



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:51 PM UTC

PDB ID : 2AWI / pdb_00002awi
Title : Structure of PrgX Y153C mutant
Authors : Shi, K.; Brown, C.K.; Gu, Z.Y.; Kozlowski, B.k.; Dunny, G.M.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2005-09-01
Resolution : 2.25 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

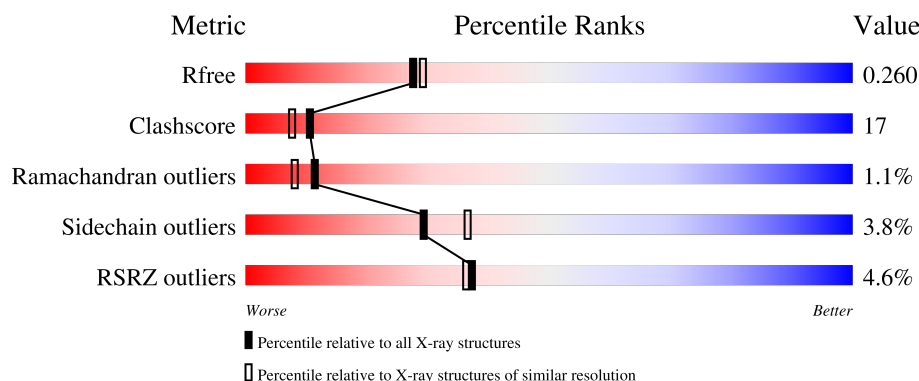
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



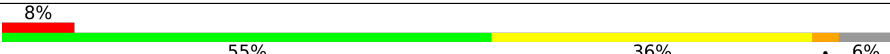
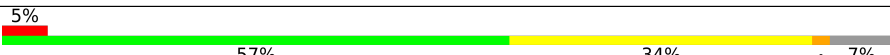
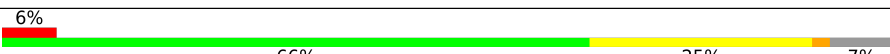
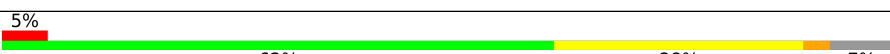
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	317	 3% 66% 26% 6%
1	B	317	 2% 62% 28% 6%
1	C	317	 3% 59% 32% 6%
1	D	317	 4% 60% 32% 6%
1	E	317	 3% 65% 25% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	317	
1	G	317	
1	H	317	
1	I	317	
1	J	317	
1	K	317	
1	L	317	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30035 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 PrgX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	Se	0	0	0
			2461	1596	397	462	2	4			
1	B	298	Total	C	N	O	S	Se	0	0	0
			2461	1596	397	462	2	4			
1	C	297	Total	C	N	O	S	Se	0	0	0
			2450	1587	396	461	2	4			
1	D	297	Total	C	N	O	S	Se	0	0	0
			2450	1587	396	461	2	4			
1	E	297	Total	C	N	O	S	Se	0	0	0
			2450	1587	396	461	2	4			
1	F	297	Total	C	N	O	S	Se	0	0	0
			2449	1587	396	460	2	4			
1	G	296	Total	C	N	O	S	Se	0	0	0
			2441	1581	394	460	2	4			
1	H	296	Total	C	N	O	S	Se	0	0	0
			2441	1581	394	460	2	4			
1	I	298	Total	C	N	O	S	Se	0	0	0
			2461	1596	397	462	2	4			
1	J	296	Total	C	N	O	S	Se	0	0	0
			2441	1581	394	460	2	4			
1	K	296	Total	C	N	O	S	Se	0	0	0
			2441	1581	394	460	2	4			
1	L	296	Total	C	N	O	S	Se	0	0	0
			2441	1581	394	460	2	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	MET	modified residue	UNP Q04114
A	67	MSE	MET	modified residue	UNP Q04114
A	153	CYS	TYR	engineered mutation	UNP Q04114
A	175	MSE	MET	modified residue	UNP Q04114
A	203	MSE	MET	modified residue	UNP Q04114

