Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:16 PM GMT

PDB ID	:	4HQC
Title	:	Crystal structure of a green-to-red photoconvertible DRONPA, pcDRONPA in the red-on-state
Authors	:	Nguyen Bich, N.; Van Meervelt, L.
Deposited on	:	2012-10-25
Resolution	:	2.05 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

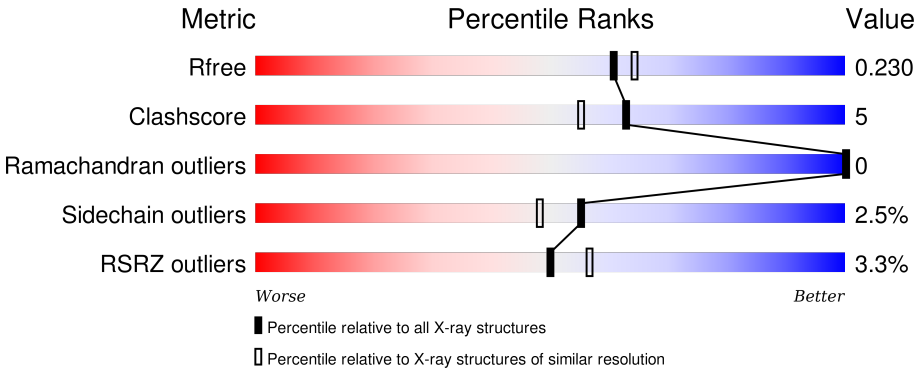
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	260	2% 73% 11% 15%
1	B	260	3% 73% 10% • 16%
1	C	260	70% 12% • 16%
1	D	260	2% 77% 7% • 16%
1	E	260	3% 74% 10% 16%

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Mol	Chain	Length	Quality of chain
1	F	260	7% 75% 10% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	A	301	-	-	-	X
2	PGE	C	301	-	-	-	X
2	PGE	E	301	-	-	-	X
4	PG4	D	301	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11645 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	6	0
			1806	1158	306	333	9			
1	B	216	Total	C	N	O	S	0	4	0
			1770	1138	295	328	9			
1	C	216	Total	C	N	O	S	0	4	0
			1746	1119	295	323	9			
1	D	217	Total	C	N	O	S	0	2	0
			1778	1141	299	329	9			
1	E	216	Total	C	N	O	S	0	3	0
			1777	1141	299	328	9			
1	F	218	Total	C	N	O	S	0	3	0
			1753	1122	296	326	9			

There are 264 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	61	NFA	PHE	MICROHETEROGENEITY	UNP Q5TLG6
A	63	IEY	CYS	CHROMOPHORE	UNP Q5TLG6
A	63	IEY	TYR	CHROMOPHORE	UNP Q5TLG6
A	63	IEY	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	THR	-	EXPRESSION TAG	UNP Q5TLG6
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	61	NFA	PHE	MICROHETEROGENEITY	UNP Q5TLG6
B	63	IEY	CYS	CHROMOPHORE	UNP Q5TLG6
B	63	IEY	TYR	CHROMOPHORE	UNP Q5TLG6
B	63	IEY	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	SER	-	EXPRESSION TAG	UNP Q5TLG6
C	-21	MET	-	EXPRESSION TAG	UNP Q5TLG6
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	61	NFA	PHE	MICROHETEROGENEITY	UNP Q5TLG6
C	63	IEY	CYS	CHROMOPHORE	UNP Q5TLG6
C	63	IEY	TYR	CHROMOPHORE	UNP Q5TLG6
C	63	IEY	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-24	MET	-	EXPRESSION TAG	UNP Q5TLG6
D	-23	ALA	-	EXPRESSION TAG	UNP Q5TLG6
D	-22	SER	-	EXPRESSION TAG	UNP Q5TLG6
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	61	NFA	PHE	MICROHETEROGENEITY	UNP Q5TLG6
D	63	IEY	CYS	CHROMOPHORE	UNP Q5TLG6
D	63	IEY	TYR	CHROMOPHORE	UNP Q5TLG6
D	63	IEY	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	61	NFA	PHE	MICROHETEROGENEITY	UNP Q5TLG6
E	63	IEY	CYS	CHROMOPHORE	UNP Q5TLG6
E	63	IEY	TYR	CHROMOPHORE	UNP Q5TLG6
E	63	IEY	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

