



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4PPK / pdb_00004ppk
Title : Crystal structure of eCGP123 T69V variant at pH 7.5
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Deposited on : 2014-02-27
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

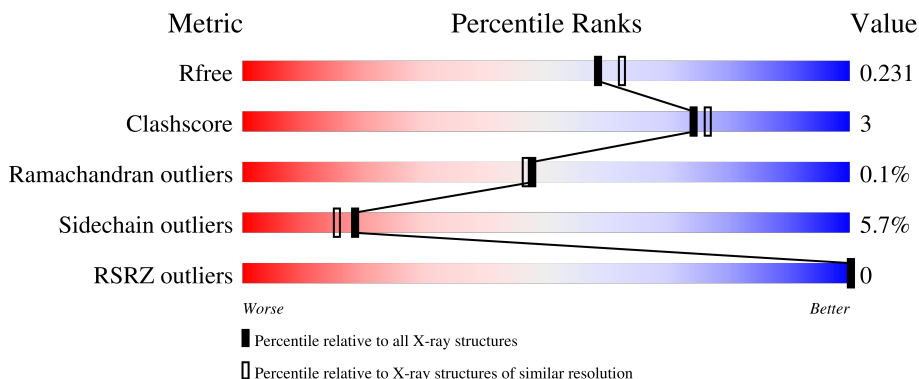
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


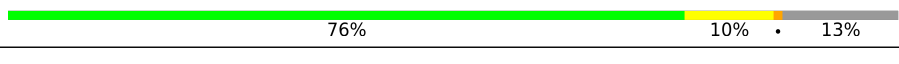
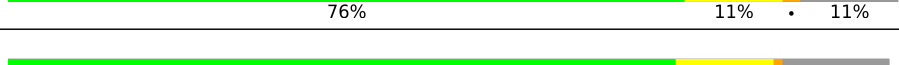

The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	245	 77% 11% • 11%
1	B	245	 76% 10% • 13%
1	C	245	 76% 11% • 11%
1	D	245	 75% 11% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7716 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 Monomeric Azami Green.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	Total 1792	C 1154	N 298	O 329	S 11	0	3	0
1	B	214	Total 1751	C 1124	N 292	O 325	S 10	0	0	0
1	C	218	Total 1815	C 1165	N 304	O 335	S 11	0	4	0
1	D	215	Total 1777	C 1139	N 299	O 329	S 10	0	2	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	164	Total 164	O 164	0	0
2	B	127	Total 127	O 127	0	0
2	C	138	Total 138	O 138	0	0
2	D	152	Total 152	O 152	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.98Å 81.33Å 73.93Å 90.00° 107.64° 90.00°	Depositor
Resolution (Å)	38.26 – 2.00 38.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.26-2.00) 98.7 (38.26-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0102, BUSTER 2.10.0	Depositor
R, R_{free}	0.194 , 0.259 0.203 , 0.231	Depositor DCC
R_{free} test set	2752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtrriage
Anisotropy	0.163	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.055 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7716	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 11.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CRQ

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	0.81	1/1823 (0.1%)	1.16	6/2455 (0.2%)
1	B	0.77	0/1772	1.13	3/2388 (0.1%)
1	C	0.73	1/1840 (0.1%)	1.13	2/2477 (0.1%)
1	D	0.75	0/1798	1.17	5/2421 (0.2%)
All	All	0.76	2/7233 (0.0%)	1.15	16/9741 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	146	MET	SD-CE	-5.66	1.65	1.79
1	A	146	MET	SD-CE	-5.33	1.66	1.79

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	PHE	CA-CB-CG	7.00	120.80	113.80
1	C	173	PHE	CA-CB-CG	6.98	120.78	113.80
1	A	114	PHE	CA-CB-CG	6.25	120.05	113.80
1	D	202	LYS	N-CA-C	6.14	118.76	111.33
1	A	173	PHE	CA-CB-CG	6.03	119.83	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1792	0	1760	8	0
1	B	1751	0	1699	12	0
1	C	1815	0	1773	16	0
1	D	1777	0	1728	14	0
2	A	164	0	0	1	0
2	B	127	0	0	0	0
2	C	138	0	0	1	0
2	D	152	0	0	0	0
All	All	7716	0	6960	44	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 3.

