W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 1, 2021 – 08:08 am BST

PDB ID	:	7A80
Title	:	rsGreen0.7-K206A-E222V in the green-on state
Authors	:	De Zitter, E.; Dedecker, P.; Van Meervelt, L.
Deposited on	:	2020-08-30
Resolution	:	2.05 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 (i) symbol.

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

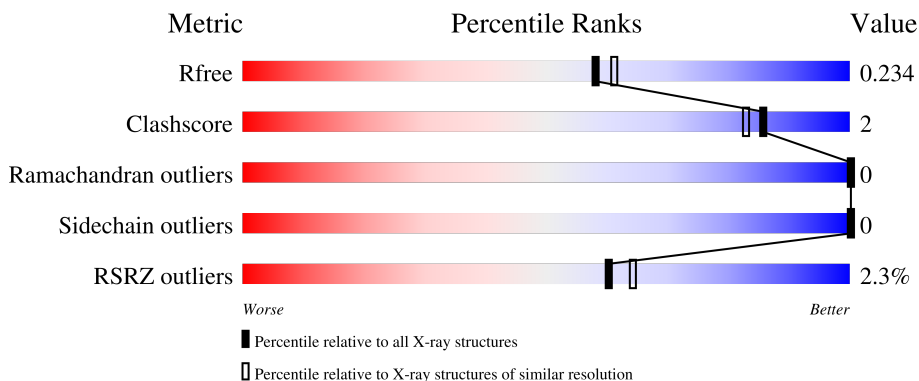|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
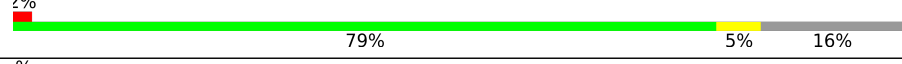*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.234
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		2.3%

Worse　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	270	.% 79% 5% 16%
1	B	270	3% 79% 6% 16%
1	C	270	2% 79% 5% 16%
1	D	270	.% 78% 6% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8063 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total 1877	C 1190	N 322	O 360	S 5	0	8	0
1	B	227	Total 1838	C 1169	N 313	O 351	S 5	0	4	0
1	C	227	Total 1844	C 1169	N 313	O 357	S 5	0	5	0
1	D	228	Total 1906	C 1208	N 327	O 366	S 5	0	10	0

