



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:12 AM EDT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

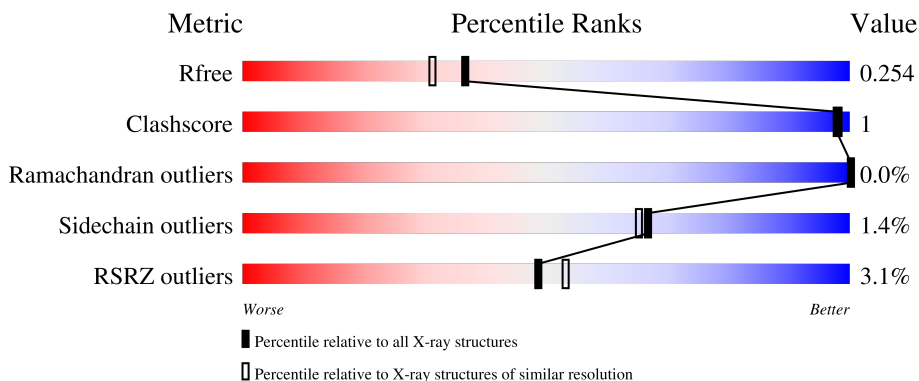
1 Overall quality at a glance

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.













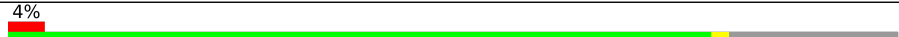
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	79% 18%
1	B	267	78% 19%
1	C	267	77% 19%
1	D	267	80% 18%
1	E	267	78% 19%

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Mol	Chain	Length	Quality of chain
1	F	267	 80% 17%
1	G	267	 79% 19%
1	H	267	 75% 5% 19%
1	I	267	 77% 19%
1	J	267	 81% 17%
1	K	267	 3% 78% 19%
1	L	267	 % 79% 19%
1	M	267	 6% 75% 22%
1	N	267	 2% 80% 19%
1	O	267	 20% 75% 21%
1	P	267	 4% 79% 19%

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

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	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	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	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	1	Total 1	Cl 1	0	0
2	P	1	Total 1	Cl 1	0	0
2	N	1	Total 1	Cl 1	0	0
2	O	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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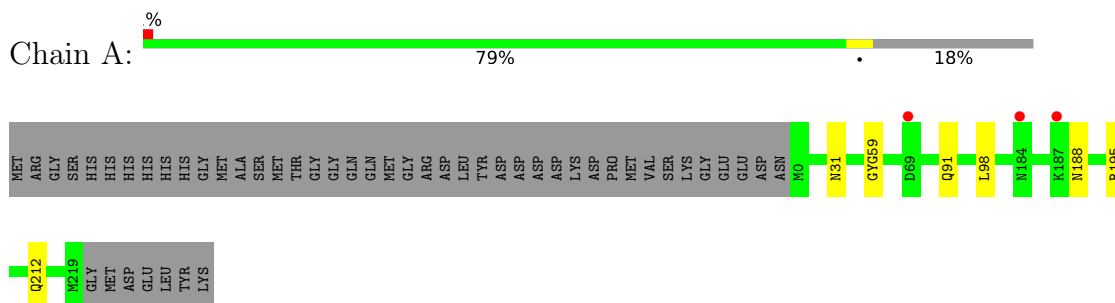
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	2	Total O 2 2	0	0

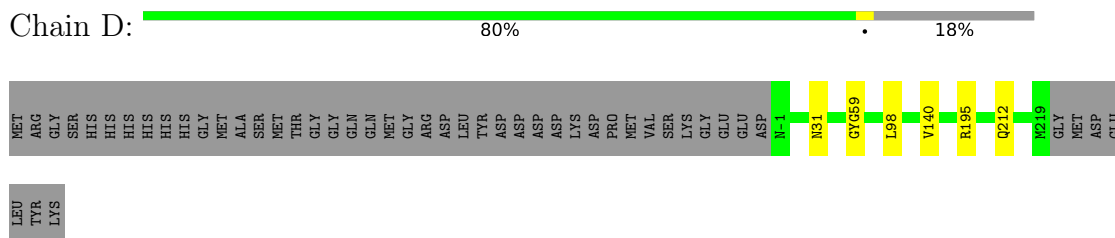
3 Residue-property plots [i](#)

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.

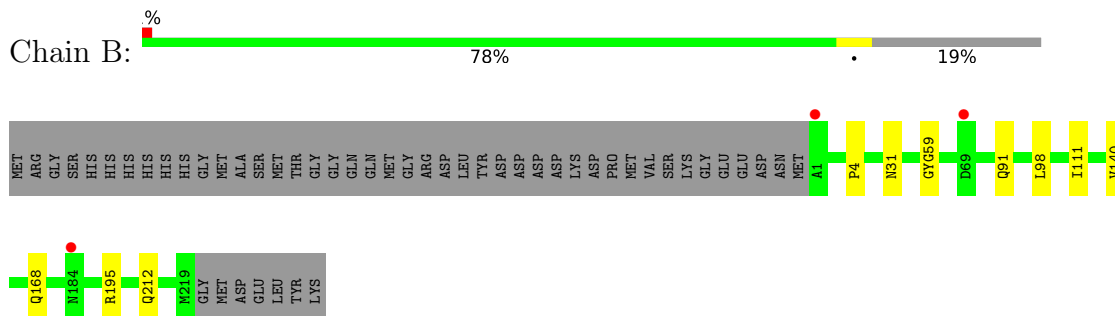
- Molecule 1: Green fluorescent protein bIFP-Y3



