



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 08:45 AM EDT

PDB ID : 3RWT
Title : Crystal structure of circular permuted Red Fluorescent Protein mKate(cp 154-153)
Authors : Wang, Q.; Sondermann, H.
Deposited on : 2011-05-09
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

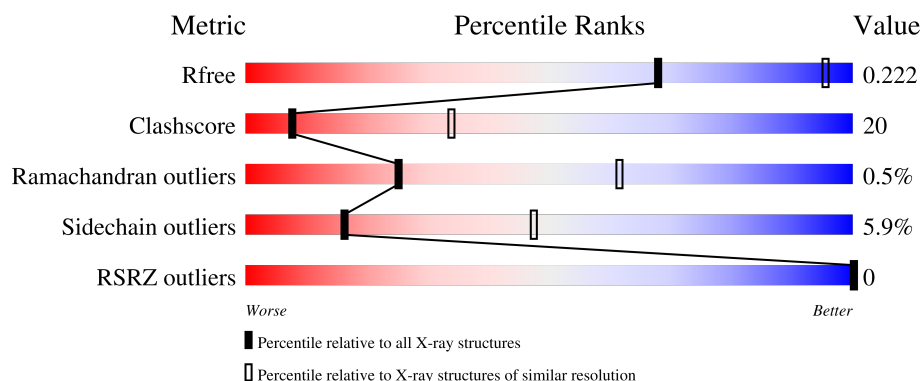
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	235	 65% 30% 5%
1	B	235	 60% 35% 5%
1	C	235	 72% 24% .
1	D	235	 69% 26% .
1	E	235	 57% 38% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	235	 68% 27% 5%
1	G	235	 67% 28% • •
1	H	235	 65% 31% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14977 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 FP480,Fluorescent protein FP480.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	235	Total	C	N	O	S	0	0	0
			1863	1181	315	353	14			
1	A	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			
1	B	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			
1	C	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			
1	D	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			
1	E	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			
1	G	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			
1	H	235	Total	C	N	O	S	0	2	0
			1873	1188	316	354	15			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLU	GLY	engineered mutation	UNP D0VX33
F	1	PHE	GLY	engineered mutation	UNP D0VX33
F	6	SER	ALA	conflict	UNP D0VX33
F	8	MET	LEU	conflict	UNP D0VX33
F	22	LEU	PHE	conflict	UNP D0VX33
F	45	ARG	TYR	conflict	UNP D0VX33
F	80	GLY	-	linker	UNP D0VX33
F	81	GLY	-	linker	UNP D0VX33
F	82	THR	-	linker	UNP D0VX33
F	83	GLY	-	linker	UNP D0VX33
F	84	GLY	-	linker	UNP D0VX33
F	85	SER	-	linker	UNP D0VX33
F	126	MET	GLN	conflict	UNP D0VX33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	MET	chromophore	UNP D0VX33
F	?	-	TYR	chromophore	UNP D0VX33
F	148	NRQ	GLY	chromophore	UNP D0VX33
F	152	LYS	HIS	conflict	UNP D0VX33
F	165	PHE	TRP	conflict	UNP D0VX33
F	228	SER	HIS	conflict	UNP D0VX33
A	0	GLU	GLY	engineered mutation	UNP D0VX33
A	1	PHE	GLY	engineered mutation	UNP D0VX33
A	6	SER	ALA	conflict	UNP D0VX33
A	8	MET	LEU	conflict	UNP D0VX33
A	22	LEU	PHE	conflict	UNP D0VX33
A	45	ARG	TYR	conflict	UNP D0VX33