There are 188 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A059PIQ0
A	-32	ARG	-	expression tag	UNP A0A059PIQ0
A	-31	GLY	-	expression tag	UNP A0A059PIQ0
A	-30	SER	-	expression tag	UNP A0A059PIQ0
A	-29	HIS	-	expression tag	UNP A0A059PIQ0
A	-28	HIS	-	expression tag	UNP A0A059PIQ0
A	-27	HIS	-	expression tag	UNP A0A059PIQ0
A	-26	HIS	-	expression tag	UNP A0A059PIQ0
A	-25	HIS	-	expression tag	UNP A0A059PIQ0
A	-24	HIS	-	expression tag	UNP A0A059PIQ0
A	-23	GLY	-	expression tag	UNP A0A059PIQ0
A	-22	MET	-	expression tag	UNP A0A059PIQ0
A	-21	ALA	-	expression tag	UNP A0A059PIQ0
A	-20	SER	-	expression tag	UNP A0A059PIQ0
A	-19	MET	-	expression tag	UNP A0A059PIQ0
A	-18	THR	-	expression tag	UNP A0A059PIQ0
A	-17	GLY	-	expression tag	UNP A0A059PIQ0
A	-16	GLY	-	expression tag	UNP A0A059PIQ0
A	-15	GLN	-	expression tag	UNP A0A059PIQ0
A	-14	GLN	-	expression tag	UNP A0A059PIQ0
A	-13	MET	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	expression tag	UNP A0A059PIQ0
A	-11	ARG	-	expression tag	UNP A0A059PIQ0
A	-10	ASP	-	expression tag	UNP A0A059PIQ0
A	-9	LEU	-	expression tag	UNP A0A059PIQ0
A	-8	TYR	-	expression tag	UNP A0A059PIQ0
A	-7	ASP	-	expression tag	UNP A0A059PIQ0
A	-6	ASP	-	expression tag	UNP A0A059PIQ0
A	-5	ASP	-	expression tag	UNP A0A059PIQ0
A	-4	ASP	-	expression tag	UNP A0A059PIQ0
A	-3	LYS	-	expression tag	UNP A0A059PIQ0
A	-2	ASP	-	expression tag	UNP A0A059PIQ0
A	-1	PRO	-	expression tag	UNP A0A059PIQ0
A	0	MET	-	expression tag	UNP A0A059PIQ0
A	1	VAL	-	expression tag	UNP A0A059PIQ0
A	2	SER	-	expression tag	UNP A0A059PIQ0
A	30	ARG	SER	conflict	UNP A0A059PIQ0
A	66	CRO	THR	chromophore	UNP A0A059PIQ0
A	66	CRO	TYR	chromophore	UNP A0A059PIQ0
A	66	CRO	GLY	chromophore	UNP A0A059PIQ0
A	69	LEU	GLN	conflict	UNP A0A059PIQ0
A	105	TYR	THR	conflict	UNP A0A059PIQ0
A	150	ALA	VAL	conflict	UNP A0A059PIQ0
A	163	SER	ALA	conflict	UNP A0A059PIQ0
A	205	ASN	SER	conflict	UNP A0A059PIQ0
A	222	VAL	GLU	engineered mutation	UNP A0A059PIQ0
A	231	LEU	HIS	conflict	UNP A0A059PIQ0
B	-33	MET	-	initiating methionine	UNP A0A059PIQ0
B	-32	ARG	-	expression tag	UNP A0A059PIQ0
B	-31	GLY	-	expression tag	UNP A0A059PIQ0
B	-30	SER	-	expression tag	UNP A0A059PIQ0
B	-29	HIS	-	expression tag	UNP A0A059PIQ0
B	-28	HIS	-	expression tag	UNP A0A059PIQ0
B	-27	HIS	-	expression tag	UNP A0A059PIQ0
B	-26	HIS	-	expression tag	UNP A0A059PIQ0
B	-25	HIS	-	expression tag	UNP A0A059PIQ0
B	-24	HIS	-	expression tag	UNP A0A059PIQ0
B	-23	GLY	-	expression tag	UNP A0A059PIQ0
B	-22	MET	-	expression tag	UNP A0A059PIQ0
B	-21	ALA	-	expression tag	UNP A0A059PIQ0
B	-20	SER	-	expression tag	UNP A0A059PIQ0
B	-19	MET	-	expression tag	UNP A0A059PIQ0
