wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2021 – 06:25 am BST

PDB ID	:	5EXB
Title	:	Wild type green fluorescent protein DendFP (Dendronephthya sp.)
Authors	:	Pletnev, V.Z.; Pletneva, N.V.; Pletnev, S.V.
Deposited on	:	2015-11-23
Resolution	:	1.81 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 (1)) were used in the production of this report:

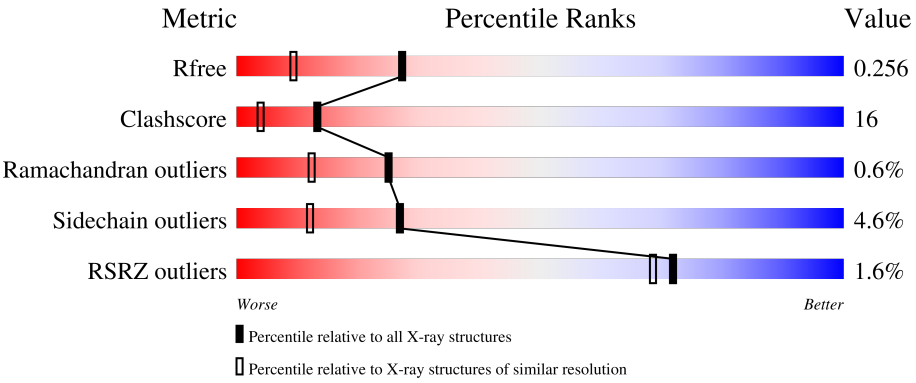
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	232	3% 59% 34% • 5%
1	B	232	66% 29% • •
1	C	232	69% 25% • •
1	D	232	% 60% 30% 5% •
1	E	232	2% 69% 25% • 5%

