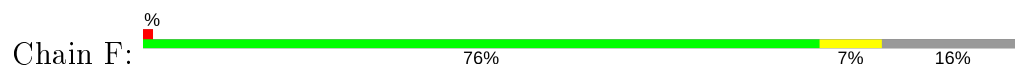




- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.54Å 103.80Å 177.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.71 – 1.95 54.71 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.71-1.95) 100.0 (54.71-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.183 , 0.232 0.179 , 0.226	Depositor DCC
$R_{free}$ test set	4728 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EPE, GYC, 1PE

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	0.47	0/1776	0.62	0/2399
1	B	0.43	0/1749	0.61	0/2365
1	C	0.48	0/1779	0.62	0/2403
1	D	0.49	0/1774	0.65	0/2396
1	E	0.47	0/1757	0.60	0/2374
1	F	0.48	0/1756	0.64	0/2371
All	All	0.47	0/10591	0.62	0/14308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1744	0	1649	17	0
1	B	1717	0	1621	31	0
1	C	1739	0	1650	11	0
1	D	1746	0	1652	17	0
1	E	1729	0	1638	9	0
1	F	1728	0	1649	14	0
2	A	15	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	15	0	17	1	0
2	D	5	0	0	0	0
2	E	15	0	17	0	0
2	F	5	0	0	0	0
3	A	16	0	22	6	0
4	B	7	0	10	0	0
4	C	14	0	20	2	0
4	D	7	0	10	0	0
4	E	7	0	10	0	0
4	F	14	0	20	1	0
5	A	155	0	0	3	0
5	B	99	0	0	4	1
5	C	153	0	0	2	0
5	D	170	0	0	1	1
5	E	155	0	0	0	0
5	F	152	0	0	2	0
All	All	11412	0	10002	103	1

