Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:16 AM EDT

PDB ID	:	4HQ8
Title	:	Crystal structure of a green-to-red photoconvertible DRONPA, pcDRONPA in the green-on-state
Authors	:	Nguyen Bich, N.; Van Meervelt, L.
Deposited on	:	2012-10-25
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

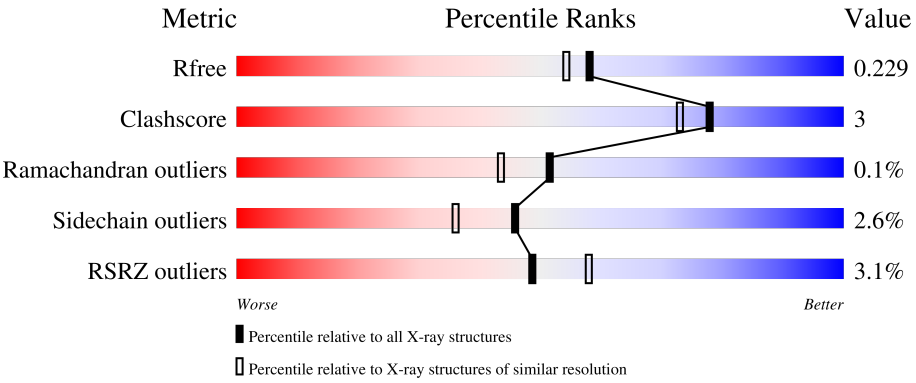
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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 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	258	3% 76% 8% 16%
1	B	258	% 79% 16%
1	C	258	3% 77% 7% 16%
1	D	258	2% 79% 5% 16%
1	E	258	5% 75% 8% 17%

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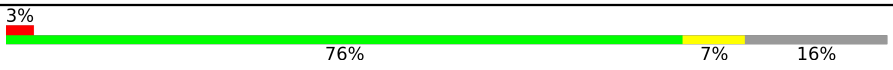
Mol	Chain	Length	Quality of chain
1	F	258	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	7	0
			1775	1137	295	333	10			
1	B	218	Total	C	N	O	S	0	2	0
			1752	1122	294	326	10			
1	C	217	Total	C	N	O	S	0	3	0
			1749	1120	293	326	10			
1	D	217	Total	C	N	O	S	0	2	0
			1751	1121	295	326	9			
1	E	215	Total	C	N	O	S	0	1	0
			1731	1109	291	322	9			
1	F	217	Total	C	N	O	S	0	2	0
			1750	1120	298	323	9			