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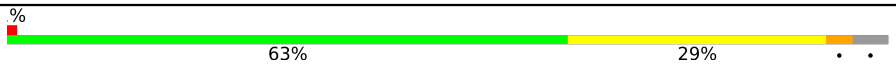
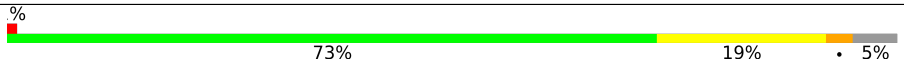
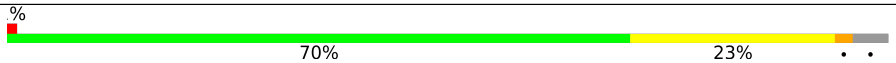
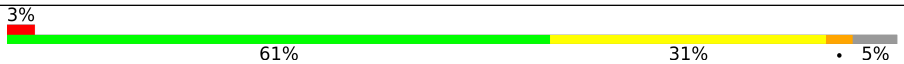
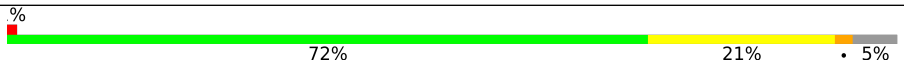
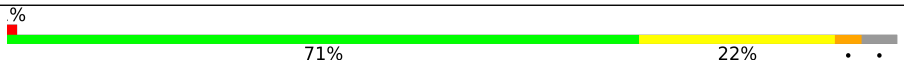
Mol	Chain	Length	Quality of chain
1	F	232	
1	G	232	
1	H	232	
1	I	232	
1	J	232	
1	K	232	
1	L	232	
1	M	232	
1	N	232	
1	O	232	
1	P	232	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	E	301	-	-	X	-
2	GOL	N	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31172 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	221	Total	C	N	O	S	0	0	0
			1802	1157	302	334	9			
1	B	225	Total	C	N	O	S	0	2	0
			1849	1186	313	341	9			
1	C	224	Total	C	N	O	S	0	1	0
			1830	1172	308	341	9			
1	D	222	Total	C	N	O	S	0	2	0
			1821	1169	305	338	9			
1	E	221	Total	C	N	O	S	0	0	0
			1802	1157	302	334	9			
1	F	222	Total	C	N	O	S	0	0	0
			1810	1161	304	336	9			
1	G	225	Total	C	N	O	S	0	6	0
			1873	1201	317	346	9			
1	H	221	Total	C	N	O	S	0	2	0
			1817	1166	305	336	10			
1	I	221	Total	C	N	O	S	0	0	0
			1802	1157	302	334	9			
1	J	222	Total	C	N	O	S	0	2	0
			1823	1171	307	336	9			
1	K	227	Total	C	N	O	S	0	6	0
			1886	1210	322	345	9			
1	L	226	Total	C	N	O	S	0	0	0
			1842	1180	313	340	9			
1	M	221	Total	C	N	O	S	0	1	0
			1808	1162	303	334	9			
1	N	221	Total	C	N	O	S	0	2	0
			1817	1167	304	337	9			
1	O	222	Total	C	N	O	S	0	2	0
			1822	1170	305	338	9			
1	P	222	Total	C	N	O	S	0	4	0
			1832	1179	307	337	9			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8T6U0
A	1	GLY	-	expression tag	UNP Q8T6U0
A	64	5SQ	HIS	chromophore	UNP Q8T6U0
A	64	5SQ	TYR	chromophore	UNP Q8T6U0
A	64	5SQ	GLY	chromophore	UNP Q8T6U0
A	226	GLY	-	expression tag	UNP Q8T6U0
A	227	SER	-	expression tag	UNP Q8T6U0
A	228	HIS	-	expression tag	UNP Q8T6U0
A	229	HIS	-	expression tag	UNP Q8T6U0
A	230	HIS	-	expression tag	UNP Q8T6U0
A	231	HIS	-	expression tag	UNP Q8T6U0
A	232	HIS	-	expression tag	UNP Q8T6U0
A	233	HIS	-	expression tag	UNP Q8T6U0
B	0	MET	-	initiating methionine	UNP Q8T6U0
B	1	GLY	-	expression tag	UNP Q8T6U0
B	64	5SQ	HIS	chromophore	UNP Q8T6U0
B	64	5SQ	TYR	chromophore	UNP Q8T6U0
B	64	5SQ	GLY	chromophore	UNP Q8T6U0
B	226	GLY	-	expression tag	UNP Q8T6U0
B	227	SER	-	expression tag	UNP Q8T6U0
B	228	HIS	-	expression tag	UNP Q8T6U0
B	229	HIS	-	expression tag	UNP Q8T6U0
B	230	HIS	-	expression tag	UNP Q8T6U0
B	231	HIS	-	expression tag	UNP Q8T6U0
B	232	HIS	-	expression tag	UNP Q8T6U0
B	233	HIS	-	expression tag	UNP Q8T6U0
C	0	MET	-	initiating methionine	UNP Q8T6U0
C	1	GLY	-	expression tag	UNP Q8T6U0
C	64	5SQ	HIS	chromophore	UNP Q8T6U0
C	64	5SQ	TYR	chromophore	UNP Q8T6U0
C	64	5SQ	GLY	chromophore	UNP Q8T6U0
C	226	GLY	-	expression tag	UNP Q8T6U0
C	227	SER	-	expression tag	UNP Q8T6U0
C	228	HIS	-	expression tag	UNP Q8T6U0
C	229	HIS	-	expression tag	UNP Q8T6U0
C	230	HIS	-	expression tag	UNP Q8T6U0
C	231	HIS	-	expression tag	UNP Q8T6U0
C	232	HIS	-	expression tag	UNP Q8T6U0
C	233	HIS	-	expression tag	UNP Q8T6U0
D	0	MET	-	initiating methionine	UNP Q8T6U0
D	1	GLY	-	expression tag	UNP Q8T6U0
D	64	5SQ	HIS	chromophore	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	64	5SQ	TYR	chromophore	UNP Q8T6U0
D	64	5SQ	GLY	chromophore	UNP Q8T6U0
D	226	GLY	-	expression tag	UNP Q8T6U0
D	227	SER	-	expression tag	UNP Q8T6U0
D	228	HIS	-	expression tag	UNP Q8T6U0
D	229	HIS	-	expression tag	UNP Q8T6U0
D	230	HIS	-	expression tag	UNP Q8T6U0
D	231	HIS	-	expression tag	UNP Q8T6U0
D	232	HIS	-	expression tag	UNP Q8T6U0
D	233	HIS	-	expression tag	UNP Q8T6U0
E	0	MET	-	initiating methionine	UNP Q8T6U0
E	1	GLY	-	expression tag	UNP Q8T6U0
E	64	5SQ	HIS	chromophore	UNP Q8T6U0
E	64	5SQ	TYR	chromophore	UNP Q8T6U0
E	64	5SQ	GLY	chromophore	UNP Q8T6U0
E	226	GLY	-	expression tag	UNP Q8T6U0
E	227	SER	-	expression tag	UNP Q8T6U0
E	228	HIS	-	expression tag	UNP Q8T6U0
E	229	HIS	-	expression tag	UNP Q8T6U0
E	230	HIS	-	expression tag	UNP Q8T6U0
E	231	HIS	-	expression tag	UNP Q8T6U0
E	232	HIS	-	expression tag	UNP Q8T6U0
E	233	HIS	-	expression tag	UNP Q8T6U0
F	0	MET	-	initiating methionine	UNP Q8T6U0
F	1	GLY	-	expression tag	UNP Q8T6U0
F	64	5SQ	HIS	chromophore	UNP Q8T6U0
F	64	5SQ	TYR	chromophore	UNP Q8T6U0
F	64	5SQ	GLY	chromophore	UNP Q8T6U0
F	226	GLY	-	expression tag	UNP Q8T6U0
F	227	SER	-	expression tag	UNP Q8T6U0
F	228	HIS	-	expression tag	UNP Q8T6U0
F	229	HIS	-	expression tag	UNP Q8T6U0
F	230	HIS	-	expression tag	UNP Q8T6U0
F	231	HIS	-	expression tag	UNP Q8T6U0
F	232	HIS	-	expression tag	UNP Q8T6U0
F	233	HIS	-	expression tag	UNP Q8T6U0
G	0	MET	-	initiating methionine	UNP Q8T6U0
G	1	GLY	-	expression tag	UNP Q8T6U0
G	64	5SQ	HIS	chromophore	UNP Q8T6U0
G	64	5SQ	TYR	chromophore	UNP Q8T6U0
G	64	5SQ	GLY	chromophore	UNP Q8T6U0
G	226	GLY	-	expression tag	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	227	SER	-	expression tag	UNP Q8T6U0
G	228	HIS	-	expression tag	UNP Q8T6U0
G	229	HIS	-	expression tag	UNP Q8T6U0
G	230	HIS	-	expression tag	UNP Q8T6U0
G	231	HIS	-	expression tag	UNP Q8T6U0
G	232	HIS	-	expression tag	UNP Q8T6U0
G	233	HIS	-	expression tag	UNP Q8T6U0
H	0	MET	-	initiating methionine	UNP Q8T6U0
H	1	GLY	-	expression tag	UNP Q8T6U0
H	64	5SQ	HIS	chromophore	UNP Q8T6U0
H	64	5SQ	TYR	chromophore	UNP Q8T6U0
H	64	5SQ	GLY	chromophore	UNP Q8T6U0
H	226	GLY	-	expression tag	UNP Q8T6U0
H	227	SER	-	expression tag	UNP Q8T6U0
H	228	HIS	-	expression tag	UNP Q8T6U0
H	229	HIS	-	expression tag	UNP Q8T6U0
H	230	HIS	-	expression tag	UNP Q8T6U0
H	231	HIS	-	expression tag	UNP Q8T6U0
H	232	HIS	-	expression tag	UNP Q8T6U0
H	233	HIS	-	expression tag	UNP Q8T6U0
I	0	MET	-	initiating methionine	UNP Q8T6U0
I	1	GLY	-	expression tag	UNP Q8T6U0
I	64	5SQ	HIS	chromophore	UNP Q8T6U0
I	64	5SQ	TYR	chromophore	UNP Q8T6U0
I	64	5SQ	GLY	chromophore	UNP Q8T6U0
I	226	GLY	-	expression tag	UNP Q8T6U0
I	227	SER	-	expression tag	UNP Q8T6U0
I	228	HIS	-	expression tag	UNP Q8T6U0
I	229	HIS	-	expression tag	UNP Q8T6U0
I	230	HIS	-	expression tag	UNP Q8T6U0
I	231	HIS	-	expression tag	UNP Q8T6U0
I	232	HIS	-	expression tag	UNP Q8T6U0
I	233	HIS	-	expression tag	UNP Q8T6U0
J	0	MET	-	initiating methionine	UNP Q8T6U0
J	1	GLY	-	expression tag	UNP Q8T6U0
J	64	5SQ	HIS	chromophore	UNP Q8T6U0
J	64	5SQ	TYR	chromophore	UNP Q8T6U0
J	64	5SQ	GLY	chromophore	UNP Q8T6U0
J	226	GLY	-	expression tag	UNP Q8T6U0
J	227	SER	-	expression tag	UNP Q8T6U0
J	228	HIS	-	expression tag	UNP Q8T6U0
J	229	HIS	-	expression tag	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	230	HIS	-	expression tag	UNP Q8T6U0
J	231	HIS	-	expression tag	UNP Q8T6U0
J	232	HIS	-	expression tag	UNP Q8T6U0
J	233	HIS	-	expression tag	UNP Q8T6U0
K	0	MET	-	initiating methionine	UNP Q8T6U0
K	1	GLY	-	expression tag	UNP Q8T6U0
K	64	5SQ	HIS	chromophore	UNP Q8T6U0
K	64	5SQ	TYR	chromophore	UNP Q8T6U0
K	64	5SQ	GLY	chromophore	UNP Q8T6U0
K	226	GLY	-	expression tag	UNP Q8T6U0
K	227	SER	-	expression tag	UNP Q8T6U0
K	228	HIS	-	expression tag	UNP Q8T6U0
K	229	HIS	-	expression tag	UNP Q8T6U0
K	230	HIS	-	expression tag	UNP Q8T6U0
K	231	HIS	-	expression tag	UNP Q8T6U0
K	232	HIS	-	expression tag	UNP Q8T6U0
K	233	HIS	-	expression tag	UNP Q8T6U0
L	0	MET	-	initiating methionine	UNP Q8T6U0
L	1	GLY	-	expression tag	UNP Q8T6U0
L	64	5SQ	HIS	chromophore	UNP Q8T6U0
L	64	5SQ	TYR	chromophore	UNP Q8T6U0
L	64	5SQ	GLY	chromophore	UNP Q8T6U0
L	226	GLY	-	expression tag	UNP Q8T6U0
L	227	SER	-	expression tag	UNP Q8T6U0
L	228	HIS	-	expression tag	UNP Q8T6U0
L	229	HIS	-	expression tag	UNP Q8T6U0
L	230	HIS	-	expression tag	UNP Q8T6U0
L	231	HIS	-	expression tag	UNP Q8T6U0
L	232	HIS	-	expression tag	UNP Q8T6U0
L	233	HIS	-	expression tag	UNP Q8T6U0
M	0	MET	-	initiating methionine	UNP Q8T6U0
M	1	GLY	-	expression tag	UNP Q8T6U0
M	64	5SQ	HIS	chromophore	UNP Q8T6U0
M	64	5SQ	TYR	chromophore	UNP Q8T6U0
M	64	5SQ	GLY	chromophore	UNP Q8T6U0
M	226	GLY	-	expression tag	UNP Q8T6U0
M	227	SER	-	expression tag	UNP Q8T6U0
M	228	HIS	-	expression tag	UNP Q8T6U0
M	229	HIS	-	expression tag	UNP Q8T6U0
M	230	HIS	-	expression tag	UNP Q8T6U0
M	231	HIS	-	expression tag	UNP Q8T6U0
M	232	HIS	-	expression tag	UNP Q8T6U0

