



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2025 – 08:20 PM JST

PDB ID : 9LSW / pdb_00009lsw
Title : Crystal structure of the calcium-free mRFP1 with a grafted calcium-binding sequence
Authors : Uehara, R.; Kamiya, Y.; Maeda, S.; Okamoto, K.; Toya, S.; Chiba, R.; Ame-saka, H.; Takano, K.; Matsumura, H.; Tanaka, S.-i.
Deposited on : 2025-02-05
Resolution : 3.16 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

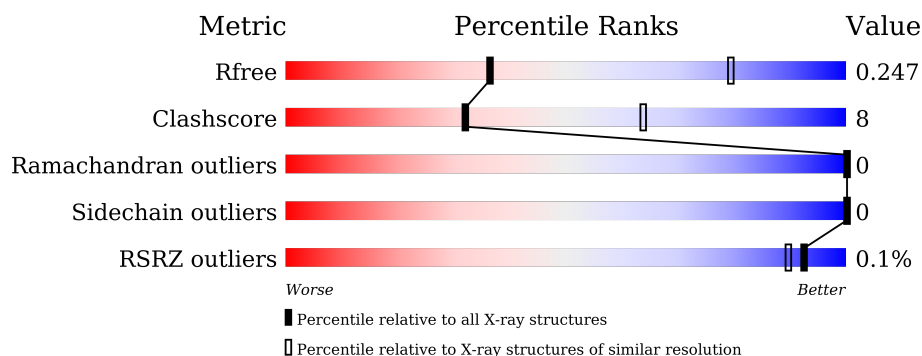
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	278	<div> <div>59%</div> <div>18%</div> <div>23%</div> </div>
1	B	278	<div> <div>62%</div> <div>15%</div> <div>23%</div> </div>
1	C	278	<div> <div>60%</div> <div>16%</div> <div>23%</div> </div>
1	D	278	<div> <div>65%</div> <div>10%</div> <div>24%</div> </div>
1	E	278	<div> <div>60%</div> <div>15%</div> <div>24%</div> </div>
1	F	278	<div> <div>65%</div> <div>11%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	278	 57% 19% 23%
1	H	278	 63% 14% 23%
1	I	278	 63% 13% 24%
1	J	278	 54% 22% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17210 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 Red fluorescent protein,grafted calcium-binding sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1727	1102	289	328	8			
1	B	213	Total	C	N	O	S	0	0	0
			1727	1102	289	328	8			
1	C	213	Total	C	N	O	S	0	0	0
			1722	1099	289	326	8			
1	D	212	Total	C	N	O	S	0	0	0
			1718	1097	288	325	8			
1	E	212	Total	C	N	O	S	0	0	0
			1718	1097	288	325	8			
1	F	212	Total	C	N	O	S	0	0	0
			1718	1097	288	325	8			
1	G	213	Total	C	N	O	S	0	0	0
			1722	1099	289	326	8			
1	H	213	Total	C	N	O	S	0	0	0
			1722	1099	289	326	8			
1	I	212	Total	C	N	O	S	0	0	0
			1718	1097	288	325	8			
1	J	212	Total	C	N	O	S	0	0	0
			1718	1097	288	325	8			

There are 530 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	initiating methionine	UNP A0A4V4ND72
A	-35	GLY	-	expression tag	UNP A0A4V4ND72
A	-34	GLY	-	expression tag	UNP A0A4V4ND72
A	-33	SER	-	expression tag	UNP A0A4V4ND72
A	-32	HIS	-	expression tag	UNP A0A4V4ND72
A	-31	HIS	-	expression tag	UNP A0A4V4ND72
A	-30	HIS	-	expression tag	UNP A0A4V4ND72
A	-29	HIS	-	expression tag	UNP A0A4V4ND72
A	-28	HIS	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	HIS	-	expression tag	UNP A0A4V4ND72
A	-26	GLY	-	expression tag	UNP A0A4V4ND72
A	-25	MET	-	expression tag	UNP A0A4V4ND72
A	-24	ALA	-	expression tag	UNP A0A4V4ND72
A	-23	SER	-	expression tag	UNP A0A4V4ND72
A	-22	MET	-	expression tag	UNP A0A4V4ND72
A	-21	THR	-	expression tag	UNP A0A4V4ND72
A	-20	GLY	-	expression tag	UNP A0A4V4ND72
A	-19	GLY	-	expression tag	UNP A0A4V4ND72
A	-18	GLN	-	expression tag	UNP A0A4V4ND72
A	-17	GLN	-	expression tag	UNP A0A4V4ND72
A	-16	MET	-	expression tag	UNP A0A4V4ND72
A	-15	GLY	-	expression tag	UNP A0A4V4ND72
A	-14	ARG	-	expression tag	UNP A0A4V4ND72
A	-13	ASP	-	expression tag	UNP A0A4V4ND72
A	-12	LEU	-	expression tag	UNP A0A4V4ND72
A	-11	TYR	-	expression tag	UNP A0A4V4ND72
A	-10	ASP	-	expression tag	UNP A0A4V4ND72
A	-9	ASP	-	expression tag	UNP A0A4V4ND72
A	-8	ASP	-	expression tag	UNP A0A4V4ND72
A	-7	ASP	-	expression tag	UNP A0A4V4ND72
A	-6	LYS	-	expression tag	UNP A0A4V4ND72
A	-5	ASP	-	expression tag	UNP A0A4V4ND72
A	-4	ARG	-	expression tag	UNP A0A4V4ND72
A	-3	TRP	-	expression tag	UNP A0A4V4ND72
A	-2	GLY	-	expression tag	UNP A0A4V4ND72
A	-1	SER	-	expression tag	UNP A0A4V4ND72
A	0	GLU	-	expression tag	UNP A0A4V4ND72
A	1	LEU	-	expression tag	UNP A0A4V4ND72
A	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
A	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
A	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
A	232	GLY	-	expression tag	UNP A0A4V4ND72
A	233	GLY	-	expression tag	UNP A0A4V4ND72
A	234	SER	-	expression tag	UNP A0A4V4ND72