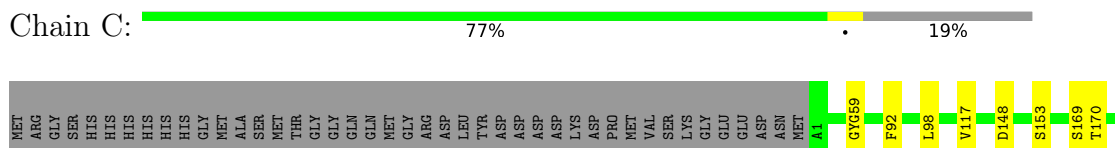
- Molecule 1: Green fluorescent protein bIFP-Y3

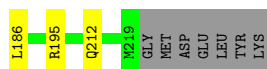


- Molecule 1: Green fluorescent protein bIFP-Y3



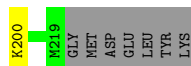
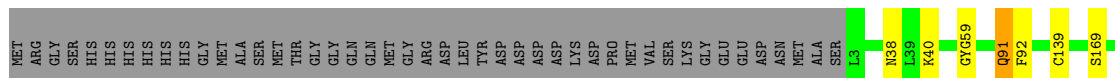
- Molecule 1: Green fluorescent protein bIFP-Y3





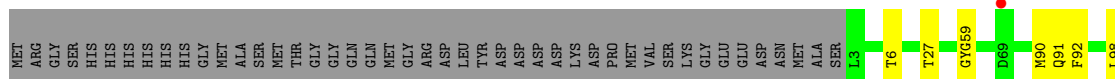
- Molecule 1: Green fluorescent protein bFP-Y3

Chain E: 78% 19%



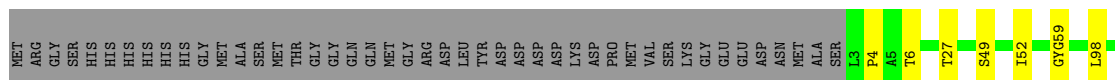
- Molecule 1: Green fluorescent protein bFP-Y3

Chain H: 75% 5% 19%



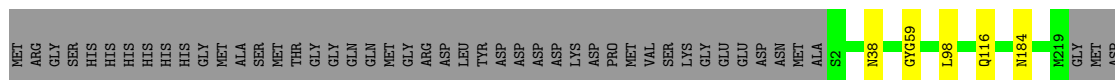
- Molecule 1: Green fluorescent protein bFP-Y3

Chain F: 80% 17%



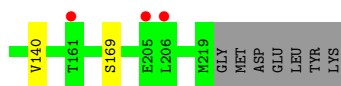
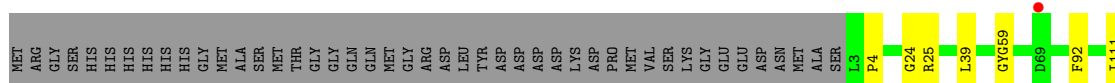
- Molecule 1: Green fluorescent protein bFP-Y3

Chain G: 79% 19%

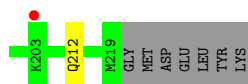
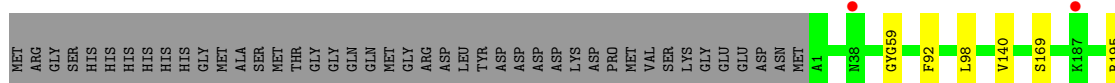
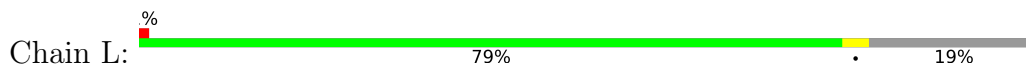


- Molecule 1: Green fluorescent protein bFP-Y3

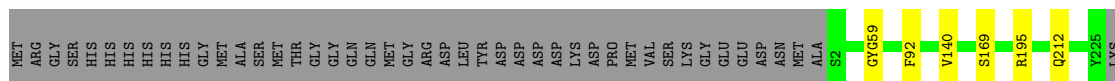
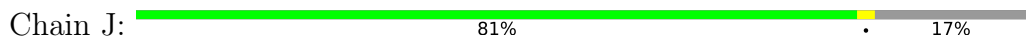
Chain I: 77% 19%



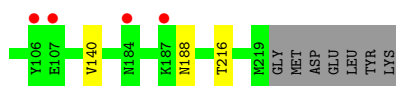
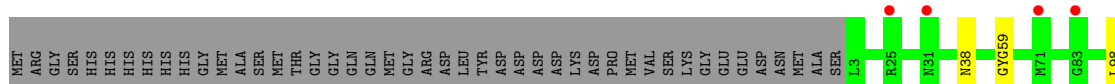
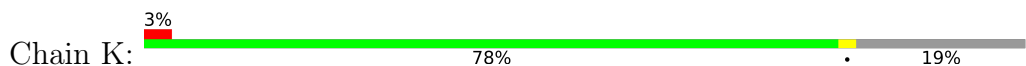
- Molecule 1: Green fluorescent protein bFP-Y3



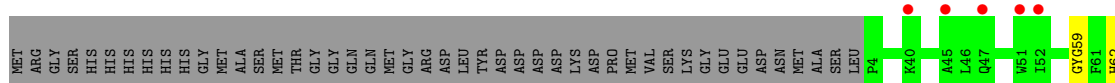
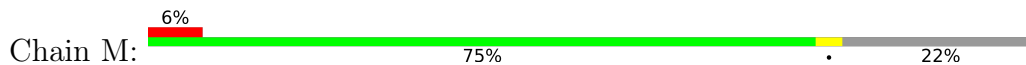
- Molecule 1: Green fluorescent protein bFP-Y3