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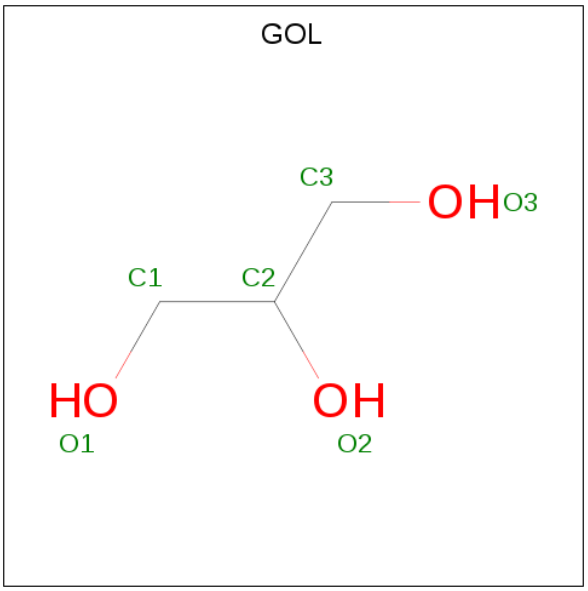
Chain	Residue	Modelled	Actual	Comment	Reference
M	233	HIS	-	expression tag	UNP Q8T6U0
N	0	MET	-	initiating methionine	UNP Q8T6U0
N	1	GLY	-	expression tag	UNP Q8T6U0
N	64	5SQ	HIS	chromophore	UNP Q8T6U0
N	64	5SQ	TYR	chromophore	UNP Q8T6U0
N	64	5SQ	GLY	chromophore	UNP Q8T6U0
N	226	GLY	-	expression tag	UNP Q8T6U0
N	227	SER	-	expression tag	UNP Q8T6U0
N	228	HIS	-	expression tag	UNP Q8T6U0
N	229	HIS	-	expression tag	UNP Q8T6U0
N	230	HIS	-	expression tag	UNP Q8T6U0
N	231	HIS	-	expression tag	UNP Q8T6U0
N	232	HIS	-	expression tag	UNP Q8T6U0
N	233	HIS	-	expression tag	UNP Q8T6U0
O	0	MET	-	initiating methionine	UNP Q8T6U0
O	1	GLY	-	expression tag	UNP Q8T6U0
O	64	5SQ	HIS	chromophore	UNP Q8T6U0
O	64	5SQ	TYR	chromophore	UNP Q8T6U0
O	64	5SQ	GLY	chromophore	UNP Q8T6U0
O	226	GLY	-	expression tag	UNP Q8T6U0
O	227	SER	-	expression tag	UNP Q8T6U0
O	228	HIS	-	expression tag	UNP Q8T6U0
O	229	HIS	-	expression tag	UNP Q8T6U0
O	230	HIS	-	expression tag	UNP Q8T6U0
O	231	HIS	-	expression tag	UNP Q8T6U0
O	232	HIS	-	expression tag	UNP Q8T6U0
O	233	HIS	-	expression tag	UNP Q8T6U0
P	0	MET	-	initiating methionine	UNP Q8T6U0
P	1	GLY	-	expression tag	UNP Q8T6U0
P	64	5SQ	HIS	chromophore	UNP Q8T6U0
P	64	5SQ	TYR	chromophore	UNP Q8T6U0
P	64	5SQ	GLY	chromophore	UNP Q8T6U0
P	226	GLY	-	expression tag	UNP Q8T6U0
P	227	SER	-	expression tag	UNP Q8T6U0
P	228	HIS	-	expression tag	UNP Q8T6U0
P	229	HIS	-	expression tag	UNP Q8T6U0
P	230	HIS	-	expression tag	UNP Q8T6U0
P	231	HIS	-	expression tag	UNP Q8T6U0
P	232	HIS	-	expression tag	UNP Q8T6U0
P	233	HIS	-	expression tag	UNP Q8T6U0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	76	Total O 76 76	0	0
3	B	140	Total O 140 140	0	0
3	C	116	Total O 116 116	0	0
3	D	123	Total O 123 123	0	0
3	E	36	Total O 36 36	0	0
3	F	135	Total O 135 135	0	0
3	G	147	Total O 147 147	0	0
3	H	156	Total O 156 156	0	0
3	I	170	Total O 170 170	0	0

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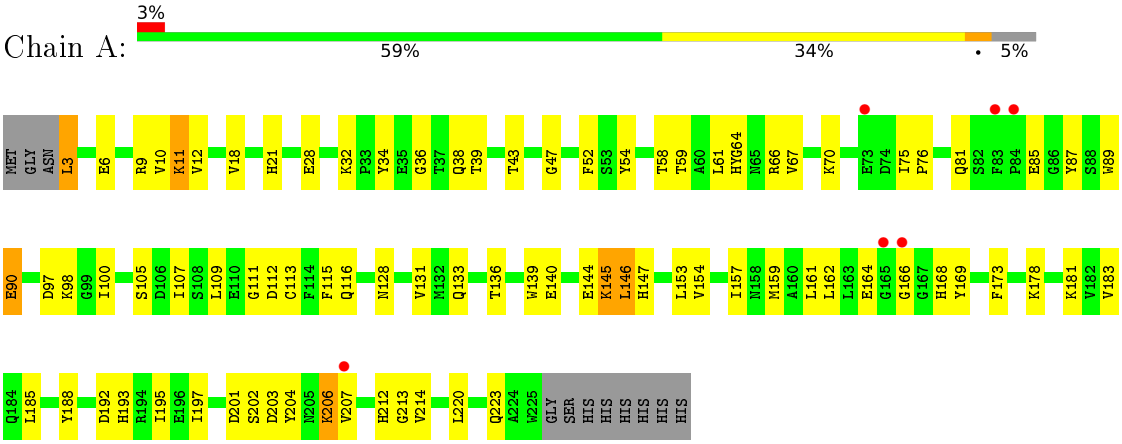
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	130	Total O 130 130	0	0
3	K	187	Total O 187 187	0	0
3	L	48	Total O 48 48	0	0
3	M	86	Total O 86 86	0	0
3	N	180	Total O 180 180	0	0
3	O	80	Total O 80 80	0	0
3	P	108	Total O 108 108	0	0

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.

