



Full wwPDB X-ray Structure Validation Report

Apr 17, 2014 – 09:37 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

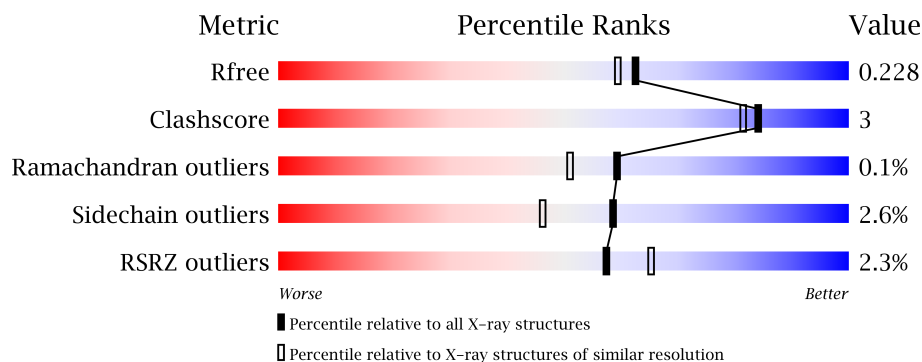
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	258	
1	B	258	
1	C	258	
1	D	258	
1	E	258	
1	F	258	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EPE	A	301	-	X
2	EPE	C	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	PGE	A	302	-	X
4	PEG	A	303	-	X
4	PEG	B	301	-	X

2 Entry composition

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

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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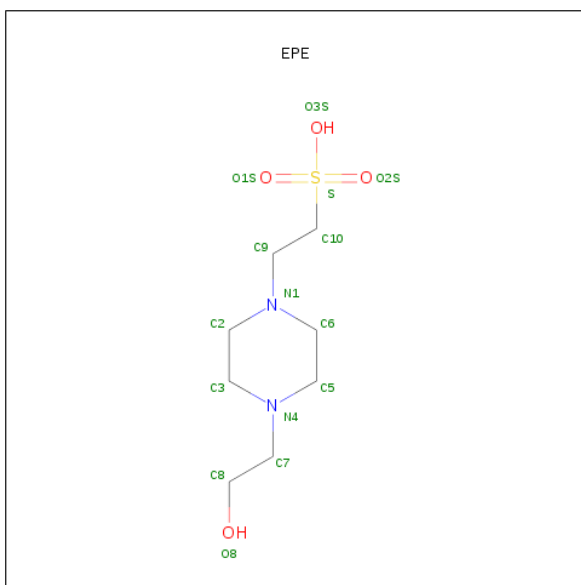
Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	SER	-	EXPRESSION TAG	UNP Q5TLG6
E	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
E	-20	THR	-	EXPRESSION TAG	UNP Q5TLG6
E	-19	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-18	GLY	-	EXPRESSION TAG	UNP Q5TLG6
E	-17	GLN	-	EXPRESSION TAG	UNP Q5TLG6
E	-16	GLN	-	EXPRESSION TAG	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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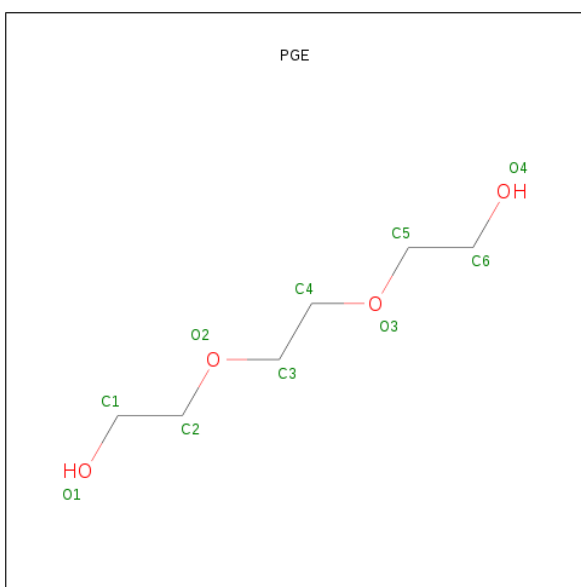
Chain	Residue	Modelled	Actual	Comment	Reference
F	-23	ALA	-	EXPRESSION TAG	UNP Q5TLG6
F	-22	SER	-	EXPRESSION TAG	UNP Q5TLG6
F	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-20	THR	-	EXPRESSION TAG	UNP Q5TLG6
F	-19	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-18	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-17	GLN	-	EXPRESSION TAG	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-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