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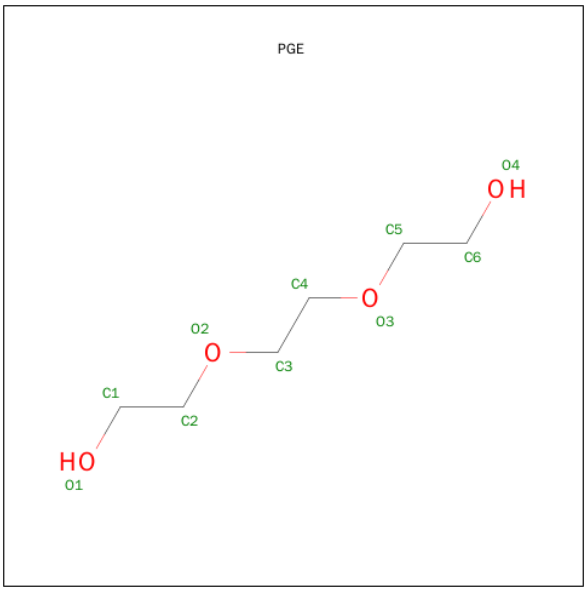
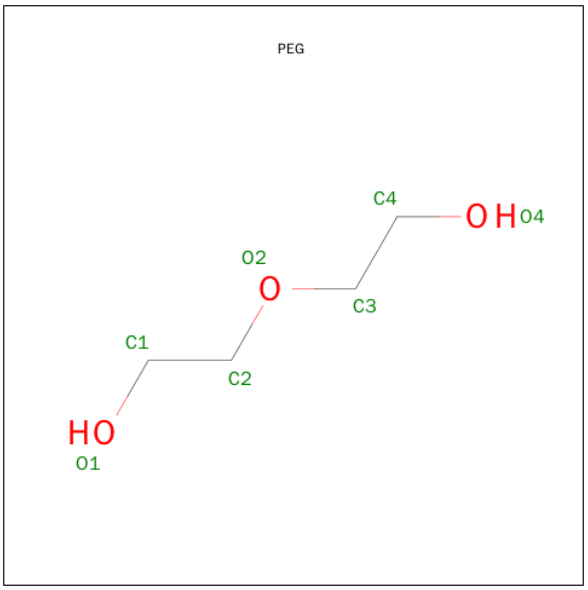
Chain	Residue	Modelled	Actual	Comment	Reference
F	-28	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-27	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-26	HIS	-	EXPRESSION TAG	UNP Q5TLG6
F	-25	GLY	-	EXPRESSION TAG	UNP Q5TLG6
F	-24	MET	-	EXPRESSION TAG	UNP Q5TLG6
F	-23	ALA	-	EXPRESSION TAG	UNP Q5TLG6
F	-22	SER	-	EXPRESSION TAG	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	61	NFA	PHE	MICROHETEROGENEITY	UNP Q5TLG6
F	63	IEY	CYS	CHROMOPHORE	UNP Q5TLG6
F	63	IEY	TYR	CHROMOPHORE	UNP Q5TLG6
F	63	IEY	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 TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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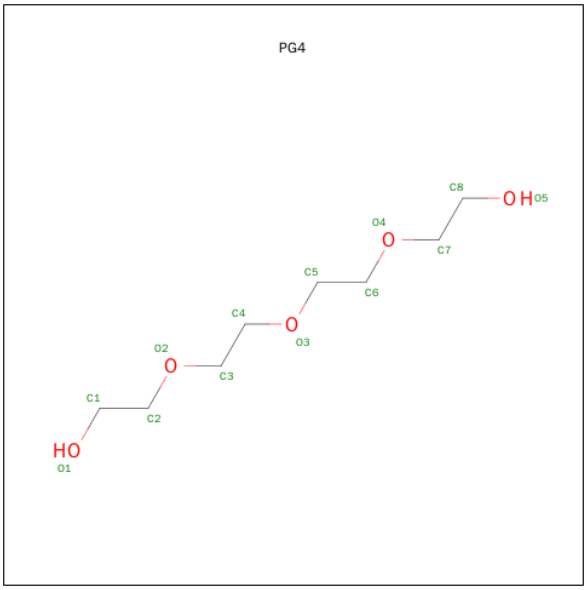
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 7 4 3	0	0

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



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

- Molecule 5 is water.

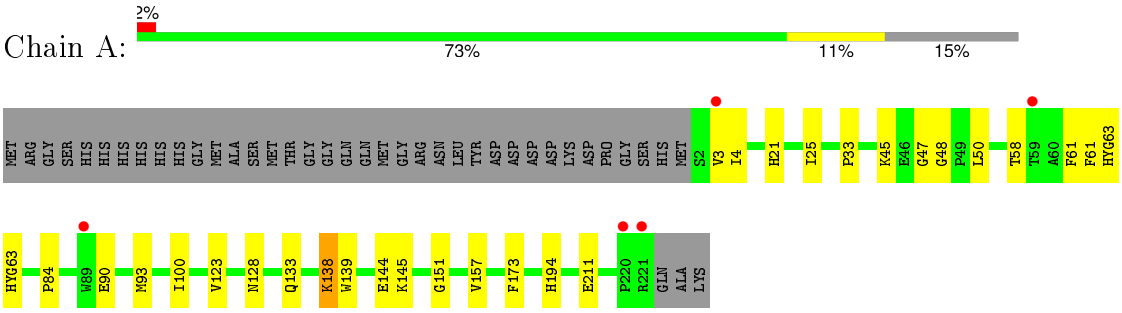
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	164	Total O 164 164	0	0
5	B	176	Total O 176 176	0	0
5	C	180	Total O 180 180	0	0
5	D	163	Total O 163 163	0	0
5	E	145	Total O 145 145	0	0
5	F	130	Total O 130 130	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

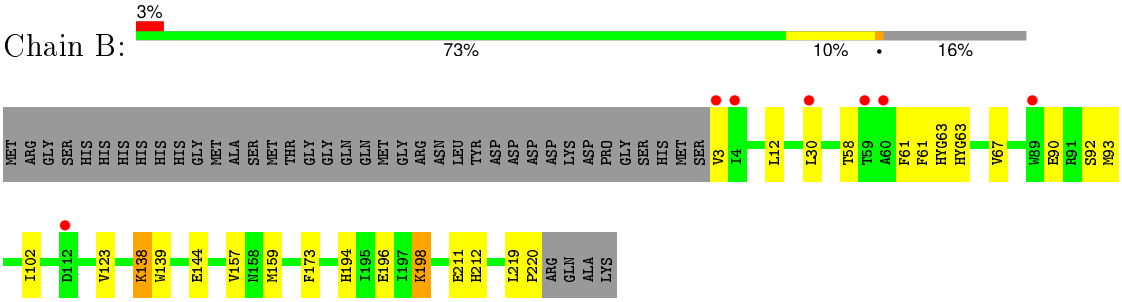
- Molecule 1: Fluorescent protein Dronpa