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 5.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ARG:HG2	1:F:135:ARG:HH11	1.40	0.86
1:B:78:TYR:O	5:B:474:HOH:O	1.95	0.83
1:B:135:ARG:HH11	1:B:164:GLU:HB3	1.51	0.73
1:B:71:TYR:OH	1:B:189:HIS:NE2	2.20	0.72
1:D:7:ASP:OD1	1:D:32:LYS:NZ	2.25	0.69
1:A:194:HIS:ND1	5:A:476:HOH:O	2.26	0.68
1:A:43:LYS:NZ	3:A:302:1PE:H242	2.12	0.64
1:F:154:LYS:NZ	5:F:545:HOH:O	2.26	0.63
1:B:135:ARG:NH1	1:B:165:GLY:H	1.96	0.63
1:D:13:ARG:NH1	1:D:26:GLU:OE2	2.32	0.63
1:D:13:ARG:HH12	1:D:45:LYS:HE3	1.62	0.63
1:D:45:LYS:NZ	1:D:46:GLU:OE2	2.26	0.62
1:A:43:LYS:HZ3	3:A:302:1PE:H232	1.63	0.61
1:B:135:ARG:HH12	1:B:165:GLY:H	1.49	0.60
1:C:187[A]:ASP:OD1	5:C:552:HOH:O	2.17	0.59
1:B:82:SER:HB2	1:B:86:GLY:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:HD2	1:B:191:VAL:HG11	1.85	0.58
1:E:65:ASN:OD1	1:E:67:VAL:HG13	2.03	0.58
1:D:187:ASP:OD1	5:D:500:HOH:O	2.17	0.58
1:B:214:GLU:OE1	5:B:476:HOH:O	2.17	0.57
1:A:13:ARG:NH1	1:A:26:GLU:OE2	2.37	0.57
1:B:4:ILE:HD13	1:B:80:LYS:HD3	1.87	0.57
1:B:82:SER:O	1:B:86:GLY:N	2.23	0.57
1:F:11:LYS:HG3	1:F:113:CYS:SG	2.45	0.56
1:A:43:LYS:NZ	3:A:302:1PE:H122	2.21	0.56
1:C:5:LYS:H	1:C:8:MET:HE2	1.72	0.54
1:A:145:ASN:ND2	5:A:492:HOH:O	2.42	0.52
1:A:137:VAL:HB	1:A:162[A]:SER:OG	2.09	0.52
1:B:67:VAL:HG22	1:B:80:LYS:HG2	1.92	0.52
1:C:11:LYS:NZ	5:C:504:HOH:O	2.43	0.52
1:B:10:ILE:HD11	1:B:68:PHE:CE1	2.45	0.52
1:F:135:ARG:CG	1:F:135:ARG:HH11	2.18	0.52
1:F:67:VAL:HG23	1:F:80:LYS:HG2	1.92	0.51
1:D:13:ARG:HH12	1:D:45:LYS:CE	2.23	0.51
1:D:93:MET:HG2	1:D:173:PHE:CE1	2.46	0.51
1:E:145:ASN:H	1:E:145:ASN:HD22	1.58	0.51
1:E:144:GLU:HA	1:E:157:VAL:HB	1.93	0.51
1:A:3:VAL:HG11	1:A:84:PRO:HB3	1.93	0.50
1:D:31:GLY:HA3	1:D:68:PHE:CE2	2.47	0.49
1:B:81:GLN:NE2	5:B:490:HOH:O	2.44	0.48
1:D:93:MET:HG2	1:D:173:PHE:CD1	2.47	0.48
1:B:77:ASP:O	1:B:81:GLN:NE2	2.45	0.48
1:A:99:GLY:O	1:A:100:ILE:HD13	2.14	0.47
1:B:184:GLN:HB3	5:B:490:HOH:O	2.13	0.47
1:E:5:LYS:HB2	1:E:8:MET:HG3	1.96	0.47
1:A:43:LYS:HZ3	3:A:302:1PE:H122	1.79	0.47
1:B:191:VAL:HA	1:B:215:ALA:HA	1.97	0.47
1:F:198:LYS:HB2	1:F:208:ASN:HD22	1.80	0.46
1:B:63:GYC:HB2	1:B:66:ARG:NH2	2.30	0.46
1:B:200:HIS:HD2	1:B:201:ASP:O	1.97	0.46
1:E:70:LYS:HE2	1:E:70:LYS:HB3	1.87	0.46
1:C:35:GLU:HB3	1:C:37:LYS:HD2	1.98	0.46
1:C:93:MET:HG2	1:C:173:PHE:CD1	2.51	0.46
1:A:128:ASN:ND2	5:A:542:HOH:O	2.46	0.45
1:B:4:ILE:HD11	1:B:33:PRO:CB	2.46	0.45
1:B:71:TYR:HA	1:B:72:PRO:HD3	1.75	0.45
1:D:13:ARG:NH1	1:D:45:LYS:HE3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:MET:HE1	1:F:109:LEU:HD11	1.99	0.44
1:B:203:ASP:N	1:B:203:ASP:OD1	2.46	0.44
1:B:72:PRO:HD2	1:B:75:ILE:HD12	1.98	0.44
1:C:45:LYS:HD2	1:C:45:LYS:HA	1.69	0.44
1:E:93:MET:HG2	1:E:173:PHE:CD1	2.52	0.44
1:A:43:LYS:HZ3	3:A:302:1PE:H242	1.83	0.44