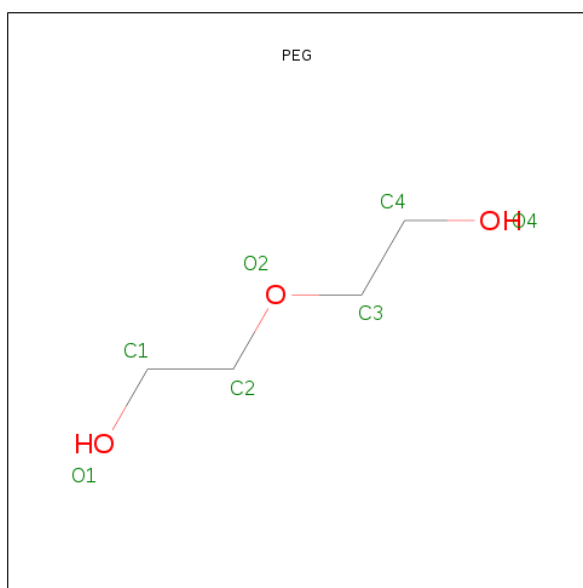
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			5	1	3	1		
2	C	1	Total	C	O	S	0	0
			5	1	3	1		
2	E	1	Total	C	O	S	0	0
			5	1	3	1		

- 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: C₄H₁₀O₃).



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

- Molecule 5 is water.

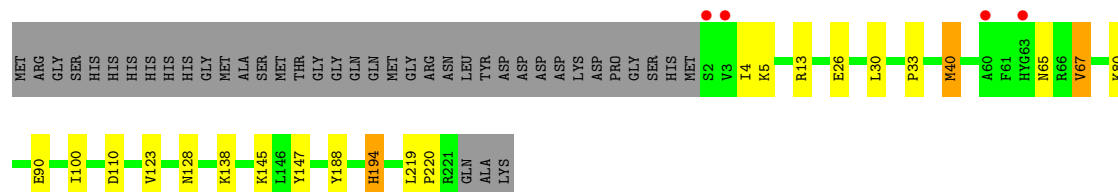
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total	O	0	0
			241	241		
5	B	271	Total	O	0	0
			271	271		
5	C	192	Total	O	0	0
			192	192		
5	D	158	Total	O	0	0
			158	158		
5	E	162	Total	O	0	0
			162	162		
5	F	168	Total	O	0	0
			168	168		

3 Residue-property plots

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

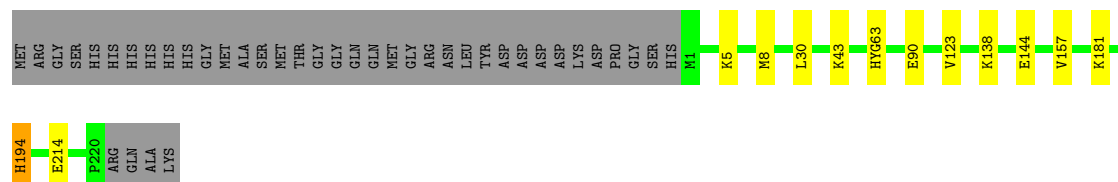
• Molecule 1: Fluorescent protein Dronpa

Chain A: 



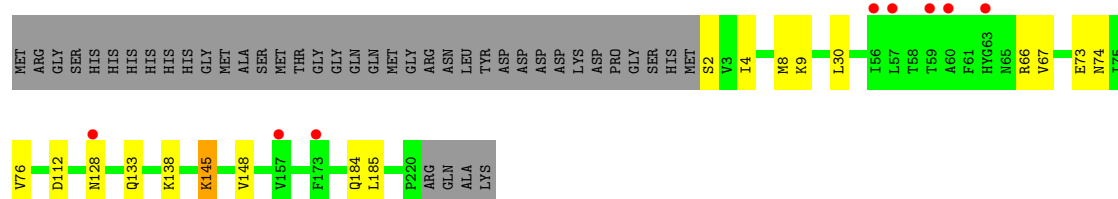
• Molecule 1: Fluorescent protein Dronpa

