



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:15 PM UTC

PDB ID : 6VIO / pdb_00006vio
Title : Crystal structure of eYFP His148Ser
Authors : Lieberman, R.L.; Hill, S.E.; Patterson-Orazem, A.C.
Deposited on : 2020-01-13
Resolution : 3.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

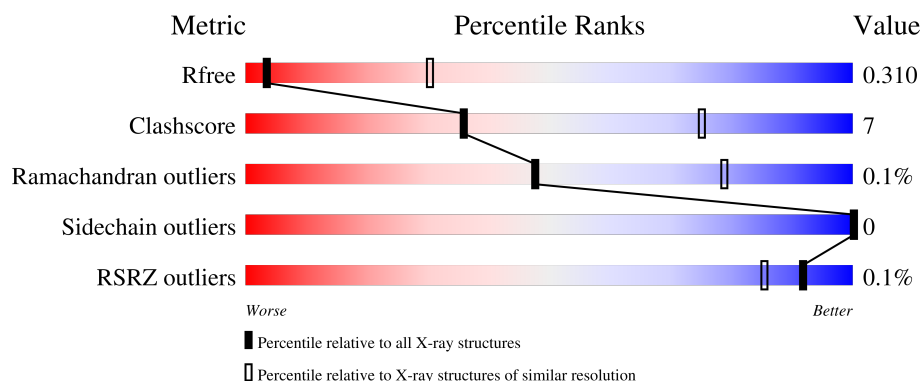
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	 75% 12% 13%
1	B	260	 70% 16% 13%
1	C	260	 72% 15% 13%
1	D	260	 73% 14% 13%
1	E	260	 72% 15% 13%

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Mol	Chain	Length	Quality of chain
1	F	260	 76% 11% 13%
1	G	260	 72% 13% 14%
1	H	260	 72% 15% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14010 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 Green fluorescent protein GFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1756	1118	292	340	6			
1	B	226	Total	C	N	O	S	0	0	0
			1750	1115	291	338	6			
1	C	225	Total	C	N	O	S	0	0	0
			1745	1112	290	337	6			
1	D	226	Total	C	N	O	S	0	0	0
			1750	1115	291	338	6			
1	E	227	Total	C	N	O	S	0	0	0
			1756	1118	292	340	6			
1	F	227	Total	C	N	O	S	0	0	0
			1756	1118	292	340	6			
1	G	224	Total	C	N	O	S	0	0	0
			1741	1110	289	336	6			
1	H	227	Total	C	N	O	S	0	0	0
			1756	1118	292	340	6			