B	-18	THR	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP A0A059PIQ0
B	-16	GLY	-	expression tag	UNP A0A059PIQ0
B	-15	GLN	-	expression tag	UNP A0A059PIQ0
B	-14	GLN	-	expression tag	UNP A0A059PIQ0
B	-13	MET	-	expression tag	UNP A0A059PIQ0
B	-12	GLY	-	expression tag	UNP A0A059PIQ0
B	-11	ARG	-	expression tag	UNP A0A059PIQ0
B	-10	ASP	-	expression tag	UNP A0A059PIQ0
B	-9	LEU	-	expression tag	UNP A0A059PIQ0
B	-8	TYR	-	expression tag	UNP A0A059PIQ0
B	-7	ASP	-	expression tag	UNP A0A059PIQ0
B	-6	ASP	-	expression tag	UNP A0A059PIQ0
B	-5	ASP	-	expression tag	UNP A0A059PIQ0
B	-4	ASP	-	expression tag	UNP A0A059PIQ0
B	-3	LYS	-	expression tag	UNP A0A059PIQ0
B	-2	ASP	-	expression tag	UNP A0A059PIQ0
B	-1	PRO	-	expression tag	UNP A0A059PIQ0
B	0	MET	-	expression tag	UNP A0A059PIQ0
B	1	VAL	-	expression tag	UNP A0A059PIQ0
B	2	SER	-	expression tag	UNP A0A059PIQ0
B	30	ARG	SER	conflict	UNP A0A059PIQ0
B	66	CRO	THR	chromophore	UNP A0A059PIQ0
B	66	CRO	TYR	chromophore	UNP A0A059PIQ0
B	66	CRO	GLY	chromophore	UNP A0A059PIQ0
B	69	LEU	GLN	conflict	UNP A0A059PIQ0
B	105	TYR	THR	conflict	UNP A0A059PIQ0
B	150	ALA	VAL	conflict	UNP A0A059PIQ0
B	163	SER	ALA	conflict	UNP A0A059PIQ0
B	205	ASN	SER	conflict	UNP A0A059PIQ0
B	222	VAL	GLU	engineered mutation	UNP A0A059PIQ0
B	231	LEU	HIS	conflict	UNP A0A059PIQ0
C	-33	MET	-	initiating methionine	UNP A0A059PIQ0
C	-32	ARG	-	expression tag	UNP A0A059PIQ0
C	-31	GLY	-	expression tag	UNP A0A059PIQ0
C	-30	SER	-	expression tag	UNP A0A059PIQ0
C	-29	HIS	-	expression tag	UNP A0A059PIQ0
C	-28	HIS	-	expression tag	UNP A0A059PIQ0
C	-27	HIS	-	expression tag	UNP A0A059PIQ0
C	-26	HIS	-	expression tag	UNP A0A059PIQ0
C	-25	HIS	-	expression tag	UNP A0A059PIQ0
C	-24	HIS	-	expression tag	UNP A0A059PIQ0
C	-23	GLY	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP A0A059PIQ0
C	-21	ALA	-	expression tag	UNP A0A059PIQ0
C	-20	SER	-	expression tag	UNP A0A059PIQ0
C	-19	MET	-	expression tag	UNP A0A059PIQ0
C	-18	THR	-	expression tag	UNP A0A059PIQ0
C	-17	GLY	-	expression tag	UNP A0A059PIQ0
C	-16	GLY	-	expression tag	UNP A0A059PIQ0
C	-15	GLN	-	expression tag	UNP A0A059PIQ0
C	-14	GLN	-	expression tag	UNP A0A059PIQ0
C	-13	MET	-	expression tag	UNP A0A059PIQ0
C	-12	GLY	-	expression tag	UNP A0A059PIQ0
C	-11	ARG	-	expression tag	UNP A0A059PIQ0
C	-10	ASP	-	expression tag	UNP A0A059PIQ0
C	-9	LEU	-	expression tag	UNP A0A059PIQ0
C	-8	TYR	-	expression tag	UNP A0A059PIQ0
C	-7	ASP	-	expression tag	UNP A0A059PIQ0
C	-6	ASP	-	expression tag	UNP A0A059PIQ0
C	-5	ASP	-	expression tag	UNP A0A059PIQ0
C	-4	ASP	-	expression tag	UNP A0A059PIQ0
C	-3	LYS	-	expression tag	UNP A0A059PIQ0