A	80	GLY	-	linker	UNP D0VX33
A	81	GLY	-	linker	UNP D0VX33
A	82	THR	-	linker	UNP D0VX33
A	83	GLY	-	linker	UNP D0VX33
A	84	GLY	-	linker	UNP D0VX33
A	85	SER	-	linker	UNP D0VX33
A	126	MET	GLN	conflict	UNP D0VX33
A	?	-	MET	chromophore	UNP D0VX33
A	?	-	TYR	chromophore	UNP D0VX33
A	148	NRQ	GLY	chromophore	UNP D0VX33
A	152	LYS	HIS	conflict	UNP D0VX33
A	165	PHE	TRP	conflict	UNP D0VX33
A	228	SER	HIS	conflict	UNP D0VX33
B	0	GLU	GLY	engineered mutation	UNP D0VX33
B	1	PHE	GLY	engineered mutation	UNP D0VX33
B	6	SER	ALA	conflict	UNP D0VX33
B	8	MET	LEU	conflict	UNP D0VX33
B	22	LEU	PHE	conflict	UNP D0VX33
B	45	ARG	TYR	conflict	UNP D0VX33
B	80	GLY	-	linker	UNP D0VX33
B	81	GLY	-	linker	UNP D0VX33
B	82	THR	-	linker	UNP D0VX33
B	83	GLY	-	linker	UNP D0VX33
B	84	GLY	-	linker	UNP D0VX33
B	85	SER	-	linker	UNP D0VX33
B	126	MET	GLN	conflict	UNP D0VX33
B	?	-	MET	chromophore	UNP D0VX33
B	?	-	TYR	chromophore	UNP D0VX33
B	148	NRQ	GLY	chromophore	UNP D0VX33
B	152	LYS	HIS	conflict	UNP D0VX33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	165	PHE	TRP	conflict	UNP D0VX33
B	228	SER	HIS	conflict	UNP D0VX33
C	0	GLU	GLY	engineered mutation	UNP D0VX33
C	1	PHE	GLY	engineered mutation	UNP D0VX33
C	6	SER	ALA	conflict	UNP D0VX33
C	8	MET	LEU	conflict	UNP D0VX33
C	22	LEU	PHE	conflict	UNP D0VX33
C	45	ARG	TYR	conflict	UNP D0VX33
C	80	GLY	-	linker	UNP D0VX33
C	81	GLY	-	linker	UNP D0VX33
C	82	THR	-	linker	UNP D0VX33
C	83	GLY	-	linker	UNP D0VX33
C	84	GLY	-	linker	UNP D0VX33
C	85	SER	-	linker	UNP D0VX33
C	126	MET	GLN	conflict	UNP D0VX33
C	?	-	MET	chromophore	UNP D0VX33
C	?	-	TYR	chromophore	UNP D0VX33
C	148	NRQ	GLY	chromophore	UNP D0VX33
C	152	LYS	HIS	conflict	UNP D0VX33
C	165	PHE	TRP	conflict	UNP D0VX33
C	228	SER	HIS	conflict	UNP D0VX33
D	0	GLU	GLY	engineered mutation	UNP D0VX33
D	1	PHE	GLY	engineered mutation	UNP D0VX33
D	6	SER	ALA	conflict	UNP D0VX33
D	8	MET	LEU	conflict	UNP D0VX33
D	22	LEU	PHE	conflict	UNP D0VX33
D	45	ARG	TYR	conflict	UNP D0VX33
D	80	GLY	-	linker	UNP D0VX33
D	81	GLY	-	linker	UNP D0VX33
D	82	THR	-	linker	UNP D0VX33
D	83	GLY	-	linker	UNP D0VX33
D	84	GLY	-	linker	UNP D0VX33
D	85	SER	-	linker	UNP D0VX33
D	126	MET	GLN	conflict	UNP D0VX33
D	?	-	MET	chromophore	UNP D0VX33