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP A0A5J6CYR6
A	-22	GLY	-	expression tag	UNP A0A5J6CYR6
A	-21	SER	-	expression tag	UNP A0A5J6CYR6
A	-20	SER	-	expression tag	UNP A0A5J6CYR6
A	-19	HIS	-	expression tag	UNP A0A5J6CYR6
A	-18	HIS	-	expression tag	UNP A0A5J6CYR6
A	-17	HIS	-	expression tag	UNP A0A5J6CYR6
A	-16	HIS	-	expression tag	UNP A0A5J6CYR6
A	-15	HIS	-	expression tag	UNP A0A5J6CYR6
A	-14	HIS	-	expression tag	UNP A0A5J6CYR6
A	-13	SER	-	expression tag	UNP A0A5J6CYR6
A	-12	SER	-	expression tag	UNP A0A5J6CYR6
A	-11	GLY	-	expression tag	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	LEU	-	expression tag	UNP A0A5J6CYR6
A	-9	VAL	-	expression tag	UNP A0A5J6CYR6
A	-8	PRO	-	expression tag	UNP A0A5J6CYR6
A	-7	ARG	-	expression tag	UNP A0A5J6CYR6
A	-6	GLY	-	expression tag	UNP A0A5J6CYR6
A	-5	SER	-	expression tag	UNP A0A5J6CYR6
A	-4	HIS	-	expression tag	UNP A0A5J6CYR6
A	-3	MET	-	expression tag	UNP A0A5J6CYR6
A	-2	ALA	-	expression tag	UNP A0A5J6CYR6
A	-1	SER	-	expression tag	UNP A0A5J6CYR6
A	0	MET	-	expression tag	UNP A0A5J6CYR6
A	1	VAL	-	expression tag	UNP A0A5J6CYR6
A	25	HIS	GLN	conflict	UNP A0A5J6CYR6
A	66	CR2	SER	chromophore	UNP A0A5J6CYR6
A	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
A	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
A	68	LEU	VAL	conflict	UNP A0A5J6CYR6
A	72	ALA	SER	conflict	UNP A0A5J6CYR6
A	100	PHE	TYR	conflict	UNP A0A5J6CYR6
A	141	LEU	MET	conflict	UNP A0A5J6CYR6
A	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
A	157	GLN	PRO	conflict	UNP A0A5J6CYR6
A	172	GLU	LYS	conflict	UNP A0A5J6CYR6
A	203	TYR	THR	conflict	UNP A0A5J6CYR6
A	219	VAL	ILE	conflict	UNP A0A5J6CYR6
A	231	LEU	HIS	conflict	UNP A0A5J6CYR6
B	-23	MET	-	expression tag	UNP A0A5J6CYR6
B	-22	GLY	-	expression tag	UNP A0A5J6CYR6
B	-21	SER	-	expression tag	UNP A0A5J6CYR6
B	-20	SER	-	expression tag	UNP A0A5J6CYR6
B	-19	HIS	-	expression tag	UNP A0A5J6CYR6
B	-18	HIS	-	expression tag	UNP A0A5J6CYR6
B	-17	HIS	-	expression tag	UNP A0A5J6CYR6
B	-16	HIS	-	expression tag	UNP A0A5J6CYR6
B	-15	HIS	-	expression tag	UNP A0A5J6CYR6
B	-14	HIS	-	expression tag	UNP A0A5J6CYR6
B	-13	SER	-	expression tag	UNP A0A5J6CYR6
B	-12	SER	-	expression tag	UNP A0A5J6CYR6
B	-11	GLY	-	expression tag	UNP A0A5J6CYR6
B	-10	LEU	-	expression tag	UNP A0A5J6CYR6
B	-9	VAL	-	expression tag	UNP A0A5J6CYR6
B	-8	PRO	-	expression tag	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	ARG	-	expression tag	UNP A0A5J6CYR6
B	-6	GLY	-	expression tag	UNP A0A5J6CYR6
B	-5	SER	-	expression tag	UNP A0A5J6CYR6
B	-4	HIS	-	expression tag	UNP A0A5J6CYR6
B	-3	MET	-	expression tag	UNP A0A5J6CYR6
B	-2	ALA	-	expression tag	UNP A0A5J6CYR6
B	-1	SER	-	expression tag	UNP A0A5J6CYR6
B	0	MET	-	expression tag	UNP A0A5J6CYR6
B	1	VAL	-	expression tag	UNP A0A5J6CYR6
B	25	HIS	GLN	conflict	UNP A0A5J6CYR6
B	66	CR2	SER	chromophore	UNP A0A5J6CYR6
B	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
B	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
B	68	LEU	VAL	conflict	UNP A0A5J6CYR6
B	72	ALA	SER	conflict	UNP A0A5J6CYR6
B	100	PHE	TYR	conflict	UNP A0A5J6CYR6
B	141	LEU	MET	conflict	UNP A0A5J6CYR6
B	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
B	157	GLN	PRO	conflict	UNP A0A5J6CYR6
B	172	GLU	LYS	conflict	UNP A0A5J6CYR6
B	203	TYR	THR	conflict	UNP A0A5J6CYR6
B	219	VAL	ILE	conflict	UNP A0A5J6CYR6
B	231	LEU	HIS	conflict	UNP A0A5J6CYR6
C	-23	MET	-	expression tag	UNP A0A5J6CYR6
C	-22	GLY	-	expression tag	UNP A0A5J6CYR6
C	-21	SER	-	expression tag	UNP A0A5J6CYR6
C	-20	SER	-	expression tag	UNP A0A5J6CYR6
C	-19	HIS	-	expression tag	UNP A0A5J6CYR6
C	-18	HIS	-	expression tag	UNP A0A5J6CYR6
C	-17	HIS	-	expression tag	UNP A0A5J6CYR6
C	-16	HIS	-	expression tag	UNP A0A5J6CYR6
C	-15	HIS	-	expression tag	UNP A0A5J6CYR6
C	-14	HIS	-	expression tag	UNP A0A5J6CYR6
C	-13	SER	-	expression tag	UNP A0A5J6CYR6
C	-12	SER	-	expression tag	UNP A0A5J6CYR6
C	-11	GLY	-	expression tag	UNP A0A5J6CYR6
C	-10	LEU	-	expression tag	UNP A0A5J6CYR6
C	-9	VAL	-	expression tag	UNP A0A5J6CYR6
C	-8	PRO	-	expression tag	UNP A0A5J6CYR6
C	-7	ARG	-	expression tag	UNP A0A5J6CYR6
C	-6	GLY	-	expression tag	UNP A0A5J6CYR6
C	-5	SER	-	expression tag	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP A0A5J6CYR6
C	-3	MET	-	expression tag	UNP A0A5J6CYR6
C	-2	ALA	-	expression tag	UNP A0A5J6CYR6
C	-1	SER	-	expression tag	UNP A0A5J6CYR6
C	0	MET	-	expression tag	UNP A0A5J6CYR6
C	1	VAL	-	expression tag	UNP A0A5J6CYR6
C	25	HIS	GLN	conflict	UNP A0A5J6CYR6
C	66	CR2	SER	chromophore	UNP A0A5J6CYR6
C	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
C	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
C	68	LEU	VAL	conflict	UNP A0A5J6CYR6
C	72	ALA	SER	conflict	UNP A0A5J6CYR6
C	100	PHE	TYR	conflict	UNP A0A5J6CYR6
C	141	LEU	MET	conflict	UNP A0A5J6CYR6
C	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
C	157	GLN	PRO	conflict	UNP A0A5J6CYR6
C	172	GLU	LYS	conflict	UNP A0A5J6CYR6
C	203	TYR	THR	conflict	UNP A0A5J6CYR6
C	219	VAL	ILE	conflict	UNP A0A5J6CYR6
C	231	LEU	HIS	conflict	UNP A0A5J6CYR6
D	-23	MET	-	expression tag	UNP A0A5J6CYR6
D	-22	GLY	-	expression tag	UNP A0A5J6CYR6
D	-21	SER	-	expression tag	UNP A0A5J6CYR6
D	-20	SER	-	expression tag	UNP A0A5J6CYR6
D	-19	HIS	-	expression tag	UNP A0A5J6CYR6
D	-18	HIS	-	expression tag	UNP A0A5J6CYR6
D	-17	HIS	-	expression tag	UNP A0A5J6CYR6
D	-16	HIS	-	expression tag	UNP A0A5J6CYR6
D	-15	HIS	-	expression tag	UNP A0A5J6CYR6
D	-14	HIS	-	expression tag	UNP A0A5J6CYR6
D	-13	SER	-	expression tag	UNP A0A5J6CYR6
D	-12	SER	-	expression tag	UNP A0A5J6CYR6
D	-11	GLY	-	expression tag	UNP A0A5J6CYR6
D	-10	LEU	-	expression tag	UNP A0A5J6CYR6
D	-9	VAL	-	expression tag	UNP A0A5J6CYR6
D	-8	PRO	-	expression tag	UNP A0A5J6CYR6
D	-7	ARG	-	expression tag	UNP A0A5J6CYR6
D	-6	GLY	-	expression tag	UNP A0A5J6CYR6
D	-5	SER	-	expression tag	UNP A0A5J6CYR6
D	-4	HIS	-	expression tag	UNP A0A5J6CYR6
D	-3	MET	-	expression tag	UNP A0A5J6CYR6
D	-2	ALA	-	expression tag	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP A0A5J6CYR6
D	0	MET	-	expression tag	UNP A0A5J6CYR6
D	1	VAL	-	expression tag	UNP A0A5J6CYR6
D	25	HIS	GLN	conflict	UNP A0A5J6CYR6
D	66	CR2	SER	chromophore	UNP A0A5J6CYR6
D	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
D	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
D	68	LEU	VAL	conflict	UNP A0A5J6CYR6
D	72	ALA	SER	conflict	UNP A0A5J6CYR6
D	100	PHE	TYR	conflict	UNP A0A5J6CYR6
D	141	LEU	MET	conflict	UNP A0A5J6CYR6
D	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
D	157	GLN	PRO	conflict	UNP A0A5J6CYR6
D	172	GLU	LYS	conflict	UNP A0A5J6CYR6
D	203	TYR	THR	conflict	UNP A0A5J6CYR6
D	219	VAL	ILE	conflict	UNP A0A5J6CYR6