1:B:144:GLU:HA	1:B:157:VAL:HB	1.99	0.44
2:C:301:EPE:H102	2:C:301:EPE:H21	1.26	0.44
1:D:13:ARG:HH12	1:D:45:LYS:CD	2.31	0.44
1:B:202:LYS:HD2	1:B:202:LYS:HA	1.83	0.44
1:C:11:LYS:HG3	1:C:113:CYS:SG	2.57	0.44
2:A:301:EPE:H52	2:A:301:EPE:H81	1.79	0.43
1:B:87:TYR:CE2	1:B:107:ILE:HD12	2.53	0.43
1:A:145:ASN:H	1:A:145:ASN:HD22	1.65	0.43
1:B:162:SER:HA	1:B:168:HIS:CD2	2.54	0.43
1:F:5:LYS:NZ	5:F:535:HOH:O	2.52	0.43
1:A:147:TYR:HB3	1:A:188:TYR:CD1	2.54	0.43
1:C:198:LYS:HB2	1:C:208:ASN:HD22	1.83	0.43
1:B:67:VAL:HG11	1:B:114:TYR:CZ	2.54	0.43
1:B:198:LYS:HB2	1:B:208:ASN:HD22	1.84	0.42
1:F:147:TYR:HB3	1:F:188:TYR:CD1	2.54	0.42
4:C:303:PEG:H32	4:C:303:PEG:H12	1.53	0.42
1:E:93:MET:HG2	1:E:173:PHE:CE1	2.54	0.42
1:C:139:TRP:CZ3	1:C:159:MET:HB3	2.55	0.42
1:F:31:GLY:HA3	1:F:68:PHE:CE2	2.55	0.42
1:F:171:CYS:HG	1:F:173:PHE:HE1	1.66	0.42
1:E:198:LYS:HD3	1:E:198:LYS:HA	1.82	0.41
1:D:211:GLU:HG2	1:D:212:HIS:N	2.35	0.41
1:F:135:ARG:NH1	1:F:135:ARG:HG2	2.20	0.41
1:D:5:LYS:HE2	1:D:112:ASP:HB3	2.03	0.41
1:C:6:PRO:O	1:C:32:LYS:HA	2.20	0.41
1:A:87:TYR:CZ	1:A:107:ILE:HD12	2.55	0.41
1:B:4:ILE:HD11	1:B:33:PRO:HB3	2.01	0.41
1:B:214:GLU:O	1:B:214:GLU:HG2	2.21	0.41
1:D:5:LYS:O	1:D:8:MET:HE2	2.21	0.41
1:A:43:LYS:HZ1	3:A:302:1PE:H242	1.86	0.40
1:D:144:GLU:O	1:D:190:PHE:HA	2.21	0.40
1:A:139:TRP:CZ3	1:A:161:LEU:HG	2.56	0.40
1:D:76:VAL:HB	1:D:186:PRO:HA	2.02	0.40
1:B:139:TRP:CZ3	1:B:159:MET:HB3	2.56	0.40
4:C:302:PEG:H41	4:C:302:PEG:H22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:GLU:HG3	1:E:73:GLU:H	1.58	0.40
1:F:170:ARG:CB	4:F:302:PEG:H31	2.51	0.40
1:D:45:LYS:HG2	1:D:46:GLU:HG3	2.03	0.40
1:F:83:PHE:HB3	1:F:84:PRO:HA	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:492:HOH:O	5:D:563:HOH:O[2_555]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/255 (85%)	215 (100%)	1 (0%)	0	100	100
1	B	213/255 (84%)	202 (95%)	11 (5%)	0	100	100
1	C	215/255 (84%)	212 (99%)	3 (1%)	0	100	100
1	D	215/255 (84%)	210 (98%)	5 (2%)	0	100	100
1	E	214/255 (84%)	210 (98%)	4 (2%)	0	100	100
1	F	212/255 (83%)	209 (99%)	3 (1%)	0	100	100
All	All	1285/1530 (84%)	1258 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/218 (85%)	183 (98%)	3 (2%)	62	58
1	B	182/218 (84%)	176 (97%)	6 (3%)	38	26
1	C	187/218 (86%)	185 (99%)	2 (1%)	73	71
1	D	186/218 (85%)	181 (97%)	5 (3%)	44	34
1	E	183/218 (84%)	181 (99%)	2 (1%)	73	71
1	F	185/218 (85%)	184 (100%)	1 (0%)	88	88
All	All	1109/1308 (85%)	1090 (98%)	19 (2%)	60	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	90	GLU
1	A	145	ASN
1	B	3	VAL
1	B	4	ILE
1	B	66	ARG
1	B	67	VAL
1	B	109	LEU
1	B	202	LYS
1	C	66	ARG
1	C	138	LYS
1	D	5	LYS
1	D	66	ARG
1	D	67	VAL
1	D	181	LYS
1	D	214	GLU
1	E	67	VAL
1	E	145	ASN
1	F	135	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	145	ASN
1	A	158	ASN