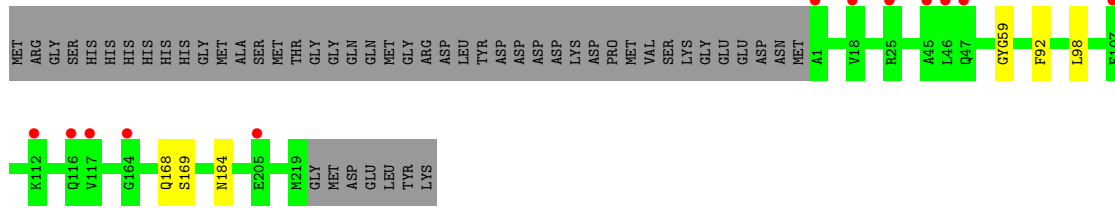
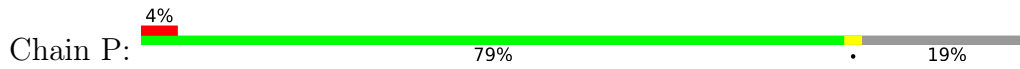
- Molecule 1: Green fluorescent protein bFP-Y3



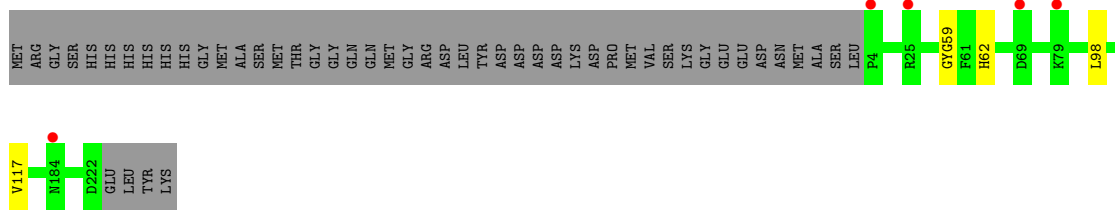
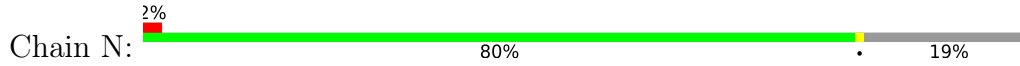
- Molecule 1: Green fluorescent protein bFP-Y3



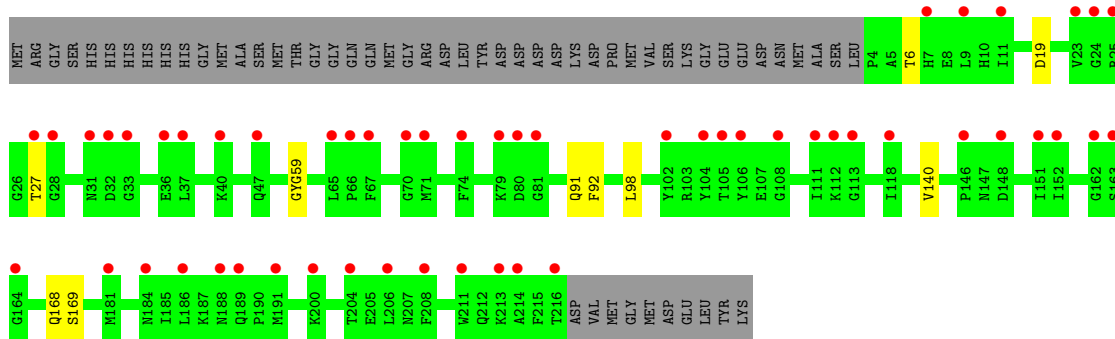
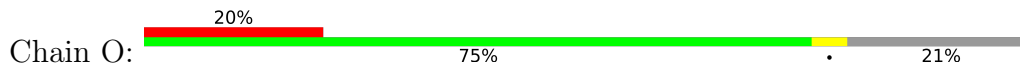
- Molecule 1: Green fluorescent protein bFP-Y3



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.05Å)	Xtrriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtrriage
Anisotropy	0.308	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28364	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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.