D	?	-	TYR	chromophore	UNP D0VX33
D	148	NRQ	GLY	chromophore	UNP D0VX33
D	152	LYS	HIS	conflict	UNP D0VX33
D	165	PHE	TRP	conflict	UNP D0VX33
D	228	SER	HIS	conflict	UNP D0VX33
E	0	GLU	GLY	engineered mutation	UNP D0VX33
E	1	PHE	GLY	engineered mutation	UNP D0VX33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	6	SER	ALA	conflict	UNP D0VX33
E	8	MET	LEU	conflict	UNP D0VX33
E	22	LEU	PHE	conflict	UNP D0VX33
E	45	ARG	TYR	conflict	UNP D0VX33
E	80	GLY	-	linker	UNP D0VX33
E	81	GLY	-	linker	UNP D0VX33
E	82	THR	-	linker	UNP D0VX33
E	83	GLY	-	linker	UNP D0VX33
E	84	GLY	-	linker	UNP D0VX33
E	85	SER	-	linker	UNP D0VX33
E	126	MET	GLN	conflict	UNP D0VX33
E	?	-	MET	chromophore	UNP D0VX33
E	?	-	TYR	chromophore	UNP D0VX33
E	148	NRQ	GLY	chromophore	UNP D0VX33
E	152	LYS	HIS	conflict	UNP D0VX33
E	165	PHE	TRP	conflict	UNP D0VX33
E	228	SER	HIS	conflict	UNP D0VX33
G	0	GLU	GLY	engineered mutation	UNP D0VX33
G	1	PHE	GLY	engineered mutation	UNP D0VX33
G	6	SER	ALA	conflict	UNP D0VX33
G	8	MET	LEU	conflict	UNP D0VX33
G	22	LEU	PHE	conflict	UNP D0VX33
G	45	ARG	TYR	conflict	UNP D0VX33
G	80	GLY	-	linker	UNP D0VX33
G	81	GLY	-	linker	UNP D0VX33
G	82	THR	-	linker	UNP D0VX33
G	83	GLY	-	linker	UNP D0VX33
G	84	GLY	-	linker	UNP D0VX33
G	85	SER	-	linker	UNP D0VX33
G	126	MET	GLN	conflict	UNP D0VX33
G	?	-	MET	chromophore	UNP D0VX33
G	?	-	TYR	chromophore	UNP D0VX33
G	148	NRQ	GLY	chromophore	UNP D0VX33
G	152	LYS	HIS	conflict	UNP D0VX33
G	165	PHE	TRP	conflict	UNP D0VX33
G	228	SER	HIS	conflict	UNP D0VX33
H	0	GLU	GLY	engineered mutation	UNP D0VX33
H	1	PHE	GLY	engineered mutation	UNP D0VX33
H	6	SER	ALA	conflict	UNP D0VX33
H	8	MET	LEU	conflict	UNP D0VX33
H	22	LEU	PHE	conflict	UNP D0VX33
H	45	ARG	TYR	conflict	UNP D0VX33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	80	GLY	-	linker	UNP D0VX33
H	81	GLY	-	linker	UNP D0VX33
H	82	THR	-	linker	UNP D0VX33
H	83	GLY	-	linker	UNP D0VX33
H	84	GLY	-	linker	UNP D0VX33
H	85	SER	-	linker	UNP D0VX33
H	126	MET	GLN	conflict	UNP D0VX33
H	?	-	MET	chromophore	UNP D0VX33
H	?	-	TYR	chromophore	UNP D0VX33
H	148	NRQ	GLY	chromophore	UNP D0VX33
H	152	LYS	HIS	conflict	UNP D0VX33
H	165	PHE	TRP	conflict	UNP D0VX33
H	228	SER	HIS	conflict	UNP D0VX33