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP Q5TLG6
A	-34	ARG	-	expression tag	UNP Q5TLG6
A	-33	GLY	-	expression tag	UNP Q5TLG6
A	-32	SER	-	expression tag	UNP Q5TLG6
A	-31	HIS	-	expression tag	UNP Q5TLG6
A	-30	HIS	-	expression tag	UNP Q5TLG6
A	-29	HIS	-	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	GLY	-	expression tag	UNP Q5TLG6
A	-24	MET	-	expression tag	UNP Q5TLG6
A	-23	ALA	-	expression tag	UNP Q5TLG6
A	-22	SER	-	expression tag	UNP Q5TLG6
A	-21	MET	-	expression tag	UNP Q5TLG6
A	-20	THR	-	expression tag	UNP Q5TLG6
A	-19	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q5TLG6
A	-17	GLN	-	expression tag	UNP Q5TLG6
A	-16	GLN	-	expression tag	UNP Q5TLG6
A	-15	MET	-	expression tag	UNP Q5TLG6
A	-14	GLY	-	expression tag	UNP Q5TLG6
A	-13	ARG	-	expression tag	UNP Q5TLG6
A	-12	ASN	-	expression tag	UNP Q5TLG6
A	-11	LEU	-	expression tag	UNP Q5TLG6
A	-10	TYR	-	expression tag	UNP Q5TLG6
A	-9	ASP	-	expression tag	UNP Q5TLG6
A	-8	ASP	-	expression tag	UNP Q5TLG6
A	-7	ASP	-	expression tag	UNP Q5TLG6
A	-6	ASP	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	ASP	-	expression tag	UNP Q5TLG6
A	-3	PRO	-	expression tag	UNP Q5TLG6
A	-2	GLY	-	expression tag	UNP Q5TLG6
A	-1	SER	-	expression tag	UNP Q5TLG6
A	0	HIS	-	expression tag	UNP Q5TLG6
A	60	ALA	VAL	engineered mutation	UNP Q5TLG6
A	63	CR8	CYS	chromophore	UNP Q5TLG6
A	63	CR8	TYR	chromophore	UNP Q5TLG6
A	63	CR8	GLY	chromophore	UNP Q5TLG6
A	94	SER	ASN	engineered mutation	UNP Q5TLG6
A	102	ILE	ASN	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	-35	MET	-	expression tag	UNP Q5TLG6
B	-34	ARG	-	expression tag	UNP Q5TLG6
B	-33	GLY	-	expression tag	UNP Q5TLG6
B	-32	SER	-	expression tag	UNP Q5TLG6
B	-31	HIS	-	expression tag	UNP Q5TLG6
B	-30	HIS	-	expression tag	UNP Q5TLG6
B	-29	HIS	-	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	GLY	-	expression tag	UNP Q5TLG6
B	-24	MET	-	expression tag	UNP Q5TLG6
B	-23	ALA	-	expression tag	UNP Q5TLG6
B	-22	SER	-	expression tag	UNP Q5TLG6
B	-21	MET	-	expression tag	UNP Q5TLG6
B	-20	THR	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP Q5TLG6
B	-18	GLY	-	expression tag	UNP Q5TLG6
B	-17	GLN	-	expression tag	UNP Q5TLG6
B	-16	GLN	-	expression tag	UNP Q5TLG6
B	-15	MET	-	expression tag	UNP Q5TLG6
B	-14	GLY	-	expression tag	UNP Q5TLG6
B	-13	ARG	-	expression tag	UNP Q5TLG6
B	-12	ASN	-	expression tag	UNP Q5TLG6
B	-11	LEU	-	expression tag	UNP Q5TLG6
B	-10	TYR	-	expression tag	UNP Q5TLG6
B	-9	ASP	-	expression tag	UNP Q5TLG6
B	-8	ASP	-	expression tag	UNP Q5TLG6
B	-7	ASP	-	expression tag	UNP Q5TLG6
B	-6	ASP	-	expression tag	UNP Q5TLG6
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	ASP	-	expression tag	UNP Q5TLG6
B	-3	PRO	-	expression tag	UNP Q5TLG6
B	-2	GLY	-	expression tag	UNP Q5TLG6
B	-1	SER	-	expression tag	UNP Q5TLG6
B	0	HIS	-	expression tag	UNP Q5TLG6
B	60	ALA	VAL	engineered mutation	UNP Q5TLG6
B	63	CR8	CYS	chromophore	UNP Q5TLG6
B	63	CR8	TYR	chromophore	UNP Q5TLG6
B	63	CR8	GLY	chromophore	UNP Q5TLG6
B	94	SER	ASN	engineered mutation	UNP Q5TLG6
B	102	ILE	ASN	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	-35	MET	-	expression tag	UNP Q5TLG6
C	-34	ARG	-	expression tag	UNP Q5TLG6
C	-33	GLY	-	expression tag	UNP Q5TLG6
C	-32	SER	-	expression tag	UNP Q5TLG6
C	-31	HIS	-	expression tag	UNP Q5TLG6
C	-30	HIS	-	expression tag	UNP Q5TLG6
C	-29	HIS	-	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	GLY	-	expression tag	UNP Q5TLG6
C	-24	MET	-	expression tag	UNP Q5TLG6
C	-23	ALA	-	expression tag	UNP Q5TLG6
C	-22	SER	-	expression tag	UNP Q5TLG6
C	-21	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	THR	-	expression tag	UNP Q5TLG6
C	-19	GLY	-	expression tag	UNP Q5TLG6
C	-18	GLY	-	expression tag	UNP Q5TLG6
C	-17	GLN	-	expression tag	UNP Q5TLG6
C	-16	GLN	-	expression tag	UNP Q5TLG6
C	-15	MET	-	expression tag	UNP Q5TLG6
C	-14	GLY	-	expression tag	UNP Q5TLG6
C	-13	ARG	-	expression tag	UNP Q5TLG6
C	-12	ASN	-	expression tag	UNP Q5TLG6
C	-11	LEU	-	expression tag	UNP Q5TLG6
C	-10	TYR	-	expression tag	UNP Q5TLG6
C	-9	ASP	-	expression tag	UNP Q5TLG6
C	-8	ASP	-	expression tag	UNP Q5TLG6
C	-7	ASP	-	expression tag	UNP Q5TLG6
C	-6	ASP	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6
C	-4	ASP	-	expression tag	UNP Q5TLG6
C	-3	PRO	-	expression tag	UNP Q5TLG6
C	-2	GLY	-	expression tag	UNP Q5TLG6
C	-1	SER	-	expression tag	UNP Q5TLG6
C	0	HIS	-	expression tag	UNP Q5TLG6
C	60	ALA	VAL	engineered mutation	UNP Q5TLG6
C	63	CR8	CYS	chromophore	UNP Q5TLG6
C	63	CR8	TYR	chromophore	UNP Q5TLG6
C	63	CR8	GLY	chromophore	UNP Q5TLG6
C	94	SER	ASN	engineered mutation	UNP Q5TLG6
C	102	ILE	ASN	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	-35	MET	-	expression tag	UNP Q5TLG6
D	-34	ARG	-	expression tag	UNP Q5TLG6
D	-33	GLY	-	expression tag	UNP Q5TLG6
D	-32	SER	-	expression tag	UNP Q5TLG6
D	-31	HIS	-	expression tag	UNP Q5TLG6
D	-30	HIS	-	expression tag	UNP Q5TLG6
D	-29	HIS	-	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	GLY	-	expression tag	UNP Q5TLG6
D	-24	MET	-	expression tag	UNP Q5TLG6
D	-23	ALA	-	expression tag	UNP Q5TLG6
D	-22	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	MET	-	expression tag	UNP Q5TLG6
D	-20	THR	-	expression tag	UNP Q5TLG6
D	-19	GLY	-	expression tag	UNP Q5TLG6
D	-18	GLY	-	expression tag	UNP Q5TLG6
D	-17	GLN	-	expression tag	UNP Q5TLG6
D	-16	GLN	-	expression tag	UNP Q5TLG6
D	-15	MET	-	expression tag	UNP Q5TLG6
D	-14	GLY	-	expression tag	UNP Q5TLG6
D	-13	ARG	-	expression tag	UNP Q5TLG6
D	-12	ASN	-	expression tag	UNP Q5TLG6
D	-11	LEU	-	expression tag	UNP Q5TLG6
D	-10	TYR	-	expression tag	UNP Q5TLG6
D	-9	ASP	-	expression tag	UNP Q5TLG6
D	-8	ASP	-	expression tag	UNP Q5TLG6
D	-7	ASP	-	expression tag	UNP Q5TLG6
D	-6	ASP	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	ASP	-	expression tag	UNP Q5TLG6
D	-3	PRO	-	expression tag	UNP Q5TLG6
D	-2	GLY	-	expression tag	UNP Q5TLG6
D	-1	SER	-	expression tag	UNP Q5TLG6
D	0	HIS	-	expression tag	UNP Q5TLG6
D	60	ALA	VAL	engineered mutation	UNP Q5TLG6
D	63	CR8	CYS	chromophore	UNP Q5TLG6
D	63	CR8	TYR	chromophore	UNP Q5TLG6
D	63	CR8	GLY	chromophore	UNP Q5TLG6
D	94	SER	ASN	engineered mutation	UNP Q5TLG6
D	102	ILE	ASN	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
E	-35	MET	-	expression tag	UNP Q5TLG6
E	-34	ARG	-	expression tag	UNP Q5TLG6
E	-33	GLY	-	expression tag	UNP Q5TLG6
E	-32	SER	-	expression tag	UNP Q5TLG6
E	-31	HIS	-	expression tag	UNP Q5TLG6
E	-30	HIS	-	expression tag	UNP Q5TLG6
E	-29	HIS	-	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	GLY	-	expression tag	UNP Q5TLG6
E	-24	MET	-	expression tag	UNP Q5TLG6
E	-23	ALA	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	SER	-	expression tag	UNP Q5TLG6
E	-21	MET	-	expression tag	UNP Q5TLG6
E	-20	THR	-	expression tag	UNP Q5TLG6
E	-19	GLY	-	expression tag	UNP Q5TLG6
E	-18	GLY	-	expression tag	UNP Q5TLG6
E	-17	GLN	-	expression tag	UNP Q5TLG6
E	-16	GLN	-	expression tag	UNP Q5TLG6
E	-15	MET	-	expression tag	UNP Q5TLG6
E	-14	GLY	-	expression tag	UNP Q5TLG6
E	-13	ARG	-	expression tag	UNP Q5TLG6
E	-12	ASN	-	expression tag	UNP Q5TLG6
E	-11	LEU	-	expression tag	UNP Q5TLG6
E	-10	TYR	-	expression tag	UNP Q5TLG6
E	-9	ASP	-	expression tag	UNP Q5TLG6
E	-8	ASP	-	expression tag	UNP Q5TLG6
E	-7	ASP	-	expression tag	UNP Q5TLG6
E	-6	ASP	-	expression tag	UNP Q5TLG6
E	-5	LYS	-	expression tag	UNP Q5TLG6
E	-4	ASP	-	expression tag	UNP Q5TLG6
E	-3	PRO	-	expression tag	UNP Q5TLG6
E	-2	GLY	-	expression tag	UNP Q5TLG6
E	-1	SER	-	expression tag	UNP Q5TLG6
E	0	HIS	-	expression tag	UNP Q5TLG6
E	60	ALA	VAL	engineered mutation	UNP Q5TLG6
E	63	CR8	CYS	chromophore	UNP Q5TLG6
E	63	CR8	TYR	chromophore	UNP Q5TLG6
E	63	CR8	GLY	chromophore	UNP Q5TLG6
E	94	SER	ASN	engineered mutation	UNP Q5TLG6
E	102	ILE	ASN	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	engineered mutation	UNP Q5TLG6
F	-35	MET	-	expression tag	UNP Q5TLG6
F	-34	ARG	-	expression tag	UNP Q5TLG6
F	-33	GLY	-	expression tag	UNP Q5TLG6
F	-32	SER	-	expression tag	UNP Q5TLG6
F	-31	HIS	-	expression tag	UNP Q5TLG6
F	-30	HIS	-	expression tag	UNP Q5TLG6
F	-29	HIS	-	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	GLY	-	expression tag	UNP Q5TLG6
F	-24	MET	-	expression tag	UNP Q5TLG6

