



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2023 – 06:36 PM EDT

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

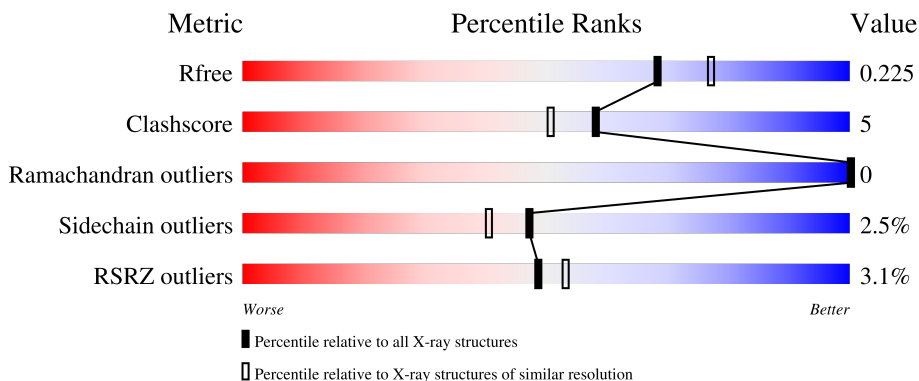
1 Overall quality at a glance

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	 2% 73% 10% 15%
1	B	260	 2% 73% 8% 16%
1	C	260	 70% 11% 16%
1	D	260	 2% 77% 6% 16%
1	E	260	 3% 74% 9% 16%

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Mol	Chain	Length	Quality of chain
1	F	260	

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
1	IEY	A	63[B]	X	-	-	-
1	IEY	B	63[B]	X	-	-	-
1	IEY	C	63[B]	X	-	-	-
1	IEY	D	63[B]	X	-	-	-
1	IEY	E	63[B]	X	-	-	-
1	IEY	F	63[B]	X	-	-	-

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	218	Total 1806	C 1158	N 306	O 333	S 9	0	6	0
1	B	216	Total 1770	C 1138	N 295	O 328	S 9	0	4	0
1	C	216	Total 1746	C 1119	N 295	O 323	S 9	0	4	0
1	D	217	Total 1778	C 1141	N 299	O 329	S 9	0	2	0
1	E	216	Total 1777	C 1141	N 299	O 328	S 9	0	3	0
1	F	218	Total 1753	C 1122	N 296	O 326	S 9	0	3	0

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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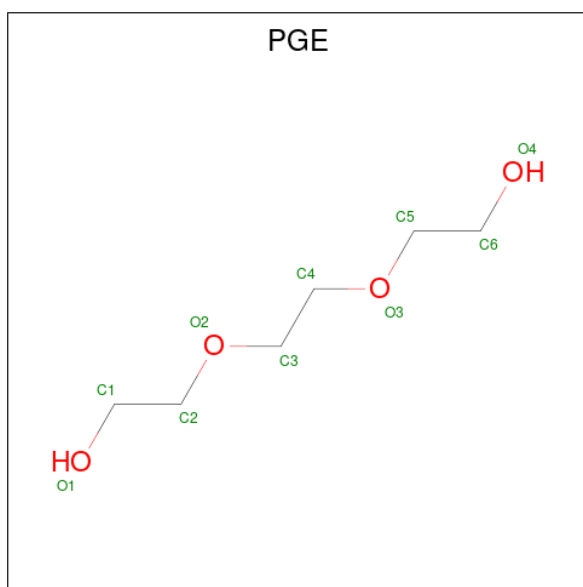
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E	-26	HIS	-	expression tag	UNP Q5TLG6
E	-25	GLY	-	expression tag	UNP Q5TLG6
E	-24	MET	-	expression tag	UNP Q5TLG6
E	-23	ALA	-	expression tag	UNP Q5TLG6
E	-22	SER	-	expression tag	UNP Q5TLG6
E	-21	MET	-	expression tag	UNP Q5TLG6
E	-20	THR	-	expression 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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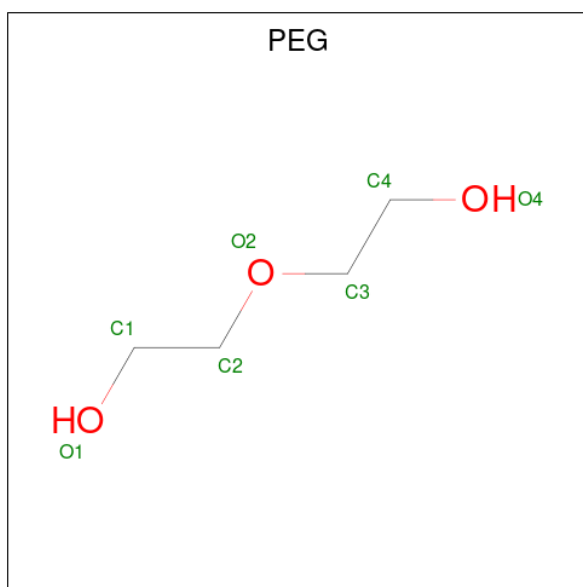
Chain	Residue	Modelled	Actual	Comment	Reference
F	-28	HIS	-	expression tag	UNP Q5TLG6
F	-27	HIS	-	expression tag	UNP Q5TLG6
F	-26	HIS	-	expression tag	UNP Q5TLG6
F	-25	GLY	-	expression tag	UNP Q5TLG6
F	-24	MET	-	expression tag	UNP Q5TLG6
F	-23	ALA	-	expression tag	UNP Q5TLG6
F	-22	SER	-	expression tag	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: C₆H₁₄O₄).