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

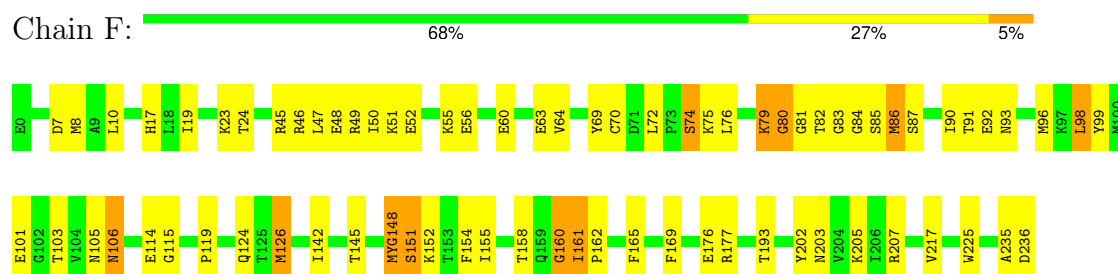
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total O 1 1	0	0
3	A	1	Total O 1 1	0	0

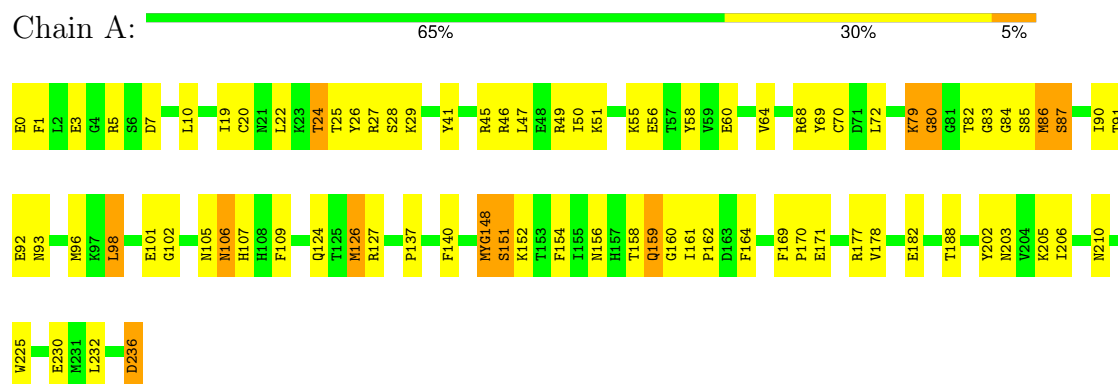
3 Residue-property plots

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.

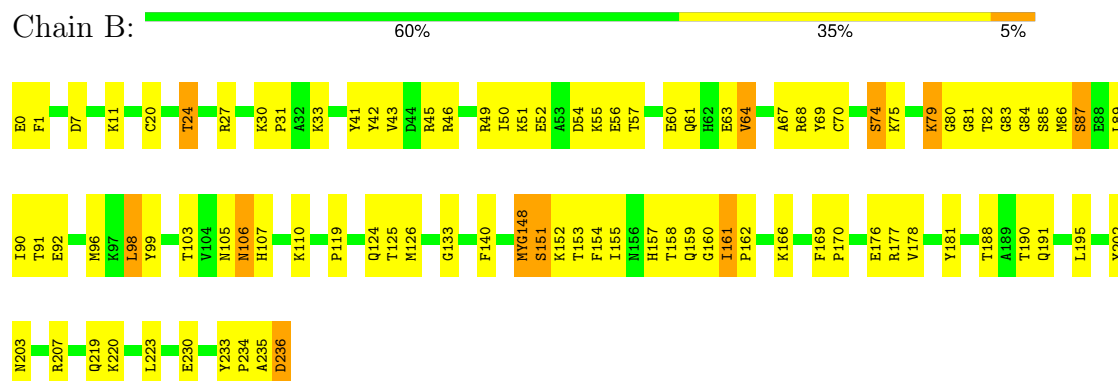
- Molecule 1: Fluorescent protein FP480, Fluorescent protein FP480



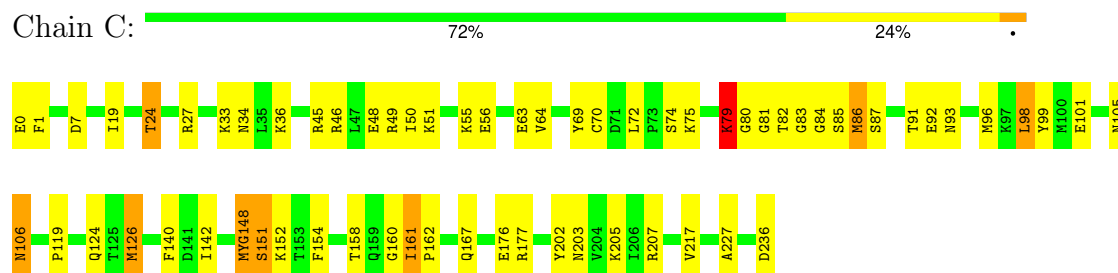
- Molecule 1: Fluorescent protein FP480, Fluorescent protein FP480