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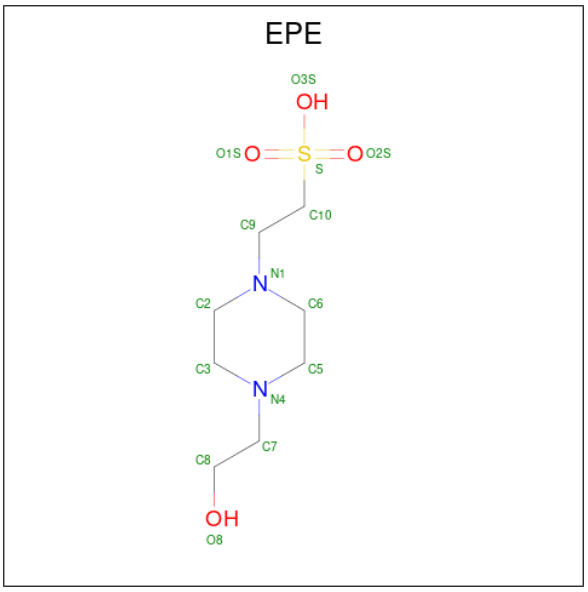
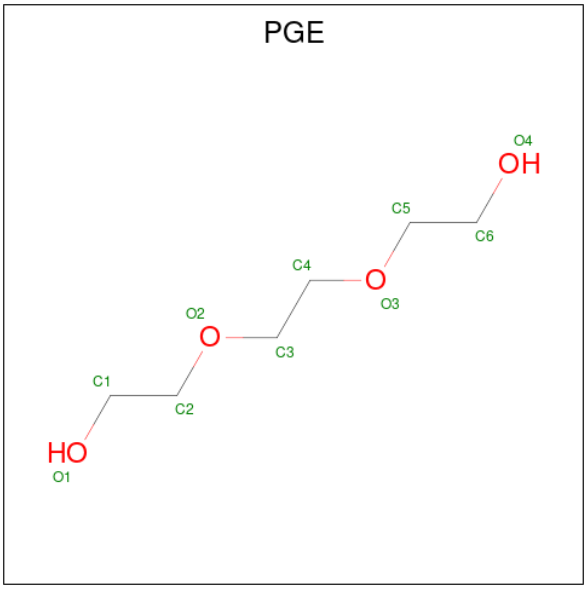
Chain	Residue	Modelled	Actual	Comment	Reference
F	-23	ALA	-	expression tag	UNP Q5TLG6
F	-22	SER	-	expression tag	UNP Q5TLG6
F	-21	MET	-	expression tag	UNP Q5TLG6
F	-20	THR	-	expression tag	UNP Q5TLG6
F	-19	GLY	-	expression tag	UNP Q5TLG6
F	-18	GLY	-	expression tag	UNP Q5TLG6
F	-17	GLN	-	expression tag	UNP Q5TLG6
F	-16	GLN	-	expression tag	UNP Q5TLG6
F	-15	MET	-	expression tag	UNP Q5TLG6
F	-14	GLY	-	expression tag	UNP Q5TLG6
F	-13	ARG	-	expression tag	UNP Q5TLG6
F	-12	ASN	-	expression tag	UNP Q5TLG6
F	-11	LEU	-	expression tag	UNP Q5TLG6
F	-10	TYR	-	expression tag	UNP Q5TLG6
F	-9	ASP	-	expression tag	UNP Q5TLG6
F	-8	ASP	-	expression tag	UNP Q5TLG6
F	-7	ASP	-	expression tag	UNP Q5TLG6
F	-6	ASP	-	expression tag	UNP Q5TLG6
F	-5	LYS	-	expression tag	UNP Q5TLG6
F	-4	ASP	-	expression tag	UNP Q5TLG6
F	-3	PRO	-	expression tag	UNP Q5TLG6
F	-2	GLY	-	expression tag	UNP Q5TLG6
F	-1	SER	-	expression tag	UNP Q5TLG6
F	0	HIS	-	expression tag	UNP Q5TLG6
F	60	ALA	VAL	engineered mutation	UNP Q5TLG6
F	63	CR8	CYS	chromophore	UNP Q5TLG6
F	63	CR8	TYR	chromophore	UNP Q5TLG6
F	63	CR8	GLY	chromophore	UNP Q5TLG6
F	94	SER	ASN	engineered mutation	UNP Q5TLG6
F	102	ILE	ASN	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	engineered mutation	UNP Q5TLG6

