



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:44 am BST

PDB ID : 5DTZ  
Title : Crystal structure of rsFolder in the fluorescent on-state  
Authors : El Khatib, M.; Colletier, J.P.; Adam, V.  
Deposited on : 2015-09-18  
Resolution : 1.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

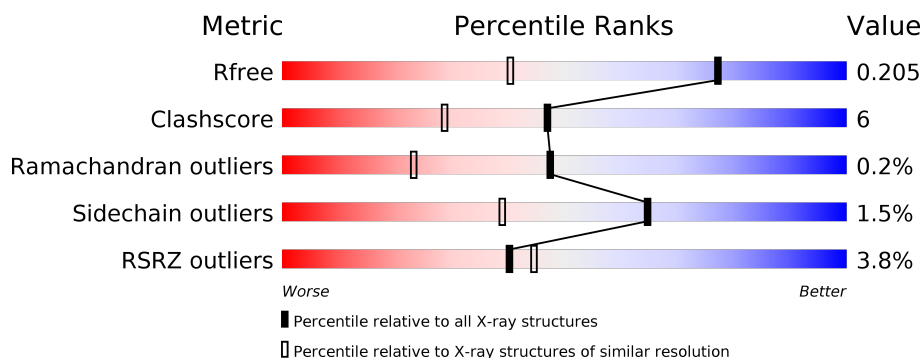
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>11%</div> </div> </div>
1	B	260	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>12%</div> </div> </div>
1	C	260	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>11%</div> </div> </div>
1	D	260	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	D	301	-	-	X	-
2	PEG	D	302	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8457 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	231	Total	C	N	O	S	0	2	0
			1856	1178	320	352	6			
1	B	230	Total	C	N	O	S	0	3	0
			1857	1179	319	353	6			
1	C	231	Total	C	N	O	S	0	3	0
			1859	1180	317	356	6			
1	D	230	Total	C	N	O	S	0	4	0
			1860	1181	319	354	6			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P42212
A	-21	GLY	-	expression tag	UNP P42212
A	-20	SER	-	expression tag	UNP P42212
A	-19	SER	-	expression tag	UNP P42212
A	-18	HIS	-	expression tag	UNP P42212
A	-17	HIS	-	expression tag	UNP P42212
A	-16	HIS	-	expression tag	UNP P42212
A	-15	HIS	-	expression tag	UNP P42212
A	-14	HIS	-	expression tag	UNP P42212
A	-13	HIS	-	expression tag	UNP P42212
A	-12	SER	-	expression tag	UNP P42212
A	-11	SER	-	expression tag	UNP P42212
A	-10	GLY	-	expression tag	UNP P42212
A	-9	LEU	-	expression tag	UNP P42212
A	-8	VAL	-	expression tag	UNP P42212
A	-7	PRO	-	expression tag	UNP P42212
A	-6	ARG	-	expression tag	UNP P42212
A	-5	GLY	-	expression tag	UNP P42212
A	-4	SER	-	expression tag	UNP P42212
A	-3	HIS	-	expression tag	UNP P42212
A	-2	MET	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P42212
A	0	THR	-	expression tag	UNP P42212
A	1	MET	-	expression tag	UNP P42212
A	2	VAL	-	expression tag	UNP P42212
A	31	ARG	SER	engineered mutation	UNP P42212
A	40	ASN	TYR	conflict	UNP P42212
A	65	LEU	PHE	conflict	UNP P42212
A	68	PIA	SER	chromophore	UNP P42212
A	68	PIA	TYR	chromophore	UNP P42212
A	68	PIA	GLY	chromophore	UNP P42212
A	70	LEU	GLN	engineered mutation	UNP P42212
A	81	ARG	GLN	engineered mutation	UNP P42212
A	100	SER	PHE	conflict	UNP P42212
A	106	THR	ASN	conflict	UNP P42212
A	146	PHE	TYR	conflict	UNP P42212
A	154	THR	MET	conflict	UNP P42212
A	164	SER	VAL	engineered mutation	UNP P42212
A	172	VAL	ILE	conflict	UNP P42212
A	207	LYS	ALA	engineered mutation	UNP P42212
B	-22	MET	-	initiating methionine	UNP P42212
B	-21	GLY	-	expression tag	UNP P42212
B	-20	SER	-	expression tag	UNP P42212
B	-19	SER	-	expression tag	UNP P42212
B	-18	HIS	-	expression tag	UNP P42212
B	-17	HIS	-	expression tag	UNP P42212
B	-16	HIS	-	expression tag	UNP P42212
B	-15	HIS	-	expression tag	UNP P42212
B	-14	HIS	-	expression tag	UNP P42212
B	-13	HIS	-	expression tag	UNP P42212
B	-12	SER	-	expression tag	UNP P42212
B	-11	SER	-	expression tag	UNP P42212
B	-10	GLY	-	expression tag	UNP P42212
B	-9	LEU	-	expression tag	UNP P42212
B	-8	VAL	-	expression tag	UNP P42212
B	-7	PRO	-	expression tag	UNP P42212
B	-6	ARG	-	expression tag	UNP P42212
B	-5	GLY	-	expression tag	UNP P42212
B	-4	SER	-	expression tag	UNP P42212
B	-3	HIS	-	expression tag	UNP P42212
B	-2	MET	-	expression tag	UNP P42212
B	-1	ALA	-	expression tag	UNP P42212
B	0	THR	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P42212
B	2	VAL	-	expression tag	UNP P42212
B	31	ARG	SER	engineered mutation	UNP P42212
B	40	ASN	TYR	conflict	UNP P42212
B	65	LEU	PHE	conflict	UNP P42212
B	68	PIA	SER	chromophore	UNP P42212
B	68	PIA	TYR	chromophore	UNP P42212
B	68	PIA	GLY	chromophore	UNP P42212
B	70	LEU	GLN	engineered mutation	UNP P42212
B	81	ARG	GLN	engineered mutation	UNP P42212
B	100	SER	PHE	conflict	UNP P42212
B	106	THR	ASN	conflict	UNP P42212
B	146	PHE	TYR	conflict	UNP P42212
B	154	THR	MET	conflict	UNP P42212
B	164	SER	VAL	engineered mutation	UNP P42212
B	172	VAL	ILE	conflict	UNP P42212
B	207	LYS	ALA	engineered mutation	UNP P42212
C	-22	MET	-	initiating methionine	UNP P42212
C	-21	GLY	-	expression tag	UNP P42212
C	-20	SER	-	expression tag	UNP P42212
C	-19	SER	-	expression tag	UNP P42212
C	-18	HIS	-	expression tag	UNP P42212
C	-17	HIS	-	expression tag	UNP P42212
C	-16	HIS	-	expression tag	UNP P42212
C	-15	HIS	-	expression tag	UNP P42212
C	-14	HIS	-	expression tag	UNP P42212
C	-13	HIS	-	expression tag	UNP P42212
C	-12	SER	-	expression tag	UNP P42212
C	-11	SER	-	expression tag	UNP P42212
C	-10	GLY	-	expression tag	UNP P42212
C	-9	LEU	-	expression tag	UNP P42212
C	-8	VAL	-	expression tag	UNP P42212
C	-7	PRO	-	expression tag	UNP P42212
C	-6	ARG	-	expression tag	UNP P42212
C	-5	GLY	-	expression tag	UNP P42212
C	-4	SER	-	expression tag	UNP P42212
C	-3	HIS	-	expression tag	UNP P42212
C	-2	MET	-	expression tag	UNP P42212
C	-1	ALA	-	expression tag	UNP P42212
C	0	THR	-	expression tag	UNP P42212
C	1	MET	-	expression tag	UNP P42212
C	2	VAL	-	expression tag	UNP P42212