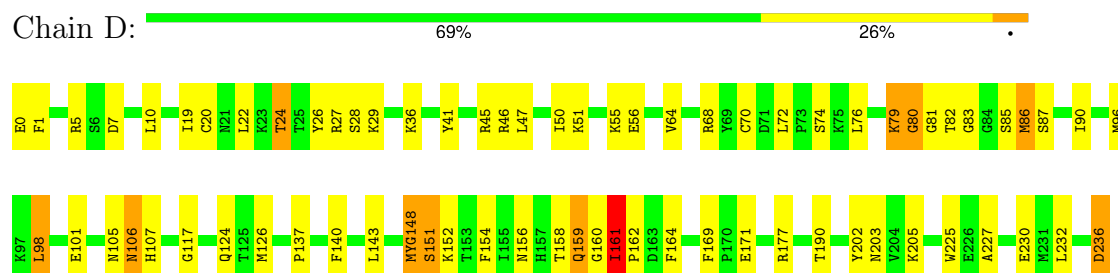
- Molecule 1: Fluorescent protein FP480, Fluorescent protein FP480



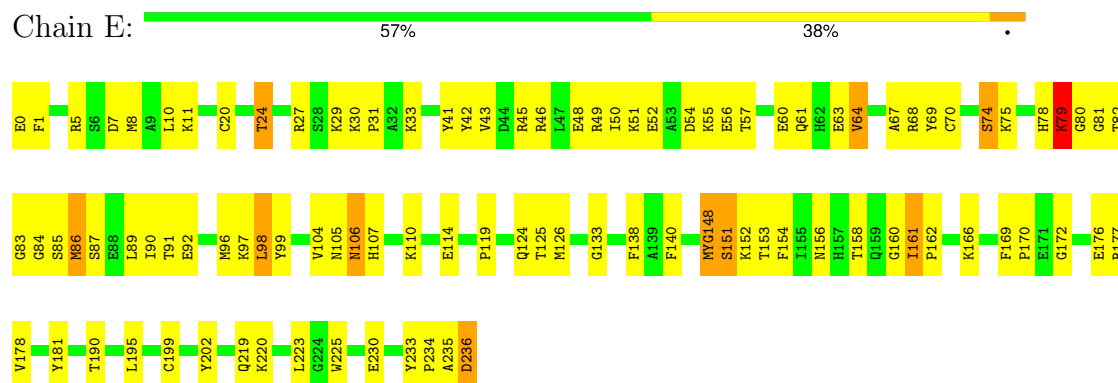
- Molecule 1: Fluorescent protein FP480,Fluorescent protein FP480



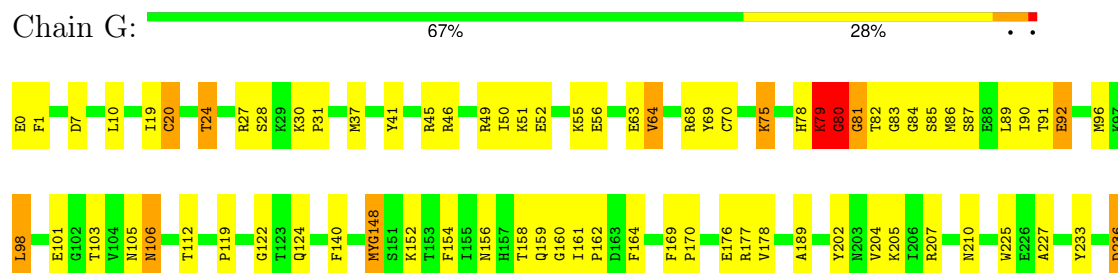
- Molecule 1: Fluorescent protein FP480,Fluorescent protein FP480



- Molecule 1: Fluorescent protein FP480,Fluorescent protein FP480



- Molecule 1: Fluorescent protein FP480,Fluorescent protein FP480



- Molecule 1: Fluorescent protein FP480,Fluorescent protein FP480



E0	F1																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
----	----	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.46Å 71.44Å 367.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.90 – 3.00 38.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.90-3.00) 99.9 (38.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.217 , 0.278 0.212 , 0.222	Depositor DCC
R_{free} test set	1948 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NRQ, MG