A	235	GLY	-	expression tag	UNP A0A4V4ND72
A	236	GLY	-	expression tag	UNP A0A4V4ND72
A	237	SER	-	expression tag	UNP A0A4V4ND72
A	238	GLU	-	expression tag	UNP A0A4V4ND72
A	239	ASN	-	expression tag	UNP A0A4V4ND72
A	240	LEU	-	expression tag	UNP A0A4V4ND72
A	241	TYR	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	242	PHE	-	expression tag	UNP A0A4V4ND72
A	243	GLN	-	expression tag	UNP A0A4V4ND72
B	-36	MET	-	initiating methionine	UNP A0A4V4ND72
B	-35	GLY	-	expression tag	UNP A0A4V4ND72
B	-34	GLY	-	expression tag	UNP A0A4V4ND72
B	-33	SER	-	expression tag	UNP A0A4V4ND72
B	-32	HIS	-	expression tag	UNP A0A4V4ND72
B	-31	HIS	-	expression tag	UNP A0A4V4ND72
B	-30	HIS	-	expression tag	UNP A0A4V4ND72
B	-29	HIS	-	expression tag	UNP A0A4V4ND72
B	-28	HIS	-	expression tag	UNP A0A4V4ND72
B	-27	HIS	-	expression tag	UNP A0A4V4ND72
B	-26	GLY	-	expression tag	UNP A0A4V4ND72
B	-25	MET	-	expression tag	UNP A0A4V4ND72
B	-24	ALA	-	expression tag	UNP A0A4V4ND72
B	-23	SER	-	expression tag	UNP A0A4V4ND72
B	-22	MET	-	expression tag	UNP A0A4V4ND72
B	-21	THR	-	expression tag	UNP A0A4V4ND72
B	-20	GLY	-	expression tag	UNP A0A4V4ND72
B	-19	GLY	-	expression tag	UNP A0A4V4ND72
B	-18	GLN	-	expression tag	UNP A0A4V4ND72
B	-17	GLN	-	expression tag	UNP A0A4V4ND72
B	-16	MET	-	expression tag	UNP A0A4V4ND72
B	-15	GLY	-	expression tag	UNP A0A4V4ND72
B	-14	ARG	-	expression tag	UNP A0A4V4ND72
B	-13	ASP	-	expression tag	UNP A0A4V4ND72
B	-12	LEU	-	expression tag	UNP A0A4V4ND72
B	-11	TYR	-	expression tag	UNP A0A4V4ND72
B	-10	ASP	-	expression tag	UNP A0A4V4ND72
B	-9	ASP	-	expression tag	UNP A0A4V4ND72
B	-8	ASP	-	expression tag	UNP A0A4V4ND72
B	-7	ASP	-	expression tag	UNP A0A4V4ND72
B	-6	LYS	-	expression tag	UNP A0A4V4ND72
B	-5	ASP	-	expression tag	UNP A0A4V4ND72
B	-4	ARG	-	expression tag	UNP A0A4V4ND72
B	-3	TRP	-	expression tag	UNP A0A4V4ND72
B	-2	GLY	-	expression tag	UNP A0A4V4ND72
B	-1	SER	-	expression tag	UNP A0A4V4ND72
B	0	GLU	-	expression tag	UNP A0A4V4ND72
B	1	LEU	-	expression tag	UNP A0A4V4ND72
B	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
B	66	CRQ	TYR	chromophore	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
B	232	GLY	-	expression tag	UNP A0A4V4ND72
B	233	GLY	-	expression tag	UNP A0A4V4ND72
B	234	SER	-	expression tag	UNP A0A4V4ND72
B	235	GLY	-	expression tag	UNP A0A4V4ND72
B	236	GLY	-	expression tag	UNP A0A4V4ND72
B	237	SER	-	expression tag	UNP A0A4V4ND72
B	238	GLU	-	expression tag	UNP A0A4V4ND72
B	239	ASN	-	expression tag	UNP A0A4V4ND72
B	240	LEU	-	expression tag	UNP A0A4V4ND72
B	241	TYR	-	expression tag	UNP A0A4V4ND72
B	242	PHE	-	expression tag	UNP A0A4V4ND72
B	243	GLN	-	expression tag	UNP A0A4V4ND72
C	-36	MET	-	initiating methionine	UNP A0A4V4ND72
C	-35	GLY	-	expression tag	UNP A0A4V4ND72
C	-34	GLY	-	expression tag	UNP A0A4V4ND72
C	-33	SER	-	expression tag	UNP A0A4V4ND72
C	-32	HIS	-	expression tag	UNP A0A4V4ND72
C	-31	HIS	-	expression tag	UNP A0A4V4ND72
C	-30	HIS	-	expression tag	UNP A0A4V4ND72
C	-29	HIS	-	expression tag	UNP A0A4V4ND72
C	-28	HIS	-	expression tag	UNP A0A4V4ND72
C	-27	HIS	-	expression tag	UNP A0A4V4ND72
C	-26	GLY	-	expression tag	UNP A0A4V4ND72
C	-25	MET	-	expression tag	UNP A0A4V4ND72
C	-24	ALA	-	expression tag	UNP A0A4V4ND72
C	-23	SER	-	expression tag	UNP A0A4V4ND72
C	-22	MET	-	expression tag	UNP A0A4V4ND72
C	-21	THR	-	expression tag	UNP A0A4V4ND72
C	-20	GLY	-	expression tag	UNP A0A4V4ND72
C	-19	GLY	-	expression tag	UNP A0A4V4ND72
C	-18	GLN	-	expression tag	UNP A0A4V4ND72
C	-17	GLN	-	expression tag	UNP A0A4V4ND72
C	-16	MET	-	expression tag	UNP A0A4V4ND72
C	-15	GLY	-	expression tag	UNP A0A4V4ND72
C	-14	ARG	-	expression tag	UNP A0A4V4ND72
C	-13	ASP	-	expression tag	UNP A0A4V4ND72
C	-12	LEU	-	expression tag	UNP A0A4V4ND72
C	-11	TYR	-	expression tag	UNP A0A4V4ND72