C	-2	ASP	-	expression tag	UNP A0A059PIQ0
C	-1	PRO	-	expression tag	UNP A0A059PIQ0
C	0	MET	-	expression tag	UNP A0A059PIQ0
C	1	VAL	-	expression tag	UNP A0A059PIQ0
C	2	SER	-	expression tag	UNP A0A059PIQ0
C	30	ARG	SER	conflict	UNP A0A059PIQ0
C	66	CRO	THR	chromophore	UNP A0A059PIQ0
C	66	CRO	TYR	chromophore	UNP A0A059PIQ0
C	66	CRO	GLY	chromophore	UNP A0A059PIQ0
C	69	LEU	GLN	conflict	UNP A0A059PIQ0
C	105	TYR	THR	conflict	UNP A0A059PIQ0
C	150	ALA	VAL	conflict	UNP A0A059PIQ0
C	163	SER	ALA	conflict	UNP A0A059PIQ0
C	205	ASN	SER	conflict	UNP A0A059PIQ0
C	222	VAL	GLU	engineered mutation	UNP A0A059PIQ0
C	231	LEU	HIS	conflict	UNP A0A059PIQ0
D	-33	MET	-	initiating methionine	UNP A0A059PIQ0
D	-32	ARG	-	expression tag	UNP A0A059PIQ0
D	-31	GLY	-	expression tag	UNP A0A059PIQ0
D	-30	SER	-	expression tag	UNP A0A059PIQ0
D	-29	HIS	-	expression tag	UNP A0A059PIQ0
D	-28	HIS	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	HIS	-	expression tag	UNP A0A059PIQ0
D	-26	HIS	-	expression tag	UNP A0A059PIQ0
D	-25	HIS	-	expression tag	UNP A0A059PIQ0
D	-24	HIS	-	expression tag	UNP A0A059PIQ0
D	-23	GLY	-	expression tag	UNP A0A059PIQ0
D	-22	MET	-	expression tag	UNP A0A059PIQ0
D	-21	ALA	-	expression tag	UNP A0A059PIQ0
D	-20	SER	-	expression tag	UNP A0A059PIQ0
D	-19	MET	-	expression tag	UNP A0A059PIQ0
D	-18	THR	-	expression tag	UNP A0A059PIQ0
D	-17	GLY	-	expression tag	UNP A0A059PIQ0
D	-16	GLY	-	expression tag	UNP A0A059PIQ0
D	-15	GLN	-	expression tag	UNP A0A059PIQ0
D	-14	GLN	-	expression tag	UNP A0A059PIQ0
D	-13	MET	-	expression tag	UNP A0A059PIQ0
D	-12	GLY	-	expression tag	UNP A0A059PIQ0
D	-11	ARG	-	expression tag	UNP A0A059PIQ0
D	-10	ASP	-	expression tag	UNP A0A059PIQ0
D	-9	LEU	-	expression tag	UNP A0A059PIQ0
D	-8	TYR	-	expression tag	UNP A0A059PIQ0
D	-7	ASP	-	expression tag	UNP A0A059PIQ0
D	-6	ASP	-	expression tag	UNP A0A059PIQ0
D	-5	ASP	-	expression tag	UNP A0A059PIQ0
D	-4	ASP	-	expression tag	UNP A0A059PIQ0
D	-3	LYS	-	expression tag	UNP A0A059PIQ0
D	-2	ASP	-	expression tag	UNP A0A059PIQ0
D	-1	PRO	-	expression tag	UNP A0A059PIQ0
D	0	MET	-	expression tag	UNP A0A059PIQ0
D	1	VAL	-	expression tag	UNP A0A059PIQ0
D	2	SER	-	expression tag	UNP A0A059PIQ0
D	30	ARG	SER	conflict	UNP A0A059PIQ0
D	66	CRO	THR	chromophore	UNP A0A059PIQ0
D	66	CRO	TYR	chromophore	UNP A0A059PIQ0
D	66	CRO	GLY	chromophore	UNP A0A059PIQ0
D	69	LEU	GLN	conflict	UNP A0A059PIQ0
D	105	TYR	THR	conflict	UNP A0A059PIQ0
D	150	ALA	VAL	conflict	UNP A0A059PIQ0
D	163	SER	ALA	conflict	UNP A0A059PIQ0
D	205	ASN	SER	conflict	UNP A0A059PIQ0
D	222	VAL	GLU	engineered mutation	UNP A0A059PIQ0
D	231	LEU	HIS	conflict	UNP A0A059PIQ0