D	231	LEU	HIS	conflict	UNP A0A5J6CYR6
E	-23	MET	-	expression tag	UNP A0A5J6CYR6
E	-22	GLY	-	expression tag	UNP A0A5J6CYR6
E	-21	SER	-	expression tag	UNP A0A5J6CYR6
E	-20	SER	-	expression tag	UNP A0A5J6CYR6
E	-19	HIS	-	expression tag	UNP A0A5J6CYR6
E	-18	HIS	-	expression tag	UNP A0A5J6CYR6
E	-17	HIS	-	expression tag	UNP A0A5J6CYR6
E	-16	HIS	-	expression tag	UNP A0A5J6CYR6
E	-15	HIS	-	expression tag	UNP A0A5J6CYR6
E	-14	HIS	-	expression tag	UNP A0A5J6CYR6
E	-13	SER	-	expression tag	UNP A0A5J6CYR6
E	-12	SER	-	expression tag	UNP A0A5J6CYR6
E	-11	GLY	-	expression tag	UNP A0A5J6CYR6
E	-10	LEU	-	expression tag	UNP A0A5J6CYR6
E	-9	VAL	-	expression tag	UNP A0A5J6CYR6
E	-8	PRO	-	expression tag	UNP A0A5J6CYR6
E	-7	ARG	-	expression tag	UNP A0A5J6CYR6
E	-6	GLY	-	expression tag	UNP A0A5J6CYR6
E	-5	SER	-	expression tag	UNP A0A5J6CYR6
E	-4	HIS	-	expression tag	UNP A0A5J6CYR6
E	-3	MET	-	expression tag	UNP A0A5J6CYR6
E	-2	ALA	-	expression tag	UNP A0A5J6CYR6
E	-1	SER	-	expression tag	UNP A0A5J6CYR6
E	0	MET	-	expression tag	UNP A0A5J6CYR6
E	1	VAL	-	expression tag	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	25	HIS	GLN	conflict	UNP A0A5J6CYR6
E	66	CR2	SER	chromophore	UNP A0A5J6CYR6
E	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
E	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
E	68	LEU	VAL	conflict	UNP A0A5J6CYR6
E	72	ALA	SER	conflict	UNP A0A5J6CYR6
E	100	PHE	TYR	conflict	UNP A0A5J6CYR6
E	141	LEU	MET	conflict	UNP A0A5J6CYR6
E	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
E	157	GLN	PRO	conflict	UNP A0A5J6CYR6
E	172	GLU	LYS	conflict	UNP A0A5J6CYR6
E	203	TYR	THR	conflict	UNP A0A5J6CYR6
E	219	VAL	ILE	conflict	UNP A0A5J6CYR6
E	231	LEU	HIS	conflict	UNP A0A5J6CYR6
F	-23	MET	-	expression tag	UNP A0A5J6CYR6
F	-22	GLY	-	expression tag	UNP A0A5J6CYR6
F	-21	SER	-	expression tag	UNP A0A5J6CYR6
F	-20	SER	-	expression tag	UNP A0A5J6CYR6
F	-19	HIS	-	expression tag	UNP A0A5J6CYR6
F	-18	HIS	-	expression tag	UNP A0A5J6CYR6
F	-17	HIS	-	expression tag	UNP A0A5J6CYR6
F	-16	HIS	-	expression tag	UNP A0A5J6CYR6
F	-15	HIS	-	expression tag	UNP A0A5J6CYR6
F	-14	HIS	-	expression tag	UNP A0A5J6CYR6
F	-13	SER	-	expression tag	UNP A0A5J6CYR6
F	-12	SER	-	expression tag	UNP A0A5J6CYR6
F	-11	GLY	-	expression tag	UNP A0A5J6CYR6
F	-10	LEU	-	expression tag	UNP A0A5J6CYR6
F	-9	VAL	-	expression tag	UNP A0A5J6CYR6
F	-8	PRO	-	expression tag	UNP A0A5J6CYR6
F	-7	ARG	-	expression tag	UNP A0A5J6CYR6
F	-6	GLY	-	expression tag	UNP A0A5J6CYR6
F	-5	SER	-	expression tag	UNP A0A5J6CYR6
F	-4	HIS	-	expression tag	UNP A0A5J6CYR6
F	-3	MET	-	expression tag	UNP A0A5J6CYR6
F	-2	ALA	-	expression tag	UNP A0A5J6CYR6
F	-1	SER	-	expression tag	UNP A0A5J6CYR6
F	0	MET	-	expression tag	UNP A0A5J6CYR6
F	1	VAL	-	expression tag	UNP A0A5J6CYR6
F	25	HIS	GLN	conflict	UNP A0A5J6CYR6
F	66	CR2	SER	chromophore	UNP A0A5J6CYR6
F	66	CR2	TYR	chromophore	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
F	68	LEU	VAL	conflict	UNP A0A5J6CYR6
F	72	ALA	SER	conflict	UNP A0A5J6CYR6
F	100	PHE	TYR	conflict	UNP A0A5J6CYR6
F	141	LEU	MET	conflict	UNP A0A5J6CYR6
F	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
F	157	GLN	PRO	conflict	UNP A0A5J6CYR6
F	172	GLU	LYS	conflict	UNP A0A5J6CYR6
F	203	TYR	THR	conflict	UNP A0A5J6CYR6
F	219	VAL	ILE	conflict	UNP A0A5J6CYR6
F	231	LEU	HIS	conflict	UNP A0A5J6CYR6
G	-23	MET	-	expression tag	UNP A0A5J6CYR6
G	-22	GLY	-	expression tag	UNP A0A5J6CYR6
G	-21	SER	-	expression tag	UNP A0A5J6CYR6
G	-20	SER	-	expression tag	UNP A0A5J6CYR6
G	-19	HIS	-	expression tag	UNP A0A5J6CYR6
G	-18	HIS	-	expression tag	UNP A0A5J6CYR6
G	-17	HIS	-	expression tag	UNP A0A5J6CYR6
G	-16	HIS	-	expression tag	UNP A0A5J6CYR6
G	-15	HIS	-	expression tag	UNP A0A5J6CYR6
G	-14	HIS	-	expression tag	UNP A0A5J6CYR6
G	-13	SER	-	expression tag	UNP A0A5J6CYR6
G	-12	SER	-	expression tag	UNP A0A5J6CYR6
G	-11	GLY	-	expression tag	UNP A0A5J6CYR6
G	-10	LEU	-	expression tag	UNP A0A5J6CYR6
G	-9	VAL	-	expression tag	UNP A0A5J6CYR6
G	-8	PRO	-	expression tag	UNP A0A5J6CYR6
G	-7	ARG	-	expression tag	UNP A0A5J6CYR6
G	-6	GLY	-	expression tag	UNP A0A5J6CYR6
G	-5	SER	-	expression tag	UNP A0A5J6CYR6
G	-4	HIS	-	expression tag	UNP A0A5J6CYR6
G	-3	MET	-	expression tag	UNP A0A5J6CYR6
G	-2	ALA	-	expression tag	UNP A0A5J6CYR6
G	-1	SER	-	expression tag	UNP A0A5J6CYR6
G	0	MET	-	expression tag	UNP A0A5J6CYR6
G	1	VAL	-	expression tag	UNP A0A5J6CYR6
G	25	HIS	GLN	conflict	UNP A0A5J6CYR6
G	66	CR2	SER	chromophore	UNP A0A5J6CYR6
G	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
G	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
G	68	LEU	VAL	conflict	UNP A0A5J6CYR6
G	72	ALA	SER	conflict	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	100	PHE	TYR	conflict	UNP A0A5J6CYR6
G	141	LEU	MET	conflict	UNP A0A5J6CYR6
G	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6
G	157	GLN	PRO	conflict	UNP A0A5J6CYR6
G	172	GLU	LYS	conflict	UNP A0A5J6CYR6
G	203	TYR	THR	conflict	UNP A0A5J6CYR6
G	219	VAL	ILE	conflict	UNP A0A5J6CYR6
G	231	LEU	HIS	conflict	UNP A0A5J6CYR6
H	-23	MET	-	expression tag	UNP A0A5J6CYR6
H	-22	GLY	-	expression tag	UNP A0A5J6CYR6
H	-21	SER	-	expression tag	UNP A0A5J6CYR6
H	-20	SER	-	expression tag	UNP A0A5J6CYR6
H	-19	HIS	-	expression tag	UNP A0A5J6CYR6
H	-18	HIS	-	expression tag	UNP A0A5J6CYR6
H	-17	HIS	-	expression tag	UNP A0A5J6CYR6
H	-16	HIS	-	expression tag	UNP A0A5J6CYR6
H	-15	HIS	-	expression tag	UNP A0A5J6CYR6
H	-14	HIS	-	expression tag	UNP A0A5J6CYR6
H	-13	SER	-	expression tag	UNP A0A5J6CYR6
H	-12	SER	-	expression tag	UNP A0A5J6CYR6
H	-11	GLY	-	expression tag	UNP A0A5J6CYR6
H	-10	LEU	-	expression tag	UNP A0A5J6CYR6
H	-9	VAL	-	expression tag	UNP A0A5J6CYR6
H	-8	PRO	-	expression tag	UNP A0A5J6CYR6
H	-7	ARG	-	expression tag	UNP A0A5J6CYR6
H	-6	GLY	-	expression tag	UNP A0A5J6CYR6
H	-5	SER	-	expression tag	UNP A0A5J6CYR6
H	-4	HIS	-	expression tag	UNP A0A5J6CYR6
H	-3	MET	-	expression tag	UNP A0A5J6CYR6
H	-2	ALA	-	expression tag	UNP A0A5J6CYR6
H	-1	SER	-	expression tag	UNP A0A5J6CYR6
H	0	MET	-	expression tag	UNP A0A5J6CYR6
H	1	VAL	-	expression tag	UNP A0A5J6CYR6
H	25	HIS	GLN	conflict	UNP A0A5J6CYR6
H	66	CR2	SER	chromophore	UNP A0A5J6CYR6
H	66	CR2	TYR	chromophore	UNP A0A5J6CYR6
H	66	CR2	GLY	chromophore	UNP A0A5J6CYR6
H	68	LEU	VAL	conflict	UNP A0A5J6CYR6
H	72	ALA	SER	conflict	UNP A0A5J6CYR6
H	100	PHE	TYR	conflict	UNP A0A5J6CYR6
H	141	LEU	MET	conflict	UNP A0A5J6CYR6
H	148	SER	HIS	engineered mutation	UNP A0A5J6CYR6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	157	GLN	PRO	conflict	UNP A0A5J6CYR6
H	172	GLU	LYS	conflict	UNP A0A5J6CYR6
H	203	TYR	THR	conflict	UNP A0A5J6CYR6
H	219	VAL	ILE	conflict	UNP A0A5J6CYR6
H	231	LEU	HIS	conflict	UNP A0A5J6CYR6



