



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2016 – 09:03 PM EST

PDB ID : 5LTQ  
Title : Structure of the Yellow Fluorescent Protein lanYFP from Branchiostoma lanceolatum at pH 7.5  
Authors : Clavel, D.; Gotthard, G.; Royant, A.  
Deposited on : 2016-09-07  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

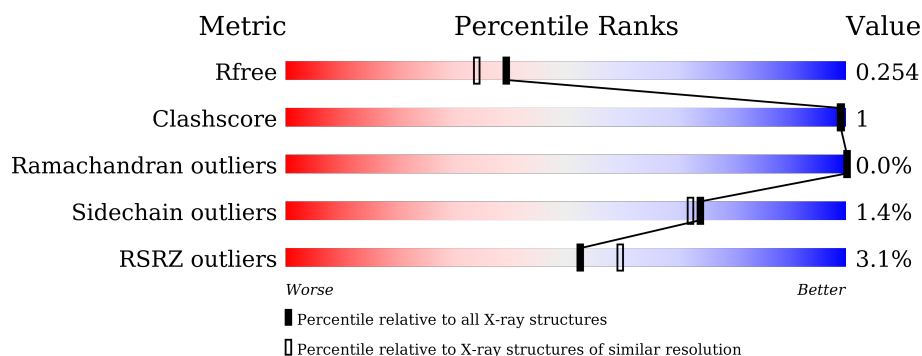
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	267	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	267	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	267	<div> <div></div> <div> <div></div> <div>78%</div> <div>•</div> <div>19%</div> </div> </div>
1	D	267	<div> <div></div> <div> <div></div> <div>80%</div> <div>•</div> <div>18%</div> </div> </div>
1	E	267	<div> <div></div> <div> <div></div> <div>78%</div> <div>•</div> <div>19%</div> </div> </div>
1	F	267	<div> <div></div> <div> <div></div> <div>80%</div> <div>•</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	267	
1	H	267	
1	I	267	
1	J	267	
1	K	267	
1	L	267	
1	M	267	
1	N	267	
1	O	267	
1	P	267	

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	CL	M	301	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28364 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 blFP-Y3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	1	0
			1746	1120	287	328	11			
1	D	219	Total	C	N	O	S	0	3	0
			1763	1130	290	331	12			
1	B	217	Total	C	N	O	S	0	3	0
			1748	1122	288	327	11			
1	C	217	Total	C	N	O	S	0	3	0
			1754	1126	290	327	11			
1	E	215	Total	C	N	O	S	0	2	0
			1732	1113	285	323	11			
1	H	215	Total	C	N	O	S	0	2	0
			1728	1109	285	323	11			
1	F	222	Total	C	N	O	S	0	1	0
			1784	1146	292	334	12			
1	G	216	Total	C	N	O	S	0	1	0
			1732	1112	285	324	11			
1	I	215	Total	C	N	O	S	0	1	0
			1725	1108	284	322	11			
1	L	217	Total	C	N	O	S	0	1	1
			1733	1112	285	325	11			
1	J	222	Total	C	N	O	S	0	1	0
			1781	1143	291	335	12			
1	K	215	Total	C	N	O	S	0	2	0
			1731	1112	285	323	11			
1	M	208	Total	C	N	O	S	0	1	0
			1676	1078	277	311	10			
1	P	217	Total	C	N	O	S	0	1	0
			1736	1114	286	325	11			
1	N	217	Total	C	N	O	S	0	1	0
			1733	1110	285	326	12			
1	O	211	Total	C	N	O	S	0	1	0
			1693	1087	280	316	10			