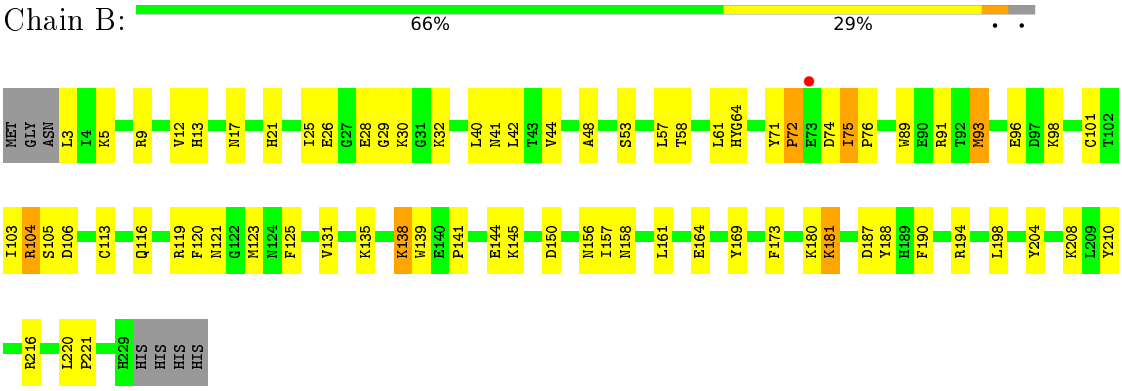
- Molecule 1: Green fluorescent protein

Chain A:



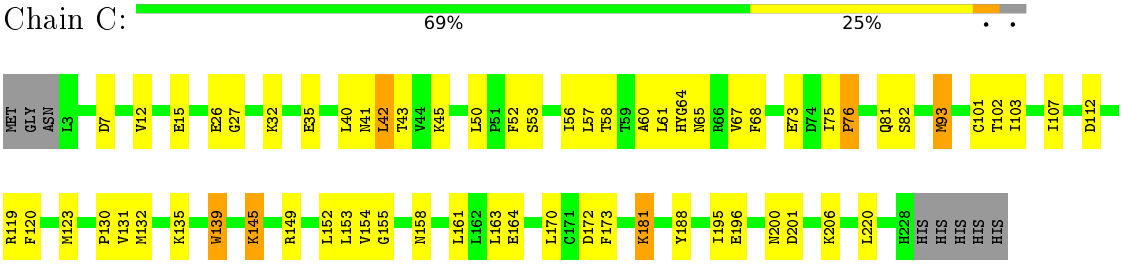
- Molecule 1: Green fluorescent protein

Chain B:



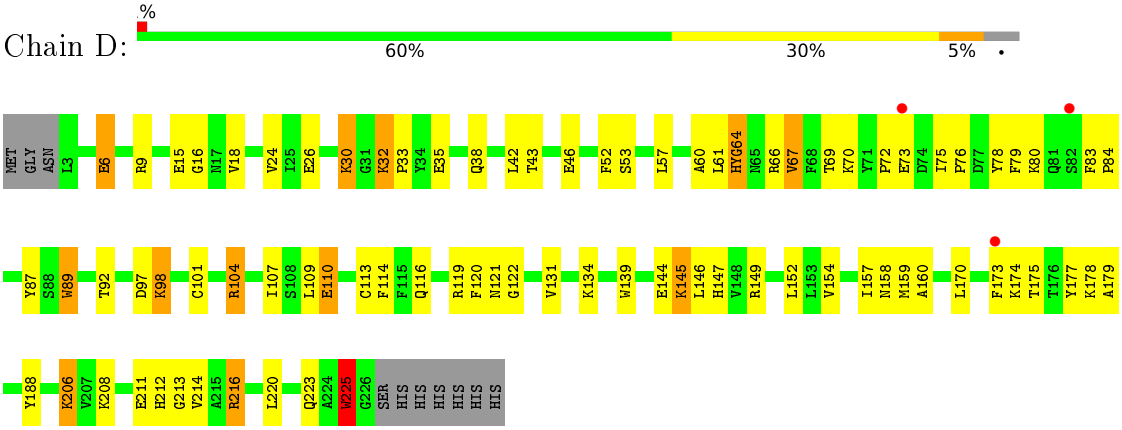
- Molecule 1: Green fluorescent protein

Chain C:



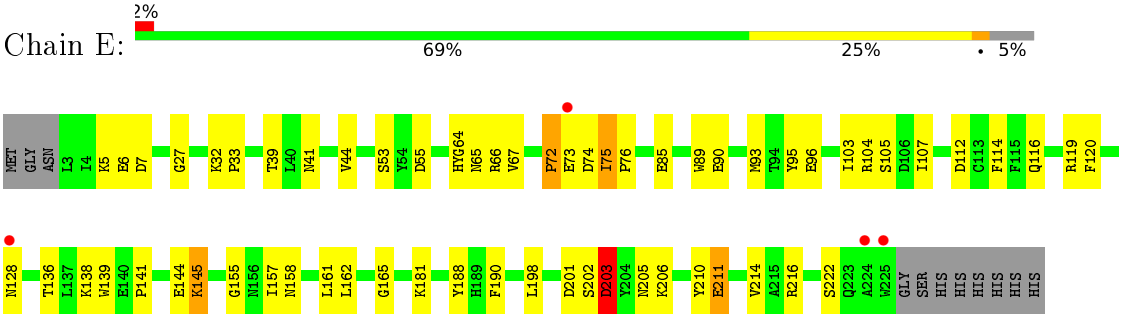
• Molecule 1: Green fluorescent protein

Chain D:



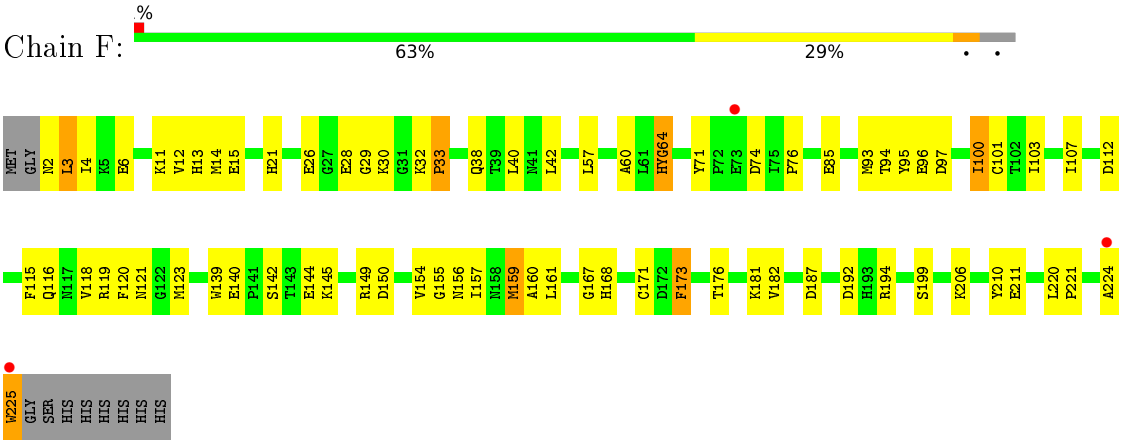
• Molecule 1: Green fluorescent protein

Chain E:



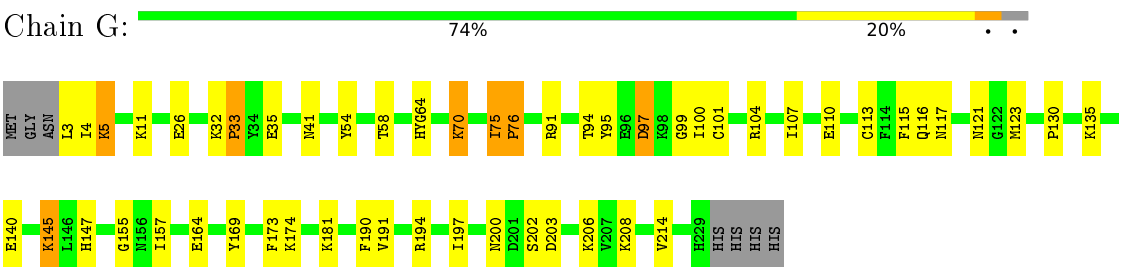
• Molecule 1: Green fluorescent protein

Chain F:



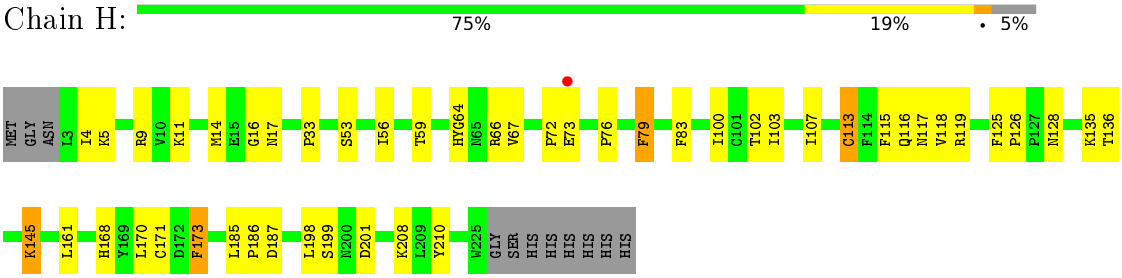
• Molecule 1: Green fluorescent protein

Chain G:



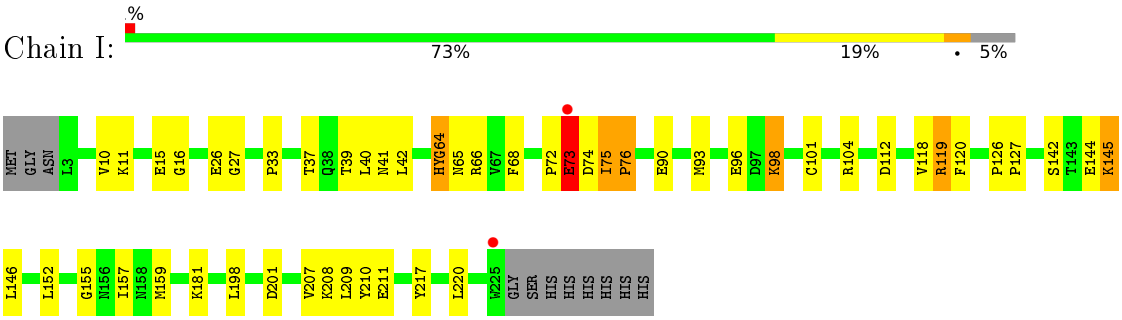
• Molecule 1: Green fluorescent protein

Chain H:



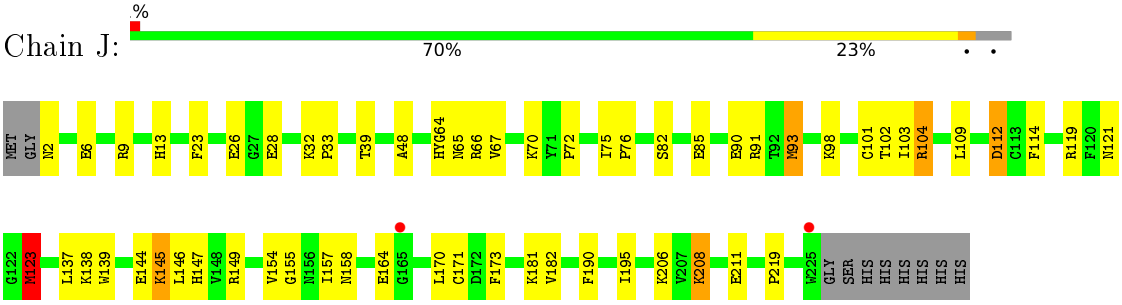
• Molecule 1: Green fluorescent protein

Chain I:



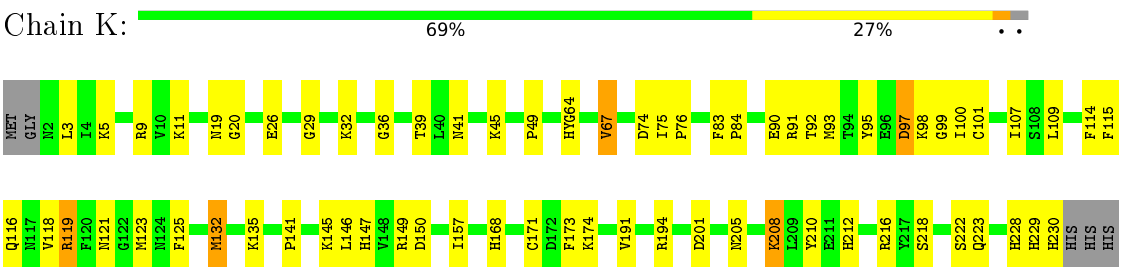
• Molecule 1: Green fluorescent protein

Chain J:



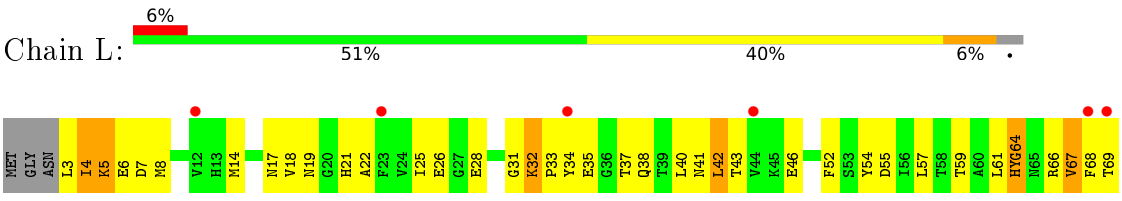
• Molecule 1: Green fluorescent protein

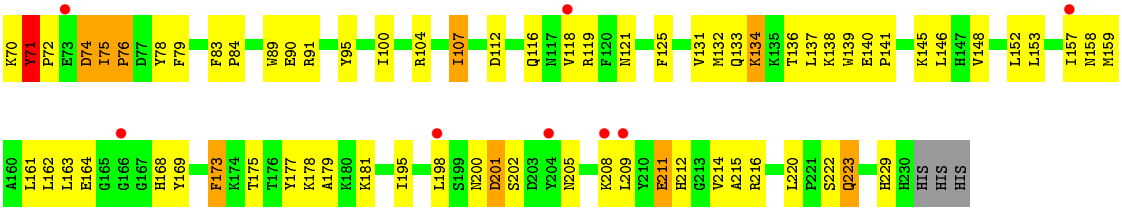
Chain K:



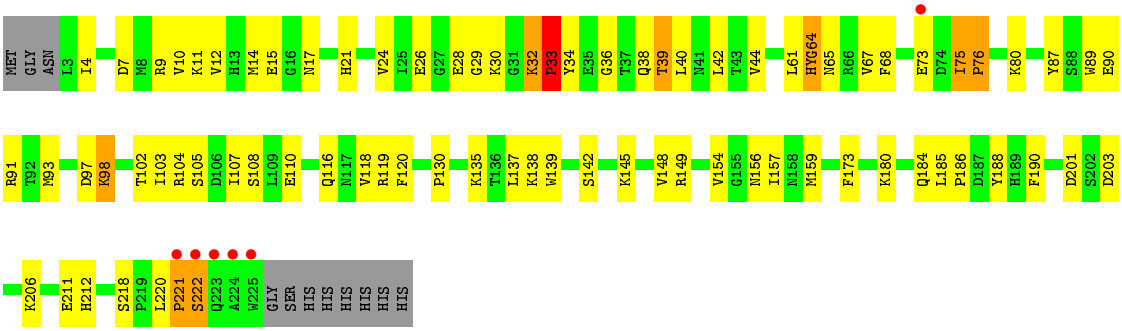
• Molecule 1: Green fluorescent protein

Chain L:

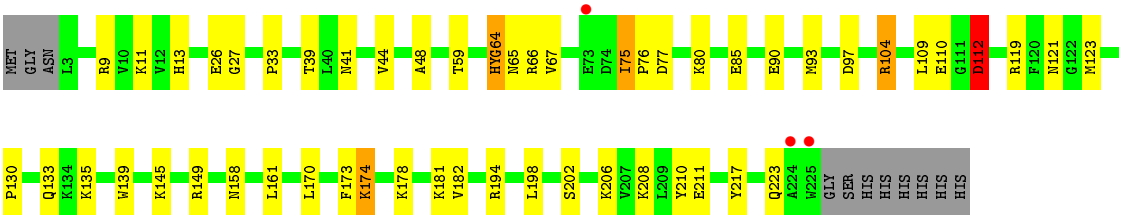




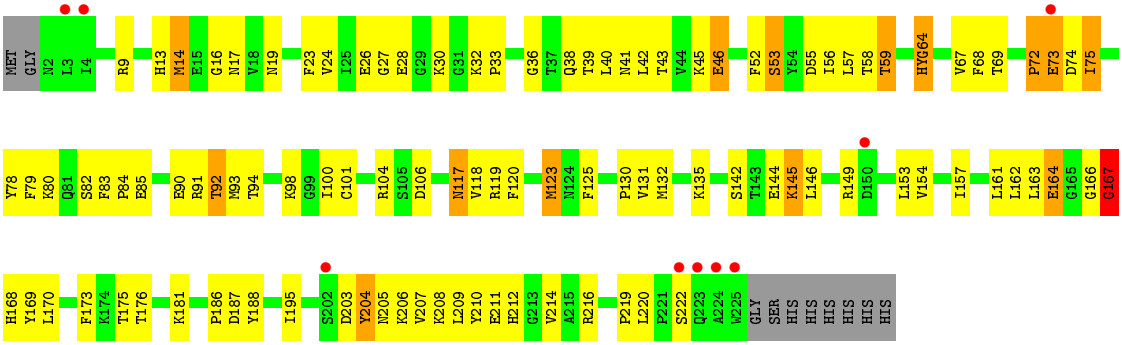
• Molecule 1: Green fluorescent protein



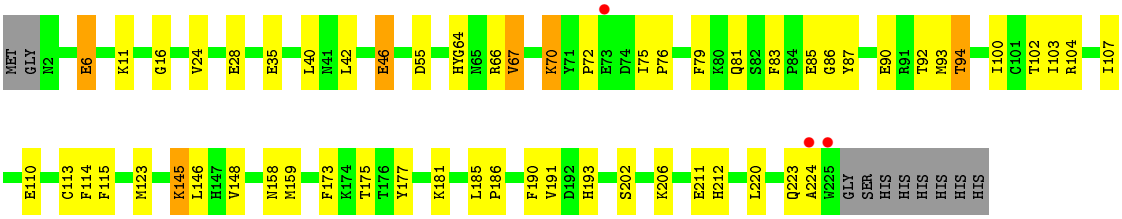
• Molecule 1: Green fluorescent protein



• Molecule 1: Green fluorescent protein



• Molecule 1: Green fluorescent protein


MET GLY M2 E6 K11 G16 V24 E28 E35 L40 N41 L42 E46 D55 HYG64 N65 R66 V67 K70 Y71 P72 E73 D74 I75 P76 F79 K80 Q81 S82 F83 P84 E85 G86 Y87 E90 A91 T92 M93 T94 I100 C101 T102 I103 R104 I107
E110 C113 F114 F115 M123 K145 L146 H147 V148 N158 M159 F173 K174 T175 T176 Y177 K181 L185 P186 F190 V191 D192 H193 S202 K206 E211 H212 L220 Q223 A224 W225 GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.38Å 106.40Å 137.21Å 109.68° 100.01° 101.72°	Depositor
Resolution (Å)	37.37 – 1.81 37.37 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.8 (37.37-1.81) 96.8 (37.37-1.81)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.182 , 0.249 0.191 , 0.256	Depositor DCC
R_{free} test set	3215 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31172	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 43.38 % 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 1.7783e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 5SQ

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	0.85	1/1824 (0.1%)	0.94	2/2467 (0.1%)
1	B	1.03	2/1873 (0.1%)	1.05	7/2532 (0.3%)
1	C	1.06	3/1853 (0.2%)	1.10	7/2506 (0.3%)
1	D	1.00	3/1843 (0.2%)	1.06	3/2493 (0.1%)
1	E	1.12	4/1824 (0.2%)	1.09	7/2467 (0.3%)
1	F	1.02	2/1832 (0.1%)	1.12	7/2478 (0.3%)
1	G	1.20	6/1913 (0.3%)	1.12	3/2585 (0.1%)
1	H	1.09	4/1839 (0.2%)	1.14	5/2486 (0.2%)
1	I	1.22	8/1824 (0.4%)	1.17	6/2467 (0.2%)
1	J	1.09	2/1851 (0.1%)	1.14	10/2503 (0.4%)
1	K	1.16	4/1929 (0.2%)	1.19	12/2607 (0.5%)
1	L	0.79	2/1867 (0.1%)	0.95	3/2525 (0.1%)
1	M	0.93	2/1833 (0.1%)	1.03	2/2478 (0.1%)
1	N	1.16	2/1842 (0.1%)	1.17	7/2490 (0.3%)
1	O	0.95	2/1847 (0.1%)	1.03	1/2499 (0.0%)
1	P	1.02	1/1866 (0.1%)	1.08	5/2524 (0.2%)
All	All	1.05	48/29660 (0.2%)	1.09	87/40107 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	O	0	2
All	All	0	3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	119[A]	ARG	N-CA	8.39	1.63	1.46
1	K	119[B]	ARG	N-CA	8.39	1.63	1.46
1	I	72	PRO	C-N	-8.24	1.15	1.34
1	O	72	PRO	C-N	-7.70	1.16	1.34
1	D	225	TRP	CB-CG	-6.46	1.38	1.50