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: C₄H₁₀O₃).



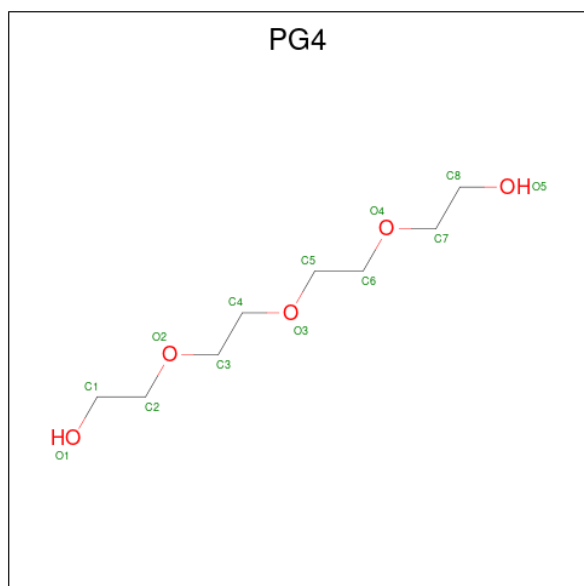
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

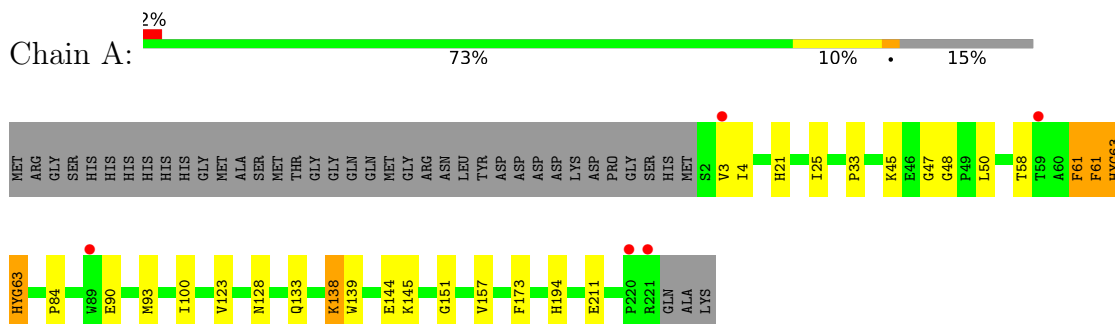
- Molecule 5 is water.

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

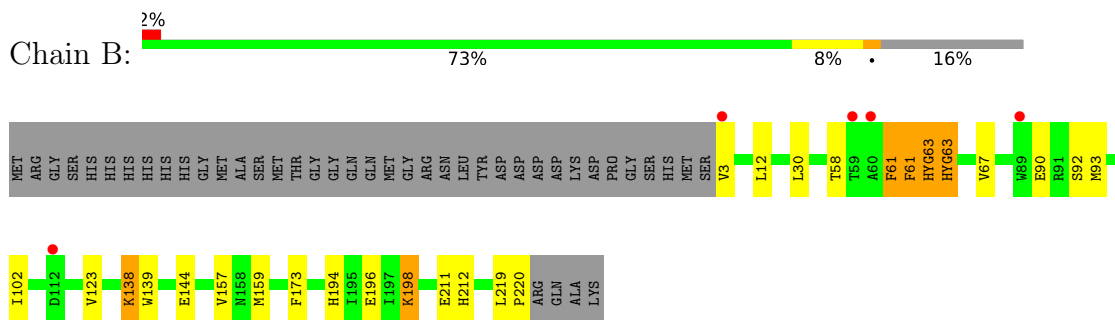
3 Residue-property plots [i](#)

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.

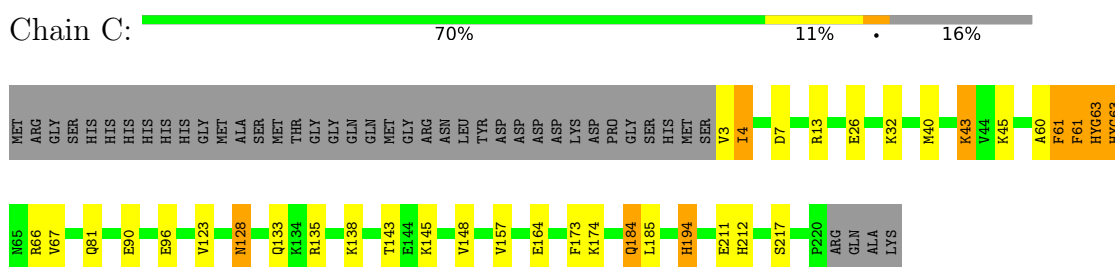
- Molecule 1: Fluorescent protein Dronpa



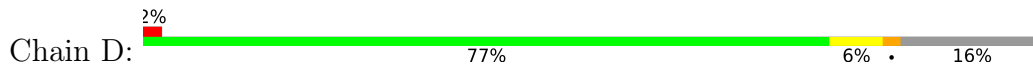
- Molecule 1: Fluorescent protein Dronpa