Chain B: 



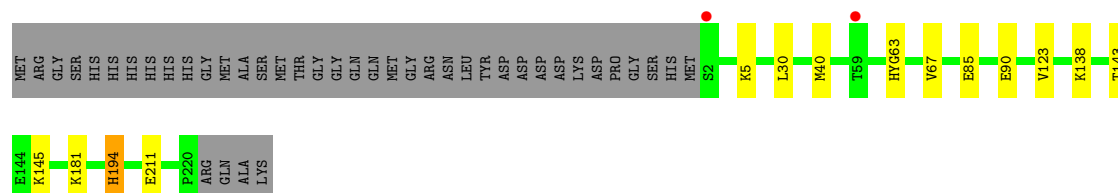
• Molecule 1: Fluorescent protein Dronpa

Chain C: 



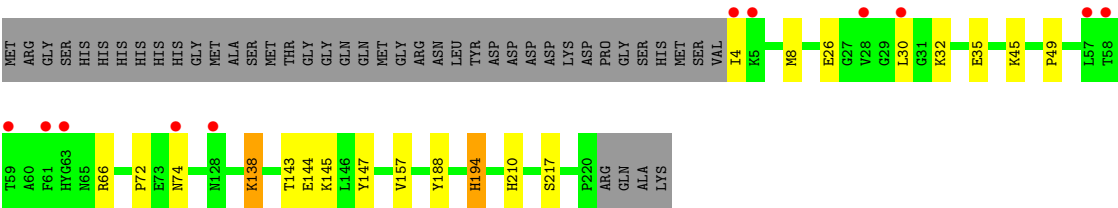
• Molecule 1: Fluorescent protein Dronpa

Chain D: 



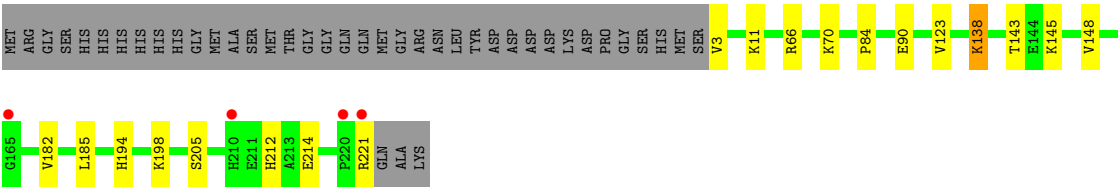
● Molecule 1: Fluorescent protein Dronpa

Chain E: 



● Molecule 1: Fluorescent protein Dronpa

Chain F: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.184 , 0.235 0.180 , 0.228	Depositor DCC
R_{free} test set	5081 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 101848 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1775	0	1697	13	0
1	B	1752	0	1672	11	0
1	C	1749	0	1664	8	0
1	D	1751	0	1675	11	0
1	E	1731	0	1655	11	0
1	F	1750	0	1678	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	1	0
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	10075	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:90:GLU:HB3	1:B:123:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:63:CR8:H23	1:D:211:GLU:HB2	1.97	0.47
1:D:40:MET:HG2	1:D:63:CR8:C10	2.43	0.47
1:E:72:PRO:HB2	1:E:74:ASN:OD1	2.15	0.46
1:F:11:LYS:HE2	1:F:11:LYS:HB2	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

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	222/258 (86%)	220 (99%)	1 (0%)	1 (0%)	38	23
1	B	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	C	217/258 (84%)	214 (99%)	3 (1%)	0	100	100
1	D	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	E	213/258 (83%)	211 (99%)	2 (1%)	0	100	100
1	F	216/258 (84%)	216 (100%)	0	0	100	100
All	All	1301/1548 (84%)	1291 (99%)	9 (1%)	1 (0%)	59	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	PRO