Chain A:



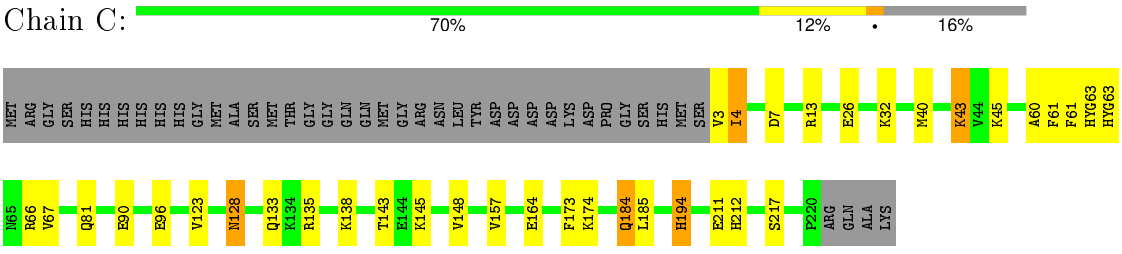
- Molecule 1: Fluorescent protein Dronpa

Chain B:



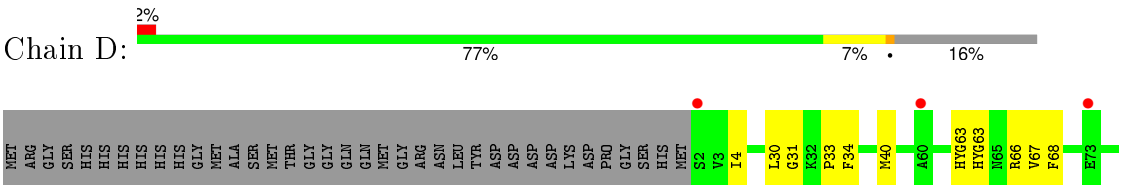
- Molecule 1: Fluorescent protein Dronpa

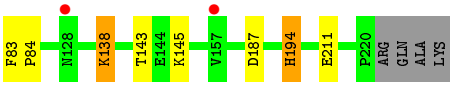
Chain C:



- Molecule 1: Fluorescent protein Dronpa

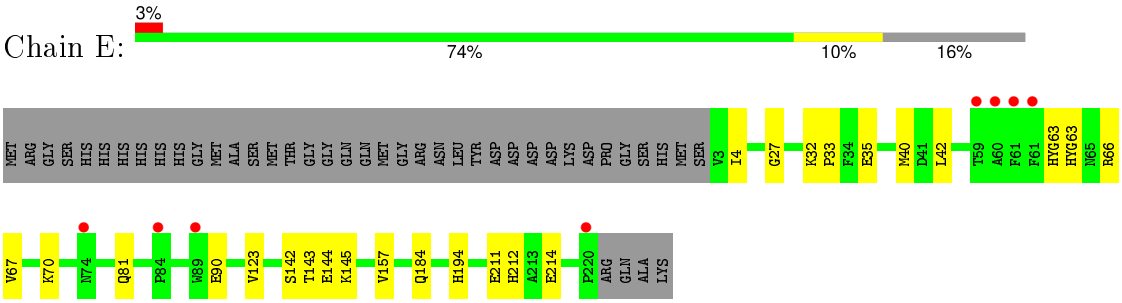
Chain D:





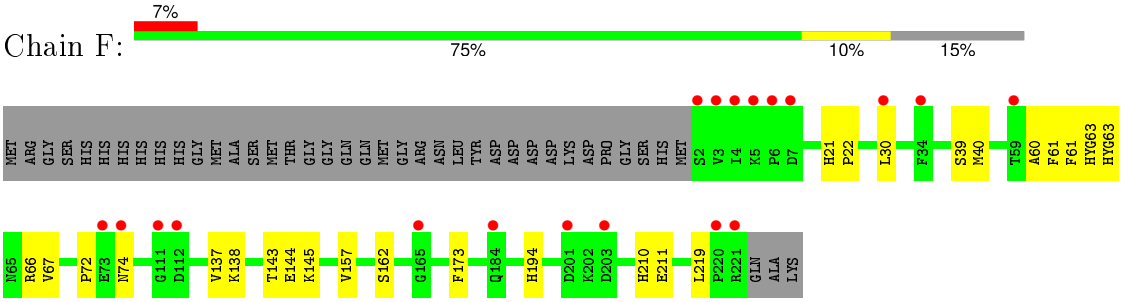
• Molecule 1: Fluorescent protein Dronpa

Chain E:



• Molecule 1: Fluorescent protein Dronpa

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.21Å 106.13Å 178.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.05 29.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.67-2.05) 100.0 (29.67-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.04Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.178 , 0.233 0.182 , 0.230	Depositor DCC
R_{free} test set	4293 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 85788 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11645	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IEY, PGE, NFA, CR8, PG4, 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	0.52	0/1804	0.62	0/2434
1	B	0.49	0/1761	0.65	0/2381
1	C	0.52	0/1761	0.65	0/2378
1	D	0.51	0/1762	0.63	0/2378
1	E	0.50	0/1764	0.64	0/2381
1	F	0.45	0/1767	0.61	0/2387
All	All	0.50	0/10619	0.63	0/14339

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	1806	0	1721	20	0
1	B	1770	0	1667	15	0
1	C	1746	0	1678	29	0
1	D	1778	0	1689	13	0
1	E	1777	0	1690	15	0
1	F	1753	0	1672	15	0
2	A	10	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	14	2	0
2	E	10	0	14	0	0
3	C	7	0	10	1	0
3	D	7	0	10	0	0
4	D	13	0	18	0	0
5	A	164	0	0	0	0
5	B	176	0	0	1	0
5	C	180	0	0	3	0
5	D	163	0	0	2	0
5	E	145	0	0	0	0
5	F	130	0	0	0	0
All	All	11645	0	10197	95	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 5.