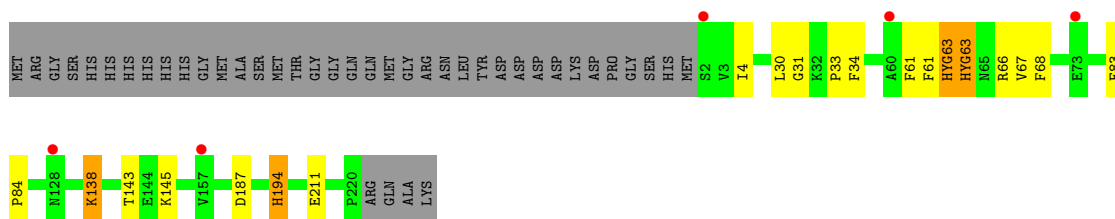


- Molecule 1: Fluorescent protein Dronpa

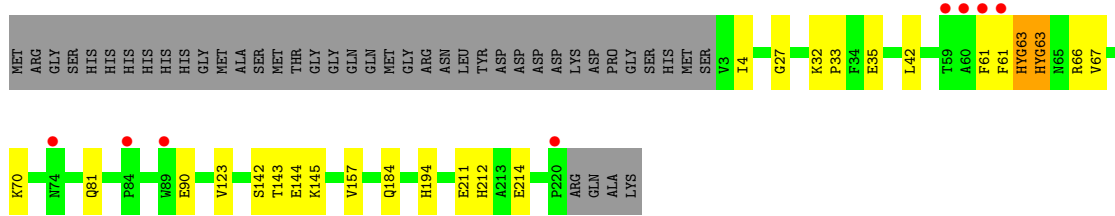
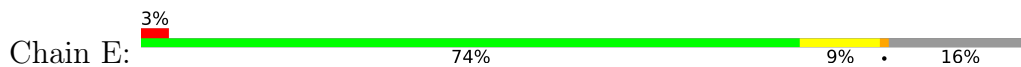


- Molecule 1: Fluorescent protein Dronpa

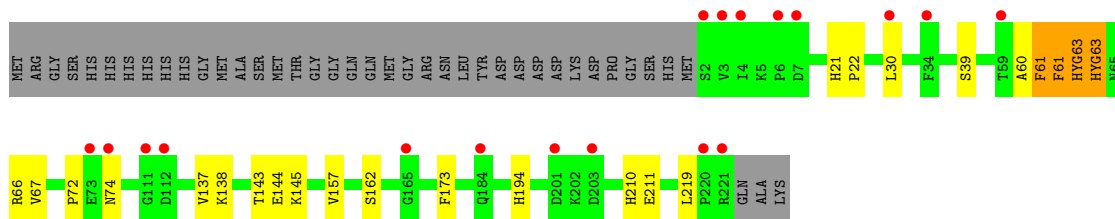
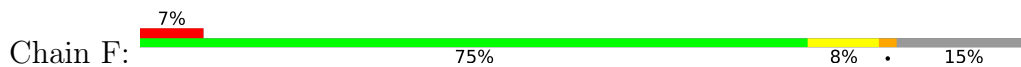




• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, 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
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.04Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.178 , 0.233 0.174 , 0.225	Depositor DCC
R_{free} test set	4293 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, IEY, PEG, CR8, NFA, 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	0.52	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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
1	E	1	0
1	F	1	0
All	All	6	0

There are no bond length outliers.

There are no bond angle outliers.

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63[B]	IEY	CA2
1	B	63[B]	IEY	CA2
1	C	63[B]	IEY	CA2

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Mol	Chain	Res	Type	Atom
1	D	63[B]	IEY	CA2
1	E	63[B]	IEY	CA2
1	F	63[B]	IEY	CA2

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	1806	0	1707	20	0
1	B	1770	0	1653	14	0
1	C	1746	0	1673	29	0
1	D	1778	0	1675	12	0
1	E	1777	0	1676	13	0
1	F	1753	0	1667	14	0
2	A	10	0	14	1	0
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	10131	90	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 (90) 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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:27:GLY:HA3	1:E:42:LEU:HD23	1.98	0.45
1:F:61[B]:NFA:HD1	1:F:61[B]:NFA:HA	1.84	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:D:138:LYS:NZ	1:D:194:HIS:HE1	2.15	0.44
1:E:32:LYS:HB2	1:E:35:GLU:HB2	1.99	0.44
1:B:139:TRP:CZ3	1:B:159:MET:HB3	2.53	0.44
1:F:39:SER:HG	1:F:210[B]:HIS:CE1	2.36	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
1:F:21:HIS:HA	1:F:22:PRO:HD3	1.82	0.43
1:C:40:MET:HG2	1:C:63[B]:IEY:C22	2.48	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:D:31:GLY:HA3	1:D:68:PHE:CE2	2.54	0.43
1:F:60:ALA:O	1:F:61[B]:NFA:NXT	2.52	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:F:63[B]:IEY:CD3	1:F:211:GLU:HB2	2.49	0.42
1:C:145:LYS:NZ	1:D:143:THR:H	2.18	0.41
1:C:43:LYS:HE2	1:C:43:LYS:HB3	1.79	0.41
1:C:61[B]:NFA:HD1	1:C:61[B]:NFA:HA	1.82	0.41
1:F:144:GLU:HA	1:F:157:VAL:HB	2.03	0.41
1:A:45:LYS:HB3	1:A:45:LYS:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HD11	1:A:50:LEU:HD11	2.02	0.40
1:C:81:GLN:HE22	1:C:184:GLN:HB2	1.85	0.40
1:A:138:LYS:HZ1	1:A:194:HIS:HE1	1.69	0.40
1:B:12:LEU:C	1:B:12:LEU:HD12	2.42	0.40
1:E:4:ILE:HD11	1:E:33:PRO:HB3	2.02	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	217/260 (84%)	213 (98%)	4 (2%)	0	100	100
1	B	213/260 (82%)	212 (100%)	1 (0%)	0	100	100
1	C	213/260 (82%)	213 (100%)	0	0	100	100
1	D	212/260 (82%)	211 (100%)	1 (0%)	0	100	100
1	E	212/260 (82%)	210 (99%)	2 (1%)	0	100	100
1	F	214/260 (82%)	212 (99%)	2 (1%)	0	100	100
All	All	1281/1560 (82%)	1271 (99%)	10 (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%)	62	59
1	B	182/218 (84%)	177 (97%)	5 (3%)	44	38
1	C	183/218 (84%)	175 (96%)	8 (4%)	28	21
1	D	184/218 (84%)	179 (97%)	5 (3%)	44	38
1	E	184/218 (84%)	181 (98%)	3 (2%)	62	59
1	F	184/218 (84%)	181 (98%)	3 (2%)	62	59
All	All	1106/1308 (85%)	1079 (98%)	27 (2%)	47	42