There are 896 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP B1PNC0
A	-41	ARG	-	expression tag	UNP B1PNC0
A	-40	GLY	-	expression tag	UNP B1PNC0
A	-39	SER	-	expression tag	UNP B1PNC0
A	-38	HIS	-	expression tag	UNP B1PNC0
A	-37	HIS	-	expression tag	UNP B1PNC0
A	-36	HIS	-	expression tag	UNP B1PNC0
A	-35	HIS	-	expression tag	UNP B1PNC0
A	-34	HIS	-	expression tag	UNP B1PNC0
A	-33	HIS	-	expression tag	UNP B1PNC0
A	-32	GLY	-	expression tag	UNP B1PNC0
A	-31	MET	-	expression tag	UNP B1PNC0
A	-30	ALA	-	expression tag	UNP B1PNC0
A	-29	SER	-	expression tag	UNP B1PNC0
A	-28	MET	-	expression tag	UNP B1PNC0
A	-27	THR	-	expression tag	UNP B1PNC0
A	-26	GLY	-	expression tag	UNP B1PNC0
A	-25	GLY	-	expression tag	UNP B1PNC0
A	-24	GLN	-	expression tag	UNP B1PNC0
A	-23	GLN	-	expression tag	UNP B1PNC0
A	-22	MET	-	expression tag	UNP B1PNC0
A	-21	GLY	-	expression tag	UNP B1PNC0
A	-20	ARG	-	expression tag	UNP B1PNC0
A	-19	ASP	-	expression tag	UNP B1PNC0
A	-18	LEU	-	expression tag	UNP B1PNC0
A	-17	TYR	-	expression tag	UNP B1PNC0
A	-16	ASP	-	expression tag	UNP B1PNC0
A	-15	ASP	-	expression tag	UNP B1PNC0
A	-14	ASP	-	expression tag	UNP B1PNC0
A	-13	ASP	-	expression tag	UNP B1PNC0
A	-12	LYS	-	expression tag	UNP B1PNC0
A	-11	ASP	-	expression tag	UNP B1PNC0
A	-10	PRO	-	expression tag	UNP B1PNC0
A	-9	MET	-	expression tag	UNP B1PNC0
A	-8	VAL	-	expression tag	UNP B1PNC0
A	-7	SER	-	expression tag	UNP B1PNC0
A	-6	LYS	-	expression tag	UNP B1PNC0
A	-5	GLY	-	expression tag	UNP B1PNC0
A	-4	GLU	-	expression tag	UNP B1PNC0
A	-3	GLU	-	expression tag	UNP B1PNC0
A	-2	ASP	-	expression tag	UNP B1PNC0
A	-1	ASN	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP B1PNC0
A	1	ALA	-	expression tag	UNP B1PNC0
A	59	CR2	GLY	chromophore	UNP B1PNC0
A	59	CR2	TYR	chromophore	UNP B1PNC0
A	59	CR2	GLY	chromophore	UNP B1PNC0
A	171	ALA	VAL	variant	UNP B1PNC0
A	174	THR	ASN	variant	UNP B1PNC0
A	220	GLY	-	expression tag	UNP B1PNC0
A	221	MET	-	expression tag	UNP B1PNC0
A	222	ASP	-	expression tag	UNP B1PNC0
A	223	GLU	-	expression tag	UNP B1PNC0
A	224	LEU	-	expression tag	UNP B1PNC0
A	225	TYR	-	expression tag	UNP B1PNC0
A	226	LYS	-	expression tag	UNP B1PNC0
D	-42	MET	-	initiating methionine	UNP B1PNC0
D	-41	ARG	-	expression tag	UNP B1PNC0
D	-40	GLY	-	expression tag	UNP B1PNC0
D	-39	SER	-	expression tag	UNP B1PNC0
D	-38	HIS	-	expression tag	UNP B1PNC0
D	-37	HIS	-	expression tag	UNP B1PNC0
D	-36	HIS	-	expression tag	UNP B1PNC0
D	-35	HIS	-	expression tag	UNP B1PNC0
D	-34	HIS	-	expression tag	UNP B1PNC0
D	-33	HIS	-	expression tag	UNP B1PNC0
D	-32	GLY	-	expression tag	UNP B1PNC0
D	-31	MET	-	expression tag	UNP B1PNC0
D	-30	ALA	-	expression tag	UNP B1PNC0
D	-29	SER	-	expression tag	UNP B1PNC0
D	-28	MET	-	expression tag	UNP B1PNC0
D	-27	THR	-	expression tag	UNP B1PNC0
D	-26	GLY	-	expression tag	UNP B1PNC0
D	-25	GLY	-	expression tag	UNP B1PNC0
D	-24	GLN	-	expression tag	UNP B1PNC0
D	-23	GLN	-	expression tag	UNP B1PNC0
D	-22	MET	-	expression tag	UNP B1PNC0
D	-21	GLY	-	expression tag	UNP B1PNC0
D	-20	ARG	-	expression tag	UNP B1PNC0
D	-19	ASP	-	expression tag	UNP B1PNC0
D	-18	LEU	-	expression tag	UNP B1PNC0
D	-17	TYR	-	expression tag	UNP B1PNC0
D	-16	ASP	-	expression tag	UNP B1PNC0
D	-15	ASP	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	ASP	-	expression tag	UNP B1PNC0
D	-13	ASP	-	expression tag	UNP B1PNC0
D	-12	LYS	-	expression tag	UNP B1PNC0
D	-11	ASP	-	expression tag	UNP B1PNC0
D	-10	PRO	-	expression tag	UNP B1PNC0
D	-9	MET	-	expression tag	UNP B1PNC0
D	-8	VAL	-	expression tag	UNP B1PNC0
D	-7	SER	-	expression tag	UNP B1PNC0
D	-6	LYS	-	expression tag	UNP B1PNC0
D	-5	GLY	-	expression tag	UNP B1PNC0
D	-4	GLU	-	expression tag	UNP B1PNC0
D	-3	GLU	-	expression tag	UNP B1PNC0
D	-2	ASP	-	expression tag	UNP B1PNC0
D	-1	ASN	-	expression tag	UNP B1PNC0
D	0	MET	-	expression tag	UNP B1PNC0
D	1	ALA	-	expression tag	UNP B1PNC0
D	59	CR2	GLY	chromophore	UNP B1PNC0
D	59	CR2	TYR	chromophore	UNP B1PNC0
D	59	CR2	GLY	chromophore	UNP B1PNC0
D	171	ALA	VAL	variant	UNP B1PNC0
D	174	THR	ASN	variant	UNP B1PNC0
D	220	GLY	-	expression tag	UNP B1PNC0
D	221	MET	-	expression tag	UNP B1PNC0
D	222	ASP	-	expression tag	UNP B1PNC0
D	223	GLU	-	expression tag	UNP B1PNC0
D	224	LEU	-	expression tag	UNP B1PNC0
D	225	TYR	-	expression tag	UNP B1PNC0
D	226	LYS	-	expression tag	UNP B1PNC0
B	-42	MET	-	initiating methionine	UNP B1PNC0
B	-41	ARG	-	expression tag	UNP B1PNC0
B	-40	GLY	-	expression tag	UNP B1PNC0
B	-39	SER	-	expression tag	UNP B1PNC0
B	-38	HIS	-	expression tag	UNP B1PNC0
B	-37	HIS	-	expression tag	UNP B1PNC0
B	-36	HIS	-	expression tag	UNP B1PNC0
B	-35	HIS	-	expression tag	UNP B1PNC0
B	-34	HIS	-	expression tag	UNP B1PNC0
B	-33	HIS	-	expression tag	UNP B1PNC0
B	-32	GLY	-	expression tag	UNP B1PNC0
B	-31	MET	-	expression tag	UNP B1PNC0
B	-30	ALA	-	expression tag	UNP B1PNC0
B	-29	SER	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-28	MET	-	expression tag	UNP B1PNC0
B	-27	THR	-	expression tag	UNP B1PNC0
B	-26	GLY	-	expression tag	UNP B1PNC0
B	-25	GLY	-	expression tag	UNP B1PNC0
B	-24	GLN	-	expression tag	UNP B1PNC0
B	-23	GLN	-	expression tag	UNP B1PNC0
B	-22	MET	-	expression tag	UNP B1PNC0
B	-21	GLY	-	expression tag	UNP B1PNC0
B	-20	ARG	-	expression tag	UNP B1PNC0
B	-19	ASP	-	expression tag	UNP B1PNC0
B	-18	LEU	-	expression tag	UNP B1PNC0
B	-17	TYR	-	expression tag	UNP B1PNC0
B	-16	ASP	-	expression tag	UNP B1PNC0
B	-15	ASP	-	expression tag	UNP B1PNC0
B	-14	ASP	-	expression tag	UNP B1PNC0
B	-13	ASP	-	expression tag	UNP B1PNC0
B	-12	LYS	-	expression tag	UNP B1PNC0
B	-11	ASP	-	expression tag	UNP B1PNC0
B	-10	PRO	-	expression tag	UNP B1PNC0
B	-9	MET	-	expression tag	UNP B1PNC0
B	-8	VAL	-	expression tag	UNP B1PNC0
B	-7	SER	-	expression tag	UNP B1PNC0
B	-6	LYS	-	expression tag	UNP B1PNC0
B	-5	GLY	-	expression tag	UNP B1PNC0
B	-4	GLU	-	expression tag	UNP B1PNC0
B	-3	GLU	-	expression tag	UNP B1PNC0
B	-2	ASP	-	expression tag	UNP B1PNC0
B	-1	ASN	-	expression tag	UNP B1PNC0
B	0	MET	-	expression tag	UNP B1PNC0
B	1	ALA	-	expression tag	UNP B1PNC0
B	59	CR2	GLY	chromophore	UNP B1PNC0
B	59	CR2	TYR	chromophore	UNP B1PNC0
B	59	CR2	GLY	chromophore	UNP B1PNC0
B	171	ALA	VAL	variant	UNP B1PNC0
B	174	THR	ASN	variant	UNP B1PNC0
B	220	GLY	-	expression tag	UNP B1PNC0
B	221	MET	-	expression tag	UNP B1PNC0
B	222	ASP	-	expression tag	UNP B1PNC0
B	223	GLU	-	expression tag	UNP B1PNC0
B	224	LEU	-	expression tag	UNP B1PNC0
B	225	TYR	-	expression tag	UNP B1PNC0
B	226	LYS	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-42	MET	-	initiating methionine	UNP B1PNC0
C	-41	ARG	-	expression tag	UNP B1PNC0
C	-40	GLY	-	expression tag	UNP B1PNC0
C	-39	SER	-	expression tag	UNP B1PNC0
C	-38	HIS	-	expression tag	UNP B1PNC0
C	-37	HIS	-	expression tag	UNP B1PNC0
C	-36	HIS	-	expression tag	UNP B1PNC0
C	-35	HIS	-	expression tag	UNP B1PNC0
C	-34	HIS	-	expression tag	UNP B1PNC0
C	-33	HIS	-	expression tag	UNP B1PNC0
C	-32	GLY	-	expression tag	UNP B1PNC0
C	-31	MET	-	expression tag	UNP B1PNC0
C	-30	ALA	-	expression tag	UNP B1PNC0
C	-29	SER	-	expression tag	UNP B1PNC0
C	-28	MET	-	expression tag	UNP B1PNC0
C	-27	THR	-	expression tag	UNP B1PNC0
C	-26	GLY	-	expression tag	UNP B1PNC0
C	-25	GLY	-	expression tag	UNP B1PNC0
C	-24	GLN	-	expression tag	UNP B1PNC0
C	-23	GLN	-	expression tag	UNP B1PNC0
C	-22	MET	-	expression tag	UNP B1PNC0
C	-21	GLY	-	expression tag	UNP B1PNC0
C	-20	ARG	-	expression tag	UNP B1PNC0
C	-19	ASP	-	expression tag	UNP B1PNC0
C	-18	LEU	-	expression tag	UNP B1PNC0
C	-17	TYR	-	expression tag	UNP B1PNC0
C	-16	ASP	-	expression tag	UNP B1PNC0
C	-15	ASP	-	expression tag	UNP B1PNC0
C	-14	ASP	-	expression tag	UNP B1PNC0
C	-13	ASP	-	expression tag	UNP B1PNC0
C	-12	LYS	-	expression tag	UNP B1PNC0
C	-11	ASP	-	expression tag	UNP B1PNC0
C	-10	PRO	-	expression tag	UNP B1PNC0
C	-9	MET	-	expression tag	UNP B1PNC0
C	-8	VAL	-	expression tag	UNP B1PNC0
C	-7	SER	-	expression tag	UNP B1PNC0
C	-6	LYS	-	expression tag	UNP B1PNC0
C	-5	GLY	-	expression tag	UNP B1PNC0
C	-4	GLU	-	expression tag	UNP B1PNC0
C	-3	GLU	-	expression tag	UNP B1PNC0
C	-2	ASP	-	expression tag	UNP B1PNC0
C	-1	ASN	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	expression tag	UNP B1PNC0
C	1	ALA	-	expression tag	UNP B1PNC0
C	59	CR2	GLY	chromophore	UNP B1PNC0
C	59	CR2	TYR	chromophore	UNP B1PNC0
C	59	CR2	GLY	chromophore	UNP B1PNC0
C	171	ALA	VAL	variant	UNP B1PNC0
C	174	THR	ASN	variant	UNP B1PNC0
C	220	GLY	-	expression tag	UNP B1PNC0
C	221	MET	-	expression tag	UNP B1PNC0
C	222	ASP	-	expression tag	UNP B1PNC0
C	223	GLU	-	expression tag	UNP B1PNC0
C	224	LEU	-	expression tag	UNP B1PNC0
C	225	TYR	-	expression tag	UNP B1PNC0
C	226	LYS	-	expression tag	UNP B1PNC0
E	-42	MET	-	initiating methionine	UNP B1PNC0
E	-41	ARG	-	expression tag	UNP B1PNC0
E	-40	GLY	-	expression tag	UNP B1PNC0
E	-39	SER	-	expression tag	UNP B1PNC0
E	-38	HIS	-	expression tag	UNP B1PNC0
E	-37	HIS	-	expression tag	UNP B1PNC0
E	-36	HIS	-	expression tag	UNP B1PNC0
E	-35	HIS	-	expression tag	UNP B1PNC0
E	-34	HIS	-	expression tag	UNP B1PNC0
E	-33	HIS	-	expression tag	UNP B1PNC0
E	-32	GLY	-	expression tag	UNP B1PNC0
E	-31	MET	-	expression tag	UNP B1PNC0
E	-30	ALA	-	expression tag	UNP B1PNC0
E	-29	SER	-	expression tag	UNP B1PNC0
E	-28	MET	-	expression tag	UNP B1PNC0
E	-27	THR	-	expression tag	UNP B1PNC0
E	-26	GLY	-	expression tag	UNP B1PNC0
E	-25	GLY	-	expression tag	UNP B1PNC0
E	-24	GLN	-	expression tag	UNP B1PNC0
E	-23	GLN	-	expression tag	UNP B1PNC0
E	-22	MET	-	expression tag	UNP B1PNC0
E	-21	GLY	-	expression tag	UNP B1PNC0
E	-20	ARG	-	expression tag	UNP B1PNC0
E	-19	ASP	-	expression tag	UNP B1PNC0
E	-18	LEU	-	expression tag	UNP B1PNC0
E	-17	TYR	-	expression tag	UNP B1PNC0
E	-16	ASP	-	expression tag	UNP B1PNC0
E	-15	ASP	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	ASP	-	expression tag	UNP B1PNC0
E	-13	ASP	-	expression tag	UNP B1PNC0
E	-12	LYS	-	expression tag	UNP B1PNC0
E	-11	ASP	-	expression tag	UNP B1PNC0
E	-10	PRO	-	expression tag	UNP B1PNC0
E	-9	MET	-	expression tag	UNP B1PNC0
E	-8	VAL	-	expression tag	UNP B1PNC0
E	-7	SER	-	expression tag	UNP B1PNC0
E	-6	LYS	-	expression tag	UNP B1PNC0
E	-5	GLY	-	expression tag	UNP B1PNC0
E	-4	GLU	-	expression tag	UNP B1PNC0
E	-3	GLU	-	expression tag	UNP B1PNC0
E	-2	ASP	-	expression tag	UNP B1PNC0
E	-1	ASN	-	expression tag	UNP B1PNC0
E	0	MET	-	expression tag	UNP B1PNC0
E	1	ALA	-	expression tag	UNP B1PNC0
E	59	CR2	GLY	chromophore	UNP B1PNC0
E	59	CR2	TYR	chromophore	UNP B1PNC0
E	59	CR2	GLY	chromophore	UNP B1PNC0
E	171	ALA	VAL	variant	UNP B1PNC0
E	174	THR	ASN	variant	UNP B1PNC0
E	220	GLY	-	expression tag	UNP B1PNC0
E	221	MET	-	expression tag	UNP B1PNC0
E	222	ASP	-	expression tag	UNP B1PNC0
E	223	GLU	-	expression tag	UNP B1PNC0
E	224	LEU	-	expression tag	UNP B1PNC0
E	225	TYR	-	expression tag	UNP B1PNC0
E	226	LYS	-	expression tag	UNP B1PNC0
H	-42	MET	-	initiating methionine	UNP B1PNC0
H	-41	ARG	-	expression tag	UNP B1PNC0
H	-40	GLY	-	expression tag	UNP B1PNC0
H	-39	SER	-	expression tag	UNP B1PNC0
H	-38	HIS	-	expression tag	UNP B1PNC0
H	-37	HIS	-	expression tag	UNP B1PNC0
H	-36	HIS	-	expression tag	UNP B1PNC0
H	-35	HIS	-	expression tag	UNP B1PNC0
H	-34	HIS	-	expression tag	UNP B1PNC0
H	-33	HIS	-	expression tag	UNP B1PNC0
H	-32	GLY	-	expression tag	UNP B1PNC0
H	-31	MET	-	expression tag	UNP B1PNC0
H	-30	ALA	-	expression tag	UNP B1PNC0
H	-29	SER	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-28	MET	-	expression tag	UNP B1PNC0
H	-27	THR	-	expression tag	UNP B1PNC0
H	-26	GLY	-	expression tag	UNP B1PNC0
H	-25	GLY	-	expression tag	UNP B1PNC0
H	-24	GLN	-	expression tag	UNP B1PNC0
H	-23	GLN	-	expression tag	UNP B1PNC0
H	-22	MET	-	expression tag	UNP B1PNC0
H	-21	GLY	-	expression tag	UNP B1PNC0
H	-20	ARG	-	expression tag	UNP B1PNC0