C	-10	ASP	-	expression tag	UNP A0A4V4ND72
C	-9	ASP	-	expression tag	UNP A0A4V4ND72
C	-8	ASP	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ASP	-	expression tag	UNP A0A4V4ND72
C	-6	LYS	-	expression tag	UNP A0A4V4ND72
C	-5	ASP	-	expression tag	UNP A0A4V4ND72
C	-4	ARG	-	expression tag	UNP A0A4V4ND72
C	-3	TRP	-	expression tag	UNP A0A4V4ND72
C	-2	GLY	-	expression tag	UNP A0A4V4ND72
C	-1	SER	-	expression tag	UNP A0A4V4ND72
C	0	GLU	-	expression tag	UNP A0A4V4ND72
C	1	LEU	-	expression tag	UNP A0A4V4ND72
C	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
C	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
C	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
C	232	GLY	-	expression tag	UNP A0A4V4ND72
C	233	GLY	-	expression tag	UNP A0A4V4ND72
C	234	SER	-	expression tag	UNP A0A4V4ND72
C	235	GLY	-	expression tag	UNP A0A4V4ND72
C	236	GLY	-	expression tag	UNP A0A4V4ND72
C	237	SER	-	expression tag	UNP A0A4V4ND72
C	238	GLU	-	expression tag	UNP A0A4V4ND72
C	239	ASN	-	expression tag	UNP A0A4V4ND72
C	240	LEU	-	expression tag	UNP A0A4V4ND72
C	241	TYR	-	expression tag	UNP A0A4V4ND72
C	242	PHE	-	expression tag	UNP A0A4V4ND72
C	243	GLN	-	expression tag	UNP A0A4V4ND72
D	-36	MET	-	initiating methionine	UNP A0A4V4ND72
D	-35	GLY	-	expression tag	UNP A0A4V4ND72
D	-34	GLY	-	expression tag	UNP A0A4V4ND72
D	-33	SER	-	expression tag	UNP A0A4V4ND72
D	-32	HIS	-	expression tag	UNP A0A4V4ND72
D	-31	HIS	-	expression tag	UNP A0A4V4ND72
D	-30	HIS	-	expression tag	UNP A0A4V4ND72
D	-29	HIS	-	expression tag	UNP A0A4V4ND72
D	-28	HIS	-	expression tag	UNP A0A4V4ND72
D	-27	HIS	-	expression tag	UNP A0A4V4ND72
D	-26	GLY	-	expression tag	UNP A0A4V4ND72
D	-25	MET	-	expression tag	UNP A0A4V4ND72
D	-24	ALA	-	expression tag	UNP A0A4V4ND72
D	-23	SER	-	expression tag	UNP A0A4V4ND72
D	-22	MET	-	expression tag	UNP A0A4V4ND72
D	-21	THR	-	expression tag	UNP A0A4V4ND72
D	-20	GLY	-	expression tag	UNP A0A4V4ND72
D	-19	GLY	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	GLN	-	expression tag	UNP A0A4V4ND72
D	-17	GLN	-	expression tag	UNP A0A4V4ND72
D	-16	MET	-	expression tag	UNP A0A4V4ND72
D	-15	GLY	-	expression tag	UNP A0A4V4ND72
D	-14	ARG	-	expression tag	UNP A0A4V4ND72
D	-13	ASP	-	expression tag	UNP A0A4V4ND72
D	-12	LEU	-	expression tag	UNP A0A4V4ND72
D	-11	TYR	-	expression tag	UNP A0A4V4ND72
D	-10	ASP	-	expression tag	UNP A0A4V4ND72
D	-9	ASP	-	expression tag	UNP A0A4V4ND72
D	-8	ASP	-	expression tag	UNP A0A4V4ND72
D	-7	ASP	-	expression tag	UNP A0A4V4ND72
D	-6	LYS	-	expression tag	UNP A0A4V4ND72
D	-5	ASP	-	expression tag	UNP A0A4V4ND72
D	-4	ARG	-	expression tag	UNP A0A4V4ND72
D	-3	TRP	-	expression tag	UNP A0A4V4ND72
D	-2	GLY	-	expression tag	UNP A0A4V4ND72
D	-1	SER	-	expression tag	UNP A0A4V4ND72
D	0	GLU	-	expression tag	UNP A0A4V4ND72
D	1	LEU	-	expression tag	UNP A0A4V4ND72
D	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
D	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
D	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
D	232	GLY	-	expression tag	UNP A0A4V4ND72
D	233	GLY	-	expression tag	UNP A0A4V4ND72
D	234	SER	-	expression tag	UNP A0A4V4ND72
D	235	GLY	-	expression tag	UNP A0A4V4ND72
D	236	GLY	-	expression tag	UNP A0A4V4ND72
D	237	SER	-	expression tag	UNP A0A4V4ND72
D	238	GLU	-	expression tag	UNP A0A4V4ND72
D	239	ASN	-	expression tag	UNP A0A4V4ND72
D	240	LEU	-	expression tag	UNP A0A4V4ND72
D	241	TYR	-	expression tag	UNP A0A4V4ND72
D	242	PHE	-	expression tag	UNP A0A4V4ND72
D	243	GLN	-	expression tag	UNP A0A4V4ND72
E	-36	MET	-	initiating methionine	UNP A0A4V4ND72
E	-35	GLY	-	expression tag	UNP A0A4V4ND72
E	-34	GLY	-	expression tag	UNP A0A4V4ND72
E	-33	SER	-	expression tag	UNP A0A4V4ND72
E	-32	HIS	-	expression tag	UNP A0A4V4ND72
E	-31	HIS	-	expression tag	UNP A0A4V4ND72