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	119	ARG	NE-CZ-NH1	-9.19	115.70	120.30
1	G	97	ASP	CB-CG-OD1	8.59	126.03	118.30
1	D	216	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	N	97	ASP	CB-CG-OD1	8.11	125.59	118.30
1	J	149	ARG	NE-CZ-NH2	-7.81	116.39	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	167	GLY	Peptide
1	O	167	GLY	Peptide
1	O	73	GLU	Mainchain

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	1802	0	1735	71	0
1	B	1849	0	1779	73	0
1	C	1830	0	1753	61	0
1	D	1821	0	1754	80	0
1	E	1802	0	1733	45	0
1	F	1810	0	1741	64	0
1	G	1873	0	1805	52	1
1	H	1817	0	1751	39	0
1	I	1802	0	1733	43	0
1	J	1823	0	1765	41	1
1	K	1886	0	1831	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1842	0	1764	99	0
1	M	1808	0	1748	59	0
1	N	1817	0	1753	47	0
1	O	1822	0	1757	109	0
1	P	1832	0	1783	48	0
2	B	6	0	8	3	0
2	E	6	0	8	4	0
2	N	6	0	8	8	0
3	A	76	0	0	20	0
3	B	140	0	0	18	0
3	C	116	0	0	13	0
3	D	123	0	0	37	0
3	E	36	0	0	6	0
3	F	135	0	0	17	0
3	G	147	0	0	14	0
3	H	156	0	0	11	0
3	I	170	0	0	15	0
3	J	130	0	0	14	0
3	K	187	0	0	15	0
3	L	48	0	0	6	0
3	M	86	0	0	11	0
3	N	180	0	0	10	0
3	O	80	0	0	43	0
3	P	108	0	0	9	0
All	All	31172	0	28209	929	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 16.

The worst 5 of 929 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:M:40:LEU:HG	3:M:326:HOH:O	1.25	1.29
1:C:56:ILE:HD11	1:C:101:CYS:SG	1.71	1.29
1:F:159:MET:SD	3:F:382:HOH:O	1.92	1.27
1:N:44:VAL:HG11	3:N:478:HOH:O	1.31	1.25
1:G:58:THR:HG21	3:G:372:HOH:O	1.39	1.23

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:11[B]:LYS:NZ	1:J:48:ALA:O[1_565]	1.85	0.35

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	218/232 (94%)	205 (94%)	11 (5%)	2 (1%)	17 6
1	B	224/232 (97%)	217 (97%)	7 (3%)	0	100 100
1	C	222/232 (96%)	214 (96%)	8 (4%)	0	100 100
1	D	221/232 (95%)	214 (97%)	5 (2%)	2 (1%)	17 6
1	E	218/232 (94%)	211 (97%)	6 (3%)	1 (0%)	29 15
1	F	219/232 (94%)	200 (91%)	18 (8%)	1 (0%)	29 15
1	G	228/232 (98%)	222 (97%)	6 (3%)	0	100 100
1	H	220/232 (95%)	214 (97%)	6 (3%)	0	100 100
1	I	218/232 (94%)	213 (98%)	4 (2%)	1 (0%)	29 15
1	J	221/232 (95%)	215 (97%)	6 (3%)	0	100 100
1	K	230/232 (99%)	222 (96%)	7 (3%)	1 (0%)	34 21
1	L	223/232 (96%)	195 (87%)	22 (10%)	6 (3%)	5 0
1	M	219/232 (94%)	198 (90%)	19 (9%)	2 (1%)	17 6
1	N	220/232 (95%)	213 (97%)	7 (3%)	0	100 100
1	O	221/232 (95%)	199 (90%)	18 (8%)	4 (2%)	8 1
1	P	223/232 (96%)	217 (97%)	5 (2%)	1 (0%)	34 21
All	All	3545/3712 (96%)	3369 (95%)	155 (4%)	21 (1%)	25 12

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	SER

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Mol	Chain	Res	Type
1	D	225	TRP
1	F	3	LEU
1	L	4	ILE
1	L	6	GLU

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	195/204 (96%)	184 (94%)	11 (6%)	21 8
1	B	200/204 (98%)	193 (96%)	7 (4%)	36 20
1	C	198/204 (97%)	193 (98%)	5 (2%)	47 33
1	D	197/204 (97%)	186 (94%)	11 (6%)	21 8
1	E	195/204 (96%)	185 (95%)	10 (5%)	24 9
1	F	196/204 (96%)	187 (95%)	9 (5%)	27 12
1	G	204/204 (100%)	194 (95%)	10 (5%)	25 10
1	H	197/204 (97%)	190 (96%)	7 (4%)	35 19
1	I	195/204 (96%)	192 (98%)	3 (2%)	65 55
1	J	198/204 (97%)	190 (96%)	8 (4%)	31 16
1	K	206/204 (101%)	203 (98%)	3 (2%)	65 55
1	L	199/204 (98%)	180 (90%)	19 (10%)	8 2
1	M	196/204 (96%)	183 (93%)	13 (7%)	16 5
1	N	197/204 (97%)	193 (98%)	4 (2%)	55 43
1	O	198/204 (97%)	179 (90%)	19 (10%)	8 2
1	P	200/204 (98%)	192 (96%)	8 (4%)	31 16
All	All	3171/3264 (97%)	3024 (95%)	147 (5%)	27 12

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	211	GLU

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Mol	Chain	Res	Type
1	P	94[A]	THR
1	N	211	GLU
1	O	92[B]	THR
1	F	159	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	124	ASN
1	M	223	GLN
1	L	19	ASN
1	O	128	ASN
1	M	116	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 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	5SQ	A	64	1	23,27,28	0.75	0	29,37,39	1.86	8 (27%)
1	5SQ	G	64	1	23,27,28	1.37	5 (21%)	29,37,39	1.53	5 (17%)
1	5SQ	M	64	1	23,27,28	1.76	3 (13%)	29,37,39	2.15	10 (34%)
1	5SQ	J	64	1	23,27,28	1.26	2 (8%)	29,37,39	2.78	11 (37%)
1	5SQ	D	64	1	23,27,28	0.90	1 (4%)	29,37,39	2.24	10 (34%)
1	5SQ	I	64	1	23,27,28	1.80	5 (21%)	29,37,39	2.20	7 (24%)
1	5SQ	C	64	1	23,27,28	1.46	3 (13%)	29,37,39	3.30	12 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5SQ	B	64	1	23,27,28	1.40	3 (13%)	29,37,39	3.88	16 (55%)
1	5SQ	L	64	1	23,27,28	1.02	2 (8%)	29,37,39	2.01	8 (27%)
1	5SQ	E	64	1	23,27,28	1.57	3 (13%)	29,37,39	2.52	9 (31%)
1	5SQ	H	64	1	23,27,28	1.69	4 (17%)	29,37,39	2.97	14 (48%)
1	5SQ	O	64	1	23,27,28	1.42	1 (4%)	29,37,39	2.26	10 (34%)
1	5SQ	P	64	1	23,27,28	1.26	2 (8%)	29,37,39	2.06	8 (27%)
1	5SQ	F	64	1	23,27,28	0.94	1 (4%)	29,37,39	1.96	6 (20%)
1	5SQ	K	64	1	23,27,28	1.88	3 (13%)	29,37,39	2.03	7 (24%)
1	5SQ	N	64	1	23,27,28	2.13	6 (26%)	29,37,39	1.97	8 (27%)