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	27	MSE	MET	modified residue	UNP Q04114
B	67	MSE	MET	modified residue	UNP Q04114
B	153	CYS	TYR	engineered mutation	UNP Q04114
B	175	MSE	MET	modified residue	UNP Q04114
B	203	MSE	MET	modified residue	UNP Q04114
C	27	MSE	MET	modified residue	UNP Q04114
C	67	MSE	MET	modified residue	UNP Q04114
C	153	CYS	TYR	engineered mutation	UNP Q04114
C	175	MSE	MET	modified residue	UNP Q04114
C	203	MSE	MET	modified residue	UNP Q04114
D	27	MSE	MET	modified residue	UNP Q04114
D	67	MSE	MET	modified residue	UNP Q04114
D	153	CYS	TYR	engineered mutation	UNP Q04114
D	175	MSE	MET	modified residue	UNP Q04114
D	203	MSE	MET	modified residue	UNP Q04114
E	27	MSE	MET	modified residue	UNP Q04114
E	67	MSE	MET	modified residue	UNP Q04114
E	153	CYS	TYR	engineered mutation	UNP Q04114
E	175	MSE	MET	modified residue	UNP Q04114
E	203	MSE	MET	modified residue	UNP Q04114
F	27	MSE	MET	modified residue	UNP Q04114
F	67	MSE	MET	modified residue	UNP Q04114
F	153	CYS	TYR	engineered mutation	UNP Q04114
F	175	MSE	MET	modified residue	UNP Q04114
F	203	MSE	MET	modified residue	UNP Q04114
G	27	MSE	MET	modified residue	UNP Q04114
G	67	MSE	MET	modified residue	UNP Q04114
G	153	CYS	TYR	engineered mutation	UNP Q04114
G	175	MSE	MET	modified residue	UNP Q04114
G	203	MSE	MET	modified residue	UNP Q04114
H	27	MSE	MET	modified residue	UNP Q04114
H	67	MSE	MET	modified residue	UNP Q04114
H	153	CYS	TYR	engineered mutation	UNP Q04114
H	175	MSE	MET	modified residue	UNP Q04114
H	203	MSE	MET	modified residue	UNP Q04114
I	27	MSE	MET	modified residue	UNP Q04114
I	67	MSE	MET	modified residue	UNP Q04114
I	153	CYS	TYR	engineered mutation	UNP Q04114
I	175	MSE	MET	modified residue	UNP Q04114
I	203	MSE	MET	modified residue	UNP Q04114
J	27	MSE	MET	modified residue	UNP Q04114
J	67	MSE	MET	modified residue	UNP Q04114

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	153	CYS	TYR	engineered mutation	UNP Q04114
J	175	MSE	MET	modified residue	UNP Q04114
J	203	MSE	MET	modified residue	UNP Q04114
K	27	MSE	MET	modified residue	UNP Q04114
K	67	MSE	MET	modified residue	UNP Q04114
K	153	CYS	TYR	engineered mutation	UNP Q04114
K	175	MSE	MET	modified residue	UNP Q04114
K	203	MSE	MET	modified residue	UNP Q04114
L	27	MSE	MET	modified residue	UNP Q04114
L	67	MSE	MET	modified residue	UNP Q04114
L	153	CYS	TYR	engineered mutation	UNP Q04114
L	175	MSE	MET	modified residue	UNP Q04114
L	203	MSE	MET	modified residue	UNP Q04114