H	-19	ASP	-	expression tag	UNP B1PNC0
H	-18	LEU	-	expression tag	UNP B1PNC0
H	-17	TYR	-	expression tag	UNP B1PNC0
H	-16	ASP	-	expression tag	UNP B1PNC0
H	-15	ASP	-	expression tag	UNP B1PNC0
H	-14	ASP	-	expression tag	UNP B1PNC0
H	-13	ASP	-	expression tag	UNP B1PNC0
H	-12	LYS	-	expression tag	UNP B1PNC0
H	-11	ASP	-	expression tag	UNP B1PNC0
H	-10	PRO	-	expression tag	UNP B1PNC0
H	-9	MET	-	expression tag	UNP B1PNC0
H	-8	VAL	-	expression tag	UNP B1PNC0
H	-7	SER	-	expression tag	UNP B1PNC0
H	-6	LYS	-	expression tag	UNP B1PNC0
H	-5	GLY	-	expression tag	UNP B1PNC0
H	-4	GLU	-	expression tag	UNP B1PNC0
H	-3	GLU	-	expression tag	UNP B1PNC0
H	-2	ASP	-	expression tag	UNP B1PNC0
H	-1	ASN	-	expression tag	UNP B1PNC0
H	0	MET	-	expression tag	UNP B1PNC0
H	1	ALA	-	expression tag	UNP B1PNC0
H	59	CR2	GLY	chromophore	UNP B1PNC0
H	59	CR2	TYR	chromophore	UNP B1PNC0
H	59	CR2	GLY	chromophore	UNP B1PNC0
H	171	ALA	VAL	variant	UNP B1PNC0
H	174	THR	ASN	variant	UNP B1PNC0
H	220	GLY	-	expression tag	UNP B1PNC0
H	221	MET	-	expression tag	UNP B1PNC0
H	222	ASP	-	expression tag	UNP B1PNC0
H	223	GLU	-	expression tag	UNP B1PNC0
H	224	LEU	-	expression tag	UNP B1PNC0
H	225	TYR	-	expression tag	UNP B1PNC0
H	226	LYS	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-42	MET	-	initiating methionine	UNP B1PNC0
F	-41	ARG	-	expression tag	UNP B1PNC0
F	-40	GLY	-	expression tag	UNP B1PNC0
F	-39	SER	-	expression tag	UNP B1PNC0
F	-38	HIS	-	expression tag	UNP B1PNC0
F	-37	HIS	-	expression tag	UNP B1PNC0
F	-36	HIS	-	expression tag	UNP B1PNC0
F	-35	HIS	-	expression tag	UNP B1PNC0
F	-34	HIS	-	expression tag	UNP B1PNC0
F	-33	HIS	-	expression tag	UNP B1PNC0
F	-32	GLY	-	expression tag	UNP B1PNC0
F	-31	MET	-	expression tag	UNP B1PNC0
F	-30	ALA	-	expression tag	UNP B1PNC0
F	-29	SER	-	expression tag	UNP B1PNC0
F	-28	MET	-	expression tag	UNP B1PNC0
F	-27	THR	-	expression tag	UNP B1PNC0
F	-26	GLY	-	expression tag	UNP B1PNC0
F	-25	GLY	-	expression tag	UNP B1PNC0
F	-24	GLN	-	expression tag	UNP B1PNC0
F	-23	GLN	-	expression tag	UNP B1PNC0
F	-22	MET	-	expression tag	UNP B1PNC0
F	-21	GLY	-	expression tag	UNP B1PNC0
F	-20	ARG	-	expression tag	UNP B1PNC0
F	-19	ASP	-	expression tag	UNP B1PNC0
F	-18	LEU	-	expression tag	UNP B1PNC0
F	-17	TYR	-	expression tag	UNP B1PNC0
F	-16	ASP	-	expression tag	UNP B1PNC0
F	-15	ASP	-	expression tag	UNP B1PNC0
F	-14	ASP	-	expression tag	UNP B1PNC0
F	-13	ASP	-	expression tag	UNP B1PNC0
F	-12	LYS	-	expression tag	UNP B1PNC0
F	-11	ASP	-	expression tag	UNP B1PNC0
F	-10	PRO	-	expression tag	UNP B1PNC0
F	-9	MET	-	expression tag	UNP B1PNC0
F	-8	VAL	-	expression tag	UNP B1PNC0
F	-7	SER	-	expression tag	UNP B1PNC0
F	-6	LYS	-	expression tag	UNP B1PNC0
F	-5	GLY	-	expression tag	UNP B1PNC0
F	-4	GLU	-	expression tag	UNP B1PNC0
F	-3	GLU	-	expression tag	UNP B1PNC0
F	-2	ASP	-	expression tag	UNP B1PNC0
F	-1	ASN	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	expression tag	UNP B1PNC0
F	1	ALA	-	expression tag	UNP B1PNC0
F	59	CR2	GLY	chromophore	UNP B1PNC0
F	59	CR2	TYR	chromophore	UNP B1PNC0
F	59	CR2	GLY	chromophore	UNP B1PNC0
F	171	ALA	VAL	variant	UNP B1PNC0
F	174	THR	ASN	variant	UNP B1PNC0
F	220	GLY	-	expression tag	UNP B1PNC0
F	221	MET	-	expression tag	UNP B1PNC0
F	222	ASP	-	expression tag	UNP B1PNC0
F	223	GLU	-	expression tag	UNP B1PNC0
F	224	LEU	-	expression tag	UNP B1PNC0
F	225	TYR	-	expression tag	UNP B1PNC0
F	226	LYS	-	expression tag	UNP B1PNC0
G	-42	MET	-	initiating methionine	UNP B1PNC0
G	-41	ARG	-	expression tag	UNP B1PNC0
G	-40	GLY	-	expression tag	UNP B1PNC0
G	-39	SER	-	expression tag	UNP B1PNC0
G	-38	HIS	-	expression tag	UNP B1PNC0
G	-37	HIS	-	expression tag	UNP B1PNC0
G	-36	HIS	-	expression tag	UNP B1PNC0
G	-35	HIS	-	expression tag	UNP B1PNC0
G	-34	HIS	-	expression tag	UNP B1PNC0
G	-33	HIS	-	expression tag	UNP B1PNC0
G	-32	GLY	-	expression tag	UNP B1PNC0
G	-31	MET	-	expression tag	UNP B1PNC0
G	-30	ALA	-	expression tag	UNP B1PNC0
G	-29	SER	-	expression tag	UNP B1PNC0
G	-28	MET	-	expression tag	UNP B1PNC0
G	-27	THR	-	expression tag	UNP B1PNC0
G	-26	GLY	-	expression tag	UNP B1PNC0
G	-25	GLY	-	expression tag	UNP B1PNC0
G	-24	GLN	-	expression tag	UNP B1PNC0
G	-23	GLN	-	expression tag	UNP B1PNC0
G	-22	MET	-	expression tag	UNP B1PNC0
G	-21	GLY	-	expression tag	UNP B1PNC0
G	-20	ARG	-	expression tag	UNP B1PNC0
G	-19	ASP	-	expression tag	UNP B1PNC0
G	-18	LEU	-	expression tag	UNP B1PNC0
G	-17	TYR	-	expression tag	UNP B1PNC0
G	-16	ASP	-	expression tag	UNP B1PNC0
G	-15	ASP	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	ASP	-	expression tag	UNP B1PNC0
G	-13	ASP	-	expression tag	UNP B1PNC0
G	-12	LYS	-	expression tag	UNP B1PNC0
G	-11	ASP	-	expression tag	UNP B1PNC0
G	-10	PRO	-	expression tag	UNP B1PNC0
G	-9	MET	-	expression tag	UNP B1PNC0
G	-8	VAL	-	expression tag	UNP B1PNC0
G	-7	SER	-	expression tag	UNP B1PNC0
G	-6	LYS	-	expression tag	UNP B1PNC0
G	-5	GLY	-	expression tag	UNP B1PNC0
G	-4	GLU	-	expression tag	UNP B1PNC0
G	-3	GLU	-	expression tag	UNP B1PNC0
G	-2	ASP	-	expression tag	UNP B1PNC0
G	-1	ASN	-	expression tag	UNP B1PNC0
G	0	MET	-	expression tag	UNP B1PNC0
G	1	ALA	-	expression tag	UNP B1PNC0
G	59	CR2	GLY	chromophore	UNP B1PNC0
G	59	CR2	TYR	chromophore	UNP B1PNC0
G	59	CR2	GLY	chromophore	UNP B1PNC0
G	171	ALA	VAL	variant	UNP B1PNC0
G	174	THR	ASN	variant	UNP B1PNC0
G	220	GLY	-	expression tag	UNP B1PNC0
G	221	MET	-	expression tag	UNP B1PNC0
G	222	ASP	-	expression tag	UNP B1PNC0
G	223	GLU	-	expression tag	UNP B1PNC0
G	224	LEU	-	expression tag	UNP B1PNC0
G	225	TYR	-	expression tag	UNP B1PNC0
G	226	LYS	-	expression tag	UNP B1PNC0
I	-42	MET	-	initiating methionine	UNP B1PNC0
I	-41	ARG	-	expression tag	UNP B1PNC0
I	-40	GLY	-	expression tag	UNP B1PNC0
I	-39	SER	-	expression tag	UNP B1PNC0
I	-38	HIS	-	expression tag	UNP B1PNC0
I	-37	HIS	-	expression tag	UNP B1PNC0
I	-36	HIS	-	expression tag	UNP B1PNC0
I	-35	HIS	-	expression tag	UNP B1PNC0
I	-34	HIS	-	expression tag	UNP B1PNC0
I	-33	HIS	-	expression tag	UNP B1PNC0
I	-32	GLY	-	expression tag	UNP B1PNC0
I	-31	MET	-	expression tag	UNP B1PNC0
I	-30	ALA	-	expression tag	UNP B1PNC0
I	-29	SER	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-28	MET	-	expression tag	UNP B1PNC0
I	-27	THR	-	expression tag	UNP B1PNC0
I	-26	GLY	-	expression tag	UNP B1PNC0
I	-25	GLY	-	expression tag	UNP B1PNC0
I	-24	GLN	-	expression tag	UNP B1PNC0
I	-23	GLN	-	expression tag	UNP B1PNC0
I	-22	MET	-	expression tag	UNP B1PNC0
I	-21	GLY	-	expression tag	UNP B1PNC0
I	-20	ARG	-	expression tag	UNP B1PNC0
I	-19	ASP	-	expression tag	UNP B1PNC0
I	-18	LEU	-	expression tag	UNP B1PNC0
I	-17	TYR	-	expression tag	UNP B1PNC0
I	-16	ASP	-	expression tag	UNP B1PNC0
I	-15	ASP	-	expression tag	UNP B1PNC0
I	-14	ASP	-	expression tag	UNP B1PNC0
I	-13	ASP	-	expression tag	UNP B1PNC0
I	-12	LYS	-	expression tag	UNP B1PNC0
I	-11	ASP	-	expression tag	UNP B1PNC0
I	-10	PRO	-	expression tag	UNP B1PNC0
I	-9	MET	-	expression tag	UNP B1PNC0
I	-8	VAL	-	expression tag	UNP B1PNC0
I	-7	SER	-	expression tag	UNP B1PNC0
I	-6	LYS	-	expression tag	UNP B1PNC0
I	-5	GLY	-	expression tag	UNP B1PNC0
I	-4	GLU	-	expression tag	UNP B1PNC0
I	-3	GLU	-	expression tag	UNP B1PNC0
I	-2	ASP	-	expression tag	UNP B1PNC0
I	-1	ASN	-	expression tag	UNP B1PNC0
I	0	MET	-	expression tag	UNP B1PNC0
I	1	ALA	-	expression tag	UNP B1PNC0
I	59	CR2	GLY	chromophore	UNP B1PNC0
I	59	CR2	TYR	chromophore	UNP B1PNC0
I	59	CR2	GLY	chromophore	UNP B1PNC0
I	171	ALA	VAL	variant	UNP B1PNC0
I	174	THR	ASN	variant	UNP B1PNC0
I	220	GLY	-	expression tag	UNP B1PNC0
I	221	MET	-	expression tag	UNP B1PNC0
I	222	ASP	-	expression tag	UNP B1PNC0
I	223	GLU	-	expression tag	UNP B1PNC0
I	224	LEU	-	expression tag	UNP B1PNC0
I	225	TYR	-	expression tag	UNP B1PNC0
I	226	LYS	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-42	MET	-	initiating methionine	UNP B1PNC0
L	-41	ARG	-	expression tag	UNP B1PNC0
L	-40	GLY	-	expression tag	UNP B1PNC0
L	-39	SER	-	expression tag	UNP B1PNC0
L	-38	HIS	-	expression tag	UNP B1PNC0
L	-37	HIS	-	expression tag	UNP B1PNC0
L	-36	HIS	-	expression tag	UNP B1PNC0
L	-35	HIS	-	expression tag	UNP B1PNC0
L	-34	HIS	-	expression tag	UNP B1PNC0
L	-33	HIS	-	expression tag	UNP B1PNC0
L	-32	GLY	-	expression tag	UNP B1PNC0
L	-31	MET	-	expression tag	UNP B1PNC0
L	-30	ALA	-	expression tag	UNP B1PNC0
L	-29	SER	-	expression tag	UNP B1PNC0
L	-28	MET	-	expression tag	UNP B1PNC0
L	-27	THR	-	expression tag	UNP B1PNC0
L	-26	GLY	-	expression tag	UNP B1PNC0
L	-25	GLY	-	expression tag	UNP B1PNC0
L	-24	GLN	-	expression tag	UNP B1PNC0
L	-23	GLN	-	expression tag	UNP B1PNC0
L	-22	MET	-	expression tag	UNP B1PNC0
L	-21	GLY	-	expression tag	UNP B1PNC0
L	-20	ARG	-	expression tag	UNP B1PNC0
L	-19	ASP	-	expression tag	UNP B1PNC0
L	-18	LEU	-	expression tag	UNP B1PNC0
L	-17	TYR	-	expression tag	UNP B1PNC0
L	-16	ASP	-	expression tag	UNP B1PNC0
L	-15	ASP	-	expression tag	UNP B1PNC0
L	-14	ASP	-	expression tag	UNP B1PNC0
L	-13	ASP	-	expression tag	UNP B1PNC0
L	-12	LYS	-	expression tag	UNP B1PNC0
L	-11	ASP	-	expression tag	UNP B1PNC0
L	-10	PRO	-	expression tag	UNP B1PNC0
L	-9	MET	-	expression tag	UNP B1PNC0
L	-8	VAL	-	expression tag	UNP B1PNC0
L	-7	SER	-	expression tag	UNP B1PNC0
L	-6	LYS	-	expression tag	UNP B1PNC0
L	-5	GLY	-	expression tag	UNP B1PNC0
L	-4	GLU	-	expression tag	UNP B1PNC0
L	-3	GLU	-	expression tag	UNP B1PNC0
L	-2	ASP	-	expression tag	UNP B1PNC0
L	-1	ASN	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	expression tag	UNP B1PNC0
L	1	ALA	-	expression tag	UNP B1PNC0
L	59	CR2	GLY	chromophore	UNP B1PNC0
L	59	CR2	TYR	chromophore	UNP B1PNC0
L	59	CR2	GLY	chromophore	UNP B1PNC0
L	171	ALA	VAL	variant	UNP B1PNC0
L	174	THR	ASN	variant	UNP B1PNC0
L	220	GLY	-	expression tag	UNP B1PNC0
L	221	MET	-	expression tag	UNP B1PNC0
L	222	ASP	-	expression tag	UNP B1PNC0
L	223	GLU	-	expression tag	UNP B1PNC0
L	224	LEU	-	expression tag	UNP B1PNC0
L	225	TYR	-	expression tag	UNP B1PNC0
L	226	LYS	-	expression tag	UNP B1PNC0
J	-42	MET	-	initiating methionine	UNP B1PNC0
J	-41	ARG	-	expression tag	UNP B1PNC0
J	-40	GLY	-	expression tag	UNP B1PNC0
J	-39	SER	-	expression tag	UNP B1PNC0
J	-38	HIS	-	expression tag	UNP B1PNC0
J	-37	HIS	-	expression tag	UNP B1PNC0
J	-36	HIS	-	expression tag	UNP B1PNC0
J	-35	HIS	-	expression tag	UNP B1PNC0
J	-34	HIS	-	expression tag	UNP B1PNC0
J	-33	HIS	-	expression tag	UNP B1PNC0
J	-32	GLY	-	expression tag	UNP B1PNC0
J	-31	MET	-	expression tag	UNP B1PNC0
J	-30	ALA	-	expression tag	UNP B1PNC0
J	-29	SER	-	expression tag	UNP B1PNC0
J	-28	MET	-	expression tag	UNP B1PNC0
J	-27	THR	-	expression tag	UNP B1PNC0
J	-26	GLY	-	expression tag	UNP B1PNC0
J	-25	GLY	-	expression tag	UNP B1PNC0
J	-24	GLN	-	expression tag	UNP B1PNC0
J	-23	GLN	-	expression tag	UNP B1PNC0
J	-22	MET	-	expression tag	UNP B1PNC0
J	-21	GLY	-	expression tag	UNP B1PNC0
J	-20	ARG	-	expression tag	UNP B1PNC0
J	-19	ASP	-	expression tag	UNP B1PNC0
J	-18	LEU	-	expression tag	UNP B1PNC0
J	-17	TYR	-	expression tag	UNP B1PNC0
J	-16	ASP	-	expression tag	UNP B1PNC0
J	-15	ASP	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-14	ASP	-	expression tag	UNP B1PNC0
J	-13	ASP	-	expression tag	UNP B1PNC0
J	-12	LYS	-	expression tag	UNP B1PNC0
J	-11	ASP	-	expression tag	UNP B1PNC0
J	-10	PRO	-	expression tag	UNP B1PNC0
J	-9	MET	-	expression tag	UNP B1PNC0
J	-8	VAL	-	expression tag	UNP B1PNC0
J	-7	SER	-	expression tag	UNP B1PNC0
J	-6	LYS	-	expression tag	UNP B1PNC0
J	-5	GLY	-	expression tag	UNP B1PNC0
J	-4	GLU	-	expression tag	UNP B1PNC0
J	-3	GLU	-	expression tag	UNP B1PNC0
J	-2	ASP	-	expression tag	UNP B1PNC0
J	-1	ASN	-	expression tag	UNP B1PNC0
J	0	MET	-	expression tag	UNP B1PNC0
J	1	ALA	-	expression tag	UNP B1PNC0
J	59	CR2	GLY	chromophore	UNP B1PNC0
J	59	CR2	TYR	chromophore	UNP B1PNC0
J	59	CR2	GLY	chromophore	UNP B1PNC0
J	171	ALA	VAL	variant	UNP B1PNC0