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	5SQ	A	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	G	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	M	64	1	-	6/12/31/32	0/3/3/3
1	5SQ	J	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	D	64	1	-	6/12/31/32	0/3/3/3
1	5SQ	I	64	1	-	2/12/31/32	0/3/3/3
1	5SQ	C	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	B	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	L	64	1	-	5/12/31/32	0/3/3/3
1	5SQ	E	64	1	-	2/12/31/32	0/3/3/3
1	5SQ	H	64	1	-	5/12/31/32	0/3/3/3
1	5SQ	O	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	P	64	1	-	2/12/31/32	0/3/3/3
1	5SQ	F	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	K	64	1	-	5/12/31/32	0/3/3/3
1	5SQ	N	64	1	-	2/12/31/32	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	64	5SQ	CB2-CA2	7.07	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	64	5SQ	CB2-CA2	5.96	1.40	1.35
1	N	64	5SQ	CB2-CA2	5.41	1.39	1.35
1	I	64	5SQ	O2-C2	-5.28	1.12	1.23
1	N	64	5SQ	CA2-C2	-5.01	1.43	1.48

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	64	5SQ	O2-C2-CA2	-9.91	125.40	130.96
1	C	64	5SQ	N3-C1-N2	9.59	118.10	111.45
1	B	64	5SQ	C2-CA2-N2	-8.25	103.16	108.93
1	H	64	5SQ	CA2-C2-N3	-7.28	99.93	103.37
1	C	64	5SQ	CA1-C1-N3	-7.19	115.47	124.85

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	5SQ	CA1-CB1-CG1-N1H
1	A	64	5SQ	C2-CA2-CB2-CG2
1	A	64	5SQ	N2-CA2-CB2-CG2
1	B	64	5SQ	C-CA3-N3-C2
1	B	64	5SQ	CA1-CB1-CG1-N1H

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	64	5SQ	1	0
1	D	64	5SQ	1	0
1	I	64	5SQ	1	0
1	L	64	5SQ	2	0
1	O	64	5SQ	3	0
1	F	64	5SQ	1	0
1	N	64	5SQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	GOL	E	301	-	5,5,5	0.61	0	5,5,5	1.16	1 (20%)
2	GOL	B	301	-	5,5,5	0.67	0	5,5,5	0.63	0
2	GOL	N	301	-	5,5,5	0.72	0	5,5,5	0.98	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	GOL	E	301	-	-	0/4/4/4	-
2	GOL	B	301	-	-	0/4/4/4	-
2	GOL	N	301	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	GOL	C3-C2-C1	-2.26	102.90	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	301	GOL	O1-C1-C2-C3
2	N	301	GOL	O1-C1-C2-O2
2	N	301	GOL	O2-C2-C3-O3
2	N	301	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	GOL	4	0
2	B	301	GOL	3	0
2	N	301	GOL	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	O	1
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	72:PRO	C	73:GLU	N	1.16
1	I	72:PRO	C	73:GLU	N	1.15

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^{th} 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	220/232 (94%)	0.04	6 (2%) 54 49	15, 29, 42, 51	2 (0%)
1	B	224/232 (96%)	-0.22	1 (0%) 92 91	10, 21, 32, 42	2 (0%)
1	C	223/232 (96%)	-0.32	0 100 100	8, 19, 30, 43	2 (0%)
1	D	221/232 (95%)	-0.07	3 (1%) 75 72	12, 24, 34, 43	2 (0%)
1	E	220/232 (94%)	-0.20	4 (1%) 68 64	9, 20, 31, 74	2 (0%)
1	F	221/232 (95%)	-0.17	3 (1%) 75 72	12, 22, 39, 88	2 (0%)
1	G	224/232 (96%)	-0.42	0 100 100	8, 15, 26, 35	1 (0%)
1	H	220/232 (94%)	-0.39	1 (0%) 91 89	6, 16, 29, 51	2 (0%)
1	I	220/232 (94%)	-0.40	2 (0%) 84 82	6, 13, 28, 72	2 (0%)
1	J	221/232 (95%)	-0.32	2 (0%) 84 82	8, 17, 29, 60	2 (0%)
1	K	226/232 (97%)	-0.44	0 100 100	6, 14, 25, 43	1 (0%)
1	L	225/232 (96%)	0.56	14 (6%) 20 16	20, 38, 58, 75	2 (0%)
1	M	220/232 (94%)	0.01	6 (2%) 54 49	13, 25, 44, 86	2 (0%)
1	N	220/232 (94%)	-0.45	3 (1%) 75 72	6, 14, 23, 67	2 (0%)
1	O	221/232 (95%)	0.19	9 (4%) 37 31	14, 30, 43, 81	2 (0%)
1	P	221/232 (95%)	-0.23	3 (1%) 75 72	9, 19, 33, 79	2 (0%)
All	All	3547/3712 (95%)	-0.18	57 (1%) 72 68	6, 20, 41, 88	30 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	225	TRP	10.3
1	O	225	TRP	8.2
1	M	225	TRP	7.4
1	P	225	TRP	7.0
1	M	224	ALA	6.7

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, 95^{th} 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	5SQ	L	64	25/26	0.79	0.14	33,42,45,47	0
1	5SQ	O	64	25/26	0.87	0.13	20,27,46,47	0
1	5SQ	D	64	25/26	0.90	0.11	14,20,22,25	0
1	5SQ	A	64	25/26	0.90	0.10	24,28,32,33	0
1	5SQ	B	64	25/26	0.90	0.10	11,15,19,20	0
1	5SQ	M	64	25/26	0.92	0.10	20,22,26,26	0
1	5SQ	F	64	25/26	0.93	0.08	12,16,20,21	0
1	5SQ	J	64	25/26	0.95	0.08	9,12,14,16	0
1	5SQ	E	64	25/26	0.95	0.07	8,12,14,15	0
1	5SQ	P	64	25/26	0.95	0.07	13,15,17,18	0
1	5SQ	G	64	25/26	0.96	0.10	9,11,13,14	0
1	5SQ	H	64	25/26	0.96	0.08	9,10,12,13	0
1	5SQ	I	64	25/26	0.96	0.08	7,8,9,10	0
1	5SQ	C	64	25/26	0.96	0.09	9,13,14,16	0
1	5SQ	K	64	25/26	0.97	0.09	7,8,10,12	0
1	5SQ	N	64	25/26	0.97	0.08	8,10,12,12	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, 95^{th} 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	GOL	E	301	6/6	0.91	0.13	21,23,23,25	0
2	GOL	N	301	6/6	0.95	0.08	17,19,23,23	0
2	GOL	B	301	6/6	0.97	0.09	22,24,24,26	0

6.5 Other polymers (i)

There are no such residues in this entry.