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	190/218 (87%)	183 (96%)	7 (4%)	45	30
1	B	185/218 (85%)	183 (99%)	2 (1%)	84	81
1	C	185/218 (85%)	179 (97%)	6 (3%)	51	37
1	D	186/218 (85%)	183 (98%)	3 (2%)	75	69
1	E	182/218 (84%)	176 (97%)	6 (3%)	50	35
1	F	184/218 (84%)	178 (97%)	6 (3%)	50	35
All	All	1112/1308 (85%)	1082 (97%)	30 (3%)	59	45

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

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	133	GLN
1	A	194	HIS
1	B	194	HIS
1	C	194	HIS
1	D	194	HIS
1	E	158	ASN
1	E	194	HIS

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

5.3.3 RNA ⓘ

There are no RNA chains 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	A	63	1	27,27,28	4.72	9 (33%)	29,37,39	1.73	5 (17%)
1	CR8	B	63	1	27,27,28	4.59	9 (33%)	29,37,39	1.60	4 (13%)
1	CR8	C	63	1	27,27,28	4.07	11 (40%)	29,37,39	1.49	5 (17%)
1	CR8	D	63	1	27,27,28	4.29	10 (37%)	29,37,39	1.73	5 (17%)
1	CR8	E	63	1	27,27,28	4.14	9 (33%)	29,37,39	1.89	6 (20%)
1	CR8	F	63	1	27,27,28	4.60	9 (33%)	29,37,39	1.62	3 (10%)

