



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:27 PM UTC

PDB ID : 2AXU / pdb_00002axu
Title : Structure of PrgX
Authors : Shi, K.; Brown, C.K.; Gu, Z.Y.; Kozlowicz, B.K.; Dunny, G.M.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2005-09-06
Resolution : 2.90 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

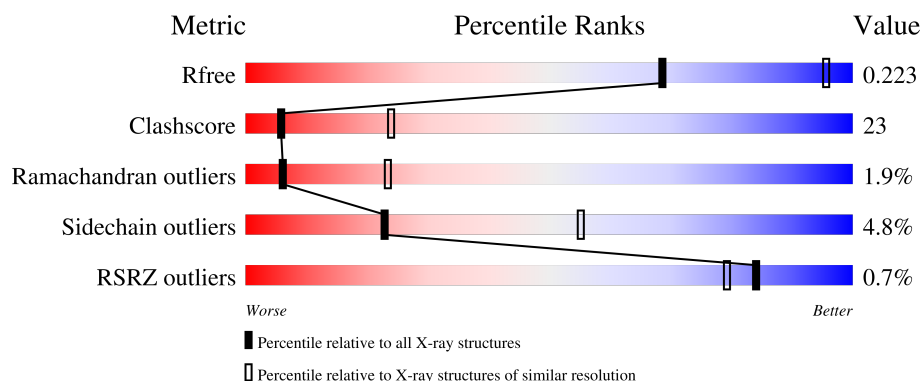
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	61% 32% • •
1	B	317	55% 37% • 5%
1	C	317	% 51% 38% • 6%
1	D	317	% 59% 32% • 6%
1	E	317	% 58% 32% • 5%

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Mol	Chain	Length	Quality of chain
1	F	317	% 56% 33% 5% • 5%
1	G	317	% 49% 39% 7% •
1	H	317	% 53% 36% 5% 6%
1	I	317	% 46% 43% 5% 5%
1	J	317	% 51% 39% • 7%
1	K	317	54% 38% • 6%
1	L	317	53% 38% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30147 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	303	Total	C	N	O	S	Se	0	0	0
			2507	1630	402	469	1	5			
1	B	300	Total	C	N	O	S	Se	0	0	0
			2486	1616	399	466	1	4			
1	C	299	Total	C	N	O	S	Se	0	0	0
			2475	1607	398	465	1	4			
1	D	298	Total	C	N	O	S	Se	0	0	0
			2468	1602	397	464	1	4			
1	E	300	Total	C	N	O	S	Se	0	0	0
			2480	1610	399	466	1	4			
1	F	301	Total	C	N	O	S	Se	0	0	0
			2488	1616	400	467	1	4			
1	G	303	Total	C	N	O	S	Se	0	0	0
			2508	1630	402	471	1	4			
1	H	298	Total	C	N	O	S	Se	0	0	0
			2468	1602	397	464	1	4			
1	I	300	Total	C	N	O	S	Se	0	0	0
			2486	1616	399	466	1	4			
1	J	296	Total	C	N	O	S	Se	0	0	0
			2447	1587	394	461	1	4			
1	K	299	Total	C	N	O	S	Se	0	0	0
			2471	1604	397	465	1	4			
1	L	299	Total	C	N	O	S	Se	0	0	0
			2479	1611	398	465	1	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q04114
A	27	MSE	MET	modified residue	UNP Q04114
A	67	MSE	MET	modified residue	UNP Q04114
A	175	MSE	MET	modified residue	UNP Q04114
A	203	MSE	MET	modified residue	UNP Q04114