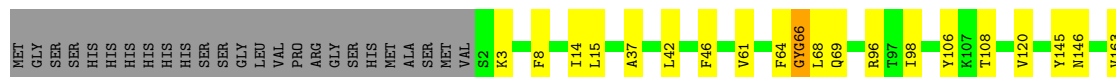
- Molecule 1: Green fluorescent protein GFP

Chain E:



- Molecule 1: Green fluorescent protein GFP

Chain F:



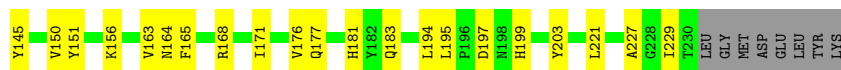
- Molecule 1: Green fluorescent protein GFP

Chain G:



- Molecule 1: Green fluorescent protein GFP

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.65Å 56.77Å 148.19Å 85.12° 85.26° 70.48°	Depositor
Resolution (Å)	37.38 – 3.60 37.38 – 3.60	Depositor EDS
% Data completeness (in resolution range)	87.8 (37.38-3.60) 87.8 (37.38-3.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.15.2	Depositor
R, R_{free}	0.237 , 0.310 0.237 , 0.310	Depositor DCC
R_{free} test set	1789 reflections (8.75%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.327 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1647e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CR2

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	0.26	0/1778	0.66	0/2417
1	B	0.25	0/1772	0.62	0/2409
1	C	0.24	0/1767	0.63	0/2402
1	D	0.24	0/1772	0.63	0/2409
1	E	0.25	0/1778	0.65	0/2417
1	F	0.27	0/1778	0.65	0/2417
1	G	0.26	0/1763	0.65	0/2397
1	H	0.26	0/1778	0.65	0/2417
All	All	0.25	0/14186	0.64	0/19285

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1756	0	1625	21	0
1	B	1750	0	1620	34	0
1	C	1745	0	1618	28	0
1	D	1750	0	1620	30	0
1	E	1756	0	1625	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1756	0	1625	18	0
1	G	1741	0	1615	28	1
1	H	1756	0	1625	26	1
All	All	14010	0	12973	198	1

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 7.

