W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 11:06 pm GMT

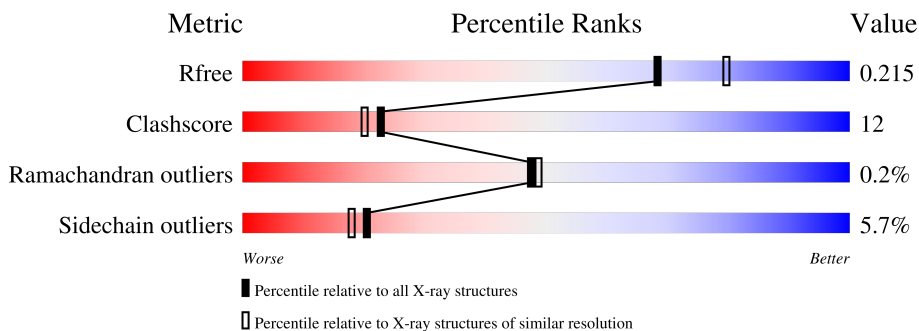|		
PDB ID	:	4B30
Title	:	Structure of the mutant V44A of the fluorescent protein KillerRed
Authors	:	Carpentier, P.; de Rosny, E.
Deposited on	:	2012-07-19
Resolution	:	2.10 Å(reported)

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 2.10 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.215
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		5.7%

Worse — *Better*

▌ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	235	76% 18% · ·
2	B	235	75% 20% · ·

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 4164 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 KILLERRED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	17	0
			1916	1210	332	358	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	VAL	engineered mutation	UNP Q2TCH5
A	65	CRQ	GLN	chromophore	UNP Q60I24
A	65	CRQ	TYR	chromophore	UNP Q60I24
A	65	CRQ	GLY	chromophore	UNP Q60I24

- Molecule 2 is a protein called KILLERRED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	19	0
			1937	1219	335	365	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	ALA	VAL	engineered mutation	UNP Q2TCH5
B	65	CRQ	GLN	chromophore	UNP Q60I24
B	65	CRQ	TYR	chromophore	UNP Q60I24
B	65	CRQ	GLY	chromophore	UNP Q60I24

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	Cl 5	0	0
4	B	3	Total 3	Cl 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Na 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	164	Total 164	O 164	0	0
7	B	96	Total 96	O 96	0	0

3 Residue-property plots ⓘ

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. 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. 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.
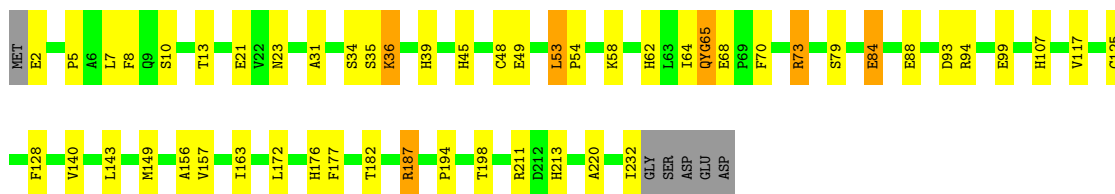
• Molecule 1: KILLERRED

Chain A:
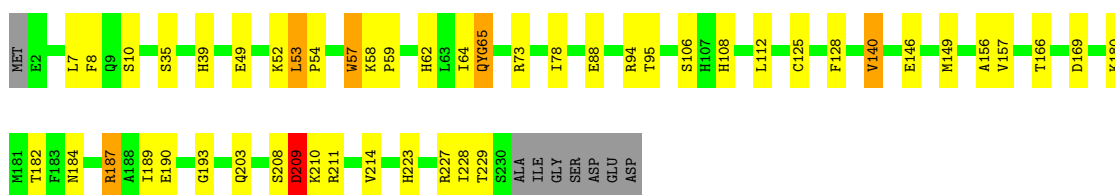
• Molecule 2: KILLERRED

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	134.31Å 134.31Å 76.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	116.32 – 2.10 46.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (116.32-2.10) 99.9 (46.24-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.165 , 0.199 0.227 , 0.215	Depositor DCC
R_{free} test set	2309 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 63.8	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, SO4, NA, CL, CRQ, GOL

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	0.79	1/1930 (0.1%)	0.84	0/2610
2	B	0.64	0/1961	0.68	0/2653
All	All	0.72	1/3891 (0.0%)	0.77	0/5263

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	TRP	CD2-CE2	5.85	1.48	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1916	0	1826	44	1
2	B	1937	0	1830	41	0
3	A	5	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	1	0
5	A	2	0	0	0	0
6	A	24	0	32	4	0
6	B	12	0	16	4	0
7	A	164	0	0	9	2
7	B	96	0	0	8	0
All	All	4164	0	3704	88	3

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 12.