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	0.54	0/1897	0.75	0/2555
1	B	0.49	0/1897	0.75	0/2555
1	C	0.52	0/1897	0.76	1/2555 (0.0%)
1	D	0.54	0/1897	0.77	0/2555
1	E	0.51	0/1897	0.73	0/2555
1	F	0.54	0/1881	0.79	3/2534 (0.1%)
1	G	0.50	1/1897 (0.1%)	0.77	2/2555 (0.1%)
1	H	0.50	1/1897 (0.1%)	0.74	0/2555
All	All	0.52	2/15160 (0.0%)	0.76	6/20419 (0.0%)

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	F	0	1
1	G	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	20	CYS	CB-SG	-6.39	1.71	1.82
1	G	20	CYS	CB-SG	-6.25	1.71	1.82

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	81	GLY	N-CA-C	-7.72	93.80	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	81	GLY	N-CA-C	-7.17	95.18	113.10
1	F	79	LYS	N-CA-C	-6.22	94.21	111.00
1	G	80	GLY	N-CA-C	-6.17	97.69	113.10
1	F	80	GLY	N-CA-C	-5.08	100.39	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	160	GLY	Mainchain
1	G	80	GLY	Peptide

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	1873	0	1840	85	0
1	B	1873	0	1840	91	0
1	C	1873	0	1840	68	0
1	D	1873	0	1840	67	0
1	E	1873	0	1840	98	0
1	F	1863	0	1825	61	0
1	G	1873	0	1840	72	0
1	H	1873	0	1840	82	0
2	A	1	0	0	0	0
3	A	1	0	0	1	0
3	F	1	0	0	0	0
All	All	14977	0	14705	586	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 20.

The worst 5 of 586 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:B:79:LYS:HG2	1:B:80:GLY:N	1.57	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:HG2	1:C:80:GLY:H	0.98	1.15
1:B:79:LYS:HG2	1:B:80:GLY:H	1.10	1.11
1:E:79:LYS:HG2	1:E:80:GLY:H	1.10	1.07
1:E:79:LYS:CG	1:E:80:GLY:H	1.66	1.07

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	232/235 (99%)	213 (92%)	17 (7%)	2 (1%)	14	49
1	B	232/235 (99%)	218 (94%)	14 (6%)	0	100	100
1	C	232/235 (99%)	217 (94%)	14 (6%)	1 (0%)	30	66
1	D	232/235 (99%)	215 (93%)	14 (6%)	3 (1%)	10	39
1	E	232/235 (99%)	217 (94%)	14 (6%)	1 (0%)	30	66
1	F	230/235 (98%)	213 (93%)	16 (7%)	1 (0%)	30	66
1	G	232/235 (99%)	217 (94%)	14 (6%)	1 (0%)	30	66
1	H	232/235 (99%)	219 (94%)	12 (5%)	1 (0%)	30	66
All	All	1854/1880 (99%)	1729 (93%)	115 (6%)	10 (0%)	25	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	C	79	LYS
1	D	80	GLY
1	A	80	GLY
1	D	161	ILE

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	202/200 (101%)	190 (94%)	12 (6%)	16	47
1	B	202/200 (101%)	188 (93%)	14 (7%)	13	42
1	C	202/200 (101%)	189 (94%)	13 (6%)	14	44
1	D	202/200 (101%)	189 (94%)	13 (6%)	14	44
1	E	202/200 (101%)	187 (93%)	15 (7%)	11	38
1	F	200/200 (100%)	190 (95%)	10 (5%)	20	53
1	G	202/200 (101%)	189 (94%)	13 (6%)	14	44
1	H	202/200 (101%)	190 (94%)	12 (6%)	16	47
All	All	1614/1600 (101%)	1512 (94%)	102 (6%)	16	45

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	106	ASN
1	E	106	ASN
1	H	106	ASN
1	D	151	SER
1	E	78	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	203	ASN
1	G	34	ASN
1	H	106	ASN
1	B	106	ASN
1	B	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	NRQ	C	148	1	24,24,25	3.99	6 (25%)	24,32,34	2.86	6 (25%)
1	NRQ	A	148	1	24,24,25	4.16	6 (25%)	24,32,34	2.84	9 (37%)
1	NRQ	E	148	1	24,24,25	3.99	7 (29%)	24,32,34	2.69	8 (33%)
1	NRQ	F	148	1	24,24,25	3.95	5 (20%)	24,32,34	2.64	4 (16%)
1	NRQ	H	148	1	24,24,25	3.77	5 (20%)	24,32,34	2.97	5 (20%)
1	NRQ	G	148	1	24,24,25	3.80	6 (25%)	24,32,34	3.02	7 (29%)
1	NRQ	D	148	1	24,24,25	4.11	7 (29%)	24,32,34	2.88	9 (37%)
1	NRQ	B	148	1	24,24,25	4.00	8 (33%)	24,32,34	2.71	7 (29%)