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
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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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	IEY	F	63[B]	1	24,26,27	2.98	4 (16%)	24,35,37	3.69	11 (45%)
1	NFA	E	61[B]	1	12,12,12	1.28	1 (8%)	15,15,15	1.24	1 (6%)
1	IEY	B	63[B]	1	24,26,27	2.82	4 (16%)	24,35,37	3.37	10 (41%)
1	NFA	C	61[B]	1	12,12,12	1.32	1 (8%)	15,15,15	1.93	4 (26%)
1	CR8	A	63[A]	1	20,27,28	2.03	7 (35%)	17,37,39	1.37	3 (17%)
1	CR8	B	63[A]	1	20,27,28	1.96	6 (30%)	17,37,39	1.33	1 (5%)

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	1.30	1 (8%)	15,15,15	1.28	3 (20%)
1	IEY	C	63[B]	1	24,26,27	2.93	5 (20%)	24,35,37	3.65	7 (29%)
1	CR8	E	63[A]	1	20,27,28	1.99	5 (25%)	17,37,39	1.50	4 (23%)
1	CR8	D	63[A]	1	20,27,28	2.02	5 (25%)	17,37,39	1.41	2 (11%)
1	IEY	E	63[B]	1	24,26,27	2.72	4 (16%)	24,35,37	3.52	10 (41%)
1	NFA	D	61[B]	1	12,12,12	1.25	1 (8%)	15,15,15	1.31	3 (20%)
1	IEY	D	63[B]	1	24,26,27	2.90	4 (16%)	24,35,37	3.36	11 (45%)
1	NFA	F	61[B]	1	12,12,12	1.26	1 (8%)	15,15,15	1.20	1 (6%)
1	NFA	B	61[B]	1	12,12,12	1.31	1 (8%)	15,15,15	1.12	2 (13%)
1	IEY	A	63[B]	1	24,26,27	2.78	4 (16%)	24,35,37	3.37	9 (37%)