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Mol	Chain	Res	Type
1	B	200	HIS
1	C	184	GLN
1	C	208	ASN
1	E	145	ASN
1	E	158	ASN
1	E	208	ASN
1	F	158	ASN
1	F	208	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	GYC	C	63	1	22,22,23	1.25	1 (4%)	26,30,32	2.14	5 (19%)
1	GYC	D	63	1	22,22,23	1.12	1 (4%)	26,30,32	2.35	6 (23%)
1	GYC	E	63	1	22,22,23	1.11	1 (4%)	26,30,32	2.61	4 (15%)
1	GYC	F	63	1	22,22,23	1.27	1 (4%)	26,30,32	2.71	7 (26%)
1	GYC	A	63	1	22,22,23	1.26	1 (4%)	26,30,32	1.69	4 (15%)
1	GYC	B	63	1	22,22,23	1.05	1 (4%)	26,30,32	2.70	7 (26%)

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	GYC	C	63	1	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	D	63	1	-	1/9/29/30	0/2/2/2
1	GYC	E	63	1	-	2/9/29/30	0/2/2/2
1	GYC	F	63	1	-	1/9/29/30	0/2/2/2
1	GYC	A	63	1	-	3/9/29/30	0/2/2/2
1	GYC	B	63	1	-	3/9/29/30	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	GYC	CB2-CA2	5.03	1.39	1.35
1	C	63	GYC	CB2-CA2	4.88	1.39	1.35
1	A	63	GYC	CB2-CA2	4.76	1.39	1.35
1	D	63	GYC	CB2-CA2	4.42	1.38	1.35
1	E	63	GYC	CB2-CA2	4.26	1.38	1.35
1	B	63	GYC	CB2-CA2	3.27	1.37	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GYC	O2-C2-CA2	-9.05	125.88	130.96
1	E	63	GYC	O2-C2-CA2	-8.89	125.97	130.96
1	F	63	GYC	O2-C2-CA2	-8.15	126.38	130.96
1	D	63	GYC	O2-C2-CA2	-7.84	126.56	130.96
1	C	63	GYC	O2-C2-CA2	-6.17	127.50	130.96
1	F	63	GYC	CA2-N2-C1	5.73	110.00	105.77
1	F	63	GYC	C2-CA2-N2	-5.60	105.01	108.93
1	E	63	GYC	CA2-C2-N3	5.45	105.95	103.37
1	B	63	GYC	CA2-C2-N3	5.26	105.86	103.37
1	F	63	GYC	CA2-C2-N3	5.12	105.79	103.37
1	E	63	GYC	CA2-N2-C1	4.92	109.39	105.77
1	A	63	GYC	O2-C2-CA2	-4.80	128.26	130.96
1	E	63	GYC	C2-CA2-N2	-4.67	105.66	108.93
1	B	63	GYC	CA2-N2-C1	4.65	109.20	105.77
1	D	63	GYC	C2-CA2-N2	-4.61	105.70	108.93
1	B	63	GYC	C2-CA2-N2	-4.55	105.75	108.93
1	C	63	GYC	CA2-N2-C1	4.54	109.12	105.77
1	D	63	GYC	CA2-C2-N3	4.16	105.34	103.37
1	D	63	GYC	CA2-N2-C1	4.12	108.81	105.77
1	C	63	GYC	CA2-C2-N3	3.80	105.17	103.37
1	C	63	GYC	C2-CA2-N2	-3.73	106.32	108.93
1	A	63	GYC	CA2-N2-C1	3.41	108.28	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GYC	CA2-C2-N3	3.40	104.98	103.37
1	C	63	GYC	CA1-CB1-SG1	-2.99	108.01	114.44
1	A	63	GYC	C2-CA2-N2	-2.91	106.89	108.93
1	F	63	GYC	CA3-N3-C1	-2.74	123.87	127.16
1	B	63	GYC	CA1-CB1-SG1	-2.59	108.86	114.44
1	B	63	GYC	O-C-CA3	-2.48	118.90	126.39
1	B	63	GYC	CG2-CB2-CA2	-2.44	126.95	129.94
1	D	63	GYC	O-C-CA3	-2.31	119.41	126.39
1	F	63	GYC	CB2-CA2-N2	2.31	132.03	128.83
1	D	63	GYC	C2-N3-C1	2.08	109.02	107.97
1	F	63	GYC	O-C-CA3	-2.04	120.23	126.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	GYC	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 ligands 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
4	PEG	D	302	-	6,6,6	0.56	0	5,5,5	0.87	0
4	PEG	E	302	-	6,6,6	0.57	0	5,5,5	0.77	0
4	PEG	B	302	-	6,6,6	0.56	0	5,5,5	0.70	0
2	EPE	B	301	-	4,4,15	1.00	0	5,6,20	2.28	2 (40%)
2	EPE	D	301	-	4,4,15	1.05	0	5,6,20	1.42	1 (20%)
2	EPE	F	301	-	4,4,15	0.98	0	5,6,20	1.48	1 (20%)
4	PEG	C	303	-	6,6,6	0.49	0	5,5,5	0.74	0
2	EPE	E	301	-	15,15,15	1.05	1 (6%)	18,20,20	1.97	5 (27%)
3	1PE	A	302	-	15,15,15	0.53	0	14,14,14	1.02	0
2	EPE	C	301	-	15,15,15	0.78	1 (6%)	18,20,20	2.36	5 (27%)
4	PEG	F	302	-	6,6,6	0.50	0	5,5,5	0.71	0
4	PEG	F	303	-	6,6,6	0.54	0	5,5,5	0.77	0
2	EPE	A	301	-	15,15,15	0.93	1 (6%)	18,20,20	1.67	5 (27%)
4	PEG	C	302	-	6,6,6	0.53	0	5,5,5	0.54	0