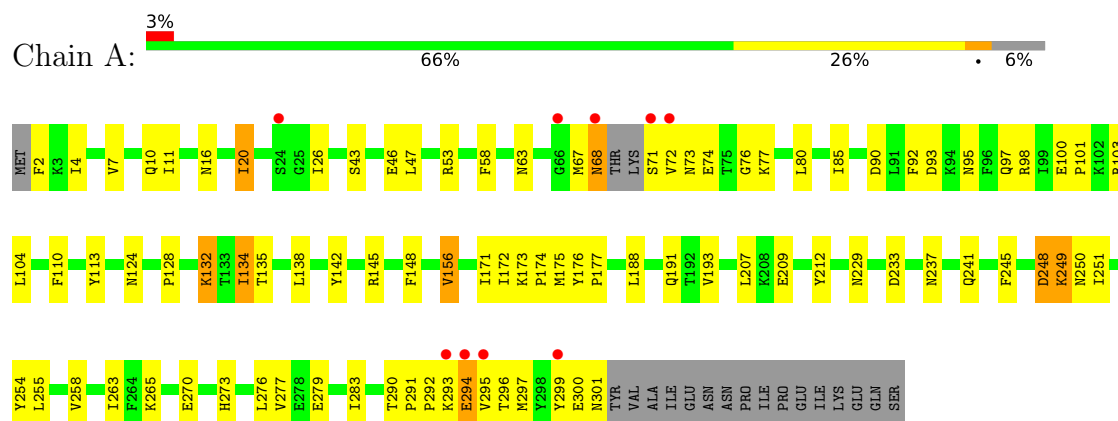
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	67	Total O 67 67	0	0
2	B	96	Total O 96 96	0	0
2	C	43	Total O 43 43	0	0
2	D	57	Total O 57 57	0	0
2	E	67	Total O 67 67	0	0
2	F	59	Total O 59 59	0	0
2	G	42	Total O 42 42	0	0
2	H	37	Total O 37 37	0	0
2	I	23	Total O 23 23	0	0
2	J	47	Total O 47 47	0	0
2	K	77	Total O 77 77	0	0
2	L	33	Total O 33 33	0	0

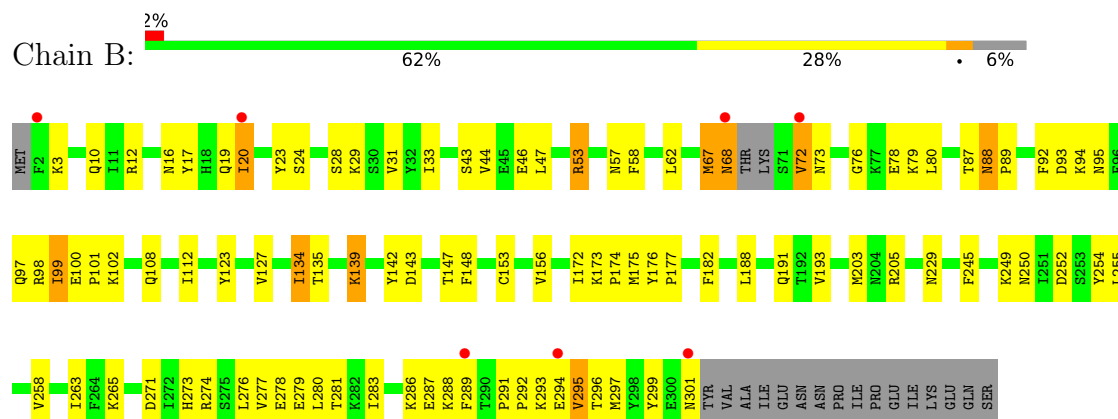
3 Residue-property plots

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 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.