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	MET	modified residue	UNP Q04114
B	27	MSE	MET	modified residue	UNP Q04114
B	67	MSE	MET	modified residue	UNP Q04114
B	175	MSE	MET	modified residue	UNP Q04114
B	203	MSE	MET	modified residue	UNP Q04114
C	1	MSE	MET	modified residue	UNP Q04114
C	27	MSE	MET	modified residue	UNP Q04114
C	67	MSE	MET	modified residue	UNP Q04114
C	175	MSE	MET	modified residue	UNP Q04114
C	203	MSE	MET	modified residue	UNP Q04114
D	1	MSE	MET	modified residue	UNP Q04114
D	27	MSE	MET	modified residue	UNP Q04114
D	67	MSE	MET	modified residue	UNP Q04114
D	175	MSE	MET	modified residue	UNP Q04114
D	203	MSE	MET	modified residue	UNP Q04114
E	1	MSE	MET	modified residue	UNP Q04114
E	27	MSE	MET	modified residue	UNP Q04114
E	67	MSE	MET	modified residue	UNP Q04114
E	175	MSE	MET	modified residue	UNP Q04114
E	203	MSE	MET	modified residue	UNP Q04114
F	1	MSE	MET	modified residue	UNP Q04114
F	27	MSE	MET	modified residue	UNP Q04114
F	67	MSE	MET	modified residue	UNP Q04114
F	175	MSE	MET	modified residue	UNP Q04114
F	203	MSE	MET	modified residue	UNP Q04114
G	1	MSE	MET	modified residue	UNP Q04114
G	27	MSE	MET	modified residue	UNP Q04114
G	67	MSE	MET	modified residue	UNP Q04114
G	175	MSE	MET	modified residue	UNP Q04114
G	203	MSE	MET	modified residue	UNP Q04114
H	1	MSE	MET	modified residue	UNP Q04114
H	27	MSE	MET	modified residue	UNP Q04114
H	67	MSE	MET	modified residue	UNP Q04114
H	175	MSE	MET	modified residue	UNP Q04114
H	203	MSE	MET	modified residue	UNP Q04114
I	1	MSE	MET	modified residue	UNP Q04114
I	27	MSE	MET	modified residue	UNP Q04114
I	67	MSE	MET	modified residue	UNP Q04114
I	175	MSE	MET	modified residue	UNP Q04114
I	203	MSE	MET	modified residue	UNP Q04114
J	1	MSE	MET	modified residue	UNP Q04114
J	27	MSE	MET	modified residue	UNP Q04114

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Chain	Residue	Modelled	Actual	Comment	Reference
J	67	MSE	MET	modified residue	UNP Q04114
J	175	MSE	MET	modified residue	UNP Q04114
J	203	MSE	MET	modified residue	UNP Q04114
K	1	MSE	MET	modified residue	UNP Q04114
K	27	MSE	MET	modified residue	UNP Q04114
K	67	MSE	MET	modified residue	UNP Q04114
K	175	MSE	MET	modified residue	UNP Q04114
K	203	MSE	MET	modified residue	UNP Q04114
L	1	MSE	MET	modified residue	UNP Q04114
L	27	MSE	MET	modified residue	UNP Q04114
L	67	MSE	MET	modified residue	UNP Q04114
L	175	MSE	MET	modified residue	UNP Q04114
L	203	MSE	MET	modified residue	UNP Q04114