All (198) 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:C:221:LEU:HD23	1:E:221:LEU:HD23	1.55	0.88
1:F:163:VAL:HB	1:F:183:GLN:HG2	1.56	0.87
1:H:163:VAL:HB	1:H:183:GLN:HG2	1.59	0.82
1:E:163:VAL:HB	1:E:183:GLN:HG2	1.62	0.81
1:B:221:LEU:HD23	1:H:221:LEU:HD23	1.59	0.81
1:D:163:VAL:HB	1:D:183:GLN:HG2	1.63	0.80
1:D:66:CR2:O2	1:D:96:ARG:NH2	2.15	0.79
1:A:163:VAL:HB	1:A:183:GLN:HG2	1.65	0.77
1:G:66:CR2:O2	1:G:96:ARG:NH2	2.17	0.76
1:E:66:CR2:O2	1:E:96:ARG:NH2	2.22	0.73
1:B:164:ASN:OD1	1:C:198:ASN:ND2	2.19	0.73
1:C:66:CR2:O2	1:C:96:ARG:NH2	2.21	0.73
1:A:66:CR2:O2	1:A:96:ARG:NH2	2.20	0.73
1:D:214:LYS:HA	1:E:122:ARG:HH21	1.55	0.70
1:B:163:VAL:HB	1:B:183:GLN:HG2	1.74	0.69
1:B:66:CR2:O2	1:B:96:ARG:NH2	2.27	0.68
1:B:168:ARG:HB3	1:B:176:VAL:HG11	1.76	0.67
1:G:163:VAL:HB	1:G:183:GLN:HG2	1.76	0.67
1:G:168:ARG:HB3	1:G:176:VAL:HG11	1.78	0.66
1:E:198:ASN:ND2	1:H:164:ASN:OD1	2.25	0.65
1:H:66:CR2:O2	1:H:96:ARG:NH2	2.29	0.65
1:D:209:LYS:NZ	1:D:217:HIS:O	2.26	0.65
1:C:163:VAL:HB	1:C:183:GLN:HG2	1.77	0.64
1:D:214:LYS:O	1:E:122:ARG:NH2	2.30	0.64
1:F:168:ARG:HB3	1:F:176:VAL:HG11	1.79	0.64
1:E:228:GLY:O	1:H:151:TYR:OH	2.15	0.63
1:D:168:ARG:HB3	1:D:176:VAL:HG11	1.79	0.63
1:C:101:LYS:HD2	1:C:178:LEU:HD12	1.81	0.62
1:H:46:PHE:CZ	1:H:64:PHE:HB3	2.35	0.62
1:F:66:CR2:O2	1:F:96:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:LYS:NZ	1:E:217:HIS:O	2.30	0.60
1:H:69:GLN:HG2	1:H:203:TYR:OH	2.02	0.60
1:E:40:GLY:O	1:E:223:PHE:HA	2.03	0.59
1:D:214:LYS:CA	1:E:122:ARG:HH21	2.15	0.58
1:G:63:THR:HA	1:G:96:ARG:HH12	1.68	0.58
1:H:98:ILE:HG12	1:H:181:HIS:CD2	2.39	0.58
1:C:63:THR:HA	1:C:96:ARG:HH12	1.68	0.58
1:G:209:LYS:NZ	1:G:217:HIS:O	2.31	0.58
1:D:68:LEU:HD21	1:D:121:ASN:HB2	1.85	0.58
1:G:168:ARG:CZ	1:G:178:LEU:HD21	2.33	0.58
1:D:221:LEU:HD12	1:D:222:GLU:N	2.19	0.57
1:B:228:GLY:O	1:C:151:TYR:OH	2.23	0.57
1:G:69:GLN:HG2	1:G:203:TYR:OH	2.05	0.57
1:F:98:ILE:HB	1:F:106:TYR:HB2	1.88	0.56
1:B:221:LEU:HD12	1:B:222:GLU:N	2.20	0.56
1:C:96:ARG:HG2	1:C:183:GLN:HB2	1.86	0.56
1:E:46:PHE:CZ	1:E:64:PHE:HB3	2.41	0.56
1:C:150:VAL:HG22	1:C:165:PHE:CG	2.42	0.55
1:D:95:GLU:HG2	1:D:109:ARG:HG3	1.89	0.55
1:D:168:ARG:CZ	1:D:178:LEU:HD21	2.36	0.55
1:D:228:GLY:O	1:G:151:TYR:OH	2.25	0.55
1:B:151:TYR:OH	1:C:228:GLY:O	2.24	0.55
1:H:142:GLU:HB3	1:H:144:ASN:ND2	2.22	0.55
1:G:46:PHE:CZ	1:G:64:PHE:HB3	2.41	0.55
1:G:66:CR2:O2	1:G:69:GLN:NE2	2.40	0.55
1:C:46:PHE:CZ	1:C:64:PHE:HB3	2.42	0.54
1:B:96:ARG:HG2	1:B:183:GLN:HB2	1.89	0.54
1:D:96:ARG:HG2	1:D:183:GLN:HB2	1.89	0.54
1:E:142:GLU:HB3	1:E:144:ASN:ND2	2.22	0.54
1:A:46:PHE:CZ	1:A:64:PHE:HB3	2.42	0.54
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.90	0.54
1:A:40:GLY:O	1:A:223:PHE:HA	2.08	0.54
1:C:168:ARG:HB3	1:C:176:VAL:HG11	1.89	0.54
1:B:18:LEU:HA	1:B:123:ILE:O	2.08	0.53
1:F:96:ARG:HG2	1:F:183:GLN:HB2	1.90	0.53
1:F:145:TYR:HD2	1:F:146:ASN:H	1.56	0.53
1:D:15:LEU:HG	1:D:118:THR:HG21	1.89	0.53
1:C:209:LYS:NZ	1:C:217:HIS:O	2.35	0.53
1:E:163:VAL:HB	1:E:183:GLN:CG	2.36	0.53
1:E:98:ILE:HG12	1:E:181:HIS:CD2	2.44	0.52
1:F:61:VAL:HB	1:F:145:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HB3	1:A:176:VAL:HG11	1.91	0.52
1:B:198:ASN:ND2	1:C:164:ASN:OD1	2.26	0.52
1:F:46:PHE:CZ	1:F:64:PHE:HB3	2.45	0.52
1:E:96:ARG:HG2	1:E:183:GLN:HB2	1.92	0.51
1:F:197:ASP:HB2	1:F:229:ILE:HD11	1.91	0.51
1:C:206:ALA:HB1	1:E:41:LYS:NZ	2.25	0.51
1:H:168:ARG:HB3	1:H:176:VAL:HG11	1.91	0.51
1:G:101:LYS:HD2	1:G:178:LEU:HD12	1.93	0.51
1:G:96:ARG:HG2	1:G:183:GLN:HB2	1.93	0.50
1:D:46:PHE:CZ	1:D:64:PHE:HB3	2.46	0.50
1:B:63:THR:HA	1:B:96:ARG:HH12	1.75	0.50
1:E:14:ILE:HD13	1:E:68:LEU:HD13	1.94	0.50
1:C:62:THR:HG21	1:C:167:ILE:HG13	1.94	0.49
1:A:98:ILE:HG12	1:A:181:HIS:CD2	2.46	0.49
1:A:63:THR:HA	1:A:96:ARG:HH12	1.77	0.49
1:A:126:LYS:NZ	1:G:109:ARG:HE	2.10	0.49
1:F:69:GLN:HG2	1:F:203:TYR:OH	2.12	0.49
1:B:98:ILE:HB	1:B:106:TYR:HB2	1.95	0.49
1:B:98:ILE:HG12	1:B:181:HIS:CD2	2.48	0.49
1:H:8:PHE:HB3	1:H:37:ALA:HB3	1.94	0.48
1:A:62:THR:HG21	1:A:167:ILE:HG13	1.94	0.48
1:B:46:PHE:CZ	1:B:64:PHE:HB3	2.48	0.48
1:E:66:CR2:HE2	1:E:167:ILE:HD11	1.95	0.48
1:H:171:ILE:HD11	1:H:177:GLN:HB2	1.96	0.48
1:G:45:LYS:HE2	1:G:47:ILE:HD11	1.95	0.48
1:D:151:TYR:OH	1:G:228:GLY:O	2.31	0.48
1:F:209:LYS:NZ	1:F:217:HIS:O	2.30	0.48
1:H:17:GLU:HG3	1:H:122:ARG:NH1	2.28	0.48
1:B:168:ARG:CZ	1:B:178:LEU:HD21	2.44	0.48
1:H:96:ARG:HG2	1:H:183:GLN:HB2	1.95	0.48
1:B:69:GLN:HG2	1:B:203:TYR:OH	2.14	0.48
1:B:68:LEU:HD21	1:B:121:ASN:HB2	1.95	0.47
1:E:156:LYS:HG2	1:E:195:LEU:HD13	1.96	0.47
1:C:68:LEU:HD21	1:C:121:ASN:HB2	1.97	0.47
1:E:62:THR:HG23	1:E:145:TYR:OH	2.14	0.47