E	-30	HIS	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-29	HIS	-	expression tag	UNP A0A4V4ND72
E	-28	HIS	-	expression tag	UNP A0A4V4ND72
E	-27	HIS	-	expression tag	UNP A0A4V4ND72
E	-26	GLY	-	expression tag	UNP A0A4V4ND72
E	-25	MET	-	expression tag	UNP A0A4V4ND72
E	-24	ALA	-	expression tag	UNP A0A4V4ND72
E	-23	SER	-	expression tag	UNP A0A4V4ND72
E	-22	MET	-	expression tag	UNP A0A4V4ND72
E	-21	THR	-	expression tag	UNP A0A4V4ND72
E	-20	GLY	-	expression tag	UNP A0A4V4ND72
E	-19	GLY	-	expression tag	UNP A0A4V4ND72
E	-18	GLN	-	expression tag	UNP A0A4V4ND72
E	-17	GLN	-	expression tag	UNP A0A4V4ND72
E	-16	MET	-	expression tag	UNP A0A4V4ND72
E	-15	GLY	-	expression tag	UNP A0A4V4ND72
E	-14	ARG	-	expression tag	UNP A0A4V4ND72
E	-13	ASP	-	expression tag	UNP A0A4V4ND72
E	-12	LEU	-	expression tag	UNP A0A4V4ND72
E	-11	TYR	-	expression tag	UNP A0A4V4ND72
E	-10	ASP	-	expression tag	UNP A0A4V4ND72
E	-9	ASP	-	expression tag	UNP A0A4V4ND72
E	-8	ASP	-	expression tag	UNP A0A4V4ND72
E	-7	ASP	-	expression tag	UNP A0A4V4ND72
E	-6	LYS	-	expression tag	UNP A0A4V4ND72
E	-5	ASP	-	expression tag	UNP A0A4V4ND72
E	-4	ARG	-	expression tag	UNP A0A4V4ND72
E	-3	TRP	-	expression tag	UNP A0A4V4ND72
E	-2	GLY	-	expression tag	UNP A0A4V4ND72
E	-1	SER	-	expression tag	UNP A0A4V4ND72
E	0	GLU	-	expression tag	UNP A0A4V4ND72
E	1	LEU	-	expression tag	UNP A0A4V4ND72
E	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
E	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
E	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
E	232	GLY	-	expression tag	UNP A0A4V4ND72
E	233	GLY	-	expression tag	UNP A0A4V4ND72
E	234	SER	-	expression tag	UNP A0A4V4ND72
E	235	GLY	-	expression tag	UNP A0A4V4ND72
E	236	GLY	-	expression tag	UNP A0A4V4ND72
E	237	SER	-	expression tag	UNP A0A4V4ND72
E	238	GLU	-	expression tag	UNP A0A4V4ND72
E	239	ASN	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
E	240	LEU	-	expression tag	UNP A0A4V4ND72
E	241	TYR	-	expression tag	UNP A0A4V4ND72
E	242	PHE	-	expression tag	UNP A0A4V4ND72
E	243	GLN	-	expression tag	UNP A0A4V4ND72
F	-36	MET	-	initiating methionine	UNP A0A4V4ND72
F	-35	GLY	-	expression tag	UNP A0A4V4ND72
F	-34	GLY	-	expression tag	UNP A0A4V4ND72
F	-33	SER	-	expression tag	UNP A0A4V4ND72
F	-32	HIS	-	expression tag	UNP A0A4V4ND72
F	-31	HIS	-	expression tag	UNP A0A4V4ND72
F	-30	HIS	-	expression tag	UNP A0A4V4ND72
F	-29	HIS	-	expression tag	UNP A0A4V4ND72
F	-28	HIS	-	expression tag	UNP A0A4V4ND72
F	-27	HIS	-	expression tag	UNP A0A4V4ND72
F	-26	GLY	-	expression tag	UNP A0A4V4ND72
F	-25	MET	-	expression tag	UNP A0A4V4ND72
F	-24	ALA	-	expression tag	UNP A0A4V4ND72
F	-23	SER	-	expression tag	UNP A0A4V4ND72
F	-22	MET	-	expression tag	UNP A0A4V4ND72
F	-21	THR	-	expression tag	UNP A0A4V4ND72
F	-20	GLY	-	expression tag	UNP A0A4V4ND72
F	-19	GLY	-	expression tag	UNP A0A4V4ND72
F	-18	GLN	-	expression tag	UNP A0A4V4ND72
F	-17	GLN	-	expression tag	UNP A0A4V4ND72
F	-16	MET	-	expression tag	UNP A0A4V4ND72
F	-15	GLY	-	expression tag	UNP A0A4V4ND72
F	-14	ARG	-	expression tag	UNP A0A4V4ND72
F	-13	ASP	-	expression tag	UNP A0A4V4ND72
F	-12	LEU	-	expression tag	UNP A0A4V4ND72
F	-11	TYR	-	expression tag	UNP A0A4V4ND72
F	-10	ASP	-	expression tag	UNP A0A4V4ND72
F	-9	ASP	-	expression tag	UNP A0A4V4ND72
F	-8	ASP	-	expression tag	UNP A0A4V4ND72
F	-7	ASP	-	expression tag	UNP A0A4V4ND72
F	-6	LYS	-	expression tag	UNP A0A4V4ND72
F	-5	ASP	-	expression tag	UNP A0A4V4ND72
F	-4	ARG	-	expression tag	UNP A0A4V4ND72
F	-3	TRP	-	expression tag	UNP A0A4V4ND72
F	-2	GLY	-	expression tag	UNP A0A4V4ND72
F	-1	SER	-	expression tag	UNP A0A4V4ND72
F	0	GLU	-	expression tag	UNP A0A4V4ND72
F	1	LEU	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
F	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