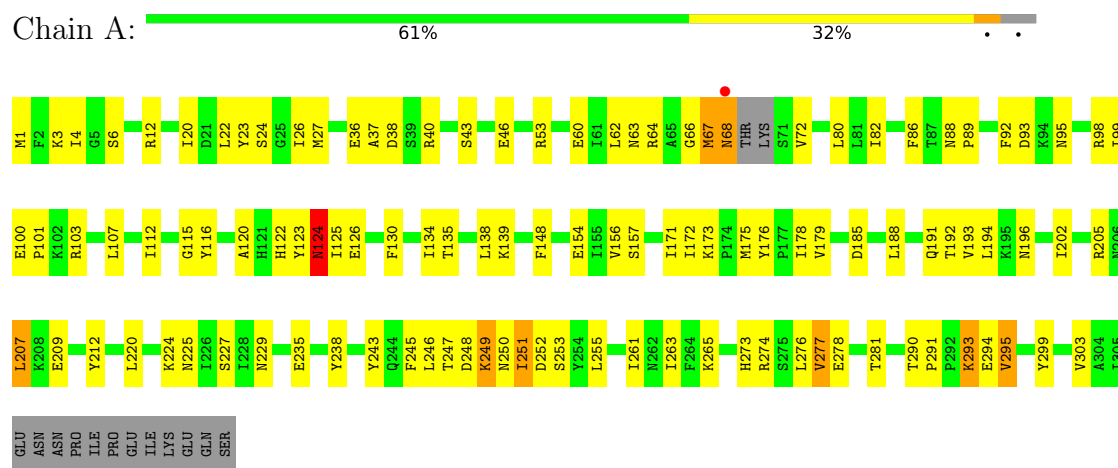
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	45	Total O 45 45	0	0
2	C	25	Total O 25 25	0	0
2	D	29	Total O 29 29	0	0
2	E	33	Total O 33 33	0	0
2	F	42	Total O 42 42	0	0
2	G	28	Total O 28 28	0	0
2	H	36	Total O 36 36	0	0
2	I	23	Total O 23 23	0	0
2	J	28	Total O 28 28	0	0
2	K	28	Total O 28 28	0	0
2	L	30	Total O 30 30	0	0