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	IEY	F	63[B]	1	1/1/4/7	6/9/28/29	0/3/3/3
1	NFA	E	61[B]	1	-	2/8/8/8	0/1/1/1
1	IEY	B	63[B]	1	1/1/4/7	7/9/28/29	0/3/3/3
1	NFA	C	61[B]	1	-	5/8/8/8	0/1/1/1
1	IEY	C	63[B]	1	1/1/4/7	4/9/28/29	0/3/3/3
1	CR8	A	63[A]	1	-	2/8/25/26	0/3/3/3
1	NFA	A	61[B]	1	-	4/8/8/8	0/1/1/1
1	CR8	B	63[A]	1	-	2/8/25/26	0/3/3/3
1	CR8	E	63[A]	1	-	2/8/25/26	0/3/3/3
1	IEY	E	63[B]	1	1/1/4/7	6/9/28/29	0/3/3/3
1	CR8	D	63[A]	1	-	2/8/25/26	0/3/3/3
1	NFA	D	61[B]	1	-	2/8/8/8	0/1/1/1
1	IEY	D	63[B]	1	1/1/4/7	6/9/28/29	0/3/3/3
1	NFA	F	61[B]	1	-	5/8/8/8	0/1/1/1
1	NFA	B	61[B]	1	-	2/8/8/8	0/1/1/1
1	IEY	A	63[B]	1	1/1/4/7	7/9/28/29	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63[B]	IEY	CB2-CA2	-10.78	1.37	1.53
1	D	63[B]	IEY	CB2-CA2	-10.72	1.37	1.53
1	B	63[B]	IEY	CB2-CA2	-10.34	1.37	1.53
1	E	63[B]	IEY	CB2-CA2	-10.24	1.38	1.53
1	A	63[B]	IEY	CB2-CA2	-10.04	1.38	1.53
1	C	63[B]	IEY	CB2-CA2	-9.90	1.38	1.53
1	C	63[B]	IEY	CA2-C2	-6.63	1.47	1.52
1	F	63[B]	IEY	CA2-C2	-6.02	1.47	1.52
1	C	63[B]	IEY	CA1-C1	5.67	1.53	1.45
1	D	63[B]	IEY	CA2-C2	-5.43	1.48	1.52
1	A	63[B]	IEY	CA2-C2	-5.06	1.48	1.52
1	A	63[B]	IEY	CA1-C1	5.02	1.52	1.45
1	D	63[B]	IEY	CA1-C1	4.98	1.52	1.45
1	B	63[B]	IEY	CA2-C2	-4.97	1.48	1.52
1	B	63[B]	IEY	CA1-C1	4.91	1.52	1.45
1	D	63[A]	CR8	O13-C11	4.83	1.39	1.24
1	F	63[B]	IEY	CA1-C1	4.83	1.52	1.45
1	F	63[B]	IEY	CA2-N2	-4.72	1.40	1.47
1	A	63[A]	CR8	O13-C11	4.65	1.38	1.24
1	E	63[B]	IEY	CA1-C1	4.65	1.51	1.45
1	B	63[B]	IEY	CA2-N2	-4.56	1.40	1.47
1	E	63[B]	IEY	CA2-N2	-4.51	1.40	1.47
1	E	63[A]	CR8	C8-C7	4.45	1.47	1.36
1	E	63[B]	IEY	CA2-C2	-4.44	1.49	1.52
1	A	63[B]	IEY	CA2-N2	-4.41	1.40	1.47
1	B	63[A]	CR8	C8-C7	4.39	1.47	1.36
1	B	63[A]	CR8	O13-C11	4.37	1.38	1.24
1	E	63[A]	CR8	O13-C11	4.36	1.37	1.24
1	D	63[B]	IEY	CA2-N2	-4.35	1.40	1.47
1	D	63[A]	CR8	C8-C7	4.33	1.46	1.36
1	C	61[B]	NFA	C-NXT	4.29	1.43	1.32
1	B	61[B]	NFA	C-NXT	4.22	1.43	1.32
1	A	63[A]	CR8	C8-C7	4.20	1.46	1.36
1	C	63[B]	IEY	CA2-N2	-4.12	1.41	1.47
1	E	61[B]	NFA	C-NXT	4.10	1.43	1.32
1	A	61[B]	NFA	C-NXT	4.09	1.43	1.32
1	D	61[B]	NFA	C-NXT	3.99	1.43	1.32
1	F	61[B]	NFA	C-NXT	3.95	1.42	1.32
1	E	63[A]	CR8	O2-C2	-2.96	1.23	1.32
1	B	63[A]	CR8	O2-C2	-2.90	1.23	1.32
1	E	63[A]	CR8	C4-C11	-2.87	1.39	1.45
1	D	63[A]	CR8	C4-C11	-2.86	1.39	1.45
1	D	63[A]	CR8	O2-C2	-2.85	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63[A]	CR8	C12-C11	-2.76	1.39	1.45
1	A	63[A]	CR8	O2-C2	-2.74	1.24	1.32
1	A	63[A]	CR8	C4-C11	-2.69	1.39	1.45
1	A	63[A]	CR8	C12-C11	-2.58	1.40	1.45
1	B	63[A]	CR8	C4-C11	-2.57	1.40	1.45
1	A	63[A]	CR8	CA3-N3	-2.42	1.44	1.49
1	D	63[A]	CR8	C12-C11	-2.42	1.40	1.45
1	B	63[A]	CR8	C12-C11	-2.42	1.40	1.45
1	A	63[A]	CR8	C1-N2	-2.15	1.31	1.34
1	C	63[B]	IEY	CA3-N3	-2.10	1.43	1.47
1	B	63[A]	CR8	CA3-N3	-2.02	1.45	1.49