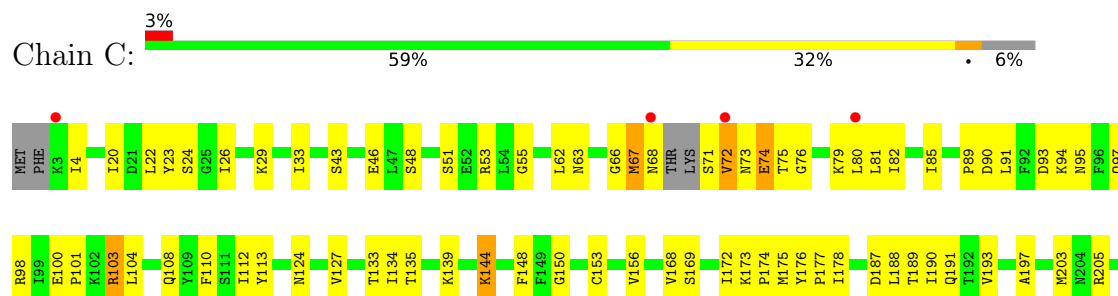
• Molecule 1: PrgX

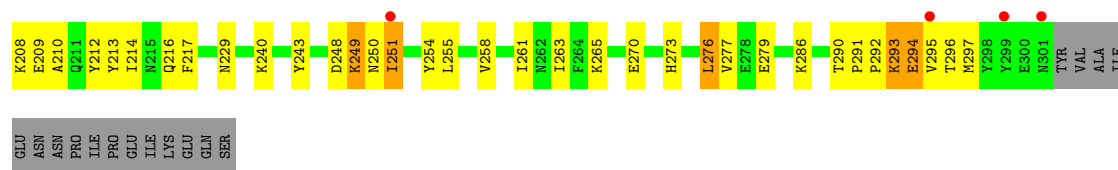


• Molecule 1: PrgX

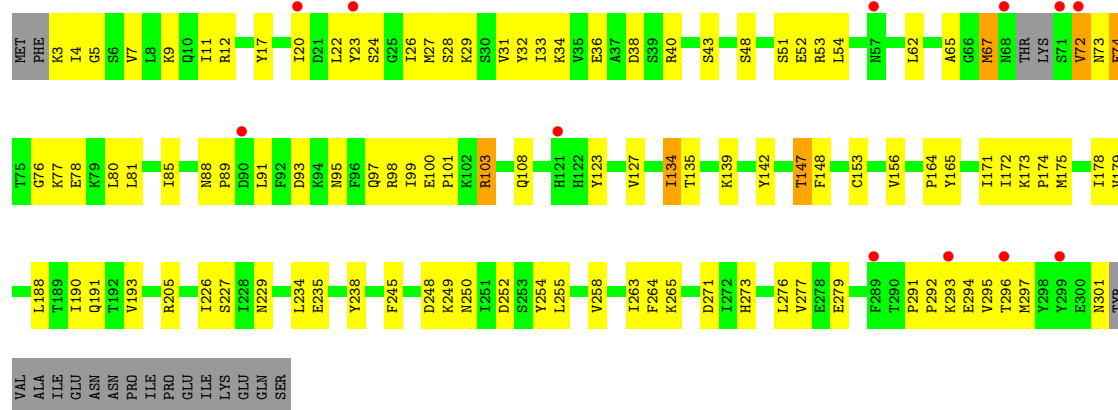


• Molecule 1: PrgX

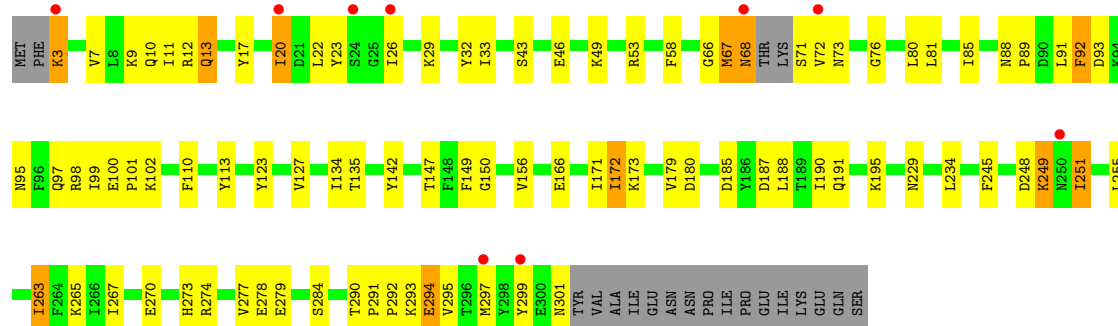




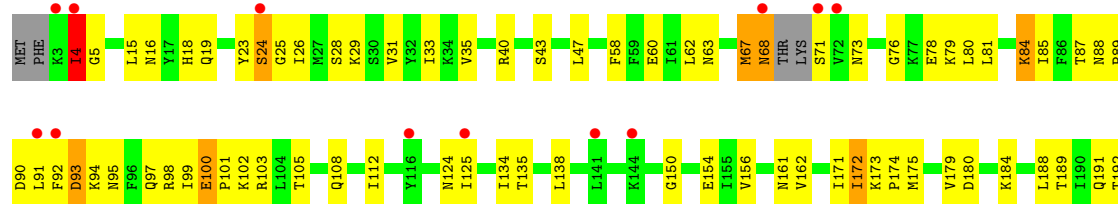
• Molecule 1: PrgX

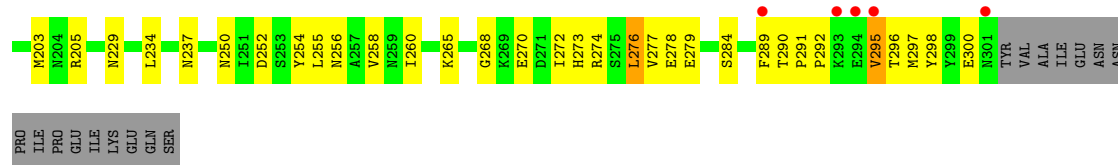


• Molecule 1: PrgX



• Molecule 1: PrgX

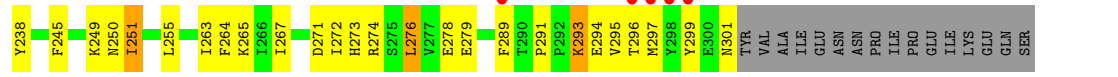




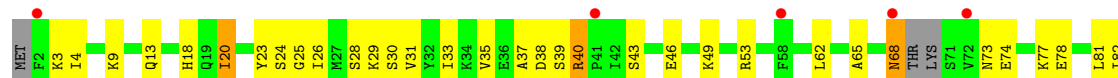
• Molecule 1: PrgX

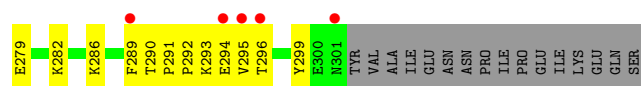


• Molecule 1: PrgX

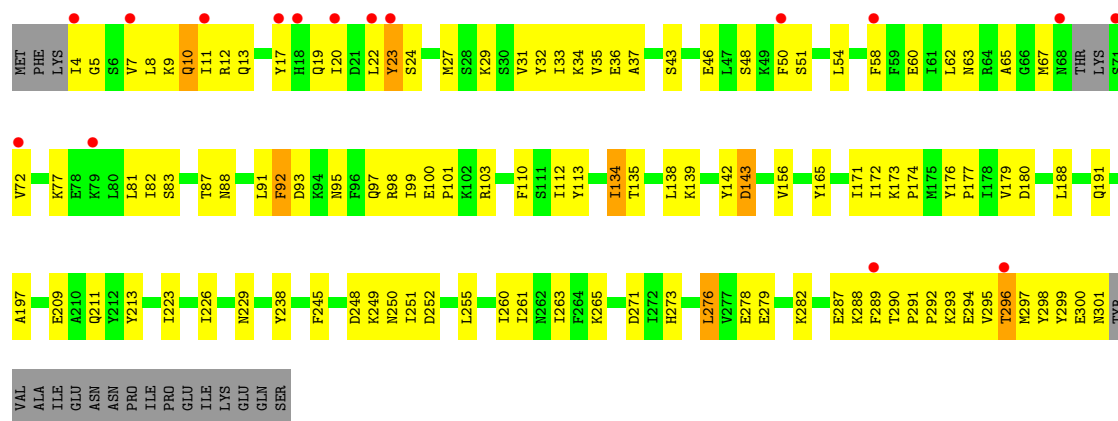


• Molecule 1: PrgX

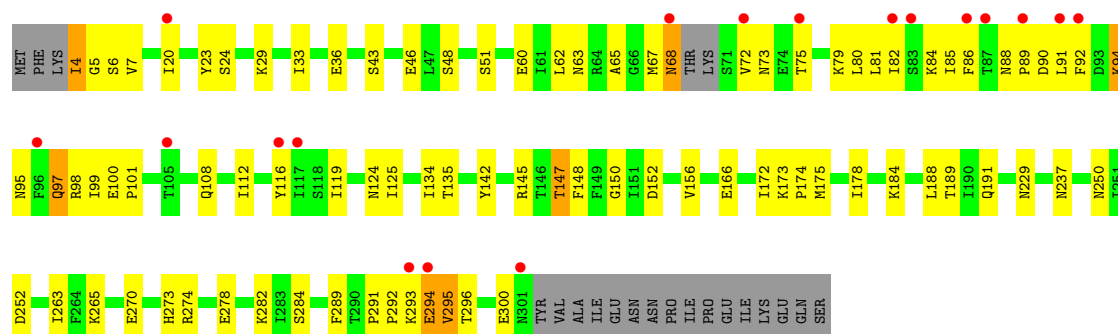




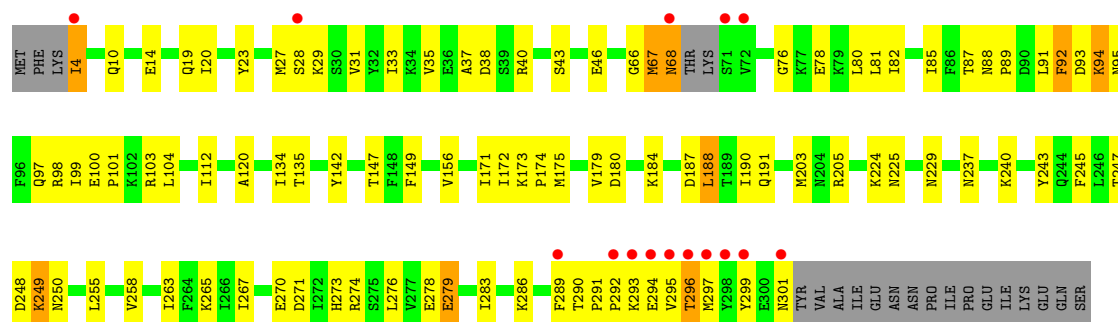
• Molecule 1: PrgX



• Molecule 1: PrgX



• Molecule 1: PrgX



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.53Å 134.37Å 195.20Å 90.00° 100.28° 90.00°	Depositor