1:B:20:GLY:HA2	1:B:125:LEU:O	2.14	0.47
1:F:96:ARG:HB2	1:F:108:THR:OG1	2.14	0.47
1:H:62:THR:HG23	1:H:145:TYR:OH	2.14	0.47
1:A:45:LYS:NZ	1:A:47:ILE:HD11	2.30	0.47
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.97	0.47
1:F:14:ILE:HD13	1:F:68:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HD2	1:B:178:LEU:HD12	1.96	0.46
1:H:98:ILE:HB	1:H:106:TYR:HB2	1.97	0.46
1:D:69:GLN:HG2	1:D:203:TYR:OH	2.15	0.46
1:C:62:THR:HG23	1:C:145:TYR:OH	2.16	0.46
1:C:69:GLN:HG2	1:C:203:TYR:OH	2.15	0.46
1:D:66:CR2:HD1	1:D:66:CR2:N2	2.31	0.46
1:F:213:GLU:HB3	1:F:217:HIS:CE1	2.50	0.46
1:E:88:MET:HE1	1:E:112:VAL:HG12	1.98	0.46
1:F:163:VAL:HB	1:F:183:GLN:CG	2.38	0.46
1:D:62:THR:HG21	1:D:167:ILE:HG13	1.96	0.46
1:E:69:GLN:HG2	1:E:203:TYR:OH	2.16	0.46
1:G:62:THR:HG23	1:G:145:TYR:OH	2.16	0.46
1:G:96:ARG:HB2	1:G:108:THR:OG1	2.16	0.45
1:H:63:THR:HA	1:H:96:ARG:HH12	1.81	0.45
1:B:16:VAL:HG22	1:B:121:ASN:HB3	1.98	0.45
1:G:14:ILE:HG21	1:G:68:LEU:HD13	1.98	0.45
1:G:63:THR:HA	1:G:96:ARG:NH1	2.31	0.45
1:D:153:MET:HE2	1:D:153:MET:HB3	1.81	0.44
1:E:44:LEU:HD13	1:E:46:PHE:HZ	1.81	0.44
1:A:70:CYS:HA	1:A:84:PHE:HB2	1.99	0.44
1:D:214:LYS:C	1:E:122:ARG:HH21	2.25	0.44
1:D:221:LEU:HD12	1:D:222:GLU:H	1.82	0.44
1:E:168:ARG:HB3	1:E:176:VAL:HG11	1.99	0.44
1:D:14:ILE:HG21	1:D:68:LEU:HD13	1.99	0.44
1:G:8:PHE:CZ	1:G:88:MET:HG3	2.52	0.44
1:B:173:ASP:O	1:B:173:ASP:OD2	2.36	0.44
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.81	0.44
1:E:98:ILE:HB	1:E:106:TYR:HB2	2.00	0.44
1:A:96:ARG:HB2	1:A:108:THR:OG1	2.18	0.44
1:A:221:LEU:HD12	1:A:222:GLU:N	2.33	0.44
1:E:150:VAL:HG22	1:E:165:PHE:CG	2.53	0.44
1:F:8:PHE:HB3	1:F:37:ALA:HB3	1.99	0.44
1:A:163:VAL:HB	1:A:183:GLN:CG	2.42	0.44
1:A:4:GLY:C	1:A:6:GLU:H	2.26	0.43
1:H:142:GLU:HB3	1:H:144:ASN:HD21	1.82	0.43
1:B:172:GLU:O	1:B:172:GLU:HG3	2.18	0.43
1:F:42:LEU:HD21	1:F:68:LEU:HB2	2.00	0.43
1:B:154:ALA:HA	1:B:161:ILE:HG22	2.00	0.43
1:B:15:LEU:HG	1:B:118:THR:HG21	2.00	0.43
1:A:62:THR:HG23	1:A:145:TYR:OH	2.18	0.43
1:H:197:ASP:HB2	1:H:229:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:NH1	1:A:176:VAL:HG11	2.34	0.43
1:G:135:ASN:ND2	1:G:177:GLN:OE1	2.37	0.43
1:C:18:LEU:HA	1:C:123:ILE:O	2.19	0.43
1:D:190:ASP:OD1	1:D:190:ASP:N	2.40	0.43
1:B:96:ARG:HG2	1:B:183:GLN:CB	2.48	0.43
1:B:66:CR2:N2	1:B:66:CR2:HD1	2.34	0.42
1:C:221:LEU:HD12	1:C:222:GLU:N	2.34	0.42
1:B:62:THR:HG23	1:B:145:TYR:OH	2.19	0.42
1:B:155:ASP:H	1:B:161:ILE:HA	1.83	0.42
1:D:198:ASN:ND2	1:G:164:ASN:OD1	2.50	0.42
1:G:98:ILE:HB	1:G:106:TYR:HB2	2.01	0.42
1:A:209:LYS:NZ	1:A:217:HIS:O	2.33	0.42
1:B:209:LYS:NZ	1:B:217:HIS:O	2.33	0.42
1:D:62:THR:HG23	1:D:145:TYR:OH	2.19	0.42
1:E:199:HIS:HB3	1:E:229:ILE:HG13	2.02	0.42
1:H:156:LYS:HG2	1:H:195:LEU:HD13	2.01	0.42
1:C:98:ILE:HB	1:C:106:TYR:HB2	2.01	0.42
1:C:147:SER:OG	1:C:204:GLN:HG2	2.20	0.42
1:H:163:VAL:HB	1:H:183:GLN:CG	2.40	0.41
1:D:143:TYR:OH	1:D:218:MET:HG3	2.20	0.41
1:C:206:ALA:HB2	1:E:223:PHE:HZ	1.85	0.41
1:E:70:CYS:HA	1:E:84:PHE:HB2	2.02	0.41
1:D:111:GLU:O	1:D:121:ASN:HA	2.20	0.41
1:G:62:THR:HG21	1:G:167:ILE:HG13	2.02	0.41
1:G:68:LEU:HD21	1:G:121:ASN:HB2	2.03	0.41
1:B:221:LEU:HD12	1:B:222:GLU:H	1.85	0.41
1:D:18:LEU:HA	1:D:123:ILE:O	2.21	0.41
1:H:110:ALA:HA	1:H:122:ARG:O	2.21	0.41
1:H:150:VAL:HG22	1:H:165:PHE:CG	2.56	0.41
1:C:14:ILE:HG21	1:C:68:LEU:HD13	2.03	0.41
1:E:156:LYS:HE2	1:E:156:LYS:HB3	1.89	0.41
1:F:15:LEU:HD12	1:F:120:VAL:HG22	2.03	0.41
1:H:86:SER:HB3	1:H:194:LEU:HD12	2.03	0.41
1:C:190:ASP:OD1	1:C:190:ASP:N	2.46	0.40
1:G:8:PHE:HZ	1:G:88:MET:HG3	1.86	0.40
1:G:168:ARG:NH2	1:G:178:LEU:HD21	2.36	0.40
1:H:199:HIS:HB2	1:H:227:ALA:O	2.21	0.40
1:A:203:TYR:CE1	1:A:224:VAL:HG22	2.56	0.40
1:B:153:MET:HE2	1:B:153:MET:HB3	1.87	0.40
1:C:203:TYR:CD1	1:C:224:VAL:HG22	2.56	0.40
1:H:44:LEU:HD13	1:H:46:PHE:HZ	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:HB3	1:B:156:LYS:HE2	1.92	0.40
1:C:172:GLU:O	1:C:172:GLU:HG3	2.22	0.40
1:D:63:THR:HA	1:D:96:ARG:HH12	1.86	0.40
1:G:98:ILE:HG12	1:G:181:HIS:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:LYS:O	1:H:122:ARG:NH2[1_556]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/260 (85%)	217 (98%)	5 (2%)	0	100	100
1	B	221/260 (85%)	216 (98%)	5 (2%)	0	100	100
1	C	220/260 (85%)	216 (98%)	4 (2%)	0	100	100
1	D	221/260 (85%)	218 (99%)	3 (1%)	0	100	100
1	E	222/260 (85%)	216 (97%)	6 (3%)	0	100	100
1	F	222/260 (85%)	217 (98%)	4 (2%)	1 (0%)	24	57
1	G	219/260 (84%)	215 (98%)	4 (2%)	0	100	100
1	H	222/260 (85%)	217 (98%)	4 (2%)	1 (0%)	24	57
All	All	1769/2080 (85%)	1732 (98%)	35 (2%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	3	LYS