F	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
F	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
F	232	GLY	-	expression tag	UNP A0A4V4ND72
F	233	GLY	-	expression tag	UNP A0A4V4ND72
F	234	SER	-	expression tag	UNP A0A4V4ND72
F	235	GLY	-	expression tag	UNP A0A4V4ND72
F	236	GLY	-	expression tag	UNP A0A4V4ND72
F	237	SER	-	expression tag	UNP A0A4V4ND72
F	238	GLU	-	expression tag	UNP A0A4V4ND72
F	239	ASN	-	expression tag	UNP A0A4V4ND72
F	240	LEU	-	expression tag	UNP A0A4V4ND72
F	241	TYR	-	expression tag	UNP A0A4V4ND72
F	242	PHE	-	expression tag	UNP A0A4V4ND72
F	243	GLN	-	expression tag	UNP A0A4V4ND72
G	-36	MET	-	initiating methionine	UNP A0A4V4ND72
G	-35	GLY	-	expression tag	UNP A0A4V4ND72
G	-34	GLY	-	expression tag	UNP A0A4V4ND72
G	-33	SER	-	expression tag	UNP A0A4V4ND72
G	-32	HIS	-	expression tag	UNP A0A4V4ND72
G	-31	HIS	-	expression tag	UNP A0A4V4ND72
G	-30	HIS	-	expression tag	UNP A0A4V4ND72
G	-29	HIS	-	expression tag	UNP A0A4V4ND72
G	-28	HIS	-	expression tag	UNP A0A4V4ND72
G	-27	HIS	-	expression tag	UNP A0A4V4ND72
G	-26	GLY	-	expression tag	UNP A0A4V4ND72
G	-25	MET	-	expression tag	UNP A0A4V4ND72
G	-24	ALA	-	expression tag	UNP A0A4V4ND72
G	-23	SER	-	expression tag	UNP A0A4V4ND72
G	-22	MET	-	expression tag	UNP A0A4V4ND72
G	-21	THR	-	expression tag	UNP A0A4V4ND72
G	-20	GLY	-	expression tag	UNP A0A4V4ND72
G	-19	GLY	-	expression tag	UNP A0A4V4ND72
G	-18	GLN	-	expression tag	UNP A0A4V4ND72
G	-17	GLN	-	expression tag	UNP A0A4V4ND72
G	-16	MET	-	expression tag	UNP A0A4V4ND72
G	-15	GLY	-	expression tag	UNP A0A4V4ND72
G	-14	ARG	-	expression tag	UNP A0A4V4ND72
G	-13	ASP	-	expression tag	UNP A0A4V4ND72
G	-12	LEU	-	expression tag	UNP A0A4V4ND72
G	-11	TYR	-	expression tag	UNP A0A4V4ND72
G	-10	ASP	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	ASP	-	expression tag	UNP A0A4V4ND72
G	-8	ASP	-	expression tag	UNP A0A4V4ND72
G	-7	ASP	-	expression tag	UNP A0A4V4ND72
G	-6	LYS	-	expression tag	UNP A0A4V4ND72
G	-5	ASP	-	expression tag	UNP A0A4V4ND72
G	-4	ARG	-	expression tag	UNP A0A4V4ND72
G	-3	TRP	-	expression tag	UNP A0A4V4ND72
G	-2	GLY	-	expression tag	UNP A0A4V4ND72
G	-1	SER	-	expression tag	UNP A0A4V4ND72
G	0	GLU	-	expression tag	UNP A0A4V4ND72
G	1	LEU	-	expression tag	UNP A0A4V4ND72
G	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
G	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
G	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
G	232	GLY	-	expression tag	UNP A0A4V4ND72
G	233	GLY	-	expression tag	UNP A0A4V4ND72
G	234	SER	-	expression tag	UNP A0A4V4ND72
G	235	GLY	-	expression tag	UNP A0A4V4ND72
G	236	GLY	-	expression tag	UNP A0A4V4ND72
G	237	SER	-	expression tag	UNP A0A4V4ND72
G	238	GLU	-	expression tag	UNP A0A4V4ND72
G	239	ASN	-	expression tag	UNP A0A4V4ND72
G	240	LEU	-	expression tag	UNP A0A4V4ND72
G	241	TYR	-	expression tag	UNP A0A4V4ND72
G	242	PHE	-	expression tag	UNP A0A4V4ND72
G	243	GLN	-	expression tag	UNP A0A4V4ND72
H	-36	MET	-	initiating methionine	UNP A0A4V4ND72
H	-35	GLY	-	expression tag	UNP A0A4V4ND72
H	-34	GLY	-	expression tag	UNP A0A4V4ND72
H	-33	SER	-	expression tag	UNP A0A4V4ND72
H	-32	HIS	-	expression tag	UNP A0A4V4ND72
H	-31	HIS	-	expression tag	UNP A0A4V4ND72
H	-30	HIS	-	expression tag	UNP A0A4V4ND72
H	-29	HIS	-	expression tag	UNP A0A4V4ND72
H	-28	HIS	-	expression tag	UNP A0A4V4ND72
H	-27	HIS	-	expression tag	UNP A0A4V4ND72
H	-26	GLY	-	expression tag	UNP A0A4V4ND72
H	-25	MET	-	expression tag	UNP A0A4V4ND72
H	-24	ALA	-	expression tag	UNP A0A4V4ND72
H	-23	SER	-	expression tag	UNP A0A4V4ND72
H	-22	MET	-	expression tag	UNP A0A4V4ND72
H	-21	THR	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	GLY	-	expression tag	UNP A0A4V4ND72
H	-19	GLY	-	expression tag	UNP A0A4V4ND72
H	-18	GLN	-	expression tag	UNP A0A4V4ND72