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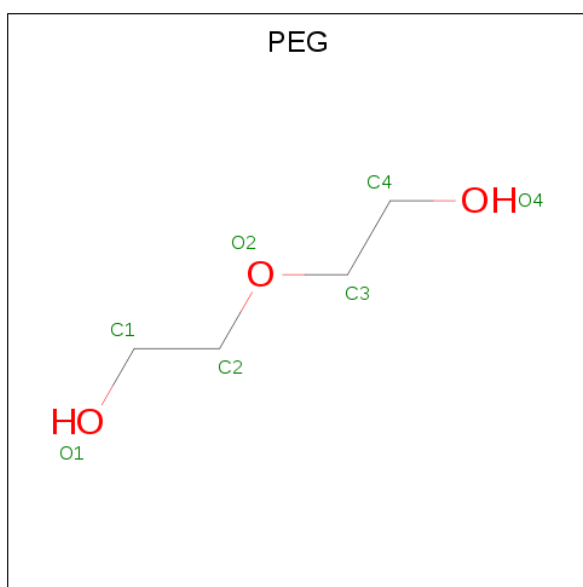
Chain	Residue	Modelled	Actual	Comment	Reference
C	31	ARG	SER	engineered mutation	UNP P42212
C	40	ASN	TYR	conflict	UNP P42212
C	65	LEU	PHE	conflict	UNP P42212
C	68	PIA	SER	chromophore	UNP P42212
C	68	PIA	TYR	chromophore	UNP P42212
C	68	PIA	GLY	chromophore	UNP P42212
C	70	LEU	GLN	engineered mutation	UNP P42212
C	81	ARG	GLN	engineered mutation	UNP P42212
C	100	SER	PHE	conflict	UNP P42212
C	106	THR	ASN	conflict	UNP P42212
C	146	PHE	TYR	conflict	UNP P42212
C	154	THR	MET	conflict	UNP P42212
C	164	SER	VAL	engineered mutation	UNP P42212
C	172	VAL	ILE	conflict	UNP P42212
C	207	LYS	ALA	engineered mutation	UNP P42212
D	-22	MET	-	initiating methionine	UNP P42212
D	-21	GLY	-	expression tag	UNP P42212
D	-20	SER	-	expression tag	UNP P42212
D	-19	SER	-	expression tag	UNP P42212
D	-18	HIS	-	expression tag	UNP P42212
D	-17	HIS	-	expression tag	UNP P42212
D	-16	HIS	-	expression tag	UNP P42212
D	-15	HIS	-	expression tag	UNP P42212
D	-14	HIS	-	expression tag	UNP P42212
D	-13	HIS	-	expression tag	UNP P42212
D	-12	SER	-	expression tag	UNP P42212
D	-11	SER	-	expression tag	UNP P42212
D	-10	GLY	-	expression tag	UNP P42212
D	-9	LEU	-	expression tag	UNP P42212
D	-8	VAL	-	expression tag	UNP P42212
D	-7	PRO	-	expression tag	UNP P42212
D	-6	ARG	-	expression tag	UNP P42212
D	-5	GLY	-	expression tag	UNP P42212
D	-4	SER	-	expression tag	UNP P42212
D	-3	HIS	-	expression tag	UNP P42212
D	-2	MET	-	expression tag	UNP P42212
D	-1	ALA	-	expression tag	UNP P42212
D	0	THR	-	expression tag	UNP P42212
D	1	MET	-	expression tag	UNP P42212
D	2	VAL	-	expression tag	UNP P42212
D	31	ARG	SER	engineered mutation	UNP P42212
D	40	ASN	TYR	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	65	LEU	PHE	conflict	UNP P42212
D	68	PIA	SER	chromophore	UNP P42212
D	68	PIA	TYR	chromophore	UNP P42212
D	68	PIA	GLY	chromophore	UNP P42212
D	70	LEU	GLN	engineered mutation	UNP P42212
D	81	ARG	GLN	engineered mutation	UNP P42212
D	100	SER	PHE	conflict	UNP P42212
D	106	THR	ASN	conflict	UNP P42212
D	146	PHE	TYR	conflict	UNP P42212
D	154	THR	MET	conflict	UNP P42212
D	164	SER	VAL	engineered mutation	UNP P42212
D	172	VAL	ILE	conflict	UNP P42212
D	207	LYS	ALA	engineered mutation	UNP P42212