The worst 5 of 88 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)
2:B:73[A]:ARG:HH11	2:B:73[A]:ARG:HG3	1.15	1.03
1:A:187[B]:ARG:NH1	1:A:189[B]:ILE:HG22	1.80	0.96
1:A:209:ASP:HB3	1:A:211:ARG:H	1.33	0.92
2:B:93:ASP:OD1	2:B:107[A]:HIS:HD2	1.51	0.91
2:B:73[A]:ARG:HH11	2:B:73[A]:ARG:CG	1.86	0.88

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2026:HOH:O	7:A:2158:HOH:O[2_544]	1.87	0.33
7:A:2026:HOH:O	7:A:2157:HOH:O[2_544]	2.01	0.19
1:A:73[A]:ARG:NH2	1:A:184:ASN:OD1[3_655]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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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	234/235 (100%)	226 (97%)	7 (3%)	1 (0%)	34	32
2	B	239/235 (102%)	232 (97%)	7 (3%)	0	100	100
All	All	473/470 (101%)	458 (97%)	14 (3%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASP

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	208/199 (104%)	195 (94%)	13 (6%)	18	15
2	B	211/200 (106%)	194 (92%)	17 (8%)	11	8
All	All	419/399 (105%)	389 (93%)	30 (7%)	20	11

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	LEU
2	B	177	PHE
2	B	36	LYS
2	B	187[B]	ARG
2	B	84[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	176	HIS
2	B	213	HIS

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Mol	Chain	Res	Type
1	A	108	HIS
2	B	39	HIS
2	B	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	CSO	A	116[B]	1	3,6,7	0.64	0	0,6,8	-	-
2	CSO	B	116[A]	2	3,6,7	0.86	0	0,6,8	-	-
1	CSO	A	215	1	3,6,7	0.57	0	0,6,8	-	-
2	CSO	B	116[B]	2	3,6,7	0.80	0	0,6,8	-	-
1	CRQ	A	65	1	24,25,26	3.26	9 (37%)	27,34,36	4.50	8 (29%)
2	CRQ	B	65	2	24,25,26	3.11	10 (41%)	27,34,36	4.77	8 (29%)
1	CSO	A	116[A]	1	3,6,7	0.68	0	0,6,8	-	-

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	CSO	A	116[B]	1	-	1/1/5/7	-
2	CSO	B	116[A]	2	-	1/1/5/7	-
1	CSO	A	215	1	-	0/1/5/7	-
2	CSO	B	116[B]	2	-	1/1/5/7	-
1	CRQ	A	65	1	-	3/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CRQ	B	65	2	-	3/10/32/33	0/2/2/2
1	CSO	A	116[A]	1	-	0/1/5/7	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	CRQ	CA1-N1	9.77	1.51	1.27
2	B	65	CRQ	CA1-N1	7.61	1.45	1.27
2	B	65	CRQ	CB2-CA2	7.60	1.41	1.35
1	A	65	CRQ	CB2-CA2	7.55	1.41	1.35
1	A	65	CRQ	CA2-C2	-5.14	1.43	1.48

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	CRQ	CA2-C2-N3	16.26	111.06	103.37
1	A	65	CRQ	CA2-C2-N3	15.91	110.90	103.37
1	A	65	CRQ	O2-C2-CA2	-11.54	124.48	130.96
2	B	65	CRQ	O2-C2-CA2	-11.49	124.51	130.96
2	B	65	CRQ	C2-CA2-N2	-9.58	102.22	108.93

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	CRQ	N2-CA2-CB2-CG2
1	A	65	CRQ	C2-CA2-CB2-CG2
2	B	65	CRQ	N2-CA2-CB2-CG2
2	B	65	CRQ	C2-CA2-CB2-CG2
2	B	116[B]	CSO	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	CRQ	1	0
2	B	65	CRQ	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

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	$\#|Z| > 2$
3	SO4	A	1231	1,5	4,4,4	0.14	0	6,6,6	0.04	0
6	GOL	B	1235	-	5,5,5	0.12	0	5,5,5	0.62	0
6	GOL	A	1241	-	5,5,5	0.49	0	5,5,5	0.41	0
6	GOL	B	1236	-	5,5,5	0.61	0	5,5,5	0.83	0
6	GOL	A	1242	-	5,5,5	0.33	0	5,5,5	0.30	0
6	GOL	A	1239	-	5,5,5	0.45	0	5,5,5	0.80	0
6	GOL	A	1240	-	5,5,5	0.25	0	5,5,5	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1235	-	-	0/4/4/4	-
6	GOL	A	1241	-	-	2/4/4/4	-
6	GOL	B	1236	-	-	2/4/4/4	-
6	GOL	A	1242	-	-	4/4/4/4	-
6	GOL	A	1239	-	-	4/4/4/4	-
6	GOL	A	1240	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1239	GOL	C1-C2-C3-O3
6	A	1240	GOL	C1-C2-C3-O3
6	A	1241	GOL	O1-C1-C2-C3
6	B	1236	GOL	C1-C2-C3-O3
6	A	1241	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1235	GOL	1	0
6	B	1236	GOL	3	0
6	A	1242	GOL	1	0
6	A	1239	GOL	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.