All (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:HE21	1:B:91[B]:GLN:HA	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
1:F:6:THR:HG22	1:F:27:THR:HG22	1.90	0.53
1:H:6:THR:HG22	1:H:27:THR:HG22	1.94	0.50
1:E:91[B]:GLN:HA	1:E:91[B]:GLN:NE2	2.24	0.50
1:L:195:ARG:HE	1:L:212:GLN:HE21	1.61	0.49
1:B:4:PRO:HB3	1:B:111:ILE:HD11	1.96	0.48
1:C:92:PHE:CD2	1:C:169:SER:HB3	2.48	0.48
1:F:4:PRO:HB3	1:F:111:ILE:HD11	1.94	0.48
1:D:140:VAL:HG11	1:B:140:VAL:HG11	1.95	0.47
1:J:92:PHE:CD2	1:J:169:SER:HB3	2.50	0.47
1:O:6:THR:HG22	1:O:27:THR:HG22	1.97	0.47
1:O:92:PHE:CD2	1:O:169:SER:HB3	2.51	0.46
1:C:148:ASP:HA	1:C:186:LEU:HD21	1.98	0.46
1:H:90[B]:MET:HE1	1:H:157:TRP:CD1	2.50	0.46
1:M:140:VAL:HG11	1:O:140:VAL:HG11	1.97	0.46
1:B:91[B]:GLN:HE21	1:B:91[B]:GLN:CA	2.28	0.46
1:H:195:ARG:HE	1:H:212:GLN:HE21	1.65	0.44
1:B:195:ARG:HE	1:B:212:GLN:HE21	1.66	0.44
1:N:98:LEU:HD21	1:N:117:VAL:HG13	2.00	0.43
1:L:92:PHE:CD2	1:L:169:SER:HB3	2.54	0.43
1:L:140:VAL:HG11	1:J:140:VAL:HG11	1.99	0.43
1:E:92:PHE:CD2	1:E:169:SER:HB3	2.54	0.43
1:H:91[B]:GLN:HA	1:H:91[B]:GLN:OE1	2.19	0.42
1:A:195:ARG:HE	1:A:212:GLN:NE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:ARG:HE	1:J:212:GLN:HE21	1.67	0.42
1:I:24:GLY:HA3	1:I:39:LEU:HD23	2.02	0.42
1:I:4:PRO:HB3	1:I:111:ILE:HD11	2.02	0.41
1:I:140:VAL:HG11	1:K:140:VAL:HG11	2.01	0.41
1:K:188:ASN:ND2	1:K:216:THR:HG21	2.36	0.41
1:H:92:PHE:CD2	1:H:169:SER:HB3	2.56	0.41
1:C:195:ARG:HE	1:C:212:GLN:HE21	1.69	0.41
1:I:92:PHE:CD2	1:I:169:SER:HB3	2.56	0.41
1:P:92:PHE:CD2	1:P:169:SER:HB3	2.55	0.41
1:F:49:SER:O	1:F:52:ILE:HG22	2.21	0.40
1:C:98:LEU:HD11	1:C:117:VAL:CG1	2.51	0.40
1:D:195:ARG:HE	1:D:212:GLN:HE21	1.67	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	18
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/226 (82%)	181 (98%)	4 (2%)	52	46
1	B	186/226 (82%)	183 (98%)	3 (2%)	62	59
1	C	187/226 (83%)	185 (99%)	2 (1%)	73	73
1	D	188/226 (83%)	186 (99%)	2 (1%)	73	73
1	E	184/226 (81%)	178 (97%)	6 (3%)	38	31
1	F	189/226 (84%)	187 (99%)	2 (1%)	73	73
1	G	184/226 (81%)	181 (98%)	3 (2%)	62	59
1	H	183/226 (81%)	180 (98%)	3 (2%)	62	59
1	I	183/226 (81%)	182 (100%)	1 (0%)	88	89
1	J	189/226 (84%)	189 (100%)	0	100	100
1	K	184/226 (81%)	182 (99%)	2 (1%)	73	73
1	L	184/226 (81%)	183 (100%)	1 (0%)	88	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	177/226 (78%)	171 (97%)	6 (3%)	37	30
1	N	183/226 (81%)	182 (100%)	1 (0%)	88	89
1	O	179/226 (79%)	175 (98%)	4 (2%)	52	46
1	P	184/226 (81%)	181 (98%)	3 (2%)	62	59
All	All	2949/3616 (82%)	2906 (98%)	43 (2%)	67	62

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	91	GLN
1	A	98	LEU
1	A	188	ASN
1	D	31	ASN
1	D	98	LEU
1	B	31	ASN
1	B	98	LEU
1	B	168	GLN
1	C	153	SER
1	C	170	THR
1	E	38	ASN
1	E	40	LYS
1	E	91[A]	GLN
1	E	91[B]	GLN
1	E	139	CYS
1	E	200	LYS
1	H	98	LEU
1	H	168	GLN
1	H	184	ASN
1	F	98	LEU
1	F	168	GLN
1	G	38	ASN
1	G	98	LEU
1	G	184	ASN
1	I	25	ARG
1	L	98	LEU
1	K	38	ASN
1	K	98	LEU
1	M	62	HIS
1	M	91	GLN
1	M	98	LEU

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Mol	Chain	Res	Type
1	M	139	CYS
1	M	165	LYS
1	M	196	LYS
1	P	98	LEU
1	P	168	GLN
1	P	184	ASN
1	N	62	HIS
1	O	19	ASP
1	O	91	GLN
1	O	98	LEU
1	O	168	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	38	ASN
1	A	47	GLN
1	A	87	HIS
1	A	189	GLN
1	A	207	ASN
1	A	212	GLN
1	D	31	ASN
1	D	189	GLN
1	D	207	ASN
1	D	212	GLN
1	B	31	ASN
1	B	38	ASN
1	B	87	HIS
1	B	168	GLN
1	B	189	GLN
1	B	207	ASN
1	B	212	GLN
1	C	38	ASN
1	C	87	HIS
1	C	189	GLN
1	C	207	ASN
1	C	212	GLN
1	E	87	HIS
1	E	212	GLN
1	H	38	ASN
1	H	87	HIS

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Mol	Chain	Res	Type
1	H	116	GLN
1	H	168	GLN
1	H	207	ASN
1	H	212	GLN
1	F	38	ASN
1	F	47	GLN
1	F	116	GLN
1	F	189	GLN
1	F	207	ASN
1	F	212	GLN
1	G	87	HIS
1	G	184	ASN
1	G	212	GLN
1	I	87	HIS
1	I	116	GLN
1	I	189	GLN
1	I	212	GLN
1	L	87	HIS
1	L	91	GLN
1	L	131	ASN
1	L	212	GLN
1	J	38	ASN
1	J	47	GLN
1	J	207	ASN
1	J	212	GLN
1	K	38	ASN
1	K	87	HIS
1	K	184	ASN
1	K	207	ASN
1	K	212	GLN
1	M	87	HIS
1	M	116	GLN
1	M	189	GLN
1	M	207	ASN
1	P	87	HIS
1	P	168	GLN
1	P	184	ASN
1	P	212	GLN
1	N	131	ASN
1	N	212	GLN
1	O	38	ASN
1	O	47	GLN

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Mol	Chain	Res	Type
1	O	189	GLN
1	O	207	ASN