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63[B]	IEY	CB2-CA2-N2	13.29	128.29	110.78
1	F	63[B]	IEY	CB2-CA2-N2	11.86	126.41	110.78
1	E	63[B]	IEY	CB2-CA2-N2	11.86	126.41	110.78
1	A	63[B]	IEY	CB2-CA2-N2	11.45	125.87	110.78
1	D	63[B]	IEY	CB2-CA2-N2	11.38	125.77	110.78
1	B	63[B]	IEY	CB2-CA2-N2	11.23	125.58	110.78
1	C	63[B]	IEY	CG2-CB2-CA2	7.55	128.56	113.40
1	F	63[B]	IEY	CG2-CB2-CA2	7.12	127.69	113.40
1	E	63[B]	IEY	CG2-CB2-CA2	6.78	127.01	113.40
1	B	63[B]	IEY	CG2-CB2-CA2	6.58	126.61	113.40
1	A	63[B]	IEY	CG2-CB2-CA2	6.29	126.04	113.40
1	D	63[B]	IEY	CG2-CB2-CA2	6.19	125.82	113.40
1	F	63[B]	IEY	CB1-CA1-C1	-5.83	113.72	122.90
1	B	63[B]	IEY	CB2-CA2-C2	5.52	123.30	110.49
1	A	63[B]	IEY	CB2-CA2-C2	5.39	122.99	110.49
1	D	63[B]	IEY	CB2-CA2-C2	5.38	122.96	110.49
1	E	63[B]	IEY	CB2-CA2-C2	5.33	122.85	110.49
1	F	63[B]	IEY	CB2-CA2-C2	5.03	122.15	110.49
1	C	63[B]	IEY	CB2-CA2-C2	4.93	121.91	110.49
1	C	61[B]	NFA	O-C-CA	4.29	126.60	120.30
1	C	61[B]	NFA	CG-CB-CA	-4.25	105.30	114.13
1	C	63[B]	IEY	CB1-CA1-C1	-4.01	116.58	122.90
1	F	63[B]	IEY	O2-C2-N3	3.88	128.88	124.14
1	F	63[B]	IEY	CA1-C1-N2	-3.87	120.26	125.17
1	D	63[B]	IEY	O2-C2-N3	3.86	128.87	124.14
1	E	63[B]	IEY	CA3-N3-C2	3.69	126.78	123.43
1	F	63[B]	IEY	CA2-N2-C1	-3.66	103.59	107.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63[B]	IEY	O2-C2-N3	3.65	128.61	124.14
1	E	63[B]	IEY	O2-C2-N3	3.62	128.57	124.14
1	C	63[B]	IEY	O2-C2-N3	3.59	128.53	124.14
1	E	63[B]	IEY	CG1-CD3-NE	-3.55	102.22	108.62
1	B	63[B]	IEY	CA1-C1-N2	-3.52	120.71	125.17
1	F	61[B]	NFA	CG-CB-CA	-3.49	106.88	114.13
1	B	63[B]	IEY	O2-C2-N3	3.48	128.40	124.14
1	E	61[B]	NFA	CG-CB-CA	-3.46	106.93	114.13
1	A	63[B]	IEY	CA1-C1-N2	-3.44	120.81	125.17
1	E	63[B]	IEY	CA2-N2-C1	-3.41	103.87	107.54
1	D	61[B]	NFA	CG-CB-CA	-3.40	107.05	114.13
1	A	63[B]	IEY	CG1-CD3-NE	-3.35	102.58	108.62
1	D	63[B]	IEY	CA2-N2-C1	-3.32	103.95	107.54
1	D	63[B]	IEY	CG1-CD3-NE	-3.32	102.64	108.62
1	A	63[B]	IEY	CA2-N2-C1	-3.25	104.03	107.54
1	C	61[B]	NFA	CB-CA-C	3.23	116.64	109.09
1	B	63[B]	IEY	CA2-N2-C1	-3.22	104.07	107.54
1	B	63[B]	IEY	CG1-CD3-NE	-3.14	102.96	108.62
1	D	63[A]	CR8	C3-CA3-N3	3.12	116.64	111.92
1	E	63[A]	CR8	C3-CA3-N3	3.09	116.60	111.92
1	A	63[A]	CR8	C3-CA3-N3	3.08	116.58	111.92
1	B	63[B]	IEY	CB1-CA1-C1	-3.02	118.14	122.90
1	E	63[B]	IEY	CB1-CA1-C1	-3.02	118.15	122.90
1	F	63[B]	IEY	CG1-CD3-NE	-2.86	103.47	108.62
1	D	63[B]	IEY	CA1-C1-N2	-2.82	121.59	125.17
1	A	61[B]	NFA	O-C-NXT	-2.80	118.13	123.00
1	B	61[B]	NFA	CG-CB-CA	-2.76	108.39	114.13
1	A	63[A]	CR8	C12-C6-C7	-2.63	119.72	121.95
1	E	63[A]	CR8	C12-C6-C7	-2.61	119.74	121.95
1	C	63[B]	IEY	CG1-CD3-NE	-2.59	103.95	108.62
1	A	63[B]	IEY	CB1-CA1-C1	-2.55	118.88	122.90
1	F	63[B]	IEY	O3-C3-CA3	-2.46	118.97	126.39
1	D	61[B]	NFA	O-C-NXT	-2.42	118.78	123.00
1	B	63[A]	CR8	C3-CA3-N3	2.41	115.58	111.92
1	C	63[B]	IEY	O3-C3-CA3	-2.41	119.12	126.39
1	D	61[B]	NFA	CA-C-NXT	2.36	120.73	116.68
1	E	63[B]	IEY	CA1-C1-N2	-2.35	122.19	125.17
1	D	63[B]	IEY	CB1-CA1-C1	-2.34	119.21	122.90
1	E	63[B]	IEY	O3-C3-CA3	-2.33	119.37	126.39
1	D	63[B]	IEY	CA3-N3-C2	2.31	125.53	123.43
1	A	61[B]	NFA	CG-CB-CA	-2.30	109.34	114.13
1	F	63[B]	IEY	CA1-C1-N3	2.27	125.19	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61[B]	NFA	CA-C-NXT	2.25	120.54	116.68
1	D	63[A]	CR8	O3-C3-CA3	-2.21	120.02	126.32
1	C	61[B]	NFA	O-C-NXT	-2.21	119.17	123.00
1	D	63[B]	IEY	O3-C3-CA3	-2.20	119.75	126.39
1	D	63[B]	IEY	CG1-CB1-CA1	-2.19	120.90	126.14
1	B	61[B]	NFA	CA-C-NXT	2.17	120.41	116.68
1	B	63[B]	IEY	O3-C3-CA3	-2.15	119.89	126.39
1	B	63[B]	IEY	CA1-C1-N3	2.08	124.98	122.76
1	A	63[B]	IEY	O3-C3-CA3	-2.08	120.12	126.39
1	F	63[B]	IEY	CA3-N3-C2	2.06	125.30	123.43
1	E	63[A]	CR8	O3-C3-CA3	-2.05	120.49	126.32
1	A	63[A]	CR8	O3-C3-CA3	-2.05	120.50	126.32
1	E	63[A]	CR8	C4-C11-C12	2.04	120.21	116.62