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3).
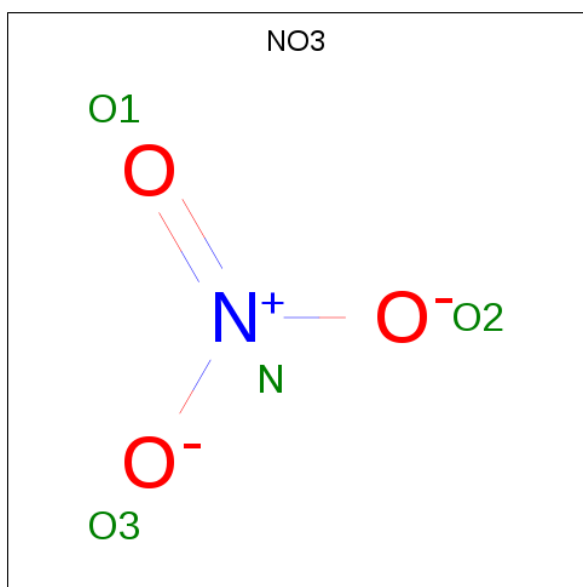
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	N 1	O 3	0	0
2	B	1	Total 4	N 1	O 3	0	0
2	C	1	Total 4	N 1	O 3	0	0
2	D	1	Total 4	N 1	O 3	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total 165	O 165	0	0
3	B	135	Total 135	O 135	0	0
3	C	131	Total 131	O 131	0	0
3	D	151	Total 151	O 151	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
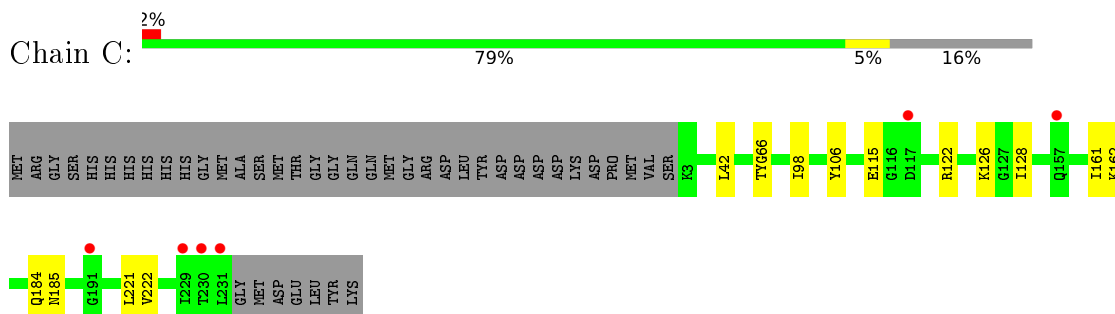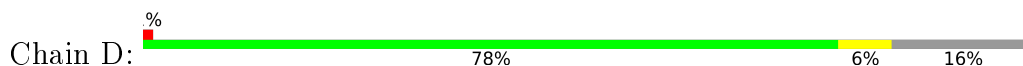
- Molecule 1: Green fluorescent protein
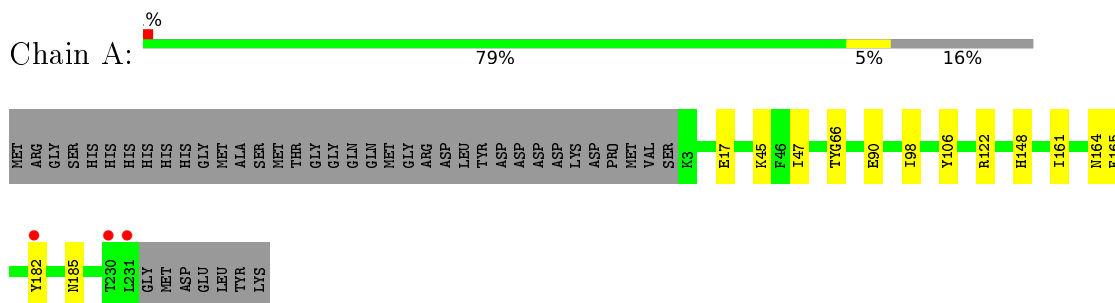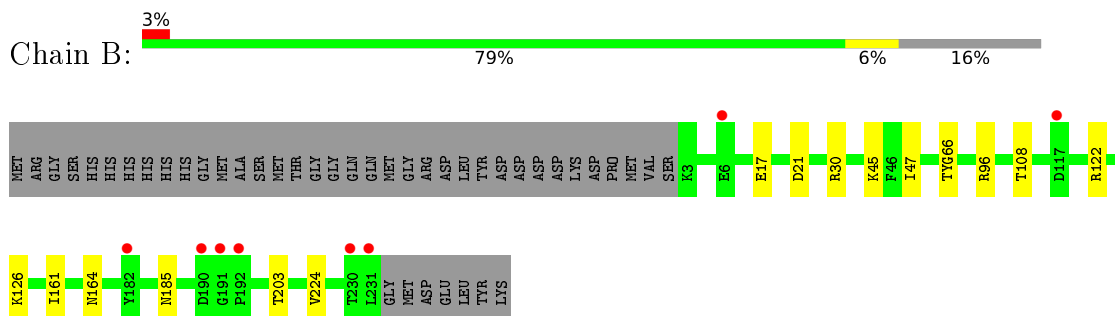
- Molecule 1: Green fluorescent protein