H	-17	GLN	-	expression tag	UNP A0A4V4ND72
H	-16	MET	-	expression tag	UNP A0A4V4ND72
H	-15	GLY	-	expression tag	UNP A0A4V4ND72
H	-14	ARG	-	expression tag	UNP A0A4V4ND72
H	-13	ASP	-	expression tag	UNP A0A4V4ND72
H	-12	LEU	-	expression tag	UNP A0A4V4ND72
H	-11	TYR	-	expression tag	UNP A0A4V4ND72
H	-10	ASP	-	expression tag	UNP A0A4V4ND72
H	-9	ASP	-	expression tag	UNP A0A4V4ND72
H	-8	ASP	-	expression tag	UNP A0A4V4ND72
H	-7	ASP	-	expression tag	UNP A0A4V4ND72
H	-6	LYS	-	expression tag	UNP A0A4V4ND72
H	-5	ASP	-	expression tag	UNP A0A4V4ND72
H	-4	ARG	-	expression tag	UNP A0A4V4ND72
H	-3	TRP	-	expression tag	UNP A0A4V4ND72
H	-2	GLY	-	expression tag	UNP A0A4V4ND72
H	-1	SER	-	expression tag	UNP A0A4V4ND72
H	0	GLU	-	expression tag	UNP A0A4V4ND72
H	1	LEU	-	expression tag	UNP A0A4V4ND72
H	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
H	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
H	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
H	232	GLY	-	expression tag	UNP A0A4V4ND72
H	233	GLY	-	expression tag	UNP A0A4V4ND72
H	234	SER	-	expression tag	UNP A0A4V4ND72
H	235	GLY	-	expression tag	UNP A0A4V4ND72
H	236	GLY	-	expression tag	UNP A0A4V4ND72
H	237	SER	-	expression tag	UNP A0A4V4ND72
H	238	GLU	-	expression tag	UNP A0A4V4ND72
H	239	ASN	-	expression tag	UNP A0A4V4ND72
H	240	LEU	-	expression tag	UNP A0A4V4ND72
H	241	TYR	-	expression tag	UNP A0A4V4ND72
H	242	PHE	-	expression tag	UNP A0A4V4ND72
H	243	GLN	-	expression tag	UNP A0A4V4ND72
I	-36	MET	-	initiating methionine	UNP A0A4V4ND72
I	-35	GLY	-	expression tag	UNP A0A4V4ND72
I	-34	GLY	-	expression tag	UNP A0A4V4ND72
I	-33	SER	-	expression tag	UNP A0A4V4ND72
I	-32	HIS	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-31	HIS	-	expression tag	UNP A0A4V4ND72
I	-30	HIS	-	expression tag	UNP A0A4V4ND72
I	-29	HIS	-	expression tag	UNP A0A4V4ND72
I	-28	HIS	-	expression tag	UNP A0A4V4ND72
I	-27	HIS	-	expression tag	UNP A0A4V4ND72
I	-26	GLY	-	expression tag	UNP A0A4V4ND72
I	-25	MET	-	expression tag	UNP A0A4V4ND72
I	-24	ALA	-	expression tag	UNP A0A4V4ND72
I	-23	SER	-	expression tag	UNP A0A4V4ND72
I	-22	MET	-	expression tag	UNP A0A4V4ND72
I	-21	THR	-	expression tag	UNP A0A4V4ND72
I	-20	GLY	-	expression tag	UNP A0A4V4ND72
I	-19	GLY	-	expression tag	UNP A0A4V4ND72
I	-18	GLN	-	expression tag	UNP A0A4V4ND72
I	-17	GLN	-	expression tag	UNP A0A4V4ND72
I	-16	MET	-	expression tag	UNP A0A4V4ND72
I	-15	GLY	-	expression tag	UNP A0A4V4ND72
I	-14	ARG	-	expression tag	UNP A0A4V4ND72
I	-13	ASP	-	expression tag	UNP A0A4V4ND72
I	-12	LEU	-	expression tag	UNP A0A4V4ND72
I	-11	TYR	-	expression tag	UNP A0A4V4ND72
I	-10	ASP	-	expression tag	UNP A0A4V4ND72
I	-9	ASP	-	expression tag	UNP A0A4V4ND72
I	-8	ASP	-	expression tag	UNP A0A4V4ND72
I	-7	ASP	-	expression tag	UNP A0A4V4ND72
I	-6	LYS	-	expression tag	UNP A0A4V4ND72
I	-5	ASP	-	expression tag	UNP A0A4V4ND72
I	-4	ARG	-	expression tag	UNP A0A4V4ND72
I	-3	TRP	-	expression tag	UNP A0A4V4ND72
I	-2	GLY	-	expression tag	UNP A0A4V4ND72
I	-1	SER	-	expression tag	UNP A0A4V4ND72
I	0	GLU	-	expression tag	UNP A0A4V4ND72
I	1	LEU	-	expression tag	UNP A0A4V4ND72
I	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
I	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
I	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
I	232	GLY	-	expression tag	UNP A0A4V4ND72
I	233	GLY	-	expression tag	UNP A0A4V4ND72
I	234	SER	-	expression tag	UNP A0A4V4ND72
I	235	GLY	-	expression tag	UNP A0A4V4ND72
I	236	GLY	-	expression tag	UNP A0A4V4ND72
I	237	SER	-	expression tag	UNP A0A4V4ND72

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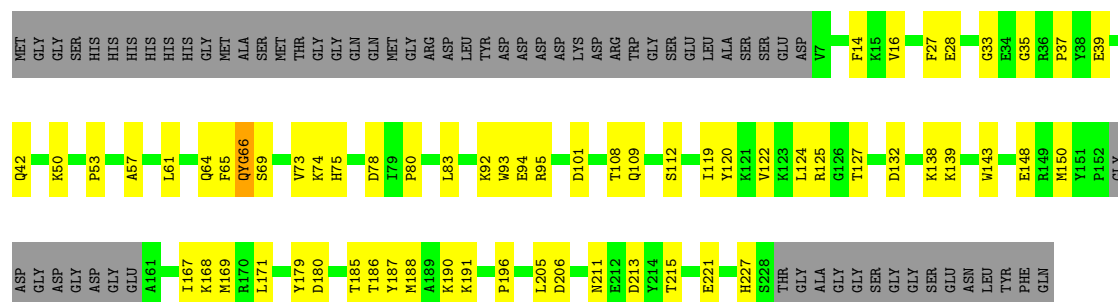
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Chain	Residue	Modelled	Actual	Comment	Reference
I	238	GLU	-	expression tag	UNP A0A4V4ND72