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	A	63	1	-	0/9/25/26	0/3/3/3
1	CR8	B	63	1	-	1/9/25/26	0/3/3/3
1	CR8	C	63	1	-	0/9/25/26	0/3/3/3
1	CR8	D	63	1	-	1/9/25/26	0/3/3/3
1	CR8	E	63	1	-	0/9/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR8	F	63	1	-	0/9/25/26	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	CR8	O19-C	22.21	1.26	1.11
1	B	63	CR8	O19-C	21.45	1.26	1.11
1	F	63	CR8	O19-C	21.42	1.26	1.11
1	D	63	CR8	O19-C	19.57	1.24	1.11
1	E	63	CR8	O19-C	18.93	1.24	1.11
1	C	63	CR8	O19-C	18.17	1.23	1.11
1	D	63	CR8	O3-C1	4.51	1.38	1.24
1	C	63	CR8	O3-C1	4.46	1.38	1.24
1	A	63	CR8	O3-C1	4.42	1.38	1.24
1	F	63	CR8	O3-C1	4.41	1.38	1.24
1	E	63	CR8	O3-C1	4.33	1.38	1.24
1	D	63	CR8	C8-C7	4.32	1.47	1.36
1	B	63	CR8	O3-C1	4.30	1.38	1.24
1	F	63	CR8	C8-C7	4.20	1.47	1.36
1	D	63	CR8	C9-C12	4.18	1.49	1.39
1	A	63	CR8	C8-C7	4.08	1.46	1.36
1	B	63	CR8	C8-C7	3.93	1.46	1.36
1	E	63	CR8	C10-N22	3.93	1.37	1.33
1	E	63	CR8	C8-C7	3.85	1.46	1.36
1	C	63	CR8	C8-C7	3.83	1.46	1.36
1	C	63	CR8	C10-N22	3.81	1.37	1.33
1	F	63	CR8	C10-N22	3.80	1.37	1.33
1	E	63	CR8	C9-C12	3.80	1.48	1.39
1	B	63	CR8	C9-C12	3.75	1.48	1.39
1	D	63	CR8	C10-N22	3.73	1.37	1.33
1	A	63	CR8	C10-N22	3.72	1.37	1.33
1	B	63	CR8	C10-N22	3.67	1.36	1.33
1	A	63	CR8	C9-C12	3.63	1.47	1.39
1	F	63	CR8	C9-C12	3.50	1.47	1.39
1	C	63	CR8	C4-C1	-3.15	1.38	1.45
1	C	63	CR8	C17-N13	-3.09	1.44	1.48
1	B	63	CR8	C21-N22	-3.08	1.34	1.38
1	B	63	CR8	C2-C1	-3.07	1.38	1.45
1	C	63	CR8	C9-C12	3.03	1.46	1.39
1	E	63	CR8	C4-C1	-3.01	1.38	1.45
1	A	63	CR8	C14-N13	2.95	1.40	1.36
1	F	63	CR8	C4-C1	-2.94	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	CR8	C17-N13	-2.94	1.44	1.48
1	A	63	CR8	C4-C1	-2.89	1.39	1.45
1	F	63	CR8	C14-N13	2.75	1.40	1.36
1	C	63	CR8	C14-N13	2.66	1.40	1.36
1	F	63	CR8	C21-N22	-2.62	1.34	1.38
1	C	63	CR8	C21-N22	-2.62	1.34	1.38
1	D	63	CR8	C4-C1	-2.60	1.39	1.45
1	B	63	CR8	C4-C1	-2.49	1.40	1.45
1	D	63	CR8	C21-N22	-2.49	1.35	1.38
1	A	63	CR8	C2-C1	-2.44	1.40	1.45
1	D	63	CR8	C14-N13	2.43	1.39	1.36
1	A	63	CR8	C21-N22	-2.35	1.35	1.38
1	C	63	CR8	C2-C1	-2.31	1.40	1.45
1	E	63	CR8	C14-N13	2.28	1.39	1.36
1	F	63	CR8	C2-C1	-2.27	1.40	1.45
1	E	63	CR8	C2-C1	-2.18	1.40	1.45
1	D	63	CR8	C2-C1	-2.18	1.40	1.45
1	C	63	CR8	C20-C21	2.17	1.51	1.49
1	D	63	CR8	C17-N13	-2.14	1.45	1.48
1	E	63	CR8	C21-N22	-2.10	1.35	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	CR8	C12-N13-C14	-6.29	107.75	111.65
1	F	63	CR8	C12-N13-C14	-5.92	107.98	111.65
1	D	63	CR8	C12-N13-C14	-5.88	108.01	111.65
1	A	63	CR8	C12-N13-C14	-5.71	108.11	111.65
1	B	63	CR8	C12-N13-C14	-4.63	108.78	111.65
1	C	63	CR8	C12-N13-C14	-4.22	109.04	111.65
1	B	63	CR8	C20-C21-C23	-3.36	124.61	130.59
1	D	63	CR8	C20-C21-C23	-3.28	124.76	130.59
1	C	63	CR8	C20-C21-C23	-3.26	124.79	130.59
1	A	63	CR8	C20-C21-C23	-3.23	124.84	130.59
1	E	63	CR8	C20-C21-C23	-3.20	124.89	130.59
1	F	63	CR8	C8-C9-N15	3.16	129.42	123.96
1	D	63	CR8	C2-C6-C7	-2.94	119.36	121.92
1	E	63	CR8	C8-C9-N15	2.77	128.75	123.96
1	F	63	CR8	C20-C21-C23	-2.68	125.82	130.59
1	E	63	CR8	C2-C6-C7	-2.58	119.68	121.92
1	C	63	CR8	C8-C9-N15	2.56	128.38	123.96
1	A	63	CR8	C8-C9-N15	2.48	128.26	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	CR8	C4-C5-C7	-2.48	119.76	121.92
1	E	63	CR8	C17-N13-C12	2.43	128.22	123.98
1	A	63	CR8	C20-C21-N22	2.36	128.37	122.96
1	B	63	CR8	C10-N22-C21	-2.31	104.65	108.29
1	C	63	CR8	C2-C6-C7	-2.31	119.91	121.92
1	B	63	CR8	C8-C9-N15	2.24	127.84	123.96
1	C	63	CR8	C20-C21-N22	2.24	128.10	122.96
1	D	63	CR8	C8-C9-N15	2.22	127.80	123.96
1	E	63	CR8	O3-C1-C4	-2.13	118.09	121.50
1	D	63	CR8	C20-C21-N22	2.13	127.84	122.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	63	CR8	C16-C20-C21-N22
1	B	63	CR8	C16-C20-C21-N22