Resolution (Å)	29.90 – 2.25 29.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.90-2.25) 95.6 (29.90-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.271 0.234 , 0.260	Depositor DCC
R_{free} test set	10751 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30035	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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](#)

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	0.38	0/2506	0.86	5/3376 (0.1%)
1	B	0.38	0/2506	0.87	7/3376 (0.2%)
1	C	0.36	0/2494	0.84	7/3360 (0.2%)
1	D	0.36	0/2494	0.83	4/3360 (0.1%)
1	E	0.36	0/2494	0.86	5/3360 (0.1%)
1	F	0.34	0/2493	0.86	6/3359 (0.2%)
1	G	0.33	0/2485	0.88	7/3349 (0.2%)
1	H	0.35	0/2485	0.85	3/3349 (0.1%)
1	I	0.33	0/2506	0.83	3/3376 (0.1%)
1	J	0.36	0/2485	0.84	4/3349 (0.1%)
1	K	0.36	0/2485	0.80	0/3349
1	L	0.36	0/2485	0.84	2/3349 (0.1%)
All	All	0.36	0/29918	0.85	53/40312 (0.1%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	VAL	CA-C-N	7.46	127.17	119.56
1	E	127	VAL	C-N-CA	7.46	127.17	119.56
1	B	134	ILE	N-CA-C	7.01	117.72	110.36
1	B	295	VAL	N-CA-C	6.62	116.75	110.53
1	B	127	VAL	CA-C-N	6.60	126.54	119.28

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	2461	0	2493	77	0
1	B	2461	0	2493	80	0
1	C	2450	0	2484	88	0
1	D	2450	0	2484	79	0
1	E	2450	0	2484	82	0
1	F	2449	0	2484	94	0
1	G	2441	0	2471	82	0
1	H	2441	0	2471	91	0
1	I	2461	0	2493	126	0
1	J	2441	0	2471	94	0
1	K	2441	0	2471	76	0
1	L	2441	0	2471	84	0
2	A	67	0	0	10	0
2	B	96	0	0	8	0
2	C	43	0	0	2	0
2	D	57	0	0	4	0
2	E	67	0	0	5	0
2	F	59	0	0	8	0
2	G	42	0	0	2	0
2	H	37	0	0	2	0
2	I	23	0	0	6	0
2	J	47	0	0	8	0
2	K	77	0	0	10	0
2	L	33	0	0	3	0
All	All	30035	0	29770	992	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 17.