All (95) 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:A:48:GLY:O	1:C:135[A]:ARG:NE	2.11	0.81
1:A:48:GLY:H	1:C:133:GLN:HE21	1.37	0.73
1:A:151:GLY:HA3	2:A:301:PGE:H6	1.71	0.72
1:A:47:GLY:HA2	1:C:135[B]:ARG:HD3	1.73	0.70
1:C:26:GLU:HB2	1:C:45:LYS:HD2	1.71	0.70
1:F:63[B]:IEY:HD3	1:F:211:GLU:HB2	1.74	0.70
1:C:40:MET:HG2	1:C:63[B]:IEY:H22	1.74	0.67
1:C:60:ALA:O	1:C:61[B]:NFA:NXT	2.30	0.65
1:D:187:ASP:OD2	5:D:515:HOH:O	2.14	0.65
1:A:21:HIS:ND1	1:C:164[A]:GLU:OE1	2.29	0.64
1:C:61[B]:NFA:O	1:C:63[B]:IEY:HA1	2.00	0.62
1:A:48:GLY:H	1:C:133:GLN:NE2	1.99	0.61
1:D:40:MET:HG2	1:D:63[B]:IEY:H22	1.82	0.60
1:B:196:GLU:OE2	1:B:198:LYS:NZ	2.29	0.59
1:C:135[B]:ARG:NH2	5:C:490:HOH:O	2.14	0.58
1:E:81:GLN:HE22	1:E:184:GLN:HB3	1.68	0.57
1:A:128[A]:ASN:OD1	1:A:133:GLN:NE2	2.38	0.57
1:A:90:GLU:HB3	1:B:123:VAL:HB	1.88	0.56
1:F:138:LYS:NZ	1:F:194:HIS:HE1	2.04	0.56
1:C:90:GLU:HB3	1:E:123:VAL:HB	1.88	0.56
1:D:4:ILE:HD11	1:D:33:PRO:HB3	1.88	0.55
1:B:3:VAL:N	5:B:451:HOH:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:HE22	1:C:184:GLN:H	1.55	0.55
1:C:174:LYS:NZ	5:C:523:HOH:O	2.40	0.53
1:E:144:GLU:HA	1:E:157:VAL:HB	1.91	0.53
1:A:3:VAL:HG11	1:A:84:PRO:HB3	1.92	0.52
1:D:4:ILE:HG23	1:D:34:PHE:HZ	1.74	0.52
1:E:40:MET:HG2	1:E:63[B]:IEY:H22	1.91	0.52
1:C:143:THR:H	1:D:145:LYS:NZ	2.08	0.51
1:C:123:VAL:HB	1:E:90:GLU:HB3	1.91	0.51
1:E:63[B]:IEY:OH	1:E:142:SER:OG	2.29	0.50
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.93	0.50
1:A:144:GLU:HA	1:A:157:VAL:HB	1.94	0.49
1:C:13:ARG:NH1	1:C:26:GLU:OE2	2.42	0.49
1:F:157:VAL:HG13	1:F:173:PHE:HB2	1.95	0.49
1:A:138:LYS:NZ	1:A:139:TRP:O	2.42	0.48
1:A:93:MET:HG2	1:A:173:PHE:CE1	2.48	0.48
1:E:32:LYS:HE2	1:E:35:GLU:OE2	2.14	0.48
1:F:72:PRO:HB2	1:F:74:ASN:OD1	2.14	0.48
1:F:40:MET:HG2	1:F:63[B]:IEY:H22	1.95	0.47
1:B:144:GLU:HA	1:B:157:VAL:HB	1.97	0.47
1:F:137:VAL:HB	1:F:162:SER:HB2	1.96	0.47
1:A:138:LYS:NZ	1:A:194:HIS:HE1	2.12	0.47
3:C:302:PEG:H22	5:C:471:HOH:O	2.16	0.46
1:D:4:ILE:HG23	1:D:34:PHE:CZ	2.51	0.46
1:B:219:LEU:HA	1:B:220:PRO:HD3	1.83	0.46
1:A:123:VAL:HB	1:B:90:GLU:HB3	1.97	0.46
1:C:138:LYS:NZ	1:C:194:HIS:HE1	2.12	0.45
1:D:138:LYS:HE2	5:D:547:HOH:O	2.16	0.45
1:F:61[B]:NFA:HD1	1:F:61[B]:NFA:HA	1.84	0.45
1:E:27:GLY:HA3	1:E:42:LEU:HD23	1.98	0.45
1:A:58:THR:HA	1:A:61[B]:NFA:HD2	1.98	0.45
1:F:61[B]:NFA:O	1:F:63[B]:IEY:HA1	2.17	0.45
1:B:58:THR:HA	1:B:61[B]:NFA:HD2	1.98	0.45
1:C:128:ASN:H	1:C:128:ASN:HD22	1.65	0.44