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	NRQ	C	148	1	-	2/9/31/32	0/2/2/2
1	NRQ	A	148	1	-	1/9/31/32	0/2/2/2
1	NRQ	E	148	1	-	2/9/31/32	0/2/2/2
1	NRQ	F	148	1	-	2/9/31/32	0/2/2/2
1	NRQ	H	148	1	-	2/9/31/32	0/2/2/2
1	NRQ	G	148	1	-	3/9/31/32	0/2/2/2
1	NRQ	D	148	1	-	1/9/31/32	0/2/2/2
1	NRQ	B	148	1	-	2/9/31/32	0/2/2/2

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	NRQ	CB2-CA2	17.28	1.51	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	148	NRQ	CB2-CA2	16.77	1.51	1.35
1	C	148	NRQ	CB2-CA2	16.58	1.51	1.35
1	F	148	NRQ	CB2-CA2	16.46	1.51	1.35
1	E	148	NRQ	CB2-CA2	15.83	1.50	1.35

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	148	NRQ	O2-C2-CA2	-11.01	123.99	131.02
1	G	148	NRQ	O2-C2-CA2	-10.76	124.15	131.02
1	C	148	NRQ	O2-C2-CA2	-9.01	125.27	131.02
1	D	148	NRQ	O2-C2-CA2	-8.82	125.39	131.02
1	A	148	NRQ	O2-C2-CA2	-8.68	125.48	131.02

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	148	NRQ	CA1-CB1-CG1-SD
1	A	148	NRQ	C1-CA1-CB1-CG1
1	C	148	NRQ	CA1-CB1-CG1-SD
1	D	148	NRQ	C1-CA1-CB1-CG1
1	E	148	NRQ	C2-CA2-CB2-CG2

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	148	NRQ	4	0
1	A	148	NRQ	2	0
1	E	148	NRQ	3	0
1	F	148	NRQ	5	0
1	H	148	NRQ	1	0
1	G	148	NRQ	1	0
1	D	148	NRQ	2	0
1	B	148	NRQ	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	234/235 (99%)	-1.52	0 100 100	36, 93, 134, 150	2 (0%)
1	B	234/235 (99%)	-1.53	0 100 100	44, 94, 145, 209	2 (0%)
1	C	234/235 (99%)	-1.54	0 100 100	46, 87, 120, 155	2 (0%)
1	D	234/235 (99%)	-1.53	0 100 100	36, 93, 132, 154	2 (0%)
1	E	234/235 (99%)	-1.51	0 100 100	40, 93, 140, 206	2 (0%)
1	F	234/235 (99%)	-1.56	0 100 100	46, 87, 122, 179	0
1	G	234/235 (99%)	-1.51	0 100 100	44, 106, 155, 199	2 (0%)
1	H	234/235 (99%)	-1.51	0 100 100	43, 108, 153, 170	2 (0%)
All	All	1872/1880 (99%)	-1.53	0 100 100	36, 94, 144, 209	14 (0%)

There are no RSRZ outliers to report.

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	NRQ	D	148	23/24	0.98	0.06	49,64,91,122	0
1	NRQ	A	148	23/24	0.99	0.04	44,59,96,110	0
1	NRQ	B	148	23/24	0.99	0.04	61,71,84,135	0
1	NRQ	C	148	23/24	0.99	0.05	53,65,80,128	0
1	NRQ	F	148	23/24	0.99	0.03	51,66,76,118	0
1	NRQ	E	148	23/24	0.99	0.04	62,70,85,138	0
1	NRQ	G	148	23/24	0.99	0.04	54,74,90,103	0
1	NRQ	H	148	23/24	0.99	0.04	55,72,91,108	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	237	1/1	0.99	0.14	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.