- Molecule 1: Green fluorescent protein

- Molecule 1: Green fluorescent protein

MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP ASP LYS ASP PRO MET VAL SER K3 T38 L42 TYG66 R73 R96 T97 I98 Y106 K126 G127 I128 K156 I161

N185 D190 G191 L195 T203 L221 V222 F223 V224 T230 L231 G232 MET ASP GLU LEU TYR LYS
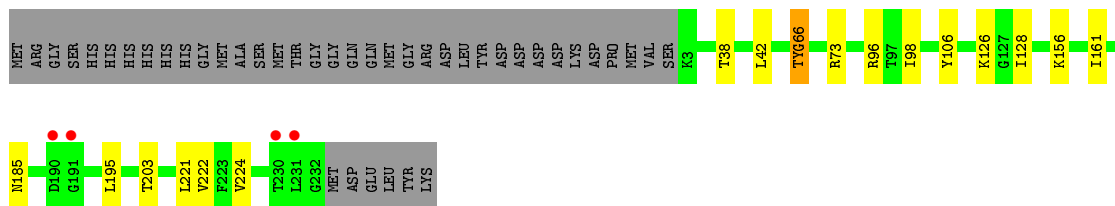
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.82Å 61.80Å 112.12Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	46.27 – 2.05 46.27 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.27-2.05) 99.9 (46.27-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.75 (at 2.05Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.234 0.183 , 0.234	Depositor DCC
R_{free} test set	3006 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.1	EDS
L-test for twinning [2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8063	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: CRO, NO3

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	0/1896	0.46	0/2565
1	B	0.25	0/1856	0.45	0/2511
1	C	0.25	0/1862	0.45	0/2521
1	D	0.25	0/1903	0.45	0/2576
All	All	0.25	0/7517	0.45	0/10173

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	1877	0	1806	7	0
1	B	1838	0	1777	9	0
1	C	1844	0	1767	7	0
1	D	1906	0	1820	11	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	165	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	135	0	0	2	0
3	C	131	0	0	0	0
3	D	151	0	0	1	0
All	All	8063	0	7170	33	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 2.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148[B]:HIS:NE2	1:A:165:PHE:HB2	2.09	0.67
1:D:66[C]:CRO:HD2	1:D:96:ARG:NH2	2.14	0.63
1:C:115:GLU:OE2	1:C:122:ARG:NH1	2.27	0.62
1:C:161:ILE:HG13	1:C:185:ASN:HB2	1.83	0.60
1:A:17:GLU:OE1	1:A:122:ARG:NH1	2.34	0.60

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	230/270 (85%)	224 (97%)	6 (3%)	0	100	100
1	B	226/270 (84%)	223 (99%)	3 (1%)	0	100	100
1	C	227/270 (84%)	224 (99%)	3 (1%)	0	100	100
1	D	232/270 (86%)	229 (99%)	3 (1%)	0	100	100
All	All	915/1080 (85%)	900 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/232 (87%)	202 (100%)	0	100	100
1	B	197/232 (85%)	197 (100%)	0	100	100
1	C	198/232 (85%)	198 (100%)	0	100	100
1	D	202/232 (87%)	202 (100%)	0	100	100
All	All	799/928 (86%)	799 (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. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 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	CRO	C	66	1	23,23,24	2.75	8 (34%)	30,32,34	2.80	7 (23%)
1	CRO	D	66[C]	1	23,23,24	2.82	8 (34%)	30,32,34	3.01	9 (30%)
1	CRO	B	66	1	23,23,24	2.71	8 (34%)	30,32,34	2.87	7 (23%)
1	CRO	A	66	1	23,23,24	2.69	8 (34%)	30,32,34	2.86	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	CRO	D	66[A]	1	23,23,24	2.74	8 (34%)	30,32,34	2.77	8 (26%)