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63[B]	IEY	CA2
1	B	63[B]	IEY	CA2
1	C	63[B]	IEY	CA2
1	D	63[B]	IEY	CA2
1	E	63[B]	IEY	CA2
1	F	63[B]	IEY	CA2

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	61[B]	NFA	O-C-CA-CB
1	A	61[B]	NFA	NXT-C-CA-CB
1	A	63[B]	IEY	N2-C1-CA1-CB1
1	A	63[B]	IEY	N3-C1-CA1-CB1
1	A	63[B]	IEY	C3-CA3-N3-C2
1	A	63[B]	IEY	N2-CA2-CB2-CG2
1	A	63[A]	CR8	CA1-C20-C21-N22
1	A	63[A]	CR8	CA1-C20-C21-C23
1	B	61[B]	NFA	O-C-CA-CB
1	B	61[B]	NFA	NXT-C-CA-CB
1	B	63[B]	IEY	N2-C1-CA1-CB1
1	B	63[B]	IEY	N3-C1-CA1-CB1
1	B	63[B]	IEY	C3-CA3-N3-C2
1	B	63[B]	IEY	N2-CA2-CB2-CG2
1	B	63[A]	CR8	CA1-C20-C21-N22

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Mol	Chain	Res	Type	Atoms
1	B	63[A]	CR8	CA1-C20-C21-C23
1	C	61[B]	NFA	NXT-C-CA-N
1	C	63[B]	IEY	C3-CA3-N3-C2
1	C	63[B]	IEY	N2-CA2-CB2-CG2
1	D	61[B]	NFA	O-C-CA-CB
1	D	61[B]	NFA	NXT-C-CA-CB
1	D	63[B]	IEY	N2-C1-CA1-CB1
1	D	63[B]	IEY	N3-C1-CA1-CB1
1	D	63[B]	IEY	C3-CA3-N3-C2
1	D	63[B]	IEY	N2-CA2-CB2-CG2
1	D	63[A]	CR8	CA1-C20-C21-N22
1	D	63[A]	CR8	CA1-C20-C21-C23
1	E	61[B]	NFA	O-C-CA-CB
1	E	61[B]	NFA	NXT-C-CA-CB
1	E	63[B]	IEY	N2-C1-CA1-CB1
1	E	63[B]	IEY	N3-C1-CA1-CB1
1	E	63[B]	IEY	C3-CA3-N3-C2
1	E	63[B]	IEY	N2-CA2-CB2-CG2
1	E	63[A]	CR8	CA1-C20-C21-N22
1	E	63[A]	CR8	CA1-C20-C21-C23
1	F	61[B]	NFA	NXT-C-CA-N
1	F	63[B]	IEY	N2-C1-CA1-CB1
1	F	63[B]	IEY	N3-C1-CA1-CB1
1	F	63[B]	IEY	C3-CA3-N3-C2
1	F	63[B]	IEY	N2-CA2-CB2-CG2
1	C	61[B]	NFA	O-C-CA-CB
1	C	61[B]	NFA	NXT-C-CA-CB
1	E	63[B]	IEY	CA2-CB2-CG2-CD1
1	E	63[B]	IEY	CA2-CB2-CG2-CD2
1	C	61[B]	NFA	O-C-CA-N
1	F	61[B]	NFA	O-C-CA-N
1	C	63[B]	IEY	CA2-CB2-CG2-CD1
1	C	63[B]	IEY	CA2-CB2-CG2-CD2
1	F	63[B]	IEY	CA2-CB2-CG2-CD2
1	B	63[B]	IEY	CA2-CB2-CG2-CD2
1	D	63[B]	IEY	CA2-CB2-CG2-CD2
1	A	63[B]	IEY	CA2-CB2-CG2-CD2
1	F	63[B]	IEY	CA2-CB2-CG2-CD1
1	B	63[B]	IEY	CA2-CB2-CG2-CD1
1	A	63[B]	IEY	CA2-CB2-CG2-CD1
1	D	63[B]	IEY	CA2-CB2-CG2-CD1
1	F	61[B]	NFA	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	F	61[B]	NFA	NXT-C-CA-CB
1	C	61[B]	NFA	C-CA-CB-CG
1	A	63[B]	IEY	C3-CA3-N3-C1
1	B	63[B]	IEY	C3-CA3-N3-C1
1	A	61[B]	NFA	CA-CB-CG-CD1
1	A	61[B]	NFA	CA-CB-CG-CD2
1	F	61[B]	NFA	CA-CB-CG-CD1

There are no ring outliers.