1:E:63[B]:IEY:HD3	1:E:211:GLU:HB2	1.99	0.44
1:E:32:LYS:HB2	1:E:35:GLU:HB2	1.99	0.44
1:D:138:LYS:NZ	1:D:194:HIS:HE1	2.15	0.44
1:F:39:SER:HG	1:F:210[B]:HIS:CE1	2.36	0.44
1:B:139:TRP:CZ3	1:B:159:MET:HB3	2.53	0.44
1:C:96:GLU:CA	2:C:301:PGE:H4	2.48	0.44
1:C:148:VAL:HG21	1:C:185:LEU:HB3	2.00	0.43
1:A:63[B]:IEY:HB1	1:A:211:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:HIS:HA	1:F:22:PRO:HD3	1.82	0.43
1:D:4:ILE:HD11	1:D:33:PRO:CB	2.48	0.43
1:B:92:SER:HA	1:B:102:ILE:HG22	2.00	0.43
1:F:60:ALA:O	1:F:61[B]:NFA:NXT	2.52	0.43
1:D:31:GLY:HA3	1:D:68:PHE:CE2	2.54	0.43
1:B:61[B]:NFA:NXT	1:B:63[B]:IEY:HA1	2.34	0.43
1:E:143:THR:H	1:F:145:LYS:NZ	2.17	0.42
1:D:63[B]:IEY:HB1	1:D:211:GLU:OE1	2.19	0.42
1:B:138:LYS:NZ	1:B:139:TRP:O	2.40	0.42
1:A:4:ILE:HD11	1:A:33:PRO:HB3	2.01	0.42
1:F:219:LEU:HD23	1:F:219:LEU:HA	1.86	0.42
1:C:3:VAL:HG13	1:C:4:ILE:HG22	2.02	0.42
1:C:145:LYS:NZ	1:D:143:THR:H	2.18	0.41
1:C:61[B]:NFA:HA	1:C:61[B]:NFA:HD1	1.82	0.41
1:C:43:LYS:HB3	1:C:43:LYS:HE2	1.79	0.41
1:F:144:GLU:HA	1:F:157:VAL:HB	2.03	0.41
1:A:45:LYS:HE3	1:A:45:LYS:HB3	1.84	0.41
1:C:96:GLU:HA	2:C:301:PGE:H4	2.02	0.41
1:C:157:VAL:CG1	1:C:173:PHE:HB2	2.51	0.41
1:B:63[B]:IEY:HD3	1:B:211:GLU:HB2	2.03	0.41
1:B:93:MET:HG2	1:B:173:PHE:CE1	2.55	0.41
1:C:7:ASP:OD1	1:C:32:LYS:NZ	2.41	0.41
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.03	0.41
1:E:145:LYS:NZ	1:F:143:THR:H	2.18	0.41
1:E:211:GLU:HG2	1:E:212:HIS:N	2.36	0.41
1:C:81:GLN:HE22	1:C:184:GLN:HB2	1.85	0.40
1:A:25:ILE:HD11	1:A:50:LEU:HD11	2.02	0.40
1:A:138:LYS:HZ1	1:A:194:HIS:HE1	1.69	0.40
1:E:4:ILE:HD11	1:E:33:PRO:HB3	2.02	0.40
1:B:12:LEU:HD12	1:B:12:LEU:C	2.42	0.40
1:C:211:GLU:HG2	1:C:212:HIS:N	2.36	0.40
1:B:211:GLU:HG2	1:B:212:HIS:N	2.36	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	218/260 (84%)	214 (98%)	4 (2%)	0	100	100
1	B	214/260 (82%)	212 (99%)	2 (1%)	0	100	100
1	C	214/260 (82%)	213 (100%)	1 (0%)	0	100	100
1	D	213/260 (82%)	211 (99%)	2 (1%)	0	100	100
1	E	213/260 (82%)	211 (99%)	2 (1%)	0	100	100
1	F	215/260 (83%)	212 (99%)	3 (1%)	0	100	100
All	All	1287/1560 (82%)	1273 (99%)	14 (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	189/218 (87%)	186 (98%)	3 (2%)	70	67
1	B	182/218 (84%)	177 (97%)	5 (3%)	52	45
1	C	183/218 (84%)	175 (96%)	8 (4%)	35	26
1	D	184/218 (84%)	179 (97%)	5 (3%)	52	45
1	E	184/218 (84%)	181 (98%)	3 (2%)	70	67
1	F	184/218 (84%)	181 (98%)	3 (2%)	70	67
All	All	1106/1308 (85%)	1079 (98%)	27 (2%)	55	50