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
4	PEG	D	302	-	-	2/4/4/4	-
4	PEG	E	302	-	-	1/4/4/4	-
4	PEG	B	302	-	-	2/4/4/4	-
4	PEG	C	303	-	-	3/4/4/4	-
2	EPE	E	301	-	-	5/9/19/19	0/1/1/1
3	1PE	A	302	-	-	8/13/13/13	-
2	EPE	C	301	-	-	5/9/19/19	0/1/1/1
4	PEG	F	302	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	F	303	-	-	1/4/4/4	-
2	EPE	A	301	-	-	1/9/19/19	0/1/1/1
4	PEG	C	302	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	EPE	C10-S	3.53	1.82	1.77
2	A	301	EPE	C10-S	3.00	1.81	1.77
2	C	301	EPE	C10-S	2.36	1.80	1.77

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	EPE	O3S-S-C10	5.29	114.33	105.77
2	C	301	EPE	C5-N4-C3	5.08	120.25	108.83
2	B	301	EPE	O2S-S-O1S	-4.38	106.20	118.02
2	C	301	EPE	C7-N4-C5	3.92	121.27	111.23
2	C	301	EPE	C3-C2-N1	-3.91	102.62	110.64
2	E	301	EPE	C5-N4-C3	3.73	117.23	108.83
2	E	301	EPE	C7-N4-C3	3.69	120.68	111.23
2	E	301	EPE	C7-N4-C5	3.42	119.99	111.23
2	A	301	EPE	C7-N4-C3	3.26	119.56	111.23
2	E	301	EPE	O3S-S-C10	3.09	110.77	105.77
2	F	301	EPE	O2S-S-O1S	-3.07	109.72	118.02
2	A	301	EPE	C7-N4-C5	3.05	119.02	111.23
2	A	301	EPE	O2S-S-C10	3.04	110.58	106.92
2	A	301	EPE	C5-N4-C3	2.94	115.45	108.83
2	D	301	EPE	O2S-S-O1S	-2.90	110.20	118.02
2	B	301	EPE	O2S-S-C10	2.50	112.74	107.54
2	E	301	EPE	O1S-S-C10	2.31	109.70	106.92
2	C	301	EPE	C7-N4-C3	2.22	116.90	111.23
2	A	301	EPE	O1S-S-C10	2.06	109.39	106.92