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 3 is water.

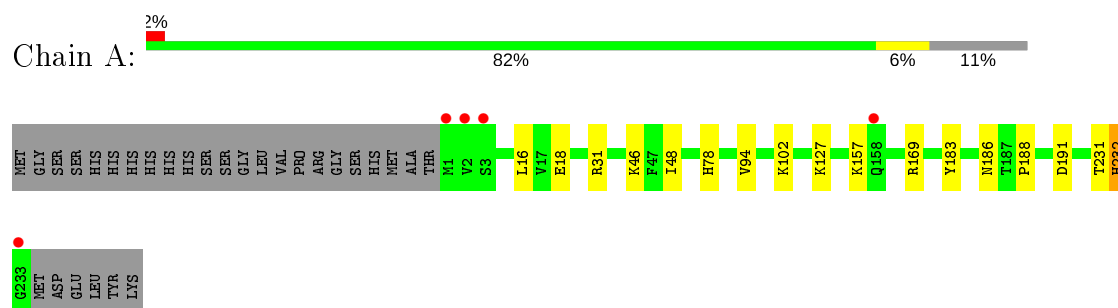


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	239	Total 239	O 239	0	0
3	B	292	Total 292	O 292	0	0
3	C	245	Total 245	O 245	0	0
3	D	228	Total 228	O 228	0	0