The worst 5 of 992 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:K:82:ILE:HD11	1:K:112:ILE:HG23	1.35	1.08
1:K:263:ILE:HG13	1:L:263:ILE:HG13	1.42	1.01
1:A:263:ILE:HG13	1:B:263:ILE:HG13	1.42	0.99
1:J:62:LEU:HB3	1:J:67:MSE:HG3	1.44	0.97
1:I:20:ILE:HD12	1:I:20:ILE:H	1.25	0.97

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	294/317 (93%)	281 (96%)	10 (3%)	3 (1%)	12	10
1	B	294/317 (93%)	281 (96%)	11 (4%)	2 (1%)	18	17
1	C	293/317 (92%)	276 (94%)	10 (3%)	7 (2%)	4	2
1	D	293/317 (92%)	274 (94%)	17 (6%)	2 (1%)	18	17
1	E	293/317 (92%)	277 (94%)	13 (4%)	3 (1%)	12	10
1	F	293/317 (92%)	269 (92%)	21 (7%)	3 (1%)	12	10
1	G	292/317 (92%)	273 (94%)	16 (6%)	3 (1%)	12	10
1	H	292/317 (92%)	278 (95%)	11 (4%)	3 (1%)	12	10
1	I	294/317 (93%)	262 (89%)	27 (9%)	5 (2%)	7	3
1	J	292/317 (92%)	271 (93%)	18 (6%)	3 (1%)	12	10
1	K	292/317 (92%)	267 (91%)	22 (8%)	3 (1%)	12	10
1	L	292/317 (92%)	272 (93%)	17 (6%)	3 (1%)	12	10
All	All	3514/3804 (92%)	3281 (93%)	193 (6%)	40 (1%)	11	8

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	C	72	VAL
1	C	249	LYS
1	E	92	PHE
1	F	24	SER

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	281/295 (95%)	270 (96%)	11 (4%)	28	35
1	B	281/295 (95%)	266 (95%)	15 (5%)	20	22
1	C	280/295 (95%)	271 (97%)	9 (3%)	34	43
1	D	280/295 (95%)	273 (98%)	7 (2%)	42	52
1	E	280/295 (95%)	269 (96%)	11 (4%)	28	35
1	F	280/295 (95%)	272 (97%)	8 (3%)	37	47
1	G	279/295 (95%)	267 (96%)	12 (4%)	26	31
1	H	279/295 (95%)	267 (96%)	12 (4%)	26	31
1	I	281/295 (95%)	272 (97%)	9 (3%)	34	43
1	J	279/295 (95%)	270 (97%)	9 (3%)	34	43
1	K	279/295 (95%)	269 (96%)	10 (4%)	31	39
1	L	279/295 (95%)	266 (95%)	13 (5%)	23	26
All	All	3358/3540 (95%)	3232 (96%)	126 (4%)	29	36

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	100	GLU
1	K	188	LEU
1	G	277	VAL
1	K	166	GLU
1	L	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	262	ASN
1	J	215	ASN
1	I	95	ASN
1	I	237	ASN
1	K	97	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	294/317 (92%)	0.07	9 (3%) 51 51	17, 40, 79, 114	0
1	B	294/317 (92%)	0.02	7 (2%) 59 61	12, 39, 75, 117	0
1	C	293/317 (92%)	0.39	8 (2%) 56 57	25, 52, 93, 113	0
1	D	293/317 (92%)	0.23	12 (4%) 41 41	20, 46, 88, 119	0
1	E	293/317 (92%)	0.24	9 (3%) 51 51	22, 45, 86, 114	0
1	F	293/317 (92%)	0.46	17 (5%) 29 27	24, 52, 98, 118	0
1	G	292/317 (92%)	0.56	16 (5%) 30 29	27, 56, 95, 112	0
1	H	292/317 (92%)	0.42	11 (3%) 44 44	25, 52, 95, 130	0
1	I	294/317 (92%)	0.67	24 (8%) 17 16	29, 64, 110, 124	0
1	J	292/317 (92%)	0.37	16 (5%) 30 29	23, 49, 98, 114	0
1	K	292/317 (92%)	0.35	18 (6%) 26 24	22, 47, 95, 112	0
1	L	292/317 (92%)	0.41	15 (5%) 33 32	23, 49, 89, 126	0
All	All	3514/3804 (92%)	0.35	162 (4%) 37 36	12, 49, 96, 130	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	289	PHE	5.6
1	L	72	VAL	5.3
1	G	4	ILE	4.9
1	H	289	PHE	4.9
1	G	72	VAL	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.