I	239	ASN	-	expression tag	UNP A0A4V4ND72
I	240	LEU	-	expression tag	UNP A0A4V4ND72
I	241	TYR	-	expression tag	UNP A0A4V4ND72
I	242	PHE	-	expression tag	UNP A0A4V4ND72
I	243	GLN	-	expression tag	UNP A0A4V4ND72
J	-36	MET	-	initiating methionine	UNP A0A4V4ND72
J	-35	GLY	-	expression tag	UNP A0A4V4ND72
J	-34	GLY	-	expression tag	UNP A0A4V4ND72
J	-33	SER	-	expression tag	UNP A0A4V4ND72
J	-32	HIS	-	expression tag	UNP A0A4V4ND72
J	-31	HIS	-	expression tag	UNP A0A4V4ND72
J	-30	HIS	-	expression tag	UNP A0A4V4ND72
J	-29	HIS	-	expression tag	UNP A0A4V4ND72
J	-28	HIS	-	expression tag	UNP A0A4V4ND72
J	-27	HIS	-	expression tag	UNP A0A4V4ND72
J	-26	GLY	-	expression tag	UNP A0A4V4ND72
J	-25	MET	-	expression tag	UNP A0A4V4ND72
J	-24	ALA	-	expression tag	UNP A0A4V4ND72
J	-23	SER	-	expression tag	UNP A0A4V4ND72
J	-22	MET	-	expression tag	UNP A0A4V4ND72
J	-21	THR	-	expression tag	UNP A0A4V4ND72
J	-20	GLY	-	expression tag	UNP A0A4V4ND72
J	-19	GLY	-	expression tag	UNP A0A4V4ND72
J	-18	GLN	-	expression tag	UNP A0A4V4ND72
J	-17	GLN	-	expression tag	UNP A0A4V4ND72
J	-16	MET	-	expression tag	UNP A0A4V4ND72
J	-15	GLY	-	expression tag	UNP A0A4V4ND72
J	-14	ARG	-	expression tag	UNP A0A4V4ND72
J	-13	ASP	-	expression tag	UNP A0A4V4ND72
J	-12	LEU	-	expression tag	UNP A0A4V4ND72
J	-11	TYR	-	expression tag	UNP A0A4V4ND72
J	-10	ASP	-	expression tag	UNP A0A4V4ND72
J	-9	ASP	-	expression tag	UNP A0A4V4ND72
J	-8	ASP	-	expression tag	UNP A0A4V4ND72
J	-7	ASP	-	expression tag	UNP A0A4V4ND72
J	-6	LYS	-	expression tag	UNP A0A4V4ND72
J	-5	ASP	-	expression tag	UNP A0A4V4ND72
J	-4	ARG	-	expression tag	UNP A0A4V4ND72
J	-3	TRP	-	expression tag	UNP A0A4V4ND72
J	-2	GLY	-	expression tag	UNP A0A4V4ND72
J	-1	SER	-	expression tag	UNP A0A4V4ND72

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	GLU	-	expression tag	UNP A0A4V4ND72
J	1	LEU	-	expression tag	UNP A0A4V4ND72
J	66	CRQ	GLN	chromophore	UNP A0A4V4ND72
J	66	CRQ	TYR	chromophore	UNP A0A4V4ND72
J	66	CRQ	GLY	chromophore	UNP A0A4V4ND72
J	232	GLY	-	expression tag	UNP A0A4V4ND72
J	233	GLY	-	expression tag	UNP A0A4V4ND72
J	234	SER	-	expression tag	UNP A0A4V4ND72
J	235	GLY	-	expression tag	UNP A0A4V4ND72
J	236	GLY	-	expression tag	UNP A0A4V4ND72
J	237	SER	-	expression tag	UNP A0A4V4ND72
J	238	GLU	-	expression tag	UNP A0A4V4ND72
J	239	ASN	-	expression tag	UNP A0A4V4ND72
J	240	LEU	-	expression tag	UNP A0A4V4ND72
J	241	TYR	-	expression tag	UNP A0A4V4ND72
J	242	PHE	-	expression tag	UNP A0A4V4ND72
J	243	GLN	-	expression tag	UNP A0A4V4ND72



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.73Å 132.28Å 227.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 3.16 49.89 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.89-3.16) 99.9 (49.89-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.185 , 0.249 0.186 , 0.247	Depositor DCC
R_{free} test set	44293 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17210	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: CRQ

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	0.50	0/1743	0.70	0/2342
1	B	0.47	0/1743	0.70	0/2342
1	C	0.46	0/1738	0.68	0/2335
1	D	0.41	0/1734	0.61	0/2330
1	E	0.43	0/1734	0.68	0/2330
1	F	0.44	0/1734	0.64	0/2330
1	G	0.46	0/1738	0.68	0/2335
1	H	0.43	0/1738	0.67	0/2335
1	I	0.42	0/1734	0.64	0/2330
1	J	0.41	0/1734	0.65	0/2330
All	All	0.44	0/17370	0.67	0/23339

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	127	THR	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	1727	0	1681	33	0
1	B	1727	0	1680	28	0
1	C	1722	0	1677	27	0
1	D	1718	0	1674	17	0
1	E	1718	0	1675	27	0
1	F	1718	0	1674	18	0
1	G	1722	0	1678	32	0
1	H	1722	0	1677	26	0
1	I	1718	0	1674	26	0
1	J	1718	0	1674	38	0
All	All	17210	0	16764	269	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 8.