J	174	THR	ASN	variant	UNP B1PNC0
J	220	GLY	-	expression tag	UNP B1PNC0
J	221	MET	-	expression tag	UNP B1PNC0
J	222	ASP	-	expression tag	UNP B1PNC0
J	223	GLU	-	expression tag	UNP B1PNC0
J	224	LEU	-	expression tag	UNP B1PNC0
J	225	TYR	-	expression tag	UNP B1PNC0
J	226	LYS	-	expression tag	UNP B1PNC0
K	-42	MET	-	initiating methionine	UNP B1PNC0
K	-41	ARG	-	expression tag	UNP B1PNC0
K	-40	GLY	-	expression tag	UNP B1PNC0
K	-39	SER	-	expression tag	UNP B1PNC0
K	-38	HIS	-	expression tag	UNP B1PNC0
K	-37	HIS	-	expression tag	UNP B1PNC0
K	-36	HIS	-	expression tag	UNP B1PNC0
K	-35	HIS	-	expression tag	UNP B1PNC0
K	-34	HIS	-	expression tag	UNP B1PNC0
K	-33	HIS	-	expression tag	UNP B1PNC0
K	-32	GLY	-	expression tag	UNP B1PNC0
K	-31	MET	-	expression tag	UNP B1PNC0
K	-30	ALA	-	expression tag	UNP B1PNC0
K	-29	SER	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-28	MET	-	expression tag	UNP B1PNC0
K	-27	THR	-	expression tag	UNP B1PNC0
K	-26	GLY	-	expression tag	UNP B1PNC0
K	-25	GLY	-	expression tag	UNP B1PNC0
K	-24	GLN	-	expression tag	UNP B1PNC0
K	-23	GLN	-	expression tag	UNP B1PNC0
K	-22	MET	-	expression tag	UNP B1PNC0
K	-21	GLY	-	expression tag	UNP B1PNC0
K	-20	ARG	-	expression tag	UNP B1PNC0
K	-19	ASP	-	expression tag	UNP B1PNC0
K	-18	LEU	-	expression tag	UNP B1PNC0
K	-17	TYR	-	expression tag	UNP B1PNC0
K	-16	ASP	-	expression tag	UNP B1PNC0
K	-15	ASP	-	expression tag	UNP B1PNC0
K	-14	ASP	-	expression tag	UNP B1PNC0
K	-13	ASP	-	expression tag	UNP B1PNC0
K	-12	LYS	-	expression tag	UNP B1PNC0
K	-11	ASP	-	expression tag	UNP B1PNC0
K	-10	PRO	-	expression tag	UNP B1PNC0
K	-9	MET	-	expression tag	UNP B1PNC0
K	-8	VAL	-	expression tag	UNP B1PNC0
K	-7	SER	-	expression tag	UNP B1PNC0
K	-6	LYS	-	expression tag	UNP B1PNC0
K	-5	GLY	-	expression tag	UNP B1PNC0
K	-4	GLU	-	expression tag	UNP B1PNC0
K	-3	GLU	-	expression tag	UNP B1PNC0
K	-2	ASP	-	expression tag	UNP B1PNC0
K	-1	ASN	-	expression tag	UNP B1PNC0
K	0	MET	-	expression tag	UNP B1PNC0
K	1	ALA	-	expression tag	UNP B1PNC0
K	59	CR2	GLY	chromophore	UNP B1PNC0
K	59	CR2	TYR	chromophore	UNP B1PNC0
K	59	CR2	GLY	chromophore	UNP B1PNC0
K	171	ALA	VAL	variant	UNP B1PNC0
K	174	THR	ASN	variant	UNP B1PNC0
K	220	GLY	-	expression tag	UNP B1PNC0
K	221	MET	-	expression tag	UNP B1PNC0
K	222	ASP	-	expression tag	UNP B1PNC0
K	223	GLU	-	expression tag	UNP B1PNC0
K	224	LEU	-	expression tag	UNP B1PNC0
K	225	TYR	-	expression tag	UNP B1PNC0
K	226	LYS	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-42	MET	-	initiating methionine	UNP B1PNC0
M	-41	ARG	-	expression tag	UNP B1PNC0
M	-40	GLY	-	expression tag	UNP B1PNC0
M	-39	SER	-	expression tag	UNP B1PNC0
M	-38	HIS	-	expression tag	UNP B1PNC0
M	-37	HIS	-	expression tag	UNP B1PNC0
M	-36	HIS	-	expression tag	UNP B1PNC0
M	-35	HIS	-	expression tag	UNP B1PNC0
M	-34	HIS	-	expression tag	UNP B1PNC0
M	-33	HIS	-	expression tag	UNP B1PNC0
M	-32	GLY	-	expression tag	UNP B1PNC0
M	-31	MET	-	expression tag	UNP B1PNC0
M	-30	ALA	-	expression tag	UNP B1PNC0
M	-29	SER	-	expression tag	UNP B1PNC0
M	-28	MET	-	expression tag	UNP B1PNC0
M	-27	THR	-	expression tag	UNP B1PNC0
M	-26	GLY	-	expression tag	UNP B1PNC0
M	-25	GLY	-	expression tag	UNP B1PNC0
M	-24	GLN	-	expression tag	UNP B1PNC0
M	-23	GLN	-	expression tag	UNP B1PNC0
M	-22	MET	-	expression tag	UNP B1PNC0
M	-21	GLY	-	expression tag	UNP B1PNC0
M	-20	ARG	-	expression tag	UNP B1PNC0
M	-19	ASP	-	expression tag	UNP B1PNC0
M	-18	LEU	-	expression tag	UNP B1PNC0
M	-17	TYR	-	expression tag	UNP B1PNC0
M	-16	ASP	-	expression tag	UNP B1PNC0
M	-15	ASP	-	expression tag	UNP B1PNC0
M	-14	ASP	-	expression tag	UNP B1PNC0
M	-13	ASP	-	expression tag	UNP B1PNC0
M	-12	LYS	-	expression tag	UNP B1PNC0
M	-11	ASP	-	expression tag	UNP B1PNC0
M	-10	PRO	-	expression tag	UNP B1PNC0
M	-9	MET	-	expression tag	UNP B1PNC0
M	-8	VAL	-	expression tag	UNP B1PNC0
M	-7	SER	-	expression tag	UNP B1PNC0
M	-6	LYS	-	expression tag	UNP B1PNC0
M	-5	GLY	-	expression tag	UNP B1PNC0
M	-4	GLU	-	expression tag	UNP B1PNC0
M	-3	GLU	-	expression tag	UNP B1PNC0
M	-2	ASP	-	expression tag	UNP B1PNC0
M	-1	ASN	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	expression tag	UNP B1PNC0
M	1	ALA	-	expression tag	UNP B1PNC0
M	59	CR2	GLY	chromophore	UNP B1PNC0
M	59	CR2	TYR	chromophore	UNP B1PNC0
M	59	CR2	GLY	chromophore	UNP B1PNC0
M	171	ALA	VAL	variant	UNP B1PNC0
M	174	THR	ASN	variant	UNP B1PNC0
M	220	GLY	-	expression tag	UNP B1PNC0
M	221	MET	-	expression tag	UNP B1PNC0
M	222	ASP	-	expression tag	UNP B1PNC0
M	223	GLU	-	expression tag	UNP B1PNC0
M	224	LEU	-	expression tag	UNP B1PNC0
M	225	TYR	-	expression tag	UNP B1PNC0
M	226	LYS	-	expression tag	UNP B1PNC0
P	-42	MET	-	initiating methionine	UNP B1PNC0
P	-41	ARG	-	expression tag	UNP B1PNC0
P	-40	GLY	-	expression tag	UNP B1PNC0
P	-39	SER	-	expression tag	UNP B1PNC0
P	-38	HIS	-	expression tag	UNP B1PNC0
P	-37	HIS	-	expression tag	UNP B1PNC0
P	-36	HIS	-	expression tag	UNP B1PNC0
P	-35	HIS	-	expression tag	UNP B1PNC0
P	-34	HIS	-	expression tag	UNP B1PNC0
P	-33	HIS	-	expression tag	UNP B1PNC0
P	-32	GLY	-	expression tag	UNP B1PNC0
P	-31	MET	-	expression tag	UNP B1PNC0
P	-30	ALA	-	expression tag	UNP B1PNC0
P	-29	SER	-	expression tag	UNP B1PNC0
P	-28	MET	-	expression tag	UNP B1PNC0
P	-27	THR	-	expression tag	UNP B1PNC0
P	-26	GLY	-	expression tag	UNP B1PNC0
P	-25	GLY	-	expression tag	UNP B1PNC0
P	-24	GLN	-	expression tag	UNP B1PNC0
P	-23	GLN	-	expression tag	UNP B1PNC0
P	-22	MET	-	expression tag	UNP B1PNC0
P	-21	GLY	-	expression tag	UNP B1PNC0
P	-20	ARG	-	expression tag	UNP B1PNC0
P	-19	ASP	-	expression tag	UNP B1PNC0
P	-18	LEU	-	expression tag	UNP B1PNC0
P	-17	TYR	-	expression tag	UNP B1PNC0
P	-16	ASP	-	expression tag	UNP B1PNC0
P	-15	ASP	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-14	ASP	-	expression tag	UNP B1PNC0
P	-13	ASP	-	expression tag	UNP B1PNC0
P	-12	LYS	-	expression tag	UNP B1PNC0
P	-11	ASP	-	expression tag	UNP B1PNC0
P	-10	PRO	-	expression tag	UNP B1PNC0
P	-9	MET	-	expression tag	UNP B1PNC0
P	-8	VAL	-	expression tag	UNP B1PNC0
P	-7	SER	-	expression tag	UNP B1PNC0
P	-6	LYS	-	expression tag	UNP B1PNC0
P	-5	GLY	-	expression tag	UNP B1PNC0
P	-4	GLU	-	expression tag	UNP B1PNC0
P	-3	GLU	-	expression tag	UNP B1PNC0
P	-2	ASP	-	expression tag	UNP B1PNC0
P	-1	ASN	-	expression tag	UNP B1PNC0
P	0	MET	-	expression tag	UNP B1PNC0
P	1	ALA	-	expression tag	UNP B1PNC0
P	59	CR2	GLY	chromophore	UNP B1PNC0
P	59	CR2	TYR	chromophore	UNP B1PNC0
P	59	CR2	GLY	chromophore	UNP B1PNC0
P	171	ALA	VAL	variant	UNP B1PNC0
P	174	THR	ASN	variant	UNP B1PNC0
P	220	GLY	-	expression tag	UNP B1PNC0
P	221	MET	-	expression tag	UNP B1PNC0
P	222	ASP	-	expression tag	UNP B1PNC0
P	223	GLU	-	expression tag	UNP B1PNC0
P	224	LEU	-	expression tag	UNP B1PNC0
P	225	TYR	-	expression tag	UNP B1PNC0
P	226	LYS	-	expression tag	UNP B1PNC0
N	-42	MET	-	initiating methionine	UNP B1PNC0
N	-41	ARG	-	expression tag	UNP B1PNC0
N	-40	GLY	-	expression tag	UNP B1PNC0
N	-39	SER	-	expression tag	UNP B1PNC0
N	-38	HIS	-	expression tag	UNP B1PNC0
N	-37	HIS	-	expression tag	UNP B1PNC0
N	-36	HIS	-	expression tag	UNP B1PNC0
N	-35	HIS	-	expression tag	UNP B1PNC0
N	-34	HIS	-	expression tag	UNP B1PNC0
N	-33	HIS	-	expression tag	UNP B1PNC0
N	-32	GLY	-	expression tag	UNP B1PNC0
N	-31	MET	-	expression tag	UNP B1PNC0
N	-30	ALA	-	expression tag	UNP B1PNC0
N	-29	SER	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-28	MET	-	expression tag	UNP B1PNC0
N	-27	THR	-	expression tag	UNP B1PNC0
N	-26	GLY	-	expression tag	UNP B1PNC0
N	-25	GLY	-	expression tag	UNP B1PNC0
N	-24	GLN	-	expression tag	UNP B1PNC0
N	-23	GLN	-	expression tag	UNP B1PNC0
N	-22	MET	-	expression tag	UNP B1PNC0
N	-21	GLY	-	expression tag	UNP B1PNC0
N	-20	ARG	-	expression tag	UNP B1PNC0
N	-19	ASP	-	expression tag	UNP B1PNC0
N	-18	LEU	-	expression tag	UNP B1PNC0
N	-17	TYR	-	expression tag	UNP B1PNC0
N	-16	ASP	-	expression tag	UNP B1PNC0
N	-15	ASP	-	expression tag	UNP B1PNC0
N	-14	ASP	-	expression tag	UNP B1PNC0
N	-13	ASP	-	expression tag	UNP B1PNC0
N	-12	LYS	-	expression tag	UNP B1PNC0
N	-11	ASP	-	expression tag	UNP B1PNC0
N	-10	PRO	-	expression tag	UNP B1PNC0
N	-9	MET	-	expression tag	UNP B1PNC0
N	-8	VAL	-	expression tag	UNP B1PNC0
N	-7	SER	-	expression tag	UNP B1PNC0
N	-6	LYS	-	expression tag	UNP B1PNC0
N	-5	GLY	-	expression tag	UNP B1PNC0
N	-4	GLU	-	expression tag	UNP B1PNC0
N	-3	GLU	-	expression tag	UNP B1PNC0
N	-2	ASP	-	expression tag	UNP B1PNC0
N	-1	ASN	-	expression tag	UNP B1PNC0
N	0	MET	-	expression tag	UNP B1PNC0
N	1	ALA	-	expression tag	UNP B1PNC0
N	59	CR2	GLY	chromophore	UNP B1PNC0
N	59	CR2	TYR	chromophore	UNP B1PNC0
N	59	CR2	GLY	chromophore	UNP B1PNC0
N	171	ALA	VAL	variant	UNP B1PNC0
N	174	THR	ASN	variant	UNP B1PNC0
N	220	GLY	-	expression tag	UNP B1PNC0
N	221	MET	-	expression tag	UNP B1PNC0
N	222	ASP	-	expression tag	UNP B1PNC0
N	223	GLU	-	expression tag	UNP B1PNC0
N	224	LEU	-	expression tag	UNP B1PNC0
N	225	TYR	-	expression tag	UNP B1PNC0
N	226	LYS	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-42	MET	-	initiating methionine	UNP B1PNC0
O	-41	ARG	-	expression tag	UNP B1PNC0
O	-40	GLY	-	expression tag	UNP B1PNC0
O	-39	SER	-	expression tag	UNP B1PNC0
O	-38	HIS	-	expression tag	UNP B1PNC0
O	-37	HIS	-	expression tag	UNP B1PNC0
O	-36	HIS	-	expression tag	UNP B1PNC0
O	-35	HIS	-	expression tag	UNP B1PNC0
O	-34	HIS	-	expression tag	UNP B1PNC0
O	-33	HIS	-	expression tag	UNP B1PNC0
O	-32	GLY	-	expression tag	UNP B1PNC0
O	-31	MET	-	expression tag	UNP B1PNC0
O	-30	ALA	-	expression tag	UNP B1PNC0
O	-29	SER	-	expression tag	UNP B1PNC0
O	-28	MET	-	expression tag	UNP B1PNC0
O	-27	THR	-	expression tag	UNP B1PNC0
O	-26	GLY	-	expression tag	UNP B1PNC0
O	-25	GLY	-	expression tag	UNP B1PNC0
O	-24	GLN	-	expression tag	UNP B1PNC0
O	-23	GLN	-	expression tag	UNP B1PNC0
O	-22	MET	-	expression tag	UNP B1PNC0
O	-21	GLY	-	expression tag	UNP B1PNC0
O	-20	ARG	-	expression tag	UNP B1PNC0
O	-19	ASP	-	expression tag	UNP B1PNC0
O	-18	LEU	-	expression tag	UNP B1PNC0
O	-17	TYR	-	expression tag	UNP B1PNC0
O	-16	ASP	-	expression tag	UNP B1PNC0
O	-15	ASP	-	expression tag	UNP B1PNC0
O	-14	ASP	-	expression tag	UNP B1PNC0
O	-13	ASP	-	expression tag	UNP B1PNC0
O	-12	LYS	-	expression tag	UNP B1PNC0
O	-11	ASP	-	expression tag	UNP B1PNC0
O	-10	PRO	-	expression tag	UNP B1PNC0
O	-9	MET	-	expression tag	UNP B1PNC0
O	-8	VAL	-	expression tag	UNP B1PNC0
O	-7	SER	-	expression tag	UNP B1PNC0
O	-6	LYS	-	expression tag	UNP B1PNC0
O	-5	GLY	-	expression tag	UNP B1PNC0
O	-4	GLU	-	expression tag	UNP B1PNC0
O	-3	GLU	-	expression tag	UNP B1PNC0
O	-2	ASP	-	expression tag	UNP B1PNC0
O	-1	ASN	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
O	0	MET	-	expression tag	UNP B1PNC0
O	1	ALA	-	expression tag	UNP B1PNC0
O	59	CR2	GLY	chromophore	UNP B1PNC0
O	59	CR2	TYR	chromophore	UNP B1PNC0
O	59	CR2	GLY	chromophore	UNP B1PNC0
O	171	ALA	VAL	variant	UNP B1PNC0
O	174	THR	ASN	variant	UNP B1PNC0
O	220	GLY	-	expression tag	UNP B1PNC0
O	221	MET	-	expression tag	UNP B1PNC0
O	222	ASP	-	expression tag	UNP B1PNC0
O	223	GLU	-	expression tag	UNP B1PNC0
O	224	LEU	-	expression tag	UNP B1PNC0
O	225	TYR	-	expression tag	UNP B1PNC0
O	226	LYS	-	expression tag	UNP B1PNC0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	N	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	1	Total 1	Cl 1	0	0
2	L	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0
2	M	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	D	53	Total 53	O 53	0	0
3	B	31	Total 31	O 31	0	0
3	C	65	Total 65	O 65	0	0
3	E	42	Total 42	O 42	0	0
3	H	31	Total 31	O 31	0	0
3	F	26	Total 26	O 26	0	0
3	G	48	Total 48	O 48	0	0
3	I	13	Total 13	O 13	0	0
3	L	60	Total 60	O 60	0	0
3	J	43	Total 43	O 43	0	0
3	K	25	Total 25	O 25	0	0
3	M	9	Total 9	O 9	0	0
3	P	25	Total 25	O 25	0	0
3	N	27	Total 27	O 27	0	0