10 monomers are involved in 14 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PG4	D	301	-	12,12,12	0.72	0	11,11,11	1.08	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PGE	A	301	-	9,9,9	0.59	0	8,8,8	0.83	0
2	PGE	E	301	-	9,9,9	0.49	0	8,8,8	0.92	0
2	PGE	C	301	-	9,9,9	0.50	0	8,8,8	0.93	0
3	PEG	C	302	-	6,6,6	0.53	0	5,5,5	0.66	0
3	PEG	D	302	-	6,6,6	0.55	0	5,5,5	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	D	301	-	-	3/10/10/10	-
2	PGE	A	301	-	-	5/7/7/7	-
2	PGE	E	301	-	-	3/7/7/7	-
2	PGE	C	301	-	-	2/7/7/7	-
3	PEG	C	302	-	-	1/4/4/4	-
3	PEG	D	302	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	PG4	C5-O3-C4	2.09	122.33	113.29
4	D	301	PG4	C7-O4-C6	2.04	122.14	113.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	PGE	O3-C5-C6-O4
2	A	301	PGE	O3-C5-C6-O4
2	E	301	PGE	O1-C1-C2-O2
2	E	301	PGE	O3-C5-C6-O4
4	D	301	PG4	O4-C7-C8-O5
4	D	301	PG4	C6-C5-O3-C4
2	A	301	PGE	O1-C1-C2-O2
3	C	302	PEG	O2-C3-C4-O4
3	D	302	PEG	O1-C1-C2-O2
2	A	301	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	E	301	PGE	C1-C2-O2-C3
4	D	301	PG4	O2-C3-C4-O3
2	A	301	PGE	C6-C5-O3-C4
2	C	301	PGE	C4-C3-O2-C2
2	A	301	PGE	O2-C3-C4-O3

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 [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	216/260 (83%)	-0.17	5 (2%) 60 64	18, 26, 45, 71	0
1	B	214/260 (82%)	-0.09	5 (2%) 60 64	18, 27, 45, 65	0
1	C	214/260 (82%)	-0.28	0 100 100	17, 25, 43, 58	0
1	D	215/260 (82%)	-0.15	5 (2%) 60 64	17, 26, 43, 63	0
1	E	214/260 (82%)	-0.08	6 (2%) 53 58	19, 28, 43, 67	0
1	F	216/260 (83%)	0.34	18 (8%) 11 11	21, 32, 53, 81	0
All	All	1289/1560 (82%)	-0.07	39 (3%) 49 54	17, 28, 45, 81	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	5.5
1	F	3	VAL	5.4
1	F	4	ILE	4.0
1	F	34	PHE	3.7
1	F	221	ARG	3.6
1	F	2	SER	3.2
1	F	220	PRO	3.0
1	F	6	PRO	3.0
1	B	89	TRP	2.9
1	F	74	ASN	2.9
1	A	220	PRO	2.9
1	E	60	ALA	2.8
1	F	73	GLU	2.8
1	D	128	ASN	2.7
1	F	165	GLY	2.6
1	A	3	VAL	2.5
1	E	89	TRP	2.5
1	F	184	GLN	2.5
1	B	59	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	60	ALA	2.4
1	F	7	ASP	2.4
1	E	59	THR	2.3
1	F	112	ASP	2.3
1	F	30	LEU	2.3
1	D	73	GLU	2.3
1	F	201	ASP	2.2
1	F	59	THR	2.2
1	F	111	GLY	2.2
1	A	89	TRP	2.2
1	A	221	ARG	2.2
1	B	112	ASP	2.1
1	D	2	SER	2.1
1	F	203	ASP	2.1
1	E	74	ASN	2.1
1	A	59	THR	2.0
1	D	60	ALA	2.0
1	E	220	PRO	2.0
1	D	157	VAL	2.0
1	E	84	PRO	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	IEY	F	63[B]	24/25	0.90	0.26	19,29,37,40	24
1	NFA	F	61[B]	12/12	0.93	0.24	22,25,38,41	12
1	CR8	D	63[A]	25/26	0.94	0.19	19,23,27,34	25
1	NFA	C	61[B]	12/12	0.94	0.18	12,15,20,27	0
1	IEY	D	63[B]	24/25	0.94	0.18	20,23,27,32	24
1	NFA	E	61[B]	12/12	0.95	0.26	21,25,26,26	12
1	CR8	B	63[A]	25/26	0.95	0.18	22,26,30,33	25
1	IEY	B	63[B]	24/25	0.95	0.17	22,26,30,31	24
1	IEY	C	63[B]	24/25	0.96	0.19	11,15,25,27	0
1	IEY	E	63[B]	24/25	0.96	0.19	21,25,31,35	24
1	CR8	E	63[A]	25/26	0.96	0.19	22,25,31,37	25
1	NFA	B	61[B]	12/12	0.96	0.21	22,24,27,27	12
1	CR8	A	63[A]	25/26	0.96	0.19	18,23,26,31	25

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	IEY	A	63[B]	24/25	0.97	0.19	18,23,27,29	24
1	NFA	D	61[B]	12/12	0.97	0.16	20,22,23,23	12
1	NFA	A	61[B]	12/12	0.97	0.18	21,23,25,26	12

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(\AA^2)	Q<0.9
3	PEG	D	302	7/7	0.81	0.14	45,49,59,62	0
2	PGE	C	301	10/10	0.85	0.22	21,46,54,58	0
4	PG4	D	301	13/13	0.87	0.21	31,44,58,62	0
3	PEG	C	302	7/7	0.88	0.14	37,46,53,54	0
2	PGE	A	301	10/10	0.89	0.15	40,54,66,69	0
2	PGE	E	301	10/10	0.92	0.20	23,40,50,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.