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	CR2	P	59	1	20,20,21	4.09	4 (20%)	25,27,29	3.99	7 (28%)
1	CR2	B	59	1	20,20,21	4.02	5 (25%)	25,27,29	4.48	6 (24%)
1	CR2	L	59	1	20,20,21	4.00	5 (25%)	25,27,29	4.49	6 (24%)
1	CR2	M	59	1	20,20,21	4.08	5 (25%)	25,27,29	4.33	6 (24%)
1	CR2	J	59	1	20,20,21	4.06	5 (25%)	25,27,29	4.37	6 (24%)
1	CR2	D	59	1	20,20,21	3.94	5 (25%)	25,27,29	4.28	7 (28%)
1	CR2	I	59	1	20,20,21	4.10	5 (25%)	25,27,29	4.17	6 (24%)
1	CR2	A	59	1	20,20,21	3.92	5 (25%)	25,27,29	4.39	7 (28%)
1	CR2	O	59	1	20,20,21	4.21	4 (20%)	25,27,29	4.08	9 (36%)
1	CR2	E	59	1	20,20,21	4.10	5 (25%)	25,27,29	4.41	6 (24%)
1	CR2	F	59	1	20,20,21	4.08	5 (25%)	25,27,29	4.31	6 (24%)
1	CR2	C	59	1	20,20,21	4.01	5 (25%)	25,27,29	4.32	6 (24%)
1	CR2	N	59	1	20,20,21	4.06	5 (25%)	25,27,29	4.49	6 (24%)
1	CR2	H	59	1	20,20,21	4.19	5 (25%)	25,27,29	4.40	6 (24%)
1	CR2	K	59	1	20,20,21	4.11	5 (25%)	25,27,29	4.06	6 (24%)
1	CR2	G	59	1	20,20,21	4.00	5 (25%)	25,27,29	4.49	7 (28%)

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	P	59	1	-	1/6/25/26	0/2/2/2
1	CR2	B	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	J	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	I	59	1	-	0/6/25/26	0/2/2/2
1	CR2	A	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	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	C	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	H	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	G	59	1	-	0/6/25/26	0/2/2/2

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	59	CR2	CB2-CA2	17.82	1.50	1.35
1	H	59	CR2	CB2-CA2	17.64	1.49	1.35
1	K	59	CR2	CB2-CA2	17.30	1.49	1.35
1	P	59	CR2	CB2-CA2	17.26	1.49	1.35
1	I	59	CR2	CB2-CA2	17.22	1.49	1.35
1	E	59	CR2	CB2-CA2	17.22	1.49	1.35
1	M	59	CR2	CB2-CA2	17.07	1.49	1.35
1	F	59	CR2	CB2-CA2	17.04	1.49	1.35
1	N	59	CR2	CB2-CA2	16.97	1.49	1.35
1	J	59	CR2	CB2-CA2	16.95	1.49	1.35
1	B	59	CR2	CB2-CA2	16.79	1.49	1.35
1	L	59	CR2	CB2-CA2	16.70	1.49	1.35
1	C	59	CR2	CB2-CA2	16.67	1.49	1.35
1	G	59	CR2	CB2-CA2	16.66	1.49	1.35
1	D	59	CR2	CB2-CA2	16.34	1.48	1.35
1	A	59	CR2	CB2-CA2	16.31	1.48	1.35
1	N	59	CR2	C1-N2	3.32	1.38	1.32
1	E	59	CR2	C1-N2	3.25	1.38	1.32
1	B	59	CR2	C1-N2	3.20	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	CR2	C1-N2	3.18	1.38	1.32
1	J	59	CR2	C1-N2	3.17	1.38	1.32
1	D	59	CR2	C1-N2	3.16	1.38	1.32
1	M	59	CR2	C1-N2	3.15	1.38	1.32
1	H	59	CR2	C1-N2	3.14	1.38	1.32
1	F	59	CR2	C1-N2	3.14	1.38	1.32
1	G	59	CR2	C2-N3	-3.09	1.32	1.39
1	I	59	CR2	C1-N2	3.08	1.38	1.32
1	N	59	CR2	C2-N3	-3.08	1.32	1.39
1	H	59	CR2	C2-N3	-3.07	1.32	1.39
1	C	59	CR2	CA2-C2	-3.07	1.45	1.48
1	A	59	CR2	C2-N3	-3.05	1.32	1.39
1	C	59	CR2	C2-N3	-3.04	1.32	1.39
1	K	59	CR2	C2-N3	-3.04	1.32	1.39
1	B	59	CR2	C2-N3	-3.03	1.32	1.39
1	A	59	CR2	CA2-C2	-3.03	1.45	1.48
1	J	59	CR2	CA2-C2	-3.03	1.45	1.48
1	F	59	CR2	C2-N3	-3.02	1.32	1.39
1	D	59	CR2	C2-N3	-3.02	1.32	1.39
1	E	59	CR2	C2-N3	-3.01	1.32	1.39
1	G	59	CR2	C1-N2	3.00	1.38	1.32
1	L	59	CR2	C1-N2	3.00	1.38	1.32
1	K	59	CR2	C1-N2	2.99	1.38	1.32
1	D	59	CR2	CA2-C2	-2.99	1.45	1.48
1	L	59	CR2	C2-N3	-2.98	1.32	1.39
1	A	59	CR2	C1-N2	2.97	1.37	1.32
1	J	59	CR2	C2-N3	-2.97	1.32	1.39
1	I	59	CR2	C2-N3	-2.95	1.32	1.39
1	F	59	CR2	CA2-C2	-2.91	1.45	1.48
1	M	59	CR2	C2-N3	-2.91	1.33	1.39
1	P	59	CR2	O2-C2	2.91	1.29	1.23
1	B	59	CR2	CA2-C2	-2.90	1.45	1.48
1	O	59	CR2	C2-N3	-2.82	1.33	1.39
1	O	59	CR2	C1-N2	2.81	1.37	1.32
1	P	59	CR2	C1-N2	2.81	1.37	1.32
1	O	59	CR2	O2-C2	2.80	1.29	1.23
1	N	59	CR2	CA2-C2	-2.79	1.45	1.48
1	L	59	CR2	CA2-C2	-2.77	1.45	1.48
1	K	59	CR2	O2-C2	2.76	1.28	1.23
1	P	59	CR2	C2-N3	-2.75	1.33	1.39
1	D	59	CR2	O2-C2	2.75	1.28	1.23
1	G	59	CR2	CA2-C2	-2.74	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	59	CR2	O2-C2	2.70	1.28	1.23
1	M	59	CR2	O2-C2	2.68	1.28	1.23
1	C	59	CR2	O2-C2	2.63	1.28	1.23
1	J	59	CR2	O2-C2	2.56	1.28	1.23
1	F	59	CR2	O2-C2	2.56	1.28	1.23
1	G	59	CR2	O2-C2	2.55	1.28	1.23
1	N	59	CR2	O2-C2	2.52	1.28	1.23
1	E	59	CR2	O2-C2	2.51	1.28	1.23
1	A	59	CR2	O2-C2	2.51	1.28	1.23
1	H	59	CR2	CA2-C2	-2.46	1.46	1.48
1	H	59	CR2	O2-C2	2.43	1.28	1.23
1	B	59	CR2	O2-C2	2.42	1.28	1.23
1	M	59	CR2	CA2-C2	-2.39	1.46	1.48
1	E	59	CR2	CA2-C2	-2.38	1.46	1.48
1	L	59	CR2	O2-C2	2.37	1.28	1.23
1	I	59	CR2	CA2-C2	-2.32	1.46	1.48
1	K	59	CR2	CA2-C2	-2.26	1.46	1.48