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Mol	Chain	Res	Type
1	H	3	LYS

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	182/225 (81%)	182 (100%)	0	100	100
1	B	181/225 (80%)	181 (100%)	0	100	100
1	C	181/225 (80%)	181 (100%)	0	100	100
1	D	181/225 (80%)	181 (100%)	0	100	100
1	E	182/225 (81%)	182 (100%)	0	100	100
1	F	182/225 (81%)	182 (100%)	0	100	100
1	G	181/225 (80%)	181 (100%)	0	100	100
1	H	182/225 (81%)	182 (100%)	0	100	100
All	All	1452/1800 (81%)	1452 (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. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	157	GLN
1	D	105	ASN
1	D	139	HIS
1	E	105	ASN
1	E	139	HIS
1	E	204	GLN
1	F	81	HIS
1	F	105	ASN
1	F	146	ASN
1	G	105	ASN
1	H	105	ASN

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Mol	Chain	Res	Type
1	H	212	ASN

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	CR2	H	66	1	20,20,21	2.79	9 (45%)	25,27,29	2.89	6 (24%)
1	CR2	G	66	1	20,20,21	2.83	9 (45%)	25,27,29	2.91	6 (24%)
1	CR2	D	66	1	20,20,21	2.79	8 (40%)	25,27,29	3.11	6 (24%)
1	CR2	A	66	1	20,20,21	2.79	9 (45%)	25,27,29	2.74	4 (16%)
1	CR2	F	66	1	20,20,21	2.76	9 (45%)	25,27,29	2.75	6 (24%)
1	CR2	C	66	1	20,20,21	2.78	9 (45%)	25,27,29	2.66	5 (20%)
1	CR2	B	66	1	20,20,21	2.81	9 (45%)	25,27,29	2.76	6 (24%)
1	CR2	E	66	1	20,20,21	2.77	9 (45%)	25,27,29	2.66	6 (24%)