The worst 5 of 44 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:C:62:CRQ:C2	1:C:66:ARG:HH22	2.05	0.69
1:A:102:ILE:HD11	1:B:100:ILE:HG22	1.74	0.69
1:B:123:THR:HG23	1:B:124:ASN:HD22	1.59	0.67
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.84	0.59
1:A:16:GLY:HA3	1:A:120:PHE:O	2.03	0.59

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	215/245 (88%)	213 (99%)	2 (1%)	0	100	100
1	B	209/245 (85%)	205 (98%)	4 (2%)	0	100	100
1	C	217/245 (89%)	211 (97%)	5 (2%)	1 (0%)	24	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	212/245 (86%)	212 (100%)	0	0	100	100
All	All	853/980 (87%)	841 (99%)	11 (1%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	GLY

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	191/212 (90%)	177 (93%)	14 (7%)	13	9
1	B	185/212 (87%)	176 (95%)	9 (5%)	22	20
1	C	193/212 (91%)	181 (94%)	12 (6%)	16	13
1	D	188/212 (89%)	179 (95%)	9 (5%)	23	21
All	All	757/848 (89%)	713 (94%)	44 (6%)	18	15

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	170	ARG
1	D	66	ARG
1	C	180	LYS
1	C	185	LEU
1	D	73	LYS

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

Mol	Chain	Res	Type
1	D	124	ASN
1	D	158	ASN
1	C	65	ASN

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Mol	Chain	Res	Type
1	C	98	GLN
1	C	124	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](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	A	62	1	25,25,26	3.96	6 (24%)	28,34,36	2.53	6 (21%)
1	CRQ	C	62	1	25,25,26	3.95	5 (20%)	28,34,36	2.32	8 (28%)
1	CRQ	D	62	1	25,25,26	4.05	7 (28%)	28,34,36	2.21	5 (17%)
1	CRQ	B	62	1	25,25,26	3.92	5 (20%)	28,34,36	2.02	6 (21%)

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	CRQ	A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	C	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	D	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	B	62	1	-	1/10/32/33	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	CRQ	CA2-C2	-11.37	1.36	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	CRQ	CA2-C2	-11.00	1.36	1.48
1	B	62	CRQ	CA2-C2	-10.72	1.37	1.48
1	A	62	CRQ	CA2-C2	-10.61	1.37	1.48
1	B	62	CRQ	CA1-N1	9.98	1.49	1.27

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	CRQ	O2-C2-CA2	-8.36	125.69	131.02
1	C	62	CRQ	O2-C2-CA2	-7.86	126.00	131.02
1	D	62	CRQ	O2-C2-CA2	-7.62	126.16	131.02
1	A	62	CRQ	CA2-C2-N3	6.99	109.37	103.50
1	C	62	CRQ	CA2-C2-N3	6.22	108.73	103.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	CRQ	C3-CA3-N3-C2
1	C	62	CRQ	C3-CA3-N3-C2
1	B	62	CRQ	C3-CA3-N3-C2
1	D	62	CRQ	C3-CA3-N3-C2
1	C	62	CRQ	C3-CA3-N3-C1

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	62	CRQ	3	0
1	D	62	CRQ	3	0
1	B	62	CRQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	216/245 (88%)	-1.45	0 100 100	16, 30, 52, 76	3 (1%)
1	B	213/245 (86%)	-1.39	0 100 100	18, 32, 53, 74	0
1	C	217/245 (88%)	-1.23	0 100 100	20, 40, 65, 87	4 (1%)
1	D	214/245 (87%)	-1.27	0 100 100	16, 41, 63, 78	2 (0%)
All	All	860/980 (87%)	-1.34	0 100 100	16, 36, 61, 87	9 (1%)

There are no RSRZ outliers to report.

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	CRQ	C	62	24/25	0.98	0.04	29,32,37,39	0
1	CRQ	B	62	24/25	0.99	0.02	14,20,23,27	0
1	CRQ	A	62	24/25	0.99	0.02	17,22,27,29	0
1	CRQ	D	62	24/25	0.99	0.03	28,31,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.