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	59	CR2	CA2-C2-N3	15.08	110.50	103.37
1	N	59	CR2	CA2-C2-N3	14.94	110.43	103.37
1	L	59	CR2	CA2-C2-N3	14.77	110.35	103.37
1	B	59	CR2	CA2-C2-N3	14.76	110.35	103.37
1	E	59	CR2	CA2-C2-N3	14.67	110.31	103.37
1	G	59	CR2	CA2-C2-N3	14.65	110.30	103.37
1	M	59	CR2	CA2-C2-N3	14.43	110.19	103.37
1	J	59	CR2	CA2-C2-N3	14.31	110.14	103.37
1	F	59	CR2	CA2-C2-N3	14.31	110.14	103.37
1	A	59	CR2	CA2-C2-N3	14.11	110.04	103.37
1	C	59	CR2	CA2-C2-N3	14.02	110.00	103.37
1	I	59	CR2	CA2-C2-N3	14.00	109.99	103.37
1	O	59	CR2	CA2-C2-N3	13.81	109.90	103.37
1	D	59	CR2	CA2-C2-N3	13.74	109.87	103.37
1	B	59	CR2	O2-C2-CA2	-13.65	123.30	130.96
1	K	59	CR2	CA2-C2-N3	13.63	109.82	103.37
1	A	59	CR2	O2-C2-CA2	-13.60	123.33	130.96
1	N	59	CR2	O2-C2-CA2	-13.49	123.38	130.96
1	G	59	CR2	O2-C2-CA2	-13.40	123.44	130.96
1	C	59	CR2	O2-C2-CA2	-13.36	123.46	130.96
1	J	59	CR2	O2-C2-CA2	-13.25	123.52	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	CR2	O2-C2-CA2	-13.09	123.61	130.96
1	E	59	CR2	O2-C2-CA2	-13.00	123.66	130.96
1	P	59	CR2	CA2-C2-N3	12.97	109.51	103.37
1	L	59	CR2	O2-C2-CA2	-12.90	123.72	130.96
1	F	59	CR2	O2-C2-CA2	-12.69	123.83	130.96
1	M	59	CR2	O2-C2-CA2	-12.56	123.91	130.96
1	H	59	CR2	O2-C2-CA2	-11.99	124.23	130.96
1	I	59	CR2	O2-C2-CA2	-11.76	124.35	130.96
1	K	59	CR2	O2-C2-CA2	-11.36	124.58	130.96
1	P	59	CR2	O2-C2-CA2	-11.05	124.76	130.96
1	O	59	CR2	O2-C2-CA2	-10.42	125.11	130.96
1	G	59	CR2	C2-N3-C1	-6.08	105.02	107.99
1	L	59	CR2	C2-N3-C1	-6.03	105.04	107.99
1	N	59	CR2	C2-N3-C1	-5.65	105.23	107.99
1	A	59	CR2	C2-N3-C1	-5.64	105.23	107.99
1	H	59	CR2	C2-CA2-N2	-5.59	105.02	108.93
1	O	59	CR2	CB2-CA2-C2	5.57	128.93	122.28
1	H	59	CR2	C2-N3-C1	-5.57	105.27	107.99
1	B	59	CR2	C2-N3-C1	-5.48	105.31	107.99
1	O	59	CR2	C2-CA2-N2	-5.45	105.11	108.93
1	I	59	CR2	C2-CA2-N2	-5.45	105.11	108.93
1	M	59	CR2	C2-N3-C1	-5.44	105.33	107.99
1	E	59	CR2	C2-N3-C1	-5.43	105.33	107.99
1	C	59	CR2	C2-N3-C1	-5.37	105.37	107.99
1	J	59	CR2	C2-N3-C1	-5.29	105.41	107.99
1	P	59	CR2	CB2-CA2-C2	5.22	128.51	122.28
1	M	59	CR2	C2-CA2-N2	-5.22	105.28	108.93
1	E	59	CR2	C2-CA2-N2	-5.14	105.33	108.93
1	L	59	CR2	C2-CA2-N2	-5.14	105.33	108.93
1	O	59	CR2	C2-N3-C1	-5.12	105.49	107.99
1	D	59	CR2	C2-N3-C1	-5.08	105.51	107.99
1	F	59	CR2	C2-N3-C1	-5.07	105.51	107.99
1	K	59	CR2	C2-CA2-N2	-5.06	105.39	108.93
1	B	59	CR2	C2-CA2-N2	-4.96	105.46	108.93
1	N	59	CR2	C2-CA2-N2	-4.93	105.48	108.93
1	F	59	CR2	C2-CA2-N2	-4.92	105.49	108.93
1	P	59	CR2	C2-CA2-N2	-4.92	105.49	108.93
1	D	59	CR2	O3-C3-CA3	-4.92	111.54	126.39
1	C	59	CR2	O3-C3-CA3	-4.78	111.95	126.39
1	P	59	CR2	C2-N3-C1	-4.76	105.67	107.99
1	G	59	CR2	C2-CA2-N2	-4.73	105.62	108.93
1	J	59	CR2	C2-CA2-N2	-4.71	105.63	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	59	CR2	O3-C3-CA3	-4.65	112.35	126.39
1	F	59	CR2	O3-C3-CA3	-4.64	112.37	126.39