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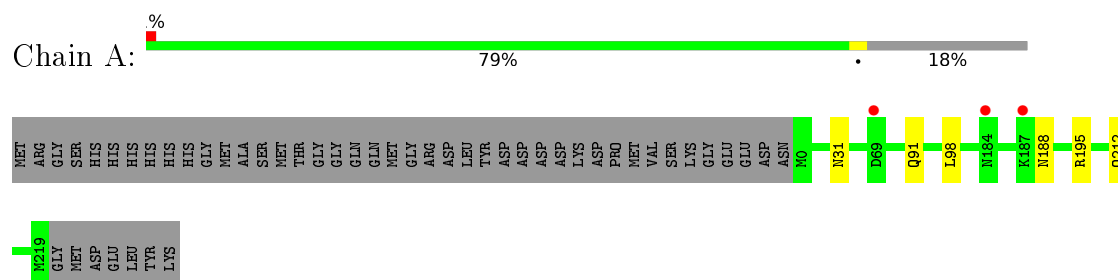
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	2	Total	O	0	0
			2	2		

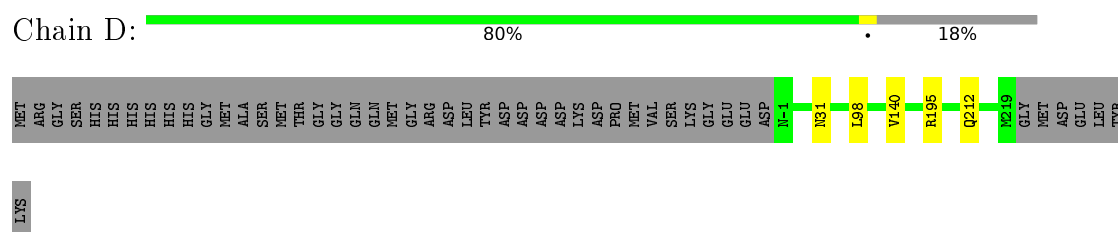
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