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	138	LYS
1	A	145	LYS

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	67	VAL
1	B	138	LYS
1	B	194	HIS
1	B	198	LYS
1	C	4	ILE
1	C	43	LYS
1	C	66	ARG
1	C	67	VAL
1	C	128	ASN
1	C	184	GLN
1	C	194	HIS
1	C	217	SER
1	D	30	LEU
1	D	66	ARG
1	D	67	VAL
1	D	138	LYS
1	D	194	HIS
1	E	66	ARG
1	E	67	VAL
1	E	194	HIS
1	F	30	LEU
1	F	66	ARG
1	F	67	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	194	HIS
1	B	133	GLN
1	B	194	HIS
1	C	81	GLN
1	C	128	ASN
1	C	133	GLN
1	C	194	HIS
1	D	21	HIS
1	D	194	HIS
1	E	194	HIS
1	F	21	HIS
1	F	158	ASN
1	F	194	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

16 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	NFA	A	61[B]	1	12,12,12	1.61	1 (8%)	15,15,15	1.35	3 (20%)
1	CR8	A	63[A]	1	20,27,28	2.04	6 (30%)	16,37,39	1.23	2 (12%)
1	IEY	A	63[B]	1	19,26,27	3.82	3 (15%)	18,35,37	1.95	3 (16%)
1	NFA	B	61[B]	1	12,12,12	1.64	1 (8%)	15,15,15	1.17	3 (20%)
1	CR8	B	63[A]	1	20,27,28	1.96	5 (25%)	16,37,39	1.18	0
1	IEY	B	63[B]	1	19,26,27	3.92	3 (15%)	18,35,37	1.99	4 (22%)
1	NFA	C	61[B]	1	12,12,12	1.66	1 (8%)	15,15,15	2.06	4 (26%)
1	IEY	C	63[B]	1	19,26,27	3.80	4 (21%)	18,35,37	2.18	4 (22%)
1	NFA	D	61[B]	1	12,12,12	1.56	1 (8%)	15,15,15	1.36	3 (20%)
1	CR8	D	63[A]	1	20,27,28	2.01	5 (25%)	16,37,39	1.14	1 (6%)
1	IEY	D	63[B]	1	19,26,27	4.08	3 (15%)	18,35,37	1.97	4 (22%)
1	NFA	E	61[B]	1	12,12,12	1.60	1 (8%)	15,15,15	1.26	2 (13%)
1	CR8	E	63[A]	1	20,27,28	2.00	5 (25%)	16,37,39	1.33	2 (12%)
1	IEY	E	63[B]	1	19,26,27	3.87	2 (10%)	18,35,37	2.24	4 (22%)
1	NFA	F	61[B]	1	12,12,12	1.55	1 (8%)	15,15,15	1.21	1 (6%)
1	IEY	F	63[B]	1	19,26,27	4.10	2 (10%)	18,35,37	2.09	3 (16%)

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	NFA	A	61[B]	1	-	0/7/8/8	0/1/1/1
1	CR8	A	63[A]	1	-	0/8/25/26	0/3/3/3
1	IEY	A	63[B]	1	-	0/3/12/13	0/3/3/3
1	NFA	B	61[B]	1	-	0/7/8/8	0/1/1/1
1	CR8	B	63[A]	1	-	0/8/25/26	0/3/3/3
1	IEY	B	63[B]	1	-	0/3/12/13	0/3/3/3
1	NFA	C	61[B]	1	-	0/7/8/8	0/1/1/1
1	IEY	C	63[B]	1	-	0/3/12/13	0/3/3/3
1	NFA	D	61[B]	1	-	0/7/8/8	0/1/1/1
1	CR8	D	63[A]	1	-	0/8/25/26	0/3/3/3
1	IEY	D	63[B]	1	-	0/3/12/13	0/3/3/3
1	NFA	E	61[B]	1	-	0/7/8/8	0/1/1/1
1	CR8	E	63[A]	1	-	0/8/25/26	0/3/3/3
1	IEY	E	63[B]	1	-	0/3/12/13	0/3/3/3
1	NFA	F	61[B]	1	-	0/7/8/8	0/1/1/1
1	IEY	F	63[B]	1	-	0/3/12/13	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63[B]	IEY	CB2-CA2	-17.27	1.37	1.51
1	D	63[B]	IEY	CB2-CA2	-17.16	1.37	1.51
1	B	63[B]	IEY	CB2-CA2	-16.46	1.37	1.51
1	E	63[B]	IEY	CB2-CA2	-16.27	1.38	1.51
1	A	63[B]	IEY	CB2-CA2	-15.89	1.38	1.51
1	C	63[B]	IEY	CB2-CA2	-15.63	1.38	1.51
1	C	63[B]	IEY	CA3-N3	-3.33	1.43	1.49
1	E	63[A]	CR8	C4-C1	-2.79	1.39	1.45
1	D	63[A]	CR8	C4-C1	-2.79	1.39	1.45
1	A	63[B]	IEY	C1-N2	-2.71	1.30	1.35
1	E	63[A]	CR8	C2-C1	-2.68	1.39	1.45
1	A	63[A]	CR8	C4-C1	-2.62	1.39	1.45
1	A	63[A]	CR8	C2-C1	-2.51	1.40	1.45
1	B	63[A]	CR8	C4-C1	-2.50	1.40	1.45
1	C	63[B]	IEY	O2-C2	-2.39	1.23	1.32
1	D	63[A]	CR8	C2-C1	-2.36	1.40	1.45
1	E	63[B]	IEY	O2-C2	-2.35	1.23	1.32
1	B	63[A]	CR8	C2-C1	-2.35	1.40	1.45
1	A	63[A]	CR8	C17-N13	-2.33	1.44	1.49
1	D	63[B]	IEY	O2-C2	-2.28	1.24	1.32
1	F	63[B]	IEY	O2-C2	-2.28	1.24	1.32
1	B	63[B]	IEY	O2-C2	-2.26	1.24	1.32
1	C	63[B]	IEY	C1-N2	-2.21	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63[B]	IEY	C1-N2	-2.20	1.31	1.35
1	A	63[B]	IEY	O2-C2	-2.19	1.24	1.32
1	D	63[B]	IEY	C1-N2	-2.07	1.31	1.35
1	D	63[A]	CR8	C9-C12	3.55	1.48	1.39
1	A	63[A]	CR8	C9-C12	3.61	1.48	1.39
1	B	63[A]	CR8	C9-C12	3.62	1.48	1.39
1	E	63[A]	CR8	C9-C12	3.70	1.48	1.39
1	A	63[A]	CR8	C8-C7	4.14	1.46	1.36
1	D	63[A]	CR8	C8-C7	4.26	1.46	1.36
1	E	63[A]	CR8	O3-C1	4.29	1.37	1.24
1	B	63[A]	CR8	O3-C1	4.30	1.38	1.24
1	B	63[A]	CR8	C8-C7	4.32	1.47	1.36
1	E	63[A]	CR8	C8-C7	4.37	1.47	1.36
1	A	63[A]	CR8	O3-C1	4.57	1.38	1.24
1	D	63[A]	CR8	O3-C1	4.75	1.39	1.24
1	F	61[B]	NFA	C-NXT	5.06	1.42	1.32
1	D	61[B]	NFA	C-NXT	5.12	1.43	1.32
1	A	61[B]	NFA	C-NXT	5.25	1.43	1.32
1	E	61[B]	NFA	C-NXT	5.26	1.43	1.32
1	B	61[B]	NFA	C-NXT	5.41	1.43	1.32
1	C	61[B]	NFA	C-NXT	5.50	1.43	1.32