1	I	59	CR2	C2-N3-C1	-4.54	105.77	107.99
1	E	59	CR2	O3-C3-CA3	-4.43	113.00	126.39
1	K	59	CR2	C2-N3-C1	-4.43	105.83	107.99
1	G	59	CR2	O3-C3-CA3	-4.39	113.14	126.39
1	H	59	CR2	O3-C3-CA3	-4.39	113.15	126.39
1	M	59	CR2	O3-C3-CA3	-4.37	113.20	126.39
1	K	59	CR2	O3-C3-CA3	-4.37	113.20	126.39
1	A	59	CR2	C2-CA2-N2	-4.36	105.88	108.93
1	N	59	CR2	O3-C3-CA3	-4.36	113.24	126.39
1	K	59	CR2	CB2-CA2-C2	4.34	127.46	122.28
1	L	59	CR2	O3-C3-CA3	-4.33	113.33	126.39
1	I	59	CR2	O3-C3-CA3	-4.33	113.33	126.39
1	H	59	CR2	CB2-CA2-C2	4.32	127.43	122.28
1	I	59	CR2	CB2-CA2-C2	4.28	127.39	122.28
1	A	59	CR2	O3-C3-CA3	-4.27	113.51	126.39
1	D	59	CR2	C2-CA2-N2	-4.26	105.95	108.93
1	L	59	CR2	CB2-CA2-C2	4.24	127.34	122.28
1	B	59	CR2	O3-C3-CA3	-4.23	113.62	126.39
1	C	59	CR2	C2-CA2-N2	-4.23	105.97	108.93
1	M	59	CR2	CB2-CA2-C2	3.85	126.87	122.28
1	G	59	CR2	CB2-CA2-C2	3.60	126.57	122.28
1	P	59	CR2	O3-C3-CA3	-3.45	115.96	126.39
1	E	59	CR2	CB2-CA2-C2	3.45	126.39	122.28
1	F	59	CR2	CB2-CA2-C2	3.43	126.37	122.28
1	N	59	CR2	CB2-CA2-C2	3.21	126.11	122.28
1	J	59	CR2	CB2-CA2-C2	3.12	126.00	122.28
1	B	59	CR2	CB2-CA2-C2	3.07	125.94	122.28
1	O	59	CR2	O3-C3-CA3	-2.93	117.55	126.39
1	A	59	CR2	CB2-CA2-C2	2.91	125.75	122.28
1	D	59	CR2	CB2-CA2-C2	2.86	125.69	122.28
1	D	59	CR2	C1-CA1-N1	-2.57	107.16	112.85
1	C	59	CR2	CB2-CA2-C2	2.55	125.32	122.28
1	O	59	CR2	CG2-CB2-CA2	-2.33	127.09	129.94
1	A	59	CR2	C1-CA1-N1	-2.27	107.83	112.85
1	G	59	CR2	C1-CA1-N1	-2.24	107.89	112.85
1	O	59	CR2	CB2-CA2-N2	-2.07	125.96	128.83
1	P	59	CR2	CB2-CA2-N2	-2.04	126.00	128.83
1	O	59	CR2	CA1-C1-N3	2.01	125.21	122.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	59	CR2	C3-CA3-N3-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/267 (81%)	-0.18	3 (1%) 75 78	21, 25, 31, 34	0
1	B	216/267 (80%)	-0.08	3 (1%) 75 78	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 92	22, 33, 45, 53	0
1	I	214/267 (80%)	0.37	4 (1%) 66 71	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%) 41 45	30, 48, 69, 74	0
1	L	216/267 (80%)	0.04	3 (1%) 75 78	24, 36, 53, 61	0
1	M	207/267 (77%)	0.66	15 (7%) 15 17	34, 53, 74, 80	0
1	N	216/267 (80%)	0.31	5 (2%) 60 64	27, 41, 66, 72	0
1	O	210/267 (78%)	1.44	54 (25%) 0 0	36, 67, 92, 98	0
1	P	216/267 (80%)	0.46	12 (5%) 24 26	26, 48, 65, 68	0
All	All	3445/4272 (80%)	0.17	108 (3%) 49 53	20, 35, 67, 98	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	71	MET	7.7
1	O	112	LYS	6.0
1	O	74	PHE	5.6
1	O	214	ALA	4.9
1	O	31	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	O	27	THR	4.7
1	M	138	TRP	4.7
1	O	81	GLY	4.6
1	O	23	VAL	4.2
1	O	70	GLY	4.1
1	O	191	MET	4.0
1	K	83	GLY	3.9
1	O	213	LYS	3.8
1	O	206	LEU	3.8
1	O	111	ILE	3.8
1	K	184	ASN	3.7
1	K	107	GLU	3.6
1	O	108	GLY	3.6
1	A	184	ASN	3.5
1	M	166	ARG	3.5
1	O	216	THR	3.4
1	O	24	GLY	3.3
1	N	69	ASP	3.3
1	N	79	LYS	3.3
1	K	71	MET	3.3