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



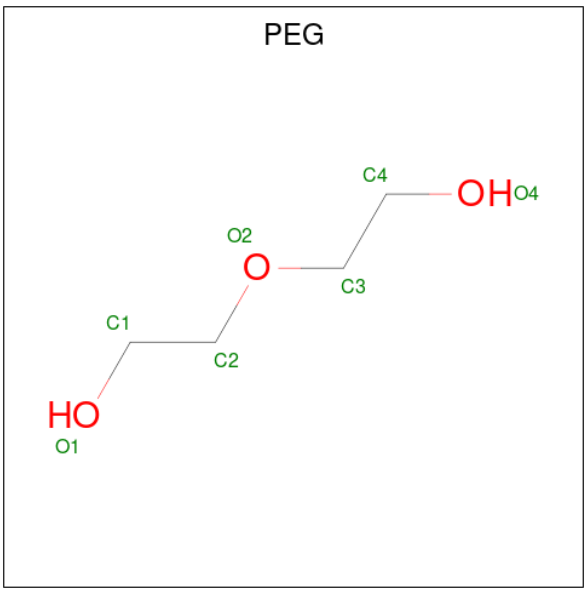
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 5 1 3 1	0	0
2	C	1	Total C O S 5 1 3 1	0	0
2	E	1	Total C O S 5 1 3 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0

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



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

- Molecule 5 is water.

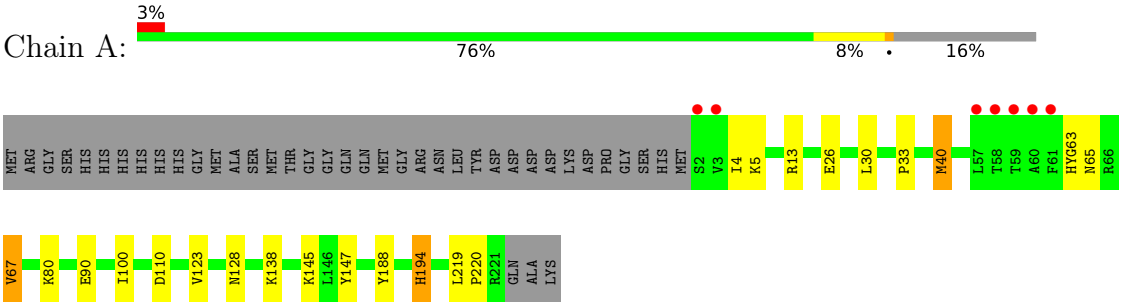
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	241	Total O 241 241	0	0
5	B	271	Total O 271 271	0	0
5	C	192	Total O 192 192	0	0
5	D	158	Total O 158 158	0	0
5	E	162	Total O 162 162	0	0
5	F	168	Total O 168 168	0	0

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.

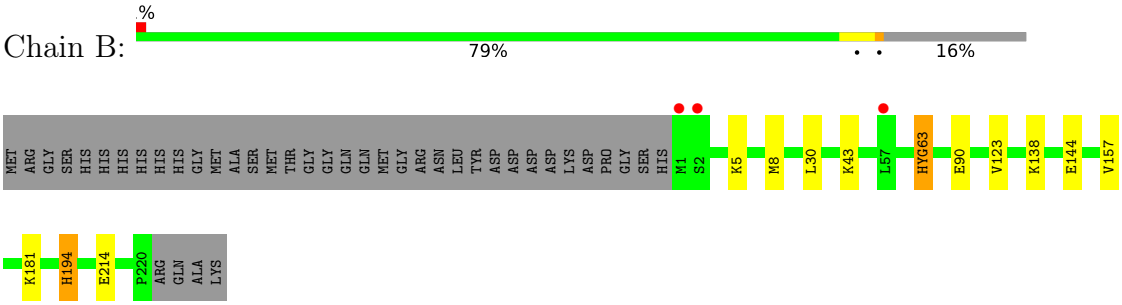
• Molecule 1: Fluorescent protein Dronpa