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	61[B]	NFA	CG-CB-CA	-3.83	105.30	114.31
1	E	63[B]	IEY	CG1-CD3-NE1	-3.55	102.22	108.62
1	A	63[B]	IEY	CG1-CD3-NE1	-3.35	102.58	108.62
1	A	61[B]	NFA	O-C-NXT	-3.34	118.13	123.08
1	D	63[B]	IEY	CG1-CD3-NE1	-3.32	102.64	108.62
1	F	61[B]	NFA	CG-CB-CA	-3.16	106.88	114.31
1	E	61[B]	NFA	CG-CB-CA	-3.14	106.93	114.31
1	B	63[B]	IEY	CG1-CD3-NE1	-3.14	102.96	108.62
1	D	61[B]	NFA	CG-CB-CA	-3.09	107.05	114.31
1	D	61[B]	NFA	O-C-NXT	-2.90	118.78	123.08
1	F	63[B]	IEY	CG1-CD3-NE1	-2.86	103.47	108.62
1	C	61[B]	NFA	O-C-NXT	-2.64	119.17	123.08
1	C	63[B]	IEY	CG1-CD3-NE1	-2.59	103.95	108.62
1	A	63[A]	CR8	C2-C6-C7	-2.57	119.72	122.00
1	E	63[A]	CR8	C2-C6-C7	-2.55	119.74	122.00
1	B	61[B]	NFA	CG-CB-CA	-2.52	108.39	114.31
1	C	63[B]	IEY	CB2-CA2-C2	-2.44	121.91	129.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	61[B]	NFA	O-C-NXT	-2.39	119.53	123.08
1	F	63[B]	IEY	CB2-CA2-C2	-2.37	122.15	129.62
1	E	63[B]	IEY	CB2-CA2-C2	-2.14	122.85	129.62
1	A	61[B]	NFA	CG-CB-CA	-2.11	109.34	114.31
1	D	63[B]	IEY	CB2-CA2-C2	-2.11	122.96	129.62
1	B	61[B]	NFA	O-C-NXT	-2.11	119.96	123.08
1	A	63[B]	IEY	CB2-CA2-C2	-2.10	122.99	129.62
1	B	63[B]	IEY	CB2-CA2-C2	-2.00	123.30	129.62
1	C	63[B]	IEY	C-CA3-N3	2.12	115.82	112.37
1	B	61[B]	NFA	CA-C-NXT	2.35	120.41	116.62
1	B	63[B]	IEY	C-CA3-N3	2.35	116.19	112.37
1	A	61[B]	NFA	CA-C-NXT	2.44	120.54	116.62
1	D	63[B]	IEY	C-CA3-N3	2.49	116.42	112.37
1	D	61[B]	NFA	CA-C-NXT	2.56	120.73	116.62
1	A	63[A]	CR8	C-C17-N13	2.59	116.58	112.37
1	E	63[A]	CR8	C-C17-N13	2.61	116.60	112.37
1	D	63[A]	CR8	C-C17-N13	2.63	116.64	112.37
1	E	63[B]	IEY	C-CA3-N3	3.82	118.58	112.37
1	C	61[B]	NFA	CB-CA-C	4.08	116.64	108.44
1	C	61[B]	NFA	O-C-CA	4.60	126.60	120.33
1	D	63[B]	IEY	CG2-CB2-CA2	6.58	125.82	112.58
1	A	63[B]	IEY	CG2-CB2-CA2	6.68	126.04	112.58
1	B	63[B]	IEY	CG2-CB2-CA2	6.97	126.61	112.58
1	E	63[B]	IEY	CG2-CB2-CA2	7.17	127.01	112.58
1	F	63[B]	IEY	CG2-CB2-CA2	7.51	127.69	112.58
1	C	63[B]	IEY	CG2-CB2-CA2	7.94	128.56	112.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	61[B]	NFA	1	0
1	A	63[B]	IEY	1	0
1	B	61[B]	NFA	2	0
1	B	63[B]	IEY	2	0
1	C	61[B]	NFA	3	0
1	C	63[B]	IEY	2	0
1	D	63[B]	IEY	2	0
1	E	63[B]	IEY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	61[B]	NFA	3	0
1	F	63[B]	IEY	3	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
2	PGE	A	301	-	9,9,9	0.60	0	8,8,8	0.84	0
2	PGE	C	301	-	9,9,9	0.50	0	8,8,8	0.92	0
3	PEG	C	302	-	6,6,6	0.53	0	5,5,5	0.64	0
4	PG4	D	301	-	12,12,12	0.72	0	11,11,11	1.08	2 (18%)
3	PEG	D	302	-	6,6,6	0.54	0	5,5,5	0.82	0
2	PGE	E	301	-	9,9,9	0.49	0	8,8,8	0.93	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	PGE	A	301	-	-	0/7/7/7	0/0/0/0
2	PGE	C	301	-	-	0/7/7/7	0/0/0/0
3	PEG	C	302	-	-	0/4/4/4	0/0/0/0