1	O	9	LEU	3.3
1	N	184	ASN	3.2
1	K	31	ASN	3.2
1	O	47	GLN	3.1
1	O	25	ARG	3.1
1	O	189	GLN	3.1
1	O	200	LYS	3.1
1	O	106	TYR	3.0
1	P	18	VAL	3.0
1	O	67	PHE	2.9
1	B	1	ALA	2.9
1	M	128	VAL	2.9
1	O	65	LEU	2.9
1	O	181	MET	2.8
1	K	106	TYR	2.8
1	O	151	ILE	2.8
1	O	164	GLY	2.7
1	L	38	ASN	2.7
1	O	28	GLY	2.7
1	O	162	GLY	2.7
1	P	47	GLN	2.7
1	M	40	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	36	GLU	2.6
1	O	7	HIS	2.6
1	O	204	THR	2.5
1	O	163	SER	2.5
1	P	45	ALA	2.5
1	O	211	TRP	2.5
1	B	69	ASP	2.5
1	M	47	GLN	2.5
1	O	32	ASP	2.5
1	P	1	ALA	2.5
1	I	161	THR	2.4
1	N	4	PRO	2.4
1	N	25	ARG	2.4
1	O	113	GLY	2.4
1	O	80	ASP	2.4
1	O	184	ASN	2.4
1	K	25	ARG	2.4
1	H	69	ASP	2.4
1	P	116	GLN	2.3
1	O	66	PRO	2.3
1	M	45	ALA	2.3
1	I	69	ASP	2.3
1	M	203	LYS	2.3
1	M	67	PHE	2.3
1	P	117	VAL	2.3
1	P	205	GLU	2.3
1	A	187	LYS	2.3
1	M	194	PHE	2.3
1	O	33	GLY	2.3
1	P	46	LEU	2.3
1	L	187	LYS	2.3
1	P	112	LYS	2.3
1	B	184	ASN	2.3
1	M	199	LEU	2.2
1	M	52	ILE	2.2
1	O	118	ILE	2.2
1	O	152	ILE	2.2
1	O	104	TYR	2.2
1	O	105	THR	2.2
1	O	186	LEU	2.2
1	O	188	ASN	2.2
1	O	102	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	205	GLU	2.2
1	O	40	LYS	2.2
1	I	206	LEU	2.1
1	O	37	LEU	2.1
1	O	208	PHE	2.1
1	M	168	GLN	2.1
1	M	202	SER	2.1
1	O	148	ASP	2.1
1	L	203	LYS	2.1
1	O	146	PRO	2.1
1	M	107	GLU	2.1
1	P	107	GLU	2.1
1	O	11	ILE	2.1
1	K	187	LYS	2.1
1	O	79	LYS	2.1
1	M	51	TRP	2.1
1	A	69	ASP	2.0
1	P	25	ARG	2.0
1	P	164	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR2	O	59	19/20	0.82	0.17	61,63,69,69	0
1	CR2	P	59	19/20	0.85	0.14	40,41,44,44	0
1	CR2	K	59	19/20	0.87	0.14	41,43,46,46	0
1	CR2	E	59	19/20	0.90	0.12	27,29,31,31	0
1	CR2	M	59	19/20	0.90	0.15	44,47,51,52	0
1	CR2	F	59	19/20	0.91	0.11	25,26,27,28	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	D	59	19/20	0.92	0.14	21,21,22,22	0
1	CR2	H	59	19/20	0.92	0.13	27,28,31,32	0
1	CR2	B	59	19/20	0.92	0.11	27,27,28,28	0
1	CR2	J	59	19/20	0.93	0.11	25,27,28,29	0
1	CR2	I	59	19/20	0.93	0.13	43,45,48,48	0
1	CR2	G	59	19/20	0.94	0.10	26,27,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CR2	C	59	19/20	0.94	0.11	22,22,23,23	0
1	CR2	A	59	19/20	0.94	0.10	21,21,22,22	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	O	301	1/1	0.78	0.18	68,68,68,68	0
2	CL	M	301	1/1	0.92	0.17	52,52,52,52	0
2	CL	N	301	1/1	0.94	0.09	55,55,55,55	0
2	CL	G	301	1/1	0.95	0.08	33,33,33,33	0
2	CL	I	301	1/1	0.95	0.08	49,49,49,49	0
2	CL	L	301	1/1	0.95	0.07	40,40,40,40	0
2	CL	P	301	1/1	0.96	0.07	43,43,43,43	0
2	CL	B	301	1/1	0.97	0.06	34,34,34,34	0
2	CL	D	301	1/1	0.97	0.11	33,33,33,33	0
2	CL	J	301	1/1	0.97	0.08	35,35,35,35	0
2	CL	K	301	1/1	0.97	0.07	49,49,49,49	0
2	CL	F	301	1/1	0.98	0.06	32,32,32,32	0
2	CL	A	301	1/1	0.98	0.05	29,29,29,29	0
2	CL	E	301	1/1	0.99	0.08	36,36,36,36	0
2	CL	H	301	1/1	0.99	0.05	39,39,39,39	0
2	CL	C	301	1/1	0.99	0.06	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.