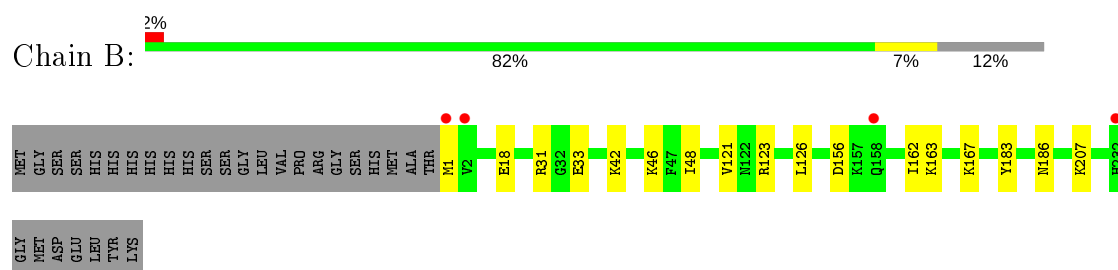
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

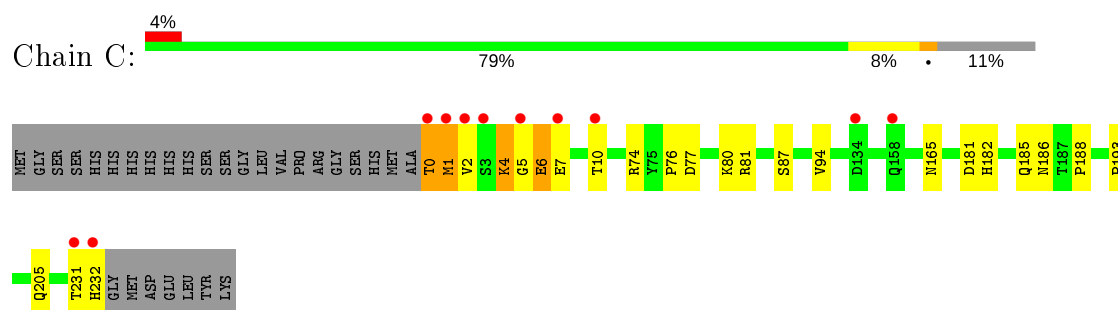
- Molecule 1: Green fluorescent protein



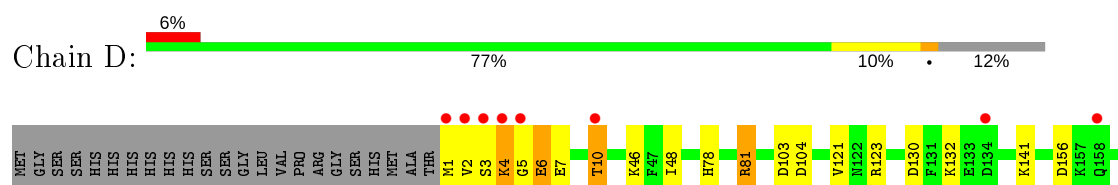
- Molecule 1: Green fluorescent protein

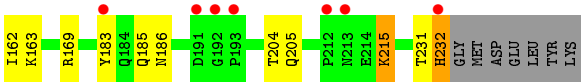


- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.47Å 134.56Å 51.72Å 90.00° 106.05° 90.00°	Depositor
Resolution (Å)	95.97 – 1.50 47.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (95.97-1.50) 97.1 (47.99-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.174 , 0.202 0.178 , 0.205	Depositor DCC
$R_{free}$ test set	7243 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 25.91 % 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 2.9035e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PIA, PEG

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	0.58	0/1882	0.67	0/2540
1	B	0.60	0/1886	0.74	0/2546
1	C	0.58	0/1888	0.71	0/2550
1	D	0.57	0/1892	0.69	0/2554
All	All	0.58	0/7548	0.70	0/10190

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	D	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	D	4	LYS	Peptide

### 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	1856	0	1825	13	0
1	B	1857	0	1825	15	1
1	C	1859	0	1824	24	0
1	D	1860	0	1831	36	0
2	C	7	0	10	0	0
2	D	14	0	19	13	0
3	A	239	0	0	6	2
3	B	292	0	0	9	1
3	C	245	0	0	5	1
3	D	228	0	0	12	1
All	All	8457	0	7334	92	4

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 6.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLU:OE1	1:B:123[A]:ARG:NH1	1.68	1.24
1:D:183[A]:TYR:CD1	3:D:496:HOH:O	2.04	1.10
1:C:181[B]:ASP:OD1	3:C:401:HOH:O	1.78	1.01
1:B:183[B]:TYR:CD1	3:B:332:HOH:O	2.19	0.94
1:A:183[B]:TYR:CD1	3:A:335:HOH:O	2.21	0.92