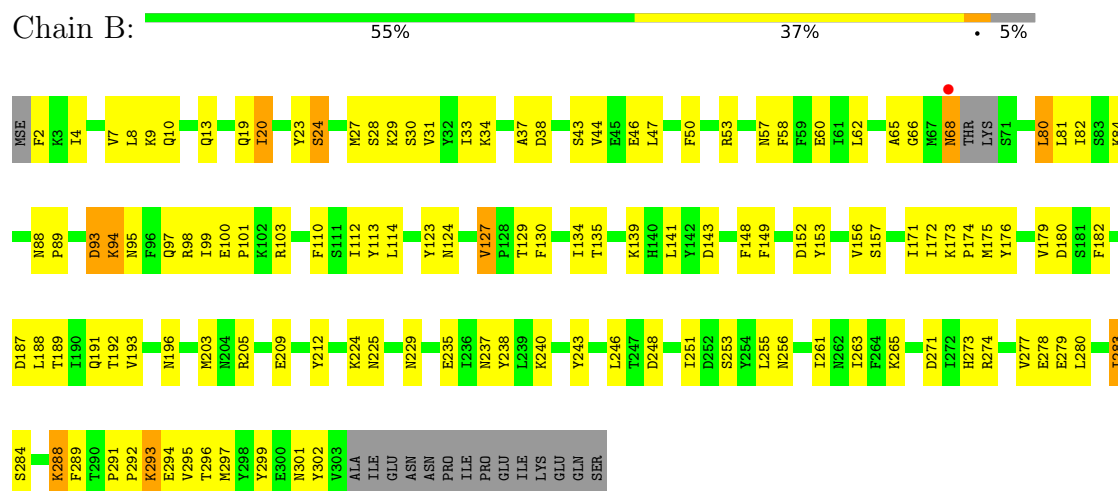
3 Residue-property plots

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

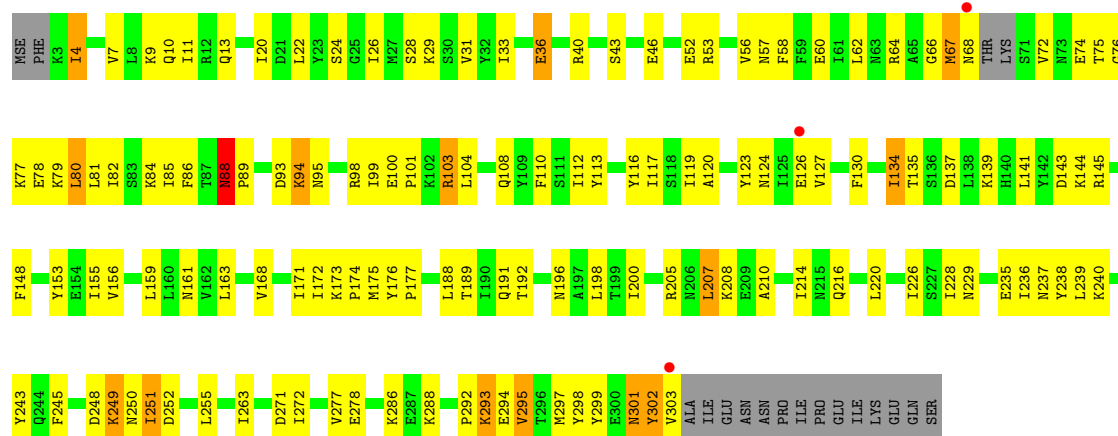


• Molecule 1: PrgX

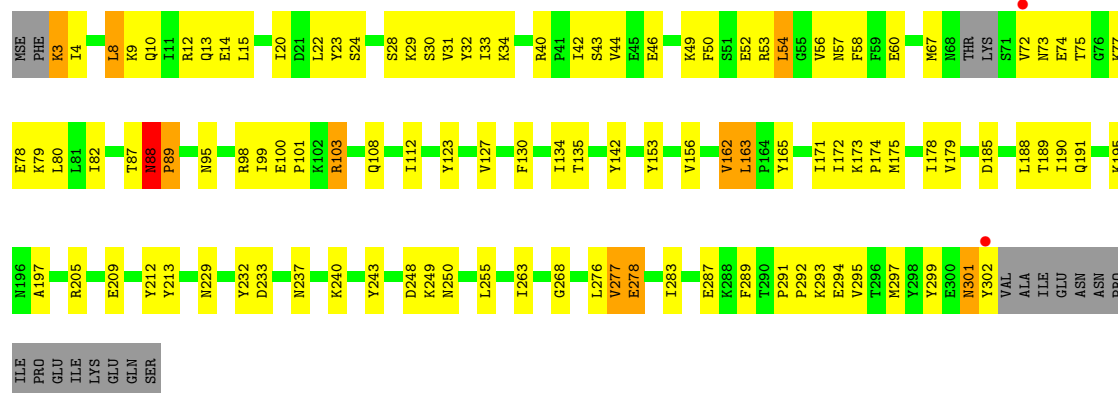


• Molecule 1: PrgX

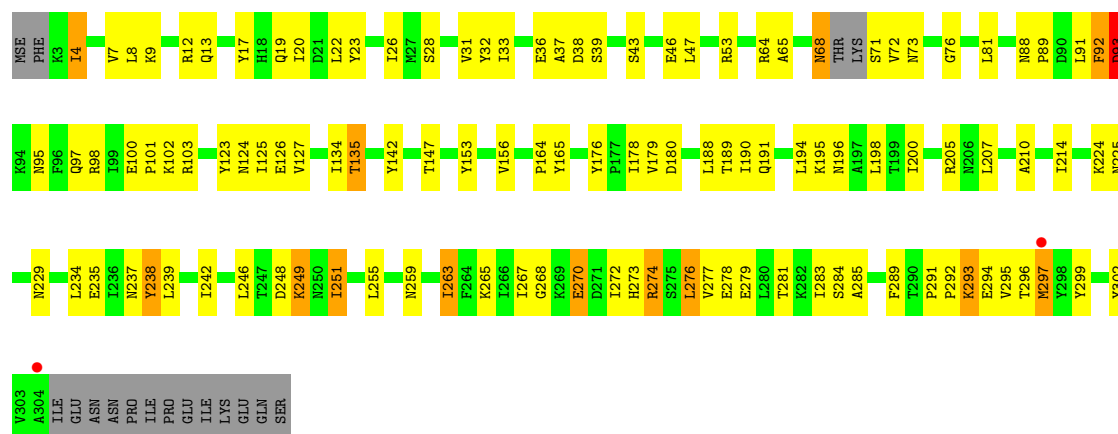