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	EPE	C10-C9-N1-C2
2	E	301	EPE	C9-C10-S-O2S
2	E	301	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
2	C	301	EPE	C10-C9-N1-C2
2	C	301	EPE	S-C10-C9-N1
2	A	301	EPE	C8-C7-N4-C5
4	C	303	PEG	C1-C2-O2-C3
3	A	302	1PE	OH5-C14-C24-OH4
4	D	302	PEG	C1-C2-O2-C3
4	C	303	PEG	O2-C3-C4-O4
4	B	302	PEG	C4-C3-O2-C2
2	C	301	EPE	N4-C7-C8-O8
4	C	303	PEG	O1-C1-C2-O2
3	A	302	1PE	OH2-C12-C22-OH3
4	C	302	PEG	O2-C3-C4-O4
3	A	302	1PE	OH4-C13-C23-OH3
3	A	302	1PE	C12-C22-OH3-C23
2	C	301	EPE	C10-C9-N1-C6
3	A	302	1PE	C23-C13-OH4-C24
3	A	302	1PE	C14-C24-OH4-C13
4	E	302	PEG	C4-C3-O2-C2
2	C	301	EPE	C8-C7-N4-C3
3	A	302	1PE	C15-C25-OH5-C14
4	C	302	PEG	C4-C3-O2-C2
4	C	302	PEG	O1-C1-C2-O2
2	E	301	EPE	C9-C10-S-O1S
4	F	303	PEG	O2-C3-C4-O4
4	B	302	PEG	O2-C3-C4-O4
4	D	302	PEG	C4-C3-O2-C2
3	A	302	1PE	C16-C26-OH6-C15
2	E	301	EPE	C10-C9-N1-C6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	PEG	1	0
3	A	302	1PE	6	0
2	C	301	EPE	1	0
4	F	302	PEG	1	0
2	A	301	EPE	1	0
4	C	302	PEG	1	0

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	214/255 (83%)	-0.21	0 100 100	16, 25, 37, 54	0
1	B	213/255 (83%)	0.57	11 (5%) 27 37	19, 39, 57, 65	0
1	C	213/255 (83%)	-0.18	1 (0%) 91 94	16, 23, 35, 45	0
1	D	214/255 (83%)	-0.17	1 (0%) 91 94	17, 24, 35, 55	1 (0%)
1	E	213/255 (83%)	-0.12	2 (0%) 84 89	18, 27, 41, 63	0
1	F	213/255 (83%)	-0.10	2 (0%) 84 89	18, 26, 38, 57	0
All	All	1280/1530 (83%)	-0.03	17 (1%) 77 83	16, 26, 46, 65	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	ALA	3.3
1	B	7	ASP	3.2
1	B	34	PHE	3.0
1	D	2	SER	2.9
1	E	2	SER	2.8
1	B	213	ALA	2.8
1	B	113	CYS	2.7
1	F	73	GLU	2.6
1	E	30	LEU	2.5
1	B	71	TYR	2.4
1	B	30	LEU	2.3
1	B	3	VAL	2.3
1	B	6	PRO	2.1
1	F	212	HIS	2.1
1	B	83	PHE	2.1
1	B	9	LYS	2.0
1	C	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	GYC	B	63	21/22	0.93	0.12	31,35,39,42	0
1	GYC	A	63	21/22	0.96	0.08	18,21,24,25	0
1	GYC	E	63	21/22	0.96	0.08	20,24,26,27	0
1	GYC	F	63	21/22	0.97	0.08	21,22,24,25	0
1	GYC	C	63	21/22	0.98	0.07	17,20,22,24	0
1	GYC	D	63	21/22	0.98	0.09	17,20,22,23	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PEG	B	302	7/7	0.75	0.15	50,51,54,56	0
4	PEG	E	302	7/7	0.80	0.17	37,42,48,52	0
4	PEG	C	303	7/7	0.81	0.23	41,44,48,53	0
4	PEG	D	302	7/7	0.86	0.16	38,39,45,47	0
3	1PE	A	302	16/16	0.86	0.17	37,43,49,50	0
4	PEG	F	303	7/7	0.87	0.29	31,38,41,41	0
2	EPE	B	301	5/15	0.89	0.20	40,43,47,48	0
4	PEG	C	302	7/7	0.91	0.10	36,39,41,45	0
2	EPE	E	301	15/15	0.92	0.18	34,45,56,57	0
2	EPE	A	301	15/15	0.92	0.22	35,44,51,55	0
2	EPE	C	301	15/15	0.92	0.23	32,46,54,55	0
4	PEG	F	302	7/7	0.93	0.14	27,29,35,37	0
2	EPE	D	301	5/15	0.96	0.13	36,37,44,45	0
2	EPE	F	301	5/15	0.96	0.13	37,40,44,50	0

## 6.5 Other polymers

There are no such residues in this entry.