All (4) 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)
3:A:389:HOH:O	3:C:459:HOH:O[1_554]	1.98	0.22
3:B:493:HOH:O	3:D:470:HOH:O[1_556]	2.08	0.12
3:A:475:HOH:O	3:A:507:HOH:O[2_556]	2.10	0.10
1:B:33:GLU:OE2	1:B:33:GLU:OE2[2_557]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/260 (88%)	225 (99%)	2 (1%)	1 (0%)	34	13
1	B	228/260 (88%)	226 (99%)	2 (1%)	0	100	100
1	C	229/260 (88%)	224 (98%)	4 (2%)	1 (0%)	34	13
1	D	229/260 (88%)	226 (99%)	3 (1%)	0	100	100
All	All	914/1040 (88%)	901 (99%)	11 (1%)	2 (0%)	47	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	C	4	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	204/227 (90%)	201 (98%)	3 (2%)	65	39
1	B	205/227 (90%)	205 (100%)	0	100	100
1	C	206/227 (91%)	202 (98%)	4 (2%)	57	27
1	D	206/227 (91%)	201 (98%)	5 (2%)	49	19
All	All	821/908 (90%)	809 (98%)	12 (2%)	65	39

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	GLU
1	C	188	PRO
1	D	81	ARG
1	C	1	MET
1	D	10	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	213	ASN
1	C	232	HIS
1	D	26	HIS
1	D	232	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	PIA	D	68	1	21,21,22	3.07	4 (19%)	27,29,31	2.61	6 (22%)
1	PIA	A	68	1	21,21,22	2.67	2 (9%)	27,29,31	2.90	5 (18%)
1	PIA	C	68	1	21,21,22	3.19	2 (9%)	27,29,31	3.10	5 (18%)
1	PIA	B	68	1	21,21,22	2.72	3 (14%)	27,29,31	2.54	6 (22%)

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	PIA	D	68	1	-	0/8/27/28	0/2/2/2
1	PIA	A	68	1	-	0/8/27/28	0/2/2/2
1	PIA	C	68	1	-	0/8/27/28	0/2/2/2
1	PIA	B	68	1	-	0/8/27/28	0/2/2/2



The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	PIA	CA2-C2	-12.77	1.36	1.48
1	D	68	PIA	CA2-C2	-12.70	1.36	1.48
1	A	68	PIA	CA2-C2	-10.98	1.37	1.48
1	B	68	PIA	CA2-C2	-10.50	1.38	1.48
1	C	68	PIA	CB2-CA2	5.23	1.39	1.35

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	PIA	CA2-C2-N3	13.79	109.89	103.37
1	A	68	PIA	CA2-C2-N3	12.37	109.22	103.37
1	D	68	PIA	CA2-C2-N3	10.69	108.42	103.37
1	B	68	PIA	CA2-C2-N3	9.25	107.75	103.37
1	B	68	PIA	C2-N3-C1	-5.26	105.31	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	PEG	D	301	-	6,6,6	1.15	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	C	301	-	6,6,6	0.91	0	5,5,5	0.34	0
2	PEG	D	302	-	6,6,6	1.27	0	5,5,5	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	D	301	-	-	3/4/4/4	-
2	PEG	C	301	-	-	2/4/4/4	-
2	PEG	D	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	302	PEG	C1-C2-O2-C3
2	D	301	PEG	O2-C3-C4-O4
2	C	301	PEG	O1-C1-C2-O2
2	D	302	PEG	O2-C3-C4-O4
2	C	301	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	PEG	8	0
2	D	302	PEG	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	230/260 (88%)	0.14	5 (2%) 62 67	13, 21, 47, 71	0
1	B	229/260 (88%)	0.10	4 (1%) 70 75	11, 18, 36, 77	0
1	C	230/260 (88%)	0.28	11 (4%) 30 33	13, 20, 49, 84	0
1	D	229/260 (88%)	0.28	15 (6%) 18 19	14, 22, 48, 80	0
All	All	918/1040 (88%)	0.20	35 (3%) 40 44	11, 20, 46, 84	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	THR	12.1
1	D	3	SER	6.4
1	A	2	VAL	6.0
1	A	1	MET	4.7
1	D	5	GLY	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PIA	D	68	20/21	0.95	0.08	13,14,19,19	0
1	PIA	A	68	20/21	0.96	0.08	12,14,17,18	0
1	PIA	C	68	20/21	0.96	0.09	12,13,16,16	0
1	PIA	B	68	20/21	0.96	0.08	10,12,13,13	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	PEG	C	301	7/7	0.51	0.24	54,62,72,72	0
2	PEG	D	302	7/7	0.71	0.27	43,45,51,54	0
2	PEG	D	301	7/7	0.72	0.29	42,50,63,71	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.