The worst 5 of 269 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:VAL:HG22	1:D:106:THR:HG22	1.57	0.86
1:H:96:VAL:HG22	1:H:106:THR:HG22	1.61	0.82
1:G:96:VAL:HG22	1:G:106:THR:HG22	1.61	0.81
1:C:170:ARG:HB2	1:C:180:ASP:OD1	1.81	0.81
1:F:96:VAL:HG22	1:F:106:THR:HG22	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/278 (74%)	200 (97%)	6 (3%)	0	100	100
1	B	206/278 (74%)	199 (97%)	7 (3%)	0	100	100
1	C	206/278 (74%)	195 (95%)	11 (5%)	0	100	100
1	D	205/278 (74%)	197 (96%)	8 (4%)	0	100	100
1	E	205/278 (74%)	195 (95%)	10 (5%)	0	100	100
1	F	205/278 (74%)	199 (97%)	6 (3%)	0	100	100
1	G	206/278 (74%)	196 (95%)	10 (5%)	0	100	100
1	H	206/278 (74%)	199 (97%)	7 (3%)	0	100	100
1	I	205/278 (74%)	191 (93%)	14 (7%)	0	100	100
1	J	205/278 (74%)	195 (95%)	10 (5%)	0	100	100
All	All	2055/2780 (74%)	1966 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	182/228 (80%)	182 (100%)	0	100	100
1	B	182/228 (80%)	182 (100%)	0	100	100
1	C	181/228 (79%)	181 (100%)	0	100	100
1	D	181/228 (79%)	181 (100%)	0	100	100
1	E	181/228 (79%)	181 (100%)	0	100	100
1	F	181/228 (79%)	181 (100%)	0	100	100
1	G	181/228 (79%)	181 (100%)	0	100	100
1	H	181/228 (79%)	181 (100%)	0	100	100
1	I	181/228 (79%)	181 (100%)	0	100	100
1	J	181/228 (79%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1812/2280 (80%)	1812 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	128	ASN
1	I	98	ASN
1	H	178	HIS
1	H	114	GLN
1	H	227	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	CRQ	B	66	1	24,25,26	1.33	2 (8%)	27,34,36	2.79	8 (29%)
1	CRQ	D	66	1	24,25,26	1.42	2 (8%)	27,34,36	2.27	6 (22%)
1	CRQ	C	66	1	24,25,26	1.23	2 (8%)	27,34,36	1.99	6 (22%)
1	CRQ	F	66	1	24,25,26	1.30	2 (8%)	27,34,36	2.33	8 (29%)
1	CRQ	I	66	1	24,25,26	1.51	2 (8%)	27,34,36	2.99	5 (18%)
1	CRQ	H	66	1	24,25,26	1.40	2 (8%)	27,34,36	3.07	9 (33%)
1	CRQ	J	66	1	24,25,26	1.45	1 (4%)	27,34,36	2.74	7 (25%)
1	CRQ	G	66	1	24,25,26	1.60	2 (8%)	27,34,36	2.39	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	A	66	1	24,25,26	1.39	2 (8%)	27,34,36	2.69	8 (29%)
1	CRQ	E	66	1	24,25,26	1.29	2 (8%)	27,34,36	3.03	8 (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	CRQ	B	66	1	-	3/10/32/33	0/2/2/2
1	CRQ	D	66	1	-	3/10/32/33	0/2/2/2
1	CRQ	C	66	1	-	4/10/32/33	0/2/2/2
1	CRQ	F	66	1	-	5/10/32/33	0/2/2/2
1	CRQ	I	66	1	-	3/10/32/33	0/2/2/2
1	CRQ	H	66	1	-	4/10/32/33	0/2/2/2
1	CRQ	J	66	1	-	6/10/32/33	0/2/2/2
1	CRQ	G	66	1	-	3/10/32/33	0/2/2/2
1	CRQ	A	66	1	-	5/10/32/33	0/2/2/2
1	CRQ	E	66	1	-	3/10/32/33	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	CRQ	CB2-CA2	6.73	1.40	1.35
1	J	66	CRQ	CB2-CA2	6.17	1.40	1.35
1	I	66	CRQ	CB2-CA2	5.84	1.40	1.35
1	D	66	CRQ	CB2-CA2	5.44	1.39	1.35
1	A	66	CRQ	CB2-CA2	5.01	1.39	1.35

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	CRQ	O2-C2-CA2	-11.29	124.62	130.96
1	E	66	CRQ	O2-C2-CA2	-10.97	124.80	130.96
1	I	66	CRQ	O2-C2-CA2	-10.07	125.30	130.96
1	B	66	CRQ	O2-C2-CA2	-9.45	125.65	130.96
1	J	66	CRQ	O2-C2-CA2	-9.44	125.66	130.96

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRQ	C3-CA3-N3-C1
1	A	66	CRQ	C3-CA3-N3-C2
1	A	66	CRQ	C2-CA2-CB2-CG2
1	B	66	CRQ	C1-CA1-CB1-CG1
1	B	66	CRQ	N2-CA2-CB2-CG2

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRQ	1	0
1	D	66	CRQ	1	0
1	C	66	CRQ	2	0
1	H	66	CRQ	2	0
1	J	66	CRQ	3	0
1	G	66	CRQ	2	0
1	E	66	CRQ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	212/278 (76%)	-0.84	0 100 100	45, 57, 73, 107	0
1	B	212/278 (76%)	-0.78	0 100 100	48, 61, 81, 114	0
1	C	212/278 (76%)	-0.76	0 100 100	51, 66, 82, 107	0
1	D	211/278 (75%)	-0.69	1 (0%) 87 77	58, 77, 93, 105	0
1	E	211/278 (75%)	-0.64	0 100 100	51, 70, 88, 100	0
1	F	211/278 (75%)	-0.72	0 100 100	50, 73, 91, 104	0
1	G	212/278 (76%)	-0.63	0 100 100	51, 75, 96, 103	0
1	H	212/278 (76%)	-0.61	1 (0%) 87 77	56, 77, 94, 102	0
1	I	211/278 (75%)	-0.56	0 100 100	62, 81, 97, 111	0
1	J	211/278 (75%)	-0.51	0 100 100	58, 85, 106, 122	0
All	All	2115/2780 (76%)	-0.67	2 (0%) 92 90	45, 72, 95, 122	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	161	ALA	2.4
1	D	161	ALA	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	CRQ	C	66	24/25	0.91	0.11	59,65,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CRQ	E	66	24/25	0.92	0.10	58,63,67,68	0
1	CRQ	D	66	24/25	0.93	0.10	65,71,76,79	0
1	CRQ	I	66	24/25	0.93	0.10	65,75,82,88	0
1	CRQ	J	66	24/25	0.93	0.09	69,80,84,90	0
1	CRQ	G	66	24/25	0.94	0.09	58,71,75,78	0
1	CRQ	H	66	24/25	0.94	0.10	59,74,78,88	0
1	CRQ	B	66	24/25	0.95	0.09	52,61,64,66	0
1	CRQ	F	66	24/25	0.95	0.10	61,68,73,76	0
1	CRQ	A	66	24/25	0.97	0.08	44,53,61,61	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.