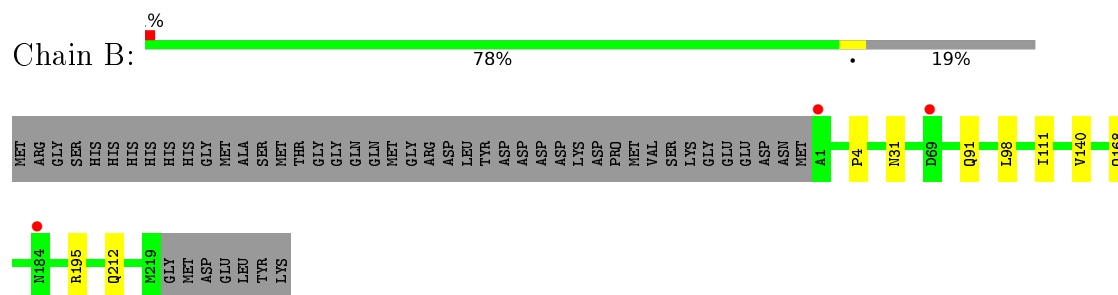
- Molecule 1: Green fluorescent protein bIFP-Y3



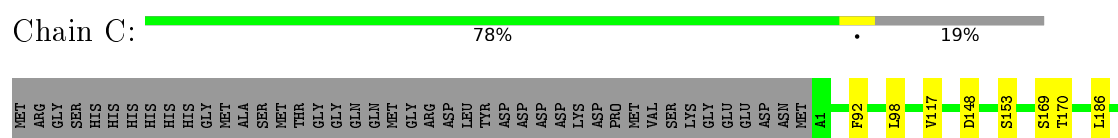
- Molecule 1: Green fluorescent protein bIFP-Y3