Chain A:



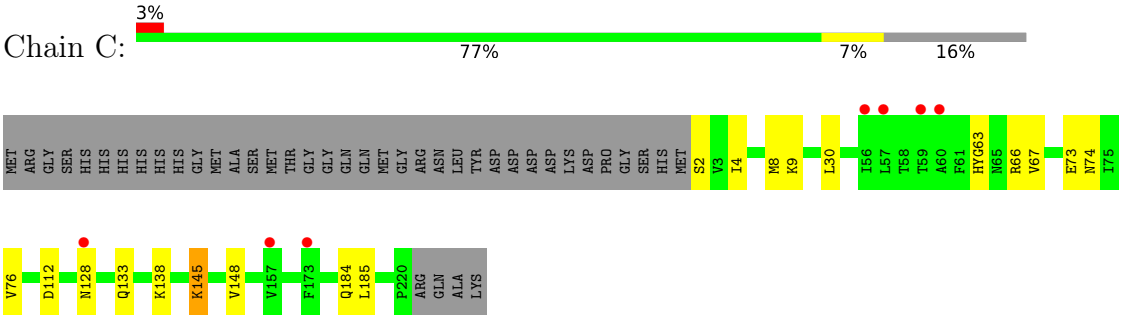
• Molecule 1: Fluorescent protein Dronpa

Chain B:



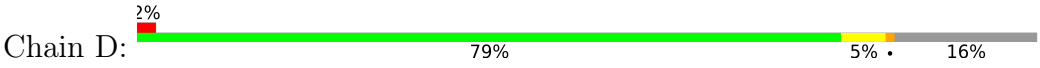
• Molecule 1: Fluorescent protein Dronpa

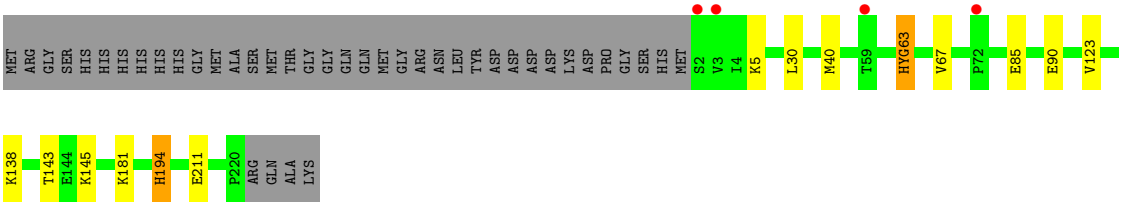
Chain C:



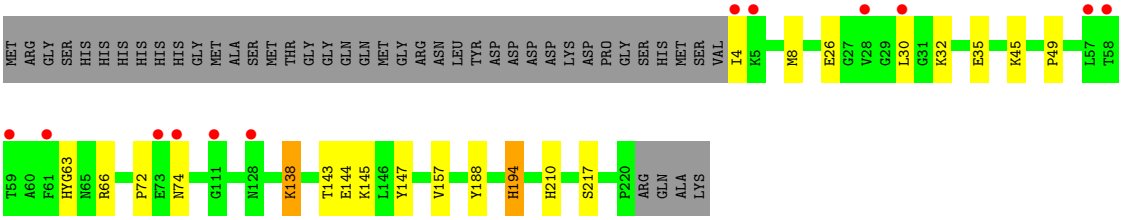
• Molecule 1: Fluorescent protein Dronpa

Chain D:

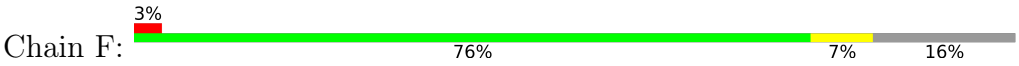


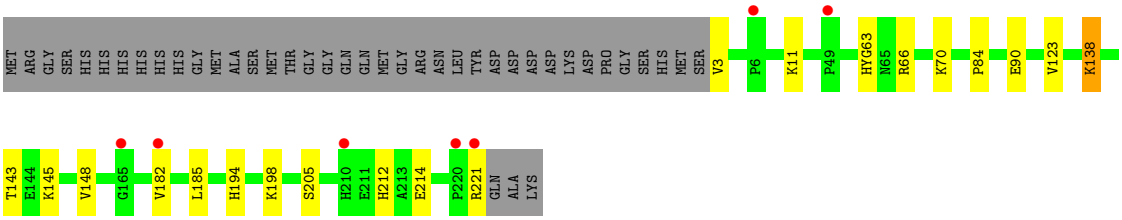


• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.38Å 107.19Å 180.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.46 – 1.95 28.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.46-1.95) 99.1 (28.46-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.184 , 0.235 0.181 , 0.229	Depositor DCC
R_{free} test set	5086 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11739	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.48	0/1819	0.64	0/2457
1	B	0.51	0/1781	0.63	0/2406
1	C	0.47	0/1781	0.63	0/2407
1	D	0.45	0/1780	0.62	0/2404
1	E	0.44	0/1755	0.62	0/2370
1	F	0.45	0/1777	0.61	0/2400
All	All	0.47	0/10693	0.63	0/14444

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1775	0	1687	13	0
1	B	1752	0	1662	11	0
1	C	1749	0	1654	8	0
1	D	1751	0	1665	11	0
1	E	1731	0	1645	11	0
1	F	1750	0	1668	11	0
2	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	E	5	0	0	0	0
3	A	10	0	14	3	0
4	A	7	0	10	0	0
4	B	7	0	10	1	0
5	A	241	0	0	4	0
5	B	271	0	0	4	0
5	C	192	0	0	1	0
5	D	158	0	0	1	0
5	E	162	0	0	2	0
5	F	168	0	0	1	0
All	All	11739	0	10015	59	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 (59) 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:C:128:ASN:OD1	1:C:133:GLN:NE2	2.25	0.70
1:B:43:LYS:HD2	4:B:301:PEG:H11	1.74	0.69
1:D:40:MET:HG2	1:D:63:CR8:H10	1.76	0.67
1:C:4:ILE:HA	1:C:8[B]:MET:HE2	1.75	0.67
1:F:138:LYS:NZ	1:F:194:HIS:HE1	1.97	0.62
1:A:13:ARG:HD3	3:A:302:PGE:H6	1.82	0.62
1:B:63:CR8:H10	5:B:446:HOH:O	2.03	0.58
1:C:138:LYS:HE3	1:F:221:ARG:HE	1.70	0.55
1:B:138:LYS:HZ1	1:B:194:HIS:HE1	1.56	0.54
1:B:214:GLU:OE1	5:B:618:HOH:O	2.19	0.54
1:F:212:HIS:ND1	5:F:396:HOH:O	2.34	0.52
1:A:26:GLU:HB3	3:A:302:PGE:H2	1.91	0.52
1:C:9:LYS:NZ	1:C:112:ASP:OD1	2.40	0.51
1:D:5:LYS:NZ	5:D:454:HOH:O	2.40	0.51
1:A:138:LYS:NZ	1:A:194:HIS:HE1	2.08	0.51
3:A:302:PGE:H32	5:A:548:HOH:O	2.10	0.51
1:C:145:LYS:NZ	1:F:143:THR:H	2.08	0.50
1:A:4:ILE:HD11	1:A:33:PRO:HB3	1.94	0.49
1:B:138:LYS:NZ	1:B:194:HIS:HE1	2.11	0.49
1:E:26:GLU:HG3	1:E:45:LYS:HG3	1.94	0.49
1:D:145:LYS:NZ	1:E:143:THR:H	2.11	0.49
1:F:138:LYS:HZ3	1:F:194:HIS:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB3	1:B:123:VAL:HB	1.94	0.48
1:D:138:LYS:NZ	1:D:194:HIS:HE1	2.12	0.48
1:B:138:LYS:HZ1	1:B:194:HIS:CE1	2.30	0.48
1:B:144:GLU:HA	1:B:157:VAL:HB	1.96	0.47
1:E:210:HIS:HD2	5:E:491:HOH:O	1.97	0.47
1:D:138:LYS:HZ1	1:D:194:HIS:HE1	1.62	0.47
1:D:143:THR:H	1:E:145:LYS:NZ	2.12	0.47
1:D:40:MET:HG2	1:D:63:CR8:C10	2.43	0.47
1:D:63:CR8:H23	1:D:211:GLU:HB2	1.97	0.47
1:E:72:PRO:HB2	1:E:74:ASN:OD1	2.15	0.46
1:F:11:LYS:HB2	1:F:11:LYS:HE2	1.71	0.46
1:A:4:ILE:HD13	1:A:80:LYS:HG2	1.98	0.45
1:E:138[A]:LYS:NZ	1:E:194:HIS:HE1	2.14	0.45
1:F:70:LYS:HB3	1:F:214:GLU:HG2	1.97	0.45
1:D:90:GLU:HB3	1:F:123:VAL:HB	1.97	0.45
1:B:5:LYS:HB2	1:B:8:MET:SD	2.58	0.44
1:A:219:LEU:O	5:A:512:HOH:O	2.21	0.44
1:B:181:LYS:N	5:B:512:HOH:O	2.35	0.44
1:A:128:ASN:HB2	5:B:601:HOH:O	2.17	0.44
1:A:65:ASN:OD1	1:A:67:VAL:HB	2.18	0.43
1:A:40:MET:HE2	1:A:40:MET:HB2	1.85	0.43
1:F:3:VAL:HG21	1:F:84:PRO:HD3	2.01	0.43
1:D:123:VAL:HB	1:F:90:GLU:HB3	2.00	0.43
1:D:85:GLU:CD	1:D:181:LYS:HD3	2.39	0.42
1:F:148:VAL:HG21	1:F:185:LEU:HB3	2.01	0.42
1:E:4:ILE:HA	1:E:8:MET:HE1	2.01	0.41
1:C:148:VAL:HG21	1:C:185:LEU:HB3	2.02	0.41
1:A:147:TYR:HB3	1:A:188:TYR:CD1	2.56	0.41
2:A:301:EPE:O2S	5:A:631:HOH:O	2.22	0.41
1:A:123:VAL:HB	1:B:90:GLU:HB3	2.03	0.41
1:E:144:GLU:HA	1:E:157:VAL:HB	2.02	0.41
1:E:147:TYR:HB3	1:E:188:TYR:CD1	2.56	0.41
1:E:49:PRO:HA	5:E:476:HOH:O	2.20	0.41
1:C:76:VAL:HG11	1:C:184:GLN:HG2	2.03	0.41
1:C:74:ASN:OD1	5:C:561:HOH:O	2.22	0.40
1:E:32:LYS:HB3	1:E:35:GLU:HG3	2.04	0.40
1:A:110:ASP:OD2	5:A:623:HOH:O	2.22	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	220/258 (85%)	219 (100%)	0	1 (0%)	29	17
1	B	215/258 (83%)	214 (100%)	1 (0%)	0	100	100
1	C	215/258 (83%)	213 (99%)	2 (1%)	0	100	100
1	D	214/258 (83%)	214 (100%)	0	0	100	100
1	E	211/258 (82%)	210 (100%)	1 (0%)	0	100	100
1	F	214/258 (83%)	214 (100%)	0	0	100	100
All	All	1289/1548 (83%)	1284 (100%)	4 (0%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	PRO

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	190/218 (87%)	183 (96%)	7 (4%)	34	22
1	B	185/218 (85%)	183 (99%)	2 (1%)	73	71
1	C	185/218 (85%)	179 (97%)	6 (3%)	39	27
1	D	186/218 (85%)	183 (98%)	3 (2%)	62	58
1	E	182/218 (84%)	176 (97%)	6 (3%)	38	26
1	F	184/218 (84%)	178 (97%)	6 (3%)	38	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1112/1308 (85%)	1082 (97%)	30 (3%)	46 34

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	30	LEU
1	A	40	MET
1	A	67	VAL
1	A	100	ILE
1	A	145	LYS
1	A	194	HIS
1	B	30	LEU
1	B	194	HIS
1	C	2	SER
1	C	30	LEU
1	C	66	ARG
1	C	67	VAL
1	C	73	GLU
1	C	145	LYS
1	D	30	LEU
1	D	67	VAL
1	D	194	HIS
1	E	30	LEU
1	E	66	ARG
1	E	138[A]	LYS
1	E	138[B]	LYS
1	E	194	HIS
1	E	217	SER
1	F	66	ARG
1	F	138	LYS
1	F	145	LYS
1	F	182	VAL
1	F	198	LYS
1	F	205	SER

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

Mol	Chain	Res	Type
1	A	133	GLN
1	A	194	HIS

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Mol	Chain	Res	Type
1	B	194	HIS
1	C	194	HIS
1	D	194	HIS
1	E	158	ASN
1	E	194	HIS
1	E	210	HIS
1	F	158	ASN
1	F	194	HIS
1	F	212	HIS

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	CR8	B	63	1	20,27,28	2.00	6 (30%)	17,37,39	1.29	1 (5%)
1	CR8	E	63	1	20,27,28	1.93	5 (25%)	17,37,39	1.54	5 (29%)
1	CR8	F	63	1	20,27,28	2.05	5 (25%)	17,37,39	1.33	2 (11%)
1	CR8	C	63	1	20,27,28	2.06	6 (30%)	17,37,39	1.33	3 (17%)
1	CR8	D	63	1	20,27,28	2.04	6 (30%)	17,37,39	1.46	3 (17%)
1	CR8	A	63	1	20,27,28	1.98	5 (25%)	17,37,39	1.55	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR8	B	63	1	-	2/8/25/26	0/3/3/3
1	CR8	E	63	1	-	2/8/25/26	0/3/3/3
1	CR8	F	63	1	-	2/8/25/26	0/3/3/3
1	CR8	C	63	1	-	2/8/25/26	0/3/3/3
1	CR8	D	63	1	-	2/8/25/26	0/3/3/3
1	CR8	A	63	1	-	2/8/25/26	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	CR8	C8-C7	4.63	1.47	1.36
1	D	63	CR8	O13-C11	4.60	1.38	1.24
1	C	63	CR8	O13-C11	4.55	1.38	1.24
1	A	63	CR8	O13-C11	4.51	1.38	1.24
1	F	63	CR8	C8-C7	4.50	1.47	1.36
1	F	63	CR8	O13-C11	4.50	1.38	1.24
1	E	63	CR8	O13-C11	4.42	1.38	1.24
1	B	63	CR8	O13-C11	4.39	1.38	1.24
1	A	63	CR8	C8-C7	4.37	1.46	1.36
1	B	63	CR8	C8-C7	4.21	1.46	1.36
1	E	63	CR8	C8-C7	4.12	1.46	1.36
1	C	63	CR8	C8-C7	4.10	1.46	1.36
1	C	63	CR8	C4-C11	-3.26	1.38	1.45
1	B	63	CR8	C12-C11	-3.18	1.38	1.45
1	F	63	CR8	O2-C2	-3.14	1.23	1.32
1	E	63	CR8	C4-C11	-3.11	1.38	1.45
1	F	63	CR8	C4-C11	-3.05	1.39	1.45
1	A	63	CR8	C4-C11	-2.99	1.39	1.45
1	D	63	CR8	O2-C2	-2.96	1.23	1.32
1	C	63	CR8	O2-C2	-2.86	1.24	1.32
1	C	63	CR8	CA3-N3	-2.79	1.44	1.49
1	E	63	CR8	O2-C2	-2.72	1.24	1.32
1	D	63	CR8	C4-C11	-2.69	1.39	1.45
1	B	63	CR8	CA3-N3	-2.68	1.44	1.49
1	B	63	CR8	C4-C11	-2.58	1.40	1.45
1	A	63	CR8	O2-C2	-2.58	1.24	1.32
1	A	63	CR8	C12-C11	-2.53	1.40	1.45
1	C	63	CR8	C12-C11	-2.40	1.40	1.45
1	F	63	CR8	C12-C11	-2.35	1.40	1.45
1	B	63	CR8	O2-C2	-2.26	1.25	1.32
1	E	63	CR8	C12-C11	-2.26	1.40	1.45
1	D	63	CR8	C12-C11	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	CR8	CA3-N3	-2.05	1.45	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	63	CR8	C3-CA3-N3	3.83	117.72	111.92
1	A	63	CR8	C3-CA3-N3	3.39	117.07	111.92
1	D	63	CR8	C12-C6-C7	-3.05	119.36	121.95
1	B	63	CR8	C3-CA3-N3	2.76	116.11	111.92
1	C	63	CR8	O3-C3-CA3	-2.69	118.68	126.32
1	E	63	CR8	C12-C6-C7	-2.68	119.68	121.95
1	A	63	CR8	C4-C5-C7	-2.57	119.76	121.95
1	D	63	CR8	C3-CA3-N3	2.53	115.76	111.92
1	C	63	CR8	C3-CA3-N3	2.46	115.66	111.92
1	C	63	CR8	C12-C6-C7	-2.40	119.91	121.95
1	E	63	CR8	CA3-N3-C2	2.39	128.22	124.32
1	F	63	CR8	O3-C3-CA3	-2.28	119.83	126.32
1	D	63	CR8	O3-C3-CA3	-2.28	119.84	126.32
1	E	63	CR8	O3-C3-CA3	-2.17	120.15	126.32
1	E	63	CR8	O13-C11-C4	-2.15	118.09	121.56
1	E	63	CR8	C3-CA3-N3	2.00	114.96	111.92

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	CR8	CA1-C20-C21-N22
1	A	63	CR8	CA1-C20-C21-C23
1	B	63	CR8	CA1-C20-C21-N22
1	B	63	CR8	CA1-C20-C21-C23
1	C	63	CR8	CA1-C20-C21-N22
1	C	63	CR8	CA1-C20-C21-C23
1	D	63	CR8	CA1-C20-C21-N22
1	D	63	CR8	CA1-C20-C21-C23
1	E	63	CR8	CA1-C20-C21-N22
1	E	63	CR8	CA1-C20-C21-C23
1	F	63	CR8	CA1-C20-C21-N22
1	F	63	CR8	CA1-C20-C21-C23

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	CR8	1	0
1	D	63	CR8	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
3	PGE	A	302	-	9,9,9	0.40	0	8,8,8	0.95	0
2	EPE	A	301	-	4,4,15	1.15	0	5,6,20	1.78	1 (20%)
2	EPE	E	301	-	4,4,15	1.00	0	5,6,20	1.44	1 (20%)
4	PEG	B	301	-	6,6,6	0.44	0	5,5,5	0.76	0
4	PEG	A	303	-	6,6,6	0.50	0	5,5,5	0.80	0
2	EPE	C	301	-	4,4,15	1.14	0	5,6,20	1.53	1 (20%)

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	B	301	-	-	3/4/4/4	-
3	PGE	A	302	-	-	5/7/7/7	-
4	PEG	A	303	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	EPE	O2S-S-O1S	-3.49	108.60	118.02
2	C	301	EPE	O2S-S-O1S	-3.01	109.91	118.02
2	E	301	EPE	O2S-S-O1S	-2.91	110.17	118.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	PGE	O1-C1-C2-O2
3	A	302	PGE	O3-C5-C6-O4
4	B	301	PEG	O2-C3-C4-O4
3	A	302	PGE	C4-C3-O2-C2
3	A	302	PGE	C3-C4-O3-C5
4	A	303	PEG	C1-C2-O2-C3
4	A	303	PEG	O1-C1-C2-O2
4	B	301	PEG	C1-C2-O2-C3
4	B	301	PEG	C4-C3-O2-C2
3	A	302	PGE	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	PGE	3	0
2	A	301	EPE	1	0
4	B	301	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^{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	217/258 (84%)	-0.03	7 (3%)	47	57	14, 22, 36, 58	0
1	B	217/258 (84%)	-0.10	3 (1%)	75	82	14, 21, 34, 43	0
1	C	216/258 (83%)	0.08	7 (3%)	47	57	16, 24, 38, 53	0
1	D	216/258 (83%)	0.07	4 (1%)	66	74	17, 26, 39, 63	0
1	E	214/258 (82%)	0.22	12 (5%)	24	33	17, 26, 41, 54	0
1	F	216/258 (83%)	0.17	7 (3%)	47	57	15, 26, 41, 56	0
All	All	1296/1548 (83%)	0.07	40 (3%)	49	58	14, 24, 39, 63	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	ILE	5.2
1	D	2	SER	4.1
1	A	2	SER	3.9
1	F	220	PRO	3.3
1	A	3	VAL	3.2
1	C	128	ASN	3.2
1	F	210	HIS	3.1
1	C	157	VAL	3.1
1	E	5	LYS	3.0
1	E	30	LEU	2.9
1	E	128	ASN	2.7
1	F	221	ARG	2.7
1	C	60	ALA	2.6
1	F	165	GLY	2.6
1	E	59	THR	2.6
1	E	74	ASN	2.6
1	A	60	ALA	2.5
1	C	173	PHE	2.5
1	C	59	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	2.3
1	E	73	GLU	2.3
1	D	59	THR	2.3
1	E	28	VAL	2.3
1	B	57	LEU	2.3
1	A	59	THR	2.3
1	E	57	LEU	2.3
1	D	72	PRO	2.3
1	B	1	MET	2.2
1	F	49	PRO	2.2
1	F	6	PRO	2.2
1	E	58	THR	2.2
1	C	56	ILE	2.2
1	E	111	GLY	2.1
1	E	61	PHE	2.1
1	C	57	LEU	2.1
1	A	58	THR	2.1
1	F	182	VAL	2.1
1	D	3	VAL	2.0
1	A	57	LEU	2.0
1	B	2	SER	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^{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	B-factors(Å^2)	Q<0.9
1	CR8	C	63	25/26	0.96	0.18	13,18,20,21	0
1	CR8	D	63	25/26	0.96	0.15	18,22,26,30	0
1	CR8	E	63	25/26	0.96	0.19	19,22,30,30	0
1	CR8	F	63	25/26	0.96	0.13	13,22,27,31	0
1	CR8	A	63	25/26	0.97	0.18	13,17,21,28	0
1	CR8	B	63	25/26	0.97	0.14	10,14,19,21	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
3	PGE	A	302	10/10	0.73	0.37	34,42,50,61	0
4	PEG	A	303	7/7	0.84	0.31	41,46,54,58	0
4	PEG	B	301	7/7	0.89	0.32	29,35,46,47	0
2	EPE	C	301	5/15	0.93	0.21	34,37,45,49	0
2	EPE	E	301	5/15	0.94	0.15	41,45,51,54	0
2	EPE	A	301	5/15	0.97	0.15	29,33,41,44	0

6.5 Other polymers

There are no such residues in this entry.