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	EPE	A	301	-	3,4,15	4.25	2 (66%)	3,6,20	0.52	0
3	PGE	A	302	-	9,9,9	0.41	0	8,8,8	0.92	0
4	PEG	A	303	-	6,6,6	0.50	0	5,5,5	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	B	301	-	6,6,6	0.44	0	5,5,5	0.73	0
2	EPE	C	301	-	3,4,15	4.26	2 (66%)	3,6,20	0.50	0
2	EPE	E	301	-	3,4,15	3.32	2 (66%)	3,6,20	0.53	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
2	EPE	A	301	-	-	0/0/0/19	0/0/0/1
3	PGE	A	302	-	-	0/7/7/7	0/0/0/0
4	PEG	A	303	-	-	0/4/4/4	0/0/0/0
4	PEG	B	301	-	-	0/4/4/4	0/0/0/0
2	EPE	C	301	-	-	0/0/0/19	0/0/0/1
2	EPE	E	301	-	-	0/0/0/19	0/0/0/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	EPE	O1S-S	5.77	1.48	1.42
2	A	301	EPE	O1S-S	5.47	1.48	1.42
2	A	301	EPE	O2S-S	4.92	1.47	1.42
2	C	301	EPE	O2S-S	4.59	1.47	1.42
2	E	301	EPE	O2S-S	4.35	1.46	1.42
2	E	301	EPE	O1S-S	3.74	1.46	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	218/258 (84%)	-0.11	4 (1%) 65 74	14, 22, 36, 58	0
1	B	218/258 (84%)	-0.20	0 100 100	14, 21, 34, 43	0
1	C	217/258 (84%)	0.00	8 (3%) 39 46	16, 24, 38, 53	0
1	D	217/258 (84%)	0.01	2 (0%) 81 88	17, 26, 39, 63	0
1	E	215/258 (83%)	0.13	11 (5%) 27 33	17, 26, 41, 54	0
1	F	217/258 (84%)	0.07	4 (1%) 65 74	15, 26, 41, 56	0
All	All	1302/1548 (84%)	-0.02	29 (2%) 57 67	14, 24, 39, 63	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	ILE	4.5
1	E	63	CR8	3.7
1	A	2	SER	3.2
1	F	210	HIS	3.1
1	F	221	ARG	2.9
1	C	128	ASN	2.9
1	D	2	SER	2.8
1	A	63	CR8	2.7
1	E	57	LEU	2.7
1	A	3	VAL	2.7
1	F	220	PRO	2.6
1	C	63	CR8	2.6
1	E	59	THR	2.5
1	E	58	THR	2.5
1	C	157	VAL	2.4
1	F	165	GLY	2.4
1	A	60	ALA	2.3
1	E	5	LYS	2.3
1	C	56	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	30	LEU	2.3
1	C	60	ALA	2.2
1	C	57	LEU	2.2
1	D	59	THR	2.2
1	C	59	THR	2.2
1	E	128	ASN	2.1
1	C	173	PHE	2.1
1	E	61	PHE	2.1
1	E	74	ASN	2.0
1	E	28	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CR8	E	63	25/26	0.20	1.56	19,22,30,30	0
1	CR8	A	63	25/26	0.17	1.03	13,17,21,28	0
1	CR8	C	63	25/26	0.17	0.78	13,18,20,21	0
1	CR8	D	63	25/26	0.15	0.63	18,22,26,30	0
1	CR8	B	63	25/26	0.14	0.38	10,14,19,21	0
1	CR8	F	63	25/26	0.12	-0.13	13,22,27,31	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PEG	B	301	7/7	0.27	13.35	29,35,46,47	0
3	PGE	A	302	10/10	0.35	9.83	34,42,50,61	0
2	EPE	C	301	5/15	0.19	3.86	34,37,45,49	0
4	PEG	A	303	7/7	0.28	3.11	41,46,54,58	0
2	EPE	A	301	5/15	0.13	2.82	29,33,41,44	0
2	EPE	E	301	5/15	0.14	1.95	41,45,51,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.