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	CR2	H	66	1	-	0/6/25/26	0/2/2/2
1	CR2	G	66	1	-	0/6/25/26	0/2/2/2
1	CR2	D	66	1	-	0/6/25/26	0/2/2/2
1	CR2	A	66	1	-	0/6/25/26	0/2/2/2
1	CR2	F	66	1	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	C	66	1	-	0/6/25/26	0/2/2/2
1	CR2	B	66	1	-	0/6/25/26	0/2/2/2
1	CR2	E	66	1	-	0/6/25/26	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	66	CR2	C1-N2	6.28	1.43	1.32
1	H	66	CR2	C1-N2	6.21	1.43	1.32
1	A	66	CR2	C1-N2	6.21	1.43	1.32
1	C	66	CR2	C1-N2	6.20	1.43	1.32
1	G	66	CR2	C1-N2	6.14	1.43	1.32
1	D	66	CR2	C1-N3	6.14	1.47	1.37
1	G	66	CR2	C1-N3	6.12	1.47	1.37
1	H	66	CR2	C1-N3	6.08	1.47	1.37
1	F	66	CR2	C1-N2	6.07	1.42	1.32
1	B	66	CR2	C1-N3	6.05	1.47	1.37
1	B	66	CR2	C1-N2	6.02	1.42	1.32
1	A	66	CR2	C1-N3	6.01	1.46	1.37
1	D	66	CR2	C1-N2	6.00	1.42	1.32
1	C	66	CR2	C1-N3	5.93	1.46	1.37
1	F	66	CR2	C1-N3	5.91	1.46	1.37
1	E	66	CR2	C1-N3	5.85	1.46	1.37
1	B	66	CR2	CA2-C2	5.23	1.54	1.48
1	G	66	CR2	CA2-C2	4.93	1.53	1.48
1	D	66	CR2	CA2-C2	4.92	1.53	1.48
1	C	66	CR2	CA2-C2	4.89	1.53	1.48
1	F	66	CR2	CA2-C2	4.86	1.53	1.48
1	A	66	CR2	CA2-C2	4.82	1.53	1.48
1	E	66	CR2	CA2-C2	4.77	1.53	1.48
1	H	66	CR2	CA2-C2	4.59	1.53	1.48
1	G	66	CR2	C2-N3	3.69	1.48	1.40
1	D	66	CR2	C2-N3	3.65	1.48	1.40
1	F	66	CR2	C2-N3	3.63	1.48	1.40
1	B	66	CR2	C2-N3	3.63	1.48	1.40
1	A	66	CR2	C2-N3	3.58	1.48	1.40
1	H	66	CR2	CB2-CA2	-3.58	1.31	1.35
1	B	66	CR2	CG2-CB2	3.46	1.53	1.46
1	C	66	CR2	CG2-CB2	3.43	1.53	1.46
1	G	66	CR2	CG2-CB2	3.42	1.53	1.46
1	E	66	CR2	C2-N3	3.42	1.47	1.40
1	H	66	CR2	C2-N3	3.40	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	CR2	CB2-CA2	-3.40	1.31	1.35
1	C	66	CR2	C2-N3	3.39	1.47	1.40
1	A	66	CR2	CG2-CB2	3.38	1.53	1.46
1	F	66	CR2	CG2-CB2	3.34	1.53	1.46
1	E	66	CR2	CG2-CB2	3.34	1.53	1.46
1	D	66	CR2	CG2-CB2	3.29	1.52	1.46
1	G	66	CR2	CB2-CA2	-3.26	1.32	1.35
1	A	66	CR2	CB2-CA2	-3.24	1.32	1.35
1	E	66	CR2	CB2-CA2	-3.20	1.32	1.35
1	C	66	CR2	CB2-CA2	-3.15	1.32	1.35
1	F	66	CR2	CB2-CA2	-3.14	1.32	1.35
1	H	66	CR2	CA1-C1	3.13	1.53	1.49
1	H	66	CR2	CG2-CB2	3.10	1.52	1.46
1	B	66	CR2	CB2-CA2	-3.08	1.32	1.35
1	G	66	CR2	CA1-C1	3.05	1.53	1.49
1	E	66	CR2	CA1-C1	3.00	1.52	1.49
1	A	66	CR2	CA1-C1	2.98	1.52	1.49
1	B	66	CR2	CA1-C1	2.96	1.52	1.49
1	C	66	CR2	CA1-C1	2.93	1.52	1.49
1	F	66	CR2	CA1-C1	2.92	1.52	1.49
1	D	66	CR2	CA1-C1	2.83	1.52	1.49
1	H	66	CR2	O2-C2	-2.31	1.18	1.23
1	D	66	CR2	O2-C2	-2.26	1.18	1.23
1	E	66	CR2	O2-C2	-2.26	1.18	1.23
1	G	66	CR2	O2-C2	-2.19	1.18	1.23
1	E	66	CR2	CA2-N2	2.18	1.43	1.38
1	B	66	CR2	O2-C2	-2.17	1.18	1.23
1	C	66	CR2	O2-C2	-2.17	1.18	1.23
1	F	66	CR2	O2-C2	-2.15	1.18	1.23
1	A	66	CR2	CA2-N2	2.14	1.43	1.38
1	A	66	CR2	O2-C2	-2.14	1.18	1.23
1	C	66	CR2	CA2-N2	2.12	1.43	1.38
1	B	66	CR2	CA2-N2	2.11	1.43	1.38
1	G	66	CR2	CA2-N2	2.08	1.43	1.38
1	H	66	CR2	CA2-N2	2.06	1.43	1.38
1	F	66	CR2	CA2-N2	2.05	1.43	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	CR2	C2-N3-C1	-9.32	103.89	108.08
1	G	66	CR2	C2-N3-C1	-8.49	104.26	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	CR2	O2-C2-CA2	-8.39	125.67	131.02
1	H	66	CR2	O2-C2-CA2	-8.21	125.78	131.02
1	H	66	CR2	C2-N3-C1	-8.17	104.41	108.08
1	D	66	CR2	O2-C2-CA2	-8.16	125.81	131.02
1	B	66	CR2	C2-N3-C1	-8.08	104.44	108.08
1	F	66	CR2	O2-C2-CA2	-8.00	125.92	131.02
1	A	66	CR2	O2-C2-CA2	-7.98	125.92	131.02
1	A	66	CR2	C2-N3-C1	-7.81	104.57	108.08
1	F	66	CR2	C2-N3-C1	-7.73	104.60	108.08
1	E	66	CR2	C2-N3-C1	-7.63	104.65	108.08
1	E	66	CR2	O2-C2-CA2	-7.56	126.19	131.02
1	C	66	CR2	C2-N3-C1	-7.46	104.73	108.08
1	C	66	CR2	O2-C2-CA2	-7.37	126.31	131.02
1	B	66	CR2	O2-C2-CA2	-7.03	126.53	131.02
1	D	66	CR2	CA2-C2-N3	5.96	108.50	103.50
1	H	66	CR2	CA2-C2-N3	5.80	108.37	103.50
1	G	66	CR2	CA2-C2-N3	5.60	108.20	103.50
1	B	66	CR2	CA2-C2-N3	5.46	108.08	103.50
1	E	66	CR2	CA2-C2-N3	5.44	108.07	103.50
1	C	66	CR2	CA2-C2-N3	5.43	108.06	103.50
1	A	66	CR2	CA2-C2-N3	5.34	107.98	103.50
1	F	66	CR2	CA2-C2-N3	5.30	107.95	103.50
1	D	66	CR2	C2-CA2-N2	-3.91	106.15	108.95
1	B	66	CR2	C2-CA2-N2	-3.83	106.21	108.95
1	H	66	CR2	C2-CA2-N2	-3.67	106.32	108.95
1	F	66	CR2	C2-CA2-N2	-3.57	106.39	108.95
1	C	66	CR2	C2-CA2-N2	-3.56	106.40	108.95
1	G	66	CR2	C2-CA2-N2	-3.54	106.41	108.95
1	D	66	CR2	CG2-CB2-CA2	-3.41	125.81	129.87
1	E	66	CR2	C2-CA2-N2	-3.32	106.58	108.95
1	A	66	CR2	C2-CA2-N2	-3.25	106.62	108.95
1	B	66	CR2	CA1-C1-N3	2.76	126.21	122.52
1	B	66	CR2	CG2-CB2-CA2	-2.75	126.60	129.87
1	D	66	CR2	CA1-C1-N3	2.57	125.96	122.52
1	G	66	CR2	CG2-CB2-CA2	-2.37	127.05	129.87
1	F	66	CR2	CG2-CB2-CA2	-2.35	127.07	129.87
1	E	66	CR2	C1-CA1-N1	-2.33	107.69	112.85
1	C	66	CR2	CA1-C1-N3	2.22	125.50	122.52
1	H	66	CR2	CB2-CA2-N2	2.20	131.75	128.76
1	F	66	CR2	CA1-C1-N3	2.15	125.40	122.52
1	E	66	CR2	CB2-CA2-N2	2.10	131.61	128.76
1	H	66	CR2	CA1-C1-N3	2.04	125.25	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	CR2	CA1-C1-N3	2.02	125.22	122.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	66	CR2	1	0
1	G	66	CR2	2	0
1	D	66	CR2	2	0
1	A	66	CR2	1	0
1	F	66	CR2	1	0
1	C	66	CR2	1	0
1	B	66	CR2	2	0
1	E	66	CR2	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	226/260 (86%)	-0.29	0 100 100	77, 104, 128, 155	0
1	B	225/260 (86%)	-0.30	0 100 100	82, 103, 131, 163	0
1	C	224/260 (86%)	-0.26	0 100 100	81, 103, 134, 159	0
1	D	225/260 (86%)	-0.35	0 100 100	75, 100, 128, 152	0
1	E	226/260 (86%)	-0.32	1 (0%) 88 70	78, 103, 131, 151	0
1	F	226/260 (86%)	-0.21	0 100 100	80, 102, 129, 162	0
1	G	223/260 (85%)	-0.31	1 (0%) 88 70	78, 100, 126, 146	0
1	H	226/260 (86%)	-0.30	0 100 100	81, 101, 133, 153	0
All	All	1801/2080 (86%)	-0.29	2 (0%) 92 85	75, 102, 132, 163	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	83	PHE	2.3
1	G	141	LEU	2.3

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	CR2	E	66	19/20	0.83	0.13	82,90,104,104	0
1	CR2	H	66	19/20	0.84	0.13	79,86,105,108	0
1	CR2	G	66	19/20	0.85	0.11	82,91,98,99	0
1	CR2	A	66	19/20	0.85	0.12	90,99,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CR2	B	66	19/20	0.86	0.11	86,94,103,106	0
1	CR2	F	66	19/20	0.86	0.11	81,96,107,109	0
1	CR2	C	66	19/20	0.86	0.10	87,94,106,109	0
1	CR2	D	66	19/20	0.86	0.12	82,88,102,103	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.