- Molecule 1: Green fluorescent protein bIFP-Y3



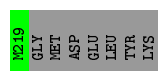
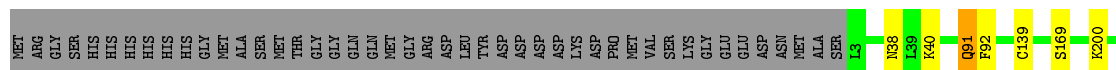
- Molecule 1: Green fluorescent protein bIFP-Y3





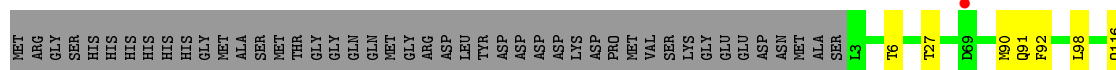
- Molecule 1: Green fluorescent protein bFP-Y3

Chain E: 78% 19%



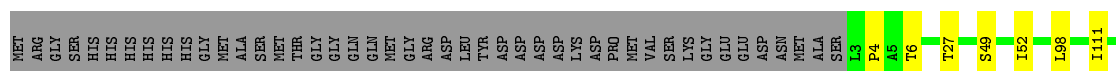
- Molecule 1: Green fluorescent protein bFP-Y3

Chain H: 76% 5% 19%



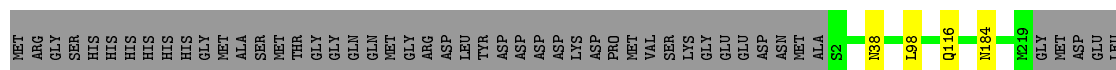
- Molecule 1: Green fluorescent protein bFP-Y3

Chain F: 80% 17%



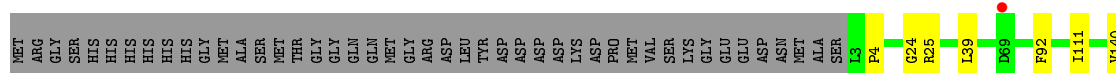
- Molecule 1: Green fluorescent protein bFP-Y3

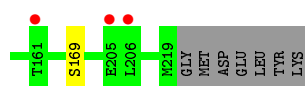
Chain G: 79% 19%



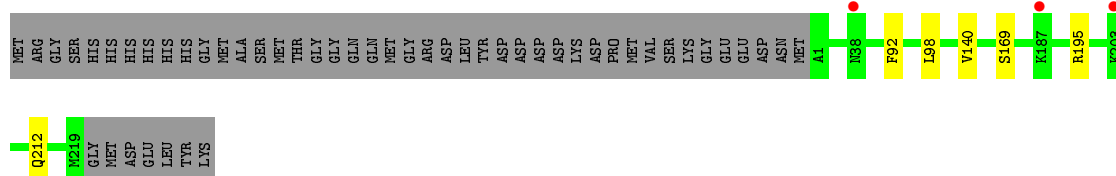
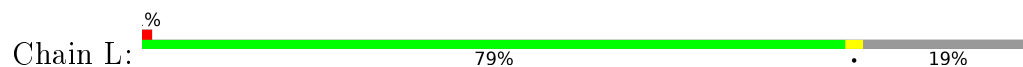
- Molecule 1: Green fluorescent protein bFP-Y3

Chain I: % 78% 19%

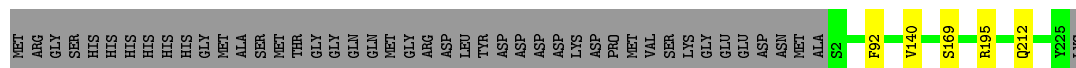
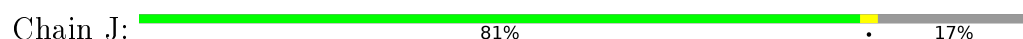




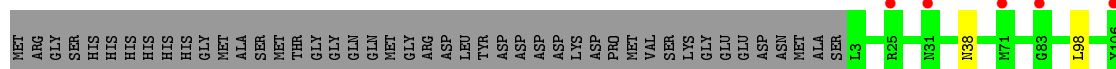
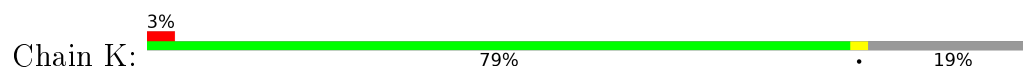
- Molecule 1: Green fluorescent protein bFP-Y3



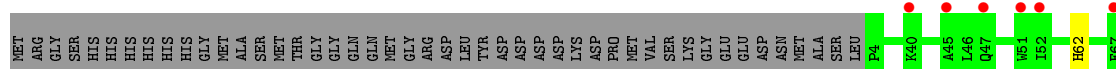
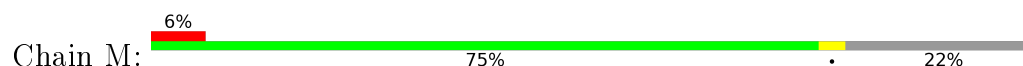
- Molecule 1: Green fluorescent protein bFP-Y3



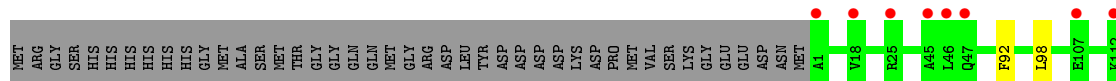
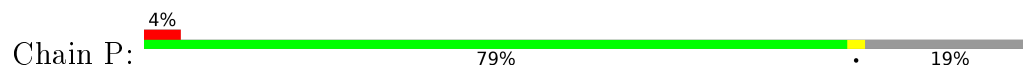
- Molecule 1: Green fluorescent protein bFP-Y3

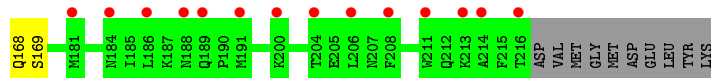


- Molecule 1: Green fluorescent protein bFP-Y3



- Molecule 1: Green fluorescent protein bFP-Y3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.66Å 197.16Å 115.09Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	49.29 – 2.05 49.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.29-2.05) 97.1 (49.29-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.225 , 0.254 0.228 , 0.254	Depositor DCC
$R_{free}$ test set	10864 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 19.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CR2, CL

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	0.36	0/1780	0.60	0/2411
1	B	0.36	0/1788	0.58	0/2422
1	C	0.36	0/1794	0.58	0/2428
1	D	0.37	0/1803	0.60	0/2442
1	E	0.36	0/1769	0.57	0/2396
1	F	0.35	0/1819	0.57	0/2462
1	G	0.35	0/1766	0.57	0/2392
1	H	0.35	0/1765	0.57	0/2391
1	I	0.36	0/1759	0.55	0/2383
1	J	0.36	0/1816	0.57	0/2459
1	K	0.36	0/1768	0.54	0/2395
1	L	0.36	0/1767	0.56	0/2393
1	M	0.36	0/1708	0.53	0/2310
1	N	0.36	0/1767	0.55	0/2393
1	O	0.37	0/1727	0.53	0/2338
1	P	0.36	0/1770	0.54	0/2398
All	All	0.36	0/28366	0.56	0/38413

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	1746	0	1660	2	0
1	B	1748	0	1668	5	0
1	C	1754	0	1682	4	0
1	D	1763	0	1679	2	0
1	E	1732	0	1649	4	0
1	F	1784	0	1696	3	0
1	G	1732	0	1646	1	0
1	H	1728	0	1638	6	0
1	I	1725	0	1639	4	0
1	J	1781	0	1688	3	0
1	K	1731	0	1647	2	0
1	L	1733	0	1645	3	0
1	M	1676	0	1594	1	0
1	N	1733	0	1634	1	0
1	O	1693	0	1606	3	0
1	P	1736	0	1652	1	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	53	0	0	0	0
3	B	31	0	0	0	0
3	C	65	0	0	0	0
3	D	53	0	0	0	0
3	E	42	0	0	0	0
3	F	26	0	0	0	0
3	G	48	0	0	0	0
3	H	31	0	0	0	0
3	I	13	0	0	0	0
3	J	43	0	0	0	0
3	K	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	60	0	0	0	0
3	M	9	0	0	0	0
3	N	27	0	0	0	0
3	O	2	0	0	0	0
3	P	25	0	0	0	0
All	All	28364	0	26423	40	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 1.

The worst 5 of 40 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:E:91[B]:GLN:HE21	1:E:91[B]:GLN:HA	1.55	0.72
1:B:91[B]:GLN:HA	1:B:91[B]:GLN:HE21	1.64	0.63
1:H:116:GLN:HE22	1:G:116:GLN:HE22	1.49	0.59
1:E:91[A]:GLN:HE21	1:E:91[A]:GLN:HA	1.70	0.56
1:A:195:ARG:HE	1:A:212:GLN:HE21	1.57	0.53

There are no symmetry-related clashes.