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	CRO	C	66	1	-	2/12/31/32	0/2/2/2
1	CRO	D	66[C]	1	-	4/12/31/32	0/2/2/2
1	CRO	B	66	1	-	1/12/31/32	0/2/2/2
1	CRO	A	66	1	-	2/12/31/32	0/2/2/2
1	CRO	D	66[A]	1	-	2/12/31/32	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66[C]	CRO	CA2-C2	6.29	1.54	1.48
1	B	66	CRO	C1-N2	6.01	1.41	1.32
1	A	66	CRO	C1-N2	6.00	1.41	1.32
1	C	66	CRO	C1-N2	5.98	1.41	1.32
1	D	66[C]	CRO	C1-N2	5.91	1.40	1.32

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	O2-C2-CA2	-9.79	125.46	130.96
1	A	66	CRO	O2-C2-CA2	-9.45	125.65	130.96
1	C	66	CRO	O2-C2-CA2	-8.84	125.99	130.96
1	D	66[A]	CRO	O2-C2-CA2	-8.34	126.28	130.96
1	A	66	CRO	CA2-C2-N3	8.23	107.26	103.37

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	C2-CA2-CB2-CG2
1	D	66[A]	CRO	C2-CA2-CB2-CG2
1	D	66[C]	CRO	N2-CA2-CB2-CG2
1	D	66[C]	CRO	C2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	A	66	CRO	N2-CA2-CB2-CG2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	66[C]	CRO	2	0
1	D	66[A]	CRO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NO3	D	301	-	1,3,3	0.68	0	0,3,3	0.00	-
2	NO3	C	301	-	1,3,3	0.64	0	0,3,3	0.00	-
2	NO3	B	301	-	1,3,3	0.64	0	0,3,3	0.00	-
2	NO3	A	301	-	1,3,3	0.65	0	0,3,3	0.00	-

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 (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(Å²)	Q<0.9
1	A	226/270 (83%)	-0.11	3 (1%)	77	79	18, 26, 38, 72	0
1	B	226/270 (83%)	-0.06	8 (3%)	44	48	17, 28, 46, 66	0
1	C	226/270 (83%)	-0.05	6 (2%)	54	59	19, 29, 48, 60	0
1	D	227/270 (84%)	-0.08	4 (1%)	68	71	18, 27, 46, 64	0
All	All	905/1080 (83%)	-0.08	21 (2%)	60	64	17, 27, 46, 72	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	5.8
1	D	191	GLY	4.1
1	B	190	ASP	3.4
1	B	230	THR	3.0
1	D	230	THR	2.9

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(Å²)	Q<0.9
1	CRO	B	66	22/23	0.91	0.13	20,26,34,37	0
1	CRO	C	66	22/23	0.92	0.12	19,28,36,44	0
1	CRO	D	66[A]	22/23	0.94	0.15	18,23,28,33	22
1	CRO	D	66[C]	22/23	0.94	0.15	19,24,28,35	22
1	CRO	A	66	22/23	0.95	0.11	14,22,30,34	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(Å^2)	Q<0.9
2	NO3	B	301	4/4	0.95	0.15	37,37,39,40	0
2	NO3	A	301	4/4	0.96	0.12	36,36,38,41	0
2	NO3	C	301	4/4	0.96	0.10	35,37,38,38	0
2	NO3	D	301	4/4	0.96	0.14	33,35,36,39	0

6.5 Other polymers (i)

There are no such residues in this entry.