4	PG4	D	301	-	-	0/10/10/10	0/0/0/0
3	PEG	D	302	-	-	0/4/4/4	0/0/0/0
2	PGE	E	301	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	301	PG4	C7-O4-C6	2.05	122.14	113.31
4	D	301	PG4	C5-O3-C4	2.10	122.33	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PGE	1	0
2	C	301	PGE	2	0
3	C	302	PEG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	216/260 (83%)	-0.12	5 (2%) 64 70	18, 26, 45, 71	0
1	B	214/260 (82%)	-0.04	7 (3%) 50 57	18, 27, 45, 65	0
1	C	214/260 (82%)	-0.24	0 100 100	17, 25, 43, 58	0
1	D	215/260 (82%)	-0.10	5 (2%) 64 70	17, 26, 43, 63	0
1	E	214/260 (82%)	-0.03	6 (2%) 56 63	19, 28, 43, 67	0
1	F	216/260 (83%)	0.40	19 (8%) 12 13	21, 32, 53, 81	0
All	All	1289/1560 (82%)	-0.02	42 (3%) 50 57	17, 28, 45, 81	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	5.9
1	F	3	VAL	5.8
1	F	4	ILE	4.3
1	F	34	PHE	3.9
1	F	221	ARG	3.7
1	F	2	SER	3.3
1	F	220	PRO	3.1
1	B	89	TRP	3.1
1	F	6	PRO	3.1
1	F	74	ASN	3.0
1	E	60	ALA	3.0
1	A	220	PRO	3.0
1	F	73	GLU	2.9
1	D	128	ASN	2.8
1	F	165	GLY	2.8
1	A	3	VAL	2.8
1	E	89	TRP	2.7
1	F	184	GLN	2.6
1	B	59	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	60	ALA	2.6
1	F	7	ASP	2.5
1	E	59	THR	2.5
1	F	112	ASP	2.4
1	F	30	LEU	2.4
1	F	59	THR	2.4
1	F	111	GLY	2.4
1	F	201	ASP	2.3
1	D	73	GLU	2.3
1	A	89	TRP	2.3
1	A	221	ARG	2.3
1	B	112	ASP	2.3
1	D	2	SER	2.2
1	F	203	ASP	2.2
1	D	157	VAL	2.2
1	D	60	ALA	2.2
1	E	74	ASN	2.2
1	A	59	THR	2.2
1	E	220	PRO	2.1
1	B	4	ILE	2.1
1	B	30	LEU	2.1
1	E	84	PRO	2.1
1	F	5	LYS	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
1	NFA	F	61[B]	12/12	0.93	0.24	-	22,25,38,41	12
1	NFA	A	61[B]	12/12	0.97	0.17	-	21,23,25,26	12
1	CR8	A	63[A]	25/26	0.96	0.19	-	18,23,26,31	25
1	IEY	A	63[B]	24/25	0.97	0.19	-	18,23,27,29	24
1	IEY	E	63[B]	24/25	0.96	0.19	-	21,25,31,35	24
1	IEY	F	63[B]	24/25	0.90	0.26	-	19,29,37,40	24
1	IEY	B	63[B]	24/25	0.95	0.17	-	22,26,30,31	24
1	NFA	B	61[B]	12/12	0.96	0.21	-	22,24,27,27	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	NFA	D	61[B]	12/12	0.97	0.16	-	20,22,23,23	12
1	NFA	C	61[B]	12/12	0.94	0.18	-	12,15,20,27	0
1	CR8	B	63[A]	25/26	0.95	0.18	-	22,26,30,33	25
1	IEY	C	63[B]	24/25	0.96	0.19	-	11,15,25,27	0
1	CR8	D	63[A]	25/26	0.94	0.19	-	19,23,27,34	25
1	IEY	D	63[B]	24/25	0.94	0.18	-	20,23,27,32	24
1	CR8	E	63[A]	25/26	0.96	0.19	-	22,25,31,37	25
1	NFA	E	61[B]	12/12	0.95	0.26	-	21,25,26,26	12

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PGE	C	301	10/10	0.85	0.22	7.55	21,46,54,58	0
4	PG4	D	301	13/13	0.87	0.21	4.72	31,44,58,62	0
2	PGE	E	301	10/10	0.92	0.20	3.75	23,40,50,53	0
2	PGE	A	301	10/10	0.89	0.14	2.12	40,54,66,69	0
3	PEG	C	302	7/7	0.88	0.14	0.87	37,46,53,54	0
3	PEG	D	302	7/7	0.81	0.14	0.69	45,49,59,62	0

6.5 Other polymers (i)

There are no such residues in this entry.