## 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	214/267 (80%)	214 (100%)	0	0	100	100
1	B	215/267 (80%)	214 (100%)	1 (0%)	0	100	100
1	C	215/267 (80%)	214 (100%)	1 (0%)	0	100	100
1	D	217/267 (81%)	216 (100%)	1 (0%)	0	100	100
1	E	212/267 (79%)	211 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	218/267 (82%)	217 (100%)	1 (0%)	0	100	100
1	G	212/267 (79%)	212 (100%)	0	0	100	100
1	H	212/267 (79%)	210 (99%)	2 (1%)	0	100	100
1	I	211/267 (79%)	206 (98%)	5 (2%)	0	100	100
1	J	218/267 (82%)	218 (100%)	0	0	100	100
1	K	212/267 (79%)	207 (98%)	5 (2%)	0	100	100
1	L	213/267 (80%)	212 (100%)	1 (0%)	0	100	100
1	M	202/267 (76%)	196 (97%)	5 (2%)	1 (0%)	34	22
1	N	213/267 (80%)	212 (100%)	1 (0%)	0	100	100
1	O	207/267 (78%)	201 (97%)	6 (3%)	0	100	100
1	P	213/267 (80%)	211 (99%)	2 (1%)	0	100	100
All	All	3404/4272 (80%)	3371 (99%)	32 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	203	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	185/226 (82%)	181 (98%)	4 (2%)	60	53
1	B	186/226 (82%)	183 (98%)	3 (2%)	70	67
1	C	187/226 (83%)	185 (99%)	2 (1%)	80	79
1	D	188/226 (83%)	186 (99%)	2 (1%)	80	79
1	E	184/226 (81%)	178 (97%)	6 (3%)	45	37
1	F	189/226 (84%)	187 (99%)	2 (1%)	80	79
1	G	184/226 (81%)	181 (98%)	3 (2%)	70	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/226 (81%)	180 (98%)	3 (2%)	70	67
1	I	183/226 (81%)	182 (100%)	1 (0%)	92	92
1	J	189/226 (84%)	189 (100%)	0	100	100
1	K	184/226 (81%)	182 (99%)	2 (1%)	80	79
1	L	184/226 (81%)	183 (100%)	1 (0%)	92	92
1	M	177/226 (78%)	171 (97%)	6 (3%)	44	36
1	N	183/226 (81%)	182 (100%)	1 (0%)	92	92
1	O	179/226 (79%)	175 (98%)	4 (2%)	60	53
1	P	184/226 (81%)	181 (98%)	3 (2%)	70	67
All	All	2949/3616 (82%)	2906 (98%)	43 (2%)	74	70

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	184	ASN
1	G	184	ASN
1	O	19	ASP
1	F	98	LEU
1	F	168	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	47	GLN
1	G	212	GLN
1	N	131	ASN
1	F	116	GLN
1	F	212	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	CR2	A	59	1	20,20,21	3.58	5 (25%)	24,27,29	4.09	4 (16%)
1	CR2	B	59	1	20,20,21	3.67	5 (25%)	24,27,29	4.20	4 (16%)
1	CR2	C	59	1	20,20,21	3.66	5 (25%)	24,27,29	4.02	4 (16%)
1	CR2	D	59	1	20,20,21	3.60	5 (25%)	24,27,29	3.96	4 (16%)
1	CR2	E	59	1	20,20,21	3.74	5 (25%)	24,27,29	4.12	4 (16%)
1	CR2	F	59	1	20,20,21	3.72	5 (25%)	24,27,29	4.01	4 (16%)
1	CR2	G	59	1	20,20,21	3.65	5 (25%)	24,27,29	4.16	4 (16%)
1	CR2	H	59	1	20,20,21	3.82	5 (25%)	24,27,29	4.09	4 (16%)
1	CR2	I	59	1	20,20,21	3.75	5 (25%)	24,27,29	3.92	5 (20%)
1	CR2	J	59	1	20,20,21	3.70	5 (25%)	24,27,29	4.07	4 (16%)
1	CR2	K	59	1	20,20,21	3.76	4 (20%)	24,27,29	3.79	5 (20%)
1	CR2	L	59	1	20,20,21	3.65	5 (25%)	24,27,29	4.16	5 (20%)
1	CR2	M	59	1	20,20,21	3.72	5 (25%)	24,27,29	4.04	4 (16%)
1	CR2	N	59	1	20,20,21	3.71	5 (25%)	24,27,29	4.20	4 (16%)
1	CR2	O	59	1	20,20,21	3.85	4 (20%)	24,27,29	3.82	6 (25%)
1	CR2	P	59	1	20,20,21	3.74	4 (20%)	24,27,29	3.73	6 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	A	59	1	-	0/6/25/26	0/2/2/2
1	CR2	B	59	1	-	0/6/25/26	0/2/2/2
1	CR2	C	59	1	-	0/6/25/26	0/2/2/2
1	CR2	D	59	1	-	0/6/25/26	0/2/2/2
1	CR2	E	59	1	-	0/6/25/26	0/2/2/2
1	CR2	F	59	1	-	0/6/25/26	0/2/2/2
1	CR2	G	59	1	-	0/6/25/26	0/2/2/2
1	CR2	H	59	1	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	I	59	1	-	0/6/25/26	0/2/2/2
1	CR2	J	59	1	-	0/6/25/26	0/2/2/2
1	CR2	K	59	1	-	0/6/25/26	0/2/2/2
1	CR2	L	59	1	-	0/6/25/26	0/2/2/2
1	CR2	M	59	1	-	0/6/25/26	0/2/2/2
1	CR2	N	59	1	-	0/6/25/26	0/2/2/2
1	CR2	O	59	1	-	0/6/25/26	0/2/2/2
1	CR2	P	59	1	-	0/6/25/26	0/2/2/2

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	59	CR2	C2-N3	-2.87	1.32	1.39
1	N	59	CR2	C2-N3	-2.86	1.32	1.39
1	H	59	CR2	C2-N3	-2.86	1.32	1.39
1	A	59	CR2	C2-N3	-2.83	1.32	1.39
1	C	59	CR2	C2-N3	-2.82	1.32	1.39

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	CR2	O2-C2-CA2	-13.35	123.30	130.97
1	A	59	CR2	O2-C2-CA2	-13.30	123.33	130.97
1	N	59	CR2	O2-C2-CA2	-13.20	123.38	130.97
1	G	59	CR2	O2-C2-CA2	-13.11	123.44	130.97
1	C	59	CR2	O2-C2-CA2	-13.07	123.46	130.97

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](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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

### 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	217/267 (81%)	-0.18	3 (1%) 78 82	21, 25, 31, 34	0
1	B	216/267 (80%)	-0.08	3 (1%) 78 82	22, 29, 39, 47	0
1	C	216/267 (80%)	-0.18	0 100 100	20, 26, 33, 37	0
1	D	218/267 (81%)	-0.21	0 100 100	20, 24, 32, 38	0
1	E	214/267 (80%)	-0.06	0 100 100	23, 33, 44, 47	0
1	F	221/267 (82%)	-0.02	0 100 100	22, 32, 42, 48	0
1	G	215/267 (80%)	-0.10	0 100 100	22, 31, 41, 45	0
1	H	214/267 (80%)	-0.07	1 (0%) 91 93	22, 33, 45, 53	0
1	I	214/267 (80%)	0.37	4 (1%) 70 75	32, 49, 66, 72	0
1	J	221/267 (82%)	-0.06	0 100 100	23, 32, 41, 45	0
1	K	214/267 (80%)	0.42	8 (3%) 45 51	30, 48, 69, 74	0
1	L	216/267 (80%)	0.04	3 (1%) 78 82	24, 36, 53, 61	0
1	M	207/267 (77%)	0.66	15 (7%) 18 22	34, 53, 74, 80	0
1	N	216/267 (80%)	0.31	5 (2%) 64 70	27, 41, 66, 72	0
1	O	210/267 (78%)	1.44	54 (25%) 1 0	36, 67, 92, 98	0
1	P	216/267 (80%)	0.46	12 (5%) 28 32	26, 48, 65, 68	0
All	All	3445/4272 (80%)	0.17	108 (3%) 52 60	20, 35, 67, 98	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	71	MET	7.8
1	O	112	LYS	6.0
1	O	74	PHE	5.6
1	O	214	ALA	4.9
1	O	31	ASN	4.8

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CR2	D	59	19/20	0.92	0.14	-	21,21,22,22	0
1	CR2	B	59	19/20	0.92	0.11	-	27,27,28,28	0
1	CR2	N	59	19/20	0.91	0.11	-	36,38,42,42	0
1	CR2	L	59	19/20	0.91	0.12	-	28,29,31,31	0
1	CR2	J	59	19/20	0.93	0.11	-	25,27,28,29	0
1	CR2	H	59	19/20	0.92	0.13	-	27,28,31,32	0
1	CR2	G	59	19/20	0.94	0.10	-	26,27,28,28	0
1	CR2	E	59	19/20	0.90	0.12	-	27,29,31,31	0
1	CR2	C	59	19/20	0.94	0.11	-	22,22,23,23	0
1	CR2	P	59	19/20	0.85	0.14	-	40,41,44,44	0
1	CR2	A	59	19/20	0.94	0.10	-	21,21,22,22	0
1	CR2	O	59	19/20	0.82	0.17	-	61,63,69,69	0
1	CR2	M	59	19/20	0.90	0.15	-	44,47,51,52	0
1	CR2	K	59	19/20	0.87	0.14	-	41,43,46,46	0
1	CR2	I	59	19/20	0.93	0.13	-	43,45,48,48	0
1	CR2	F	59	19/20	0.91	0.11	-	25,26,27,28	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	M	301	1/1	0.92	0.17	2.59	52,52,52,52	0
2	CL	D	301	1/1	0.97	0.11	0.64	33,33,33,33	0
2	CL	O	301	1/1	0.78	0.18	0.27	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	N	301	1/1	0.94	0.09	-1.17	55,55,55,55	0
2	CL	J	301	1/1	0.97	0.08	-1.28	35,35,35,35	0
2	CL	E	301	1/1	0.99	0.08	-1.49	36,36,36,36	0
2	CL	I	301	1/1	0.95	0.08	-1.57	49,49,49,49	0
2	CL	K	301	1/1	0.97	0.07	-2.33	49,49,49,49	0
2	CL	L	301	1/1	0.95	0.07	-2.45	40,40,40,40	0
2	CL	P	301	1/1	0.96	0.07	-2.64	43,43,43,43	0
2	CL	G	301	1/1	0.94	0.08	-3.63	33,33,33,33	0
2	CL	B	301	1/1	0.97	0.06	-3.94	34,34,34,34	0
2	CL	C	301	1/1	0.99	0.06	-4.15	33,33,33,33	0
2	CL	H	301	1/1	0.99	0.05	-6.34	39,39,39,39	0
2	CL	F	301	1/1	0.98	0.06	-7.30	32,32,32,32	0
2	CL	A	301	1/1	0.98	0.05	-9.13	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.