Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2023 – 11:06 PM EDT

PDB ID	:	4HQ9
Title	:	Crystal structure of a green-to-red photoconvertible DRONPA, pcDRONPA in the green-off-state
Authors	:	Nguyen Bich, N.; Van Meervelt, L.
Deposited on	:	2012-10-25
Resolution	:	2.07 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:

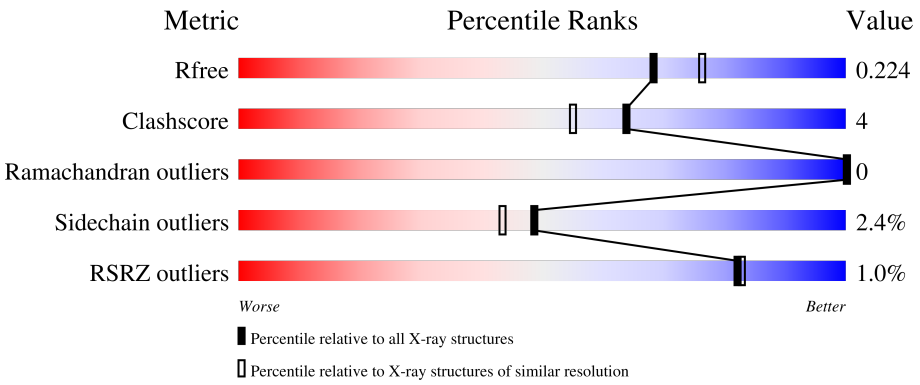
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	78% 6% 16%
1	B	258	76% 8% 16%
1	C	258	79% 5% 16%
1	D	258	72% 11% 16%
1	E	258	2% 74% 10% 16%

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Mol	Chain	Length	Quality of chain
1	F	258	2% 66% 15% • 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11101 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	N	O	S			
1	A	217	1756	1124	298	325	9	0	2	0
1	B	216	1734	1112	292	321	9	0	1	0
1	C	218	1763	1128	295	330	10	0	3	0
1	D	216	1730	1108	290	323	9	0	0	0
1	E	217	1732	1111	289	323	9	0	0	0
1	F	214	1721	1101	290	321	9	0	0	0

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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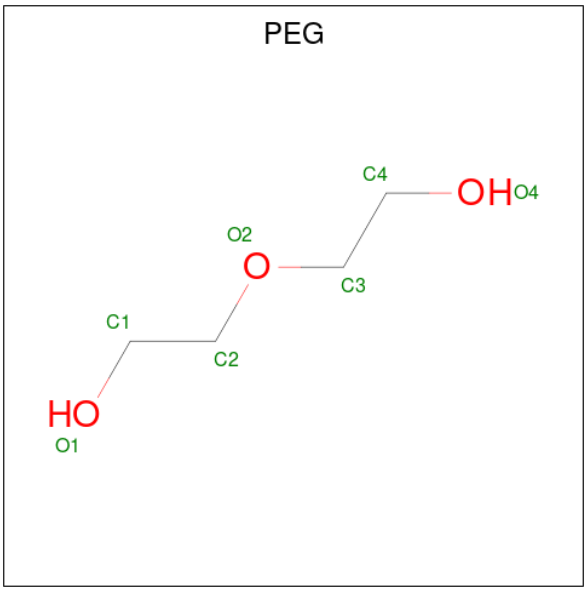
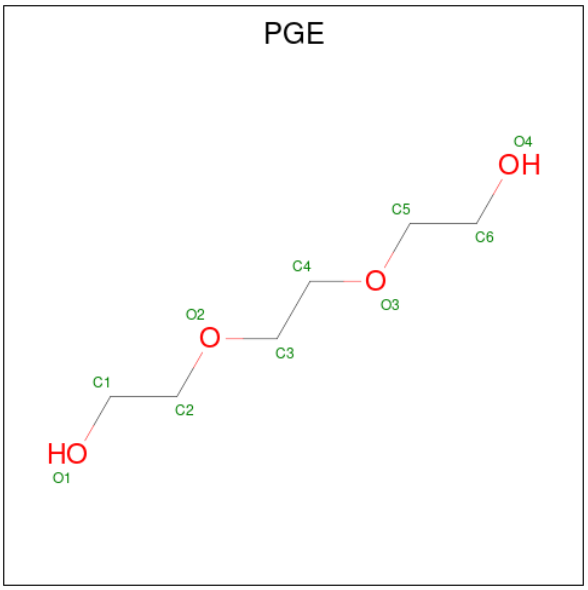
Chain	Residue	Modelled	Actual	Comment	Reference
F	-23	ALA	-	expression tag	UNP Q5TLG6
F	-22	SER	-	expression tag	UNP Q5TLG6
F	-21	MET	-	expression tag	UNP Q5TLG6
F	-20	THR	-	expression tag	UNP Q5TLG6
F	-19	GLY	-	expression tag	UNP Q5TLG6
F	-18	GLY	-	expression tag	UNP Q5TLG6
F	-17	GLN	-	expression tag	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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



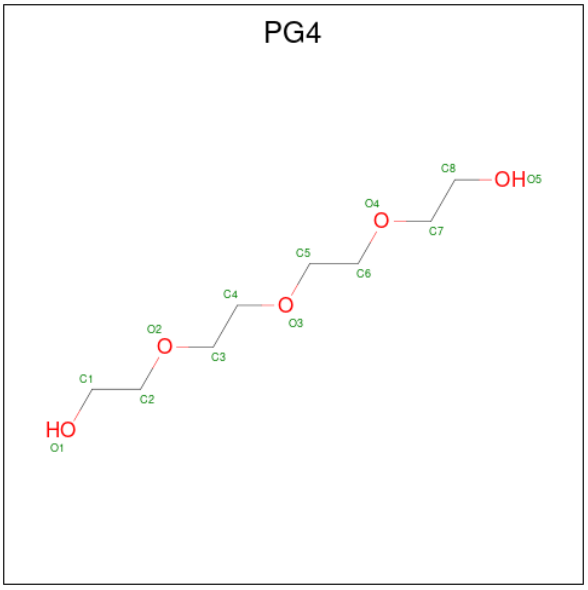
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	4	3	0	0
2	B	1	7	4	3	0	0
2	D	1	7	4	3	0	0
2	F	1	7	4	3	0	0

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



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	C	1	13	8	5	0	0
			Total	C	O		
4	F	1	13	8	5	0	0

- Molecule 5 is water.

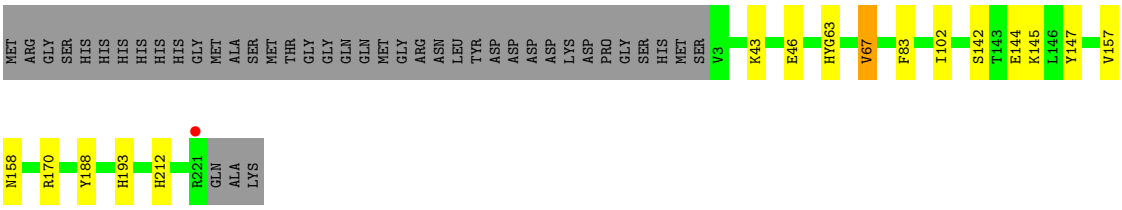
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	126	126	126	0	0
			Total	O		
5	B	84	84	84	0	0
			Total	O		
5	C	111	111	111	0	0
			Total	O		
5	D	98	98	98	0	0
			Total	O		
5	E	83	83	83	0	0
			Total	O		
5	F	99	99	99	0	0

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.

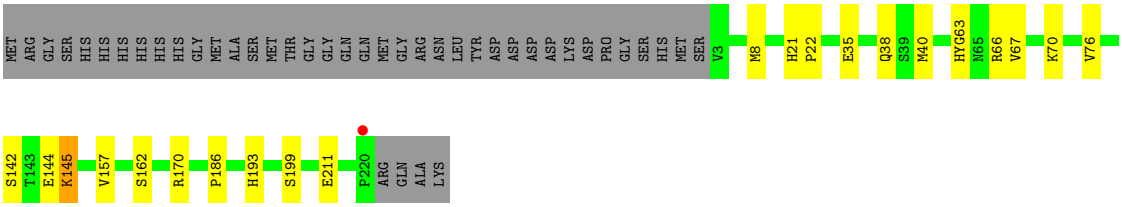
• Molecule 1: Fluorescent protein Dronpa

Chain A: 78% 6% 16%



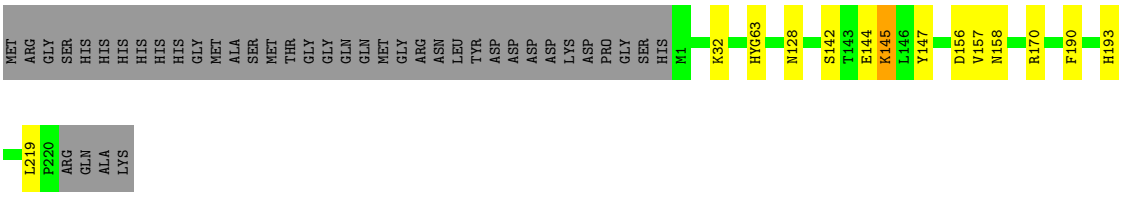
• Molecule 1: Fluorescent protein Dronpa

Chain B: 76% 8% 16%



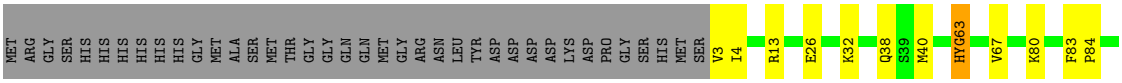
• Molecule 1: Fluorescent protein Dronpa

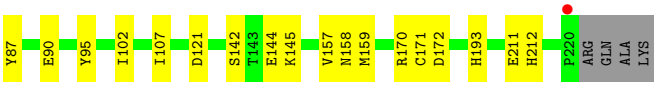
Chain C: 79% 5% 16%



• Molecule 1: Fluorescent protein Dronpa

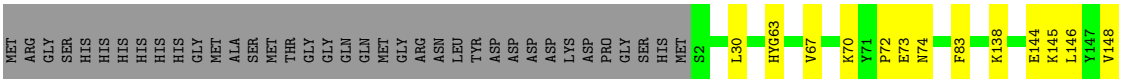
Chain D: 72% 11% 16%





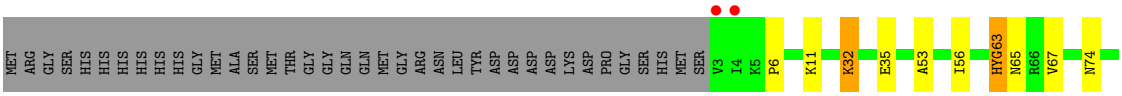
• Molecule 1: Fluorescent protein Dronpa

Chain E:



• Molecule 1: Fluorescent protein Dronpa

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.18Å 103.55Å 176.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.43 – 2.07 64.43 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.4 (64.43-2.07) 98.4 (64.43-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.189 , 0.234 0.184 , 0.224	Depositor DCC
R_{free} test set	3879 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11101	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.36% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PGE, CR8, 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	0.56	0/1785	0.64	0/2410
1	B	0.51	0/1759	0.63	0/2379
1	C	0.53	0/1794	0.61	0/2422
1	D	0.56	0/1751	0.65	0/2367
1	E	0.52	0/1753	0.63	0/2369
1	F	0.53	0/1741	0.68	1/2350 (0.0%)
All	All	0.54	0/10583	0.64	1/14297 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	150	ASP	CB-CA-C	-6.83	96.74	110.40

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	1756	0	1673	12	0
1	B	1734	0	1639	11	0
1	C	1763	0	1682	9	0
1	D	1730	0	1634	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1732	0	1639	11	0
1	F	1721	0	1634	29	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
2	D	7	0	10	0	0
2	F	7	0	10	2	0
3	A	10	0	14	3	0
4	C	13	0	18	0	0
4	F	13	0	18	0	0
5	A	126	0	0	2	0
5	B	84	0	0	2	0
5	C	111	0	0	2	0
5	D	98	0	0	2	0
5	E	83	0	0	0	0
5	F	99	0	0	3	0
All	All	11101	0	9991	87	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 4.

All (87) 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:D:170:ARG:NH1	5:D:488:HOH:O	2.19	0.76
1:D:158:ASN:ND2	1:D:172:ASP:OD2	2.19	0.75
1:F:128:ASN:ND2	5:F:459:HOH:O	2.20	0.75
1:C:219:LEU:HD13	1:D:212:HIS:HD2	1.52	0.74
1:D:142:SER:OG	1:D:193:HIS:NE2	2.23	0.71
1:A:43:LYS:HZ1	3:A:302:PGE:H32	1.54	0.70
1:D:142:SER:HG	1:D:193:HIS:HE2	1.38	0.69
1:F:133:GLN:OE1	1:F:135:ARG:NH2	2.24	0.69
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.76	0.66
1:D:38:GLN:OE1	5:D:498:HOH:O	2.14	0.64
1:B:38:GLN:OE1	5:B:481:HOH:O	2.15	0.63
1:E:73:GLU:H	1:E:73:GLU:CD	2.02	0.63
1:A:212:HIS:ND1	5:A:504:HOH:O	2.31	0.61
1:C:142:SER:OG	1:C:193:HIS:NE2	2.34	0.60
1:E:146:LEU:HD23	1:E:153:LEU:HD21	1.83	0.60
1:B:145:LYS:HD3	5:B:471:HOH:O	2.02	0.59
1:F:67:VAL:HG11	1:F:83:PHE:CE1	2.37	0.59
1:E:158:ASN:ND2	1:E:172:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:VAL:HG11	1:F:83:PHE:HE1	1.68	0.58
1:F:81:GLN:O	1:F:181:LYS:NZ	2.34	0.58
1:F:112:ASP:OD2	1:F:112:ASP:N	2.36	0.57
1:F:144:GLU:HA	1:F:157:VAL:HB	1.85	0.57
1:A:43:LYS:NZ	3:A:302:PGE:H5	2.20	0.55
1:D:144:GLU:HA	1:D:157:VAL:HB	1.87	0.55
1:B:38:GLN:NE2	1:B:211:GLU:OE1	2.39	0.55
1:E:67:VAL:HG11	1:E:83:PHE:CE1	2.42	0.54
1:E:149:ARG:HG2	1:E:154:LYS:HE2	1.91	0.53
1:F:85:GLU:CD	1:F:181:LYS:HD3	2.28	0.53
1:F:11:LYS:HG3	1:F:113:CYS:SG	2.49	0.53
1:B:142:SER:OG	1:B:193:HIS:NE2	2.42	0.52
1:C:147:TYR:OH	1:D:170:ARG:NE	2.36	0.52
1:C:145:LYS:HG3	1:C:190:PHE:CE2	2.44	0.52
1:D:13:ARG:NH1	1:D:26:GLU:OE2	2.41	0.51
1:A:43:LYS:HE3	3:A:302:PGE:H4	1.93	0.51
1:E:144:GLU:HA	1:E:157:VAL:HB	1.93	0.51
1:A:142:SER:OG	1:A:193:HIS:NE2	2.44	0.50
1:F:6:PRO:O	5:F:466:HOH:O	2.19	0.50
1:B:35:GLU:HA	1:B:70:LYS:HD3	1.93	0.49
1:D:142:SER:HG	1:D:193:HIS:CD2	2.30	0.49
1:F:149:ARG:O	1:F:150:ASP:HB2	2.13	0.49
1:A:158:ASN:HB3	1:A:170:ARG:CZ	2.42	0.49
1:A:144:GLU:HA	1:A:157:VAL:HB	1.94	0.49
1:D:142:SER:OG	1:D:159:MET:SD	2.71	0.49
1:A:158:ASN:HB3	1:A:170:ARG:NH2	2.29	0.48
1:C:144:GLU:HA	1:C:157:VAL:HB	1.95	0.48
1:F:137:VAL:HB	1:F:162:SER:HB3	1.96	0.48
1:F:65:ASN:OD1	1:F:67:VAL:HG13	2.14	0.48
1:B:144:GLU:HA	1:B:157:VAL:HB	1.95	0.47
1:B:145:LYS:N	1:B:145:LYS:HE2	2.30	0.47
1:A:147:TYR:HB3	1:A:188:TYR:CD1	2.51	0.46
1:F:142:SER:OG	1:F:193:HIS:NE2	2.47	0.46
1:F:163:LEU:HD11	1:F:169:TYR:HB2	1.96	0.46
1:F:96:GLU:HA	2:F:301:PEG:H32	1.97	0.46
1:C:128:ASN:ND2	5:C:497:HOH:O	2.48	0.46
1:C:32:LYS:HE2	1:C:32:LYS:HB3	1.74	0.46
1:C:219:LEU:CD1	1:D:212:HIS:HD2	2.26	0.45
1:D:95:TYR:CD2	1:D:171:CYS:HB2	2.51	0.45
1:F:79:PHE:O	1:F:82:SER:OG	2.31	0.45
1:E:72:PRO:HB2	1:E:74:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:HG21	1:A:83:PHE:CE1	2.53	0.43
1:B:170:ARG:HB3	1:B:170:ARG:CZ	2.48	0.43
1:F:53:ALA:O	1:F:56:ILE:HG12	2.18	0.43
1:F:96:GLU:HB3	2:F:301:PEG:H21	2.00	0.42
1:F:210:HIS:HB2	5:F:487:HOH:O	2.19	0.42
5:C:507:HOH:O	1:D:142:SER:HB3	2.19	0.42
1:D:4:ILE:HD13	1:D:80:LYS:HB3	2.00	0.42
1:A:46:GLU:OE1	5:A:438:HOH:O	2.22	0.42
1:F:87:TYR:CZ	1:F:107:ILE:HD12	2.54	0.42
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.01	0.42
1:F:63:CR8:H23	1:F:211:GLU:HB2	2.01	0.42
1:D:102:ILE:HD13	1:F:102:ILE:HG23	2.02	0.41
1:F:136:THR:HG21	1:F:161:LEU:HD13	2.01	0.41
1:E:201:ASP:OD2	1:E:206:ASN:HB2	2.20	0.41
1:E:148:VAL:HG21	1:E:185:LEU:HB3	2.02	0.41
1:D:90:GLU:HB3	1:F:123:VAL:HB	2.01	0.41
1:E:196:GLU:HG3	1:E:198:LYS:HD3	2.03	0.41
1:D:121:ASP:C	1:F:102:ILE:HD11	2.41	0.41
1:B:21[A]:HIS:HA	1:B:22:PRO:HD3	1.76	0.41
1:B:170:ARG:HB3	1:B:170:ARG:NH1	2.36	0.41
1:F:74:ASN:OD1	1:F:74:ASN:N	2.48	0.41
1:F:32:LYS:HG2	1:F:35:GLU:OE2	2.21	0.40
1:A:102:ILE:HD13	1:A:102:ILE:HG21	1.85	0.40
1:C:158:ASN:HB3	1:C:170:ARG:CZ	2.51	0.40
1:D:87:TYR:CZ	1:D:107:ILE:HD12	2.57	0.40
1:F:198:LYS:HB3	1:F:198:LYS:HE3	1.69	0.40
1:B:76:VAL:HB	1:B:186:PRO:HB3	2.03	0.40
1:D:40:MET:HG2	1:D:63:CR8:C10	2.51	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	214/258 (83%)	210 (98%)	4 (2%)	0	100	100
1	B	212/258 (82%)	211 (100%)	1 (0%)	0	100	100
1	C	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	D	211/258 (82%)	209 (99%)	2 (1%)	0	100	100
1	E	212/258 (82%)	210 (99%)	2 (1%)	0	100	100
1	F	209/258 (81%)	208 (100%)	1 (0%)	0	100	100
All	All	1274/1548 (82%)	1262 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/218 (85%)	184 (99%)	2 (1%)	73	72
1	B	181/218 (83%)	174 (96%)	7 (4%)	32	25
1	C	188/218 (86%)	186 (99%)	2 (1%)	73	72
1	D	181/218 (83%)	176 (97%)	5 (3%)	43	37
1	E	181/218 (83%)	178 (98%)	3 (2%)	60	57
1	F	181/218 (83%)	174 (96%)	7 (4%)	32	25
All	All	1098/1308 (84%)	1072 (98%)	26 (2%)	49	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	145	LYS
1	B	8	MET
1	B	40	MET
1	B	66	ARG
1	B	67	VAL
1	B	145	LYS

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Mol	Chain	Res	Type
1	B	162	SER
1	B	199	SER
1	C	145	LYS
1	C	156	ASP
1	D	3	VAL
1	D	32	LYS
1	D	67	VAL
1	D	145	LYS
1	D	211	GLU
1	E	30	LEU
1	E	138	LYS
1	E	145	LYS
1	F	32	LYS
1	F	102	ILE
1	F	112	ASP
1	F	145	LYS
1	F	162	SER
1	F	196	GLU
1	F	217	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	194	HIS
1	D	38	GLN
1	D	74	ASN
1	D	206	ASN
1	E	158	ASN
1	E	194	HIS
1	E	212	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	D	63	1	20,27,28	1.94	7 (35%)	17,37,39	1.95	7 (41%)
1	CR8	C	63	1	20,27,28	1.99	7 (35%)	17,37,39	1.93	6 (35%)
1	CR8	B	63	1	20,27,28	1.96	7 (35%)	17,37,39	2.00	7 (41%)
1	CR8	F	63	1	20,27,28	1.91	8 (40%)	17,37,39	1.82	7 (41%)
1	CR8	A	63	1	20,27,28	1.96	5 (25%)	17,37,39	1.43	3 (17%)
1	CR8	E	63	1	20,27,28	2.03	7 (35%)	17,37,39	1.49	3 (17%)

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	D	63	1	-	5/8/25/26	0/3/3/3
1	CR8	C	63	1	-	6/8/25/26	0/3/3/3
1	CR8	B	63	1	-	6/8/25/26	0/3/3/3
1	CR8	F	63	1	-	7/8/25/26	0/3/3/3
1	CR8	A	63	1	-	6/8/25/26	0/3/3/3
1	CR8	E	63	1	-	6/8/25/26	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	CR8	O13-C11	4.81	1.39	1.24
1	C	63	CR8	O13-C11	4.48	1.38	1.24
1	A	63	CR8	O13-C11	4.45	1.38	1.24
1	B	63	CR8	O13-C11	4.34	1.37	1.24
1	D	63	CR8	O13-C11	4.27	1.37	1.24
1	F	63	CR8	O13-C11	4.09	1.37	1.24
1	E	63	CR8	C8-C7	3.99	1.46	1.36
1	C	63	CR8	C8-C7	3.94	1.45	1.36
1	A	63	CR8	C8-C7	3.85	1.45	1.36
1	B	63	CR8	C8-C7	3.52	1.44	1.36
1	F	63	CR8	C8-C7	3.47	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	CR8	C8-C7	3.16	1.44	1.36
1	D	63	CR8	C1-N2	-3.11	1.30	1.34
1	A	63	CR8	C4-C11	-3.05	1.39	1.45
1	B	63	CR8	C4-C11	-3.04	1.39	1.45
1	D	63	CR8	C4-C11	-2.99	1.39	1.45
1	E	63	CR8	C4-C11	-2.97	1.39	1.45
1	A	63	CR8	O2-C2	-2.93	1.23	1.32
1	B	63	CR8	O2-C2	-2.92	1.23	1.32
1	C	63	CR8	C4-C11	-2.87	1.39	1.45
1	C	63	CR8	O2-C2	-2.81	1.24	1.32
1	E	63	CR8	O2-C2	-2.70	1.24	1.32
1	F	63	CR8	C4-C11	-2.70	1.39	1.45
1	F	63	CR8	O2-C2	-2.60	1.24	1.32
1	D	63	CR8	O2-C2	-2.59	1.24	1.32
1	F	63	CR8	C1-N2	-2.55	1.31	1.34
1	C	63	CR8	C2-N3	2.55	1.40	1.36
1	B	63	CR8	C1-N2	-2.53	1.31	1.34
1	A	63	CR8	C12-C11	-2.51	1.40	1.45
1	F	63	CR8	C12-C11	-2.43	1.40	1.45
1	E	63	CR8	C2-N3	2.42	1.40	1.36
1	E	63	CR8	C1-N2	-2.38	1.31	1.34
1	C	63	CR8	C12-C11	-2.36	1.40	1.45
1	E	63	CR8	C12-C11	-2.33	1.40	1.45
1	D	63	CR8	C12-C11	-2.32	1.40	1.45
1	F	63	CR8	CA3-N3	-2.31	1.45	1.49
1	B	63	CR8	C12-C11	-2.15	1.41	1.45
1	C	63	CR8	C1-N2	-2.15	1.31	1.34
1	F	63	CR8	C2-N3	2.14	1.39	1.36
1	D	63	CR8	CA3-N3	-2.13	1.45	1.49
1	B	63	CR8	C2-N3	2.07	1.39	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	CR8	C3-CA3-N3	3.94	117.89	111.92
1	C	63	CR8	C3-CA3-N3	3.79	117.67	111.92
1	B	63	CR8	C12-C6-C7	-3.22	119.22	121.95
1	D	63	CR8	C12-C6-C7	-3.16	119.26	121.95
1	D	63	CR8	CA1-C1-N2	-3.13	118.76	124.99
1	B	63	CR8	CA1-C1-N2	-3.01	119.00	124.99
1	F	63	CR8	O3-C3-CA3	-2.94	117.97	126.32
1	C	63	CR8	C20-CA1-C1	-2.93	105.89	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	CR8	CA1-C1-N2	-2.92	119.18	124.99
1	D	63	CR8	O3-C3-CA3	-2.86	118.20	126.32
1	C	63	CR8	O3-C3-CA3	-2.76	118.48	126.32
1	B	63	CR8	O13-C11-C4	-2.68	117.24	121.56
1	D	63	CR8	C4-C11-C12	2.67	121.33	116.62
1	E	63	CR8	C3-CA3-N3	2.55	115.78	111.92
1	F	63	CR8	C4-C5-C7	-2.55	119.79	121.95
1	C	63	CR8	CA3-N3-C2	2.51	128.41	124.32
1	E	63	CR8	CA3-N3-C2	2.50	128.40	124.32
1	F	63	CR8	CA1-C1-N2	-2.46	120.10	124.99
1	C	63	CR8	C12-C6-C7	-2.45	119.87	121.95
1	E	63	CR8	CA1-C1-N2	-2.45	120.11	124.99
1	B	63	CR8	O3-C3-CA3	-2.45	119.36	126.32
1	F	63	CR8	C4-C11-C12	2.43	120.91	116.62
1	F	63	CR8	CA3-N3-C2	2.42	128.27	124.32
1	B	63	CR8	CA3-N3-C2	2.41	128.25	124.32
1	D	63	CR8	O13-C11-C4	-2.40	117.69	121.56
1	F	63	CR8	C3-CA3-N3	2.31	115.42	111.92
1	A	63	CR8	CA1-C1-N2	-2.29	120.44	124.99
1	F	63	CR8	C12-C6-C7	-2.28	120.01	121.95
1	A	63	CR8	C3-CA3-N3	2.27	115.37	111.92
1	B	63	CR8	C4-C11-C12	2.22	120.54	116.62
1	A	63	CR8	O3-C3-CA3	-2.18	120.11	126.32
1	D	63	CR8	C4-C5-C7	-2.10	120.17	121.95
1	D	63	CR8	C6-C7-C5	2.05	120.50	116.20

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	CR8	C5-C7-C8-CA2
1	A	63	CR8	C6-C7-C8-CA2
1	A	63	CR8	C7-C8-CA2-C2
1	A	63	CR8	C7-C8-CA2-N2
1	A	63	CR8	CA1-C20-C21-N22
1	A	63	CR8	CA1-C20-C21-C23
1	B	63	CR8	C5-C7-C8-CA2
1	B	63	CR8	C6-C7-C8-CA2
1	B	63	CR8	C7-C8-CA2-C2
1	B	63	CR8	C7-C8-CA2-N2
1	B	63	CR8	CA1-C20-C21-N22
1	B	63	CR8	CA1-C20-C21-C23

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Mol	Chain	Res	Type	Atoms
1	C	63	CR8	C5-C7-C8-CA2
1	C	63	CR8	C6-C7-C8-CA2
1	C	63	CR8	C7-C8-CA2-C2
1	C	63	CR8	C7-C8-CA2-N2
1	C	63	CR8	CA1-C20-C21-N22
1	D	63	CR8	C5-C7-C8-CA2
1	D	63	CR8	C6-C7-C8-CA2
1	D	63	CR8	C7-C8-CA2-N2
1	D	63	CR8	CA1-C20-C21-N22
1	D	63	CR8	CA1-C20-C21-C23
1	E	63	CR8	C5-C7-C8-CA2
1	E	63	CR8	C6-C7-C8-CA2
1	E	63	CR8	C7-C8-CA2-C2
1	E	63	CR8	C7-C8-CA2-N2
1	E	63	CR8	CA1-C20-C21-N22
1	F	63	CR8	C5-C7-C8-CA2
1	F	63	CR8	C6-C7-C8-CA2
1	F	63	CR8	C7-C8-CA2-C2
1	F	63	CR8	C7-C8-CA2-N2
1	F	63	CR8	CA1-C20-C21-N22
1	F	63	CR8	CA1-C20-C21-C23
1	F	63	CR8	C21-C20-CA1-N1
1	C	63	CR8	CA1-C20-C21-C23
1	E	63	CR8	CA1-C20-C21-C23

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	PG4	C	301	-	12,12,12	0.71	0	11,11,11	0.73	0
2	PEG	A	301	-	6,6,6	0.50	0	5,5,5	0.70	0
2	PEG	B	301	-	6,6,6	0.44	0	5,5,5	1.17	1 (20%)
4	PG4	F	302	-	12,12,12	0.72	0	11,11,11	0.99	1 (9%)
2	PEG	F	301	-	6,6,6	0.52	0	5,5,5	0.77	0
2	PEG	D	301	-	6,6,6	0.43	0	5,5,5	0.74	0
3	PGE	A	302	-	9,9,9	0.54	0	8,8,8	0.97	1 (12%)

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	PG4	C	301	-	-	4/10/10/10	-
2	PEG	A	301	-	-	1/4/4/4	-
2	PEG	B	301	-	-	3/4/4/4	-
4	PG4	F	302	-	-	4/10/10/10	-
2	PEG	F	301	-	-	2/4/4/4	-
2	PEG	D	301	-	-	2/4/4/4	-
3	PGE	A	302	-	-	3/7/7/7	-

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	B	301	PEG	C3-O2-C2	2.50	124.10	113.29
4	F	302	PG4	C5-O3-C4	2.31	123.32	113.29
3	A	302	PGE	C5-O3-C4	2.14	122.57	113.29

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	PEG	C4-C3-O2-C2
4	F	302	PG4	O2-C3-C4-O3
2	B	301	PEG	O2-C3-C4-O4
2	A	301	PEG	O1-C1-C2-O2
2	B	301	PEG	O1-C1-C2-O2
2	D	301	PEG	O1-C1-C2-O2
2	F	301	PEG	O1-C1-C2-O2
3	A	302	PGE	C4-C3-O2-C2
4	C	301	PG4	O3-C5-C6-O4
3	A	302	PGE	C1-C2-O2-C3
2	F	301	PEG	O2-C3-C4-O4
4	C	301	PG4	C3-C4-O3-C5
4	F	302	PG4	C4-C3-O2-C2
3	A	302	PGE	O2-C3-C4-O3
4	C	301	PG4	O1-C1-C2-O2
4	F	302	PG4	O1-C1-C2-O2
4	C	301	PG4	C8-C7-O4-C6
2	B	301	PEG	C4-C3-O2-C2
4	F	302	PG4	C8-C7-O4-C6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	PEG	2	0
3	A	302	PGE	3	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 (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	216/258 (83%)	-0.34	1 (0%)	91	91	21, 31, 49, 73	0
1	B	215/258 (83%)	-0.20	1 (0%)	91	91	21, 34, 54, 79	0
1	C	217/258 (84%)	-0.25	0	100	100	20, 31, 49, 69	0
1	D	215/258 (83%)	-0.23	1 (0%)	91	91	22, 32, 51, 66	0
1	E	216/258 (83%)	-0.24	4 (1%)	66	68	22, 34, 52, 77	0
1	F	213/258 (82%)	-0.18	6 (2%)	53	56	22, 34, 51, 65	0
All	All	1292/1548 (83%)	-0.24	13 (1%)	82	83	20, 33, 52, 79	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	112	ASP	5.0
1	F	110	ASP	2.8
1	E	220	PRO	2.8
1	F	4	ILE	2.7
1	D	220	PRO	2.4
1	E	219	LEU	2.4
1	A	221	ARG	2.4
1	F	3	VAL	2.3
1	B	220	PRO	2.3
1	E	218	GLY	2.1
1	F	86	GLY	2.1
1	F	113	CYS	2.1
1	E	165	GLY	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	CR8	E	63	25/26	0.94	0.13	25,34,43,50	0
1	CR8	C	63	25/26	0.95	0.10	20,29,45,51	0
1	CR8	D	63	25/26	0.95	0.12	20,34,45,57	0
1	CR8	B	63	25/26	0.95	0.12	24,35,51,57	0
1	CR8	F	63	25/26	0.95	0.11	22,35,45,47	0
1	CR8	A	63	25/26	0.96	0.10	21,31,43,49	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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
2	PEG	B	301	7/7	0.73	0.21	43,45,55,65	0
2	PEG	D	301	7/7	0.82	0.17	47,50,59,59	0
4	PG4	F	302	13/13	0.83	0.14	40,52,57,65	0
4	PG4	C	301	13/13	0.84	0.23	40,48,56,56	0
3	PGE	A	302	10/10	0.85	0.22	48,57,60,61	0
2	PEG	A	301	7/7	0.88	0.14	46,52,55,57	0
2	PEG	F	301	7/7	0.89	0.14	38,41,50,52	0

6.5 Other polymers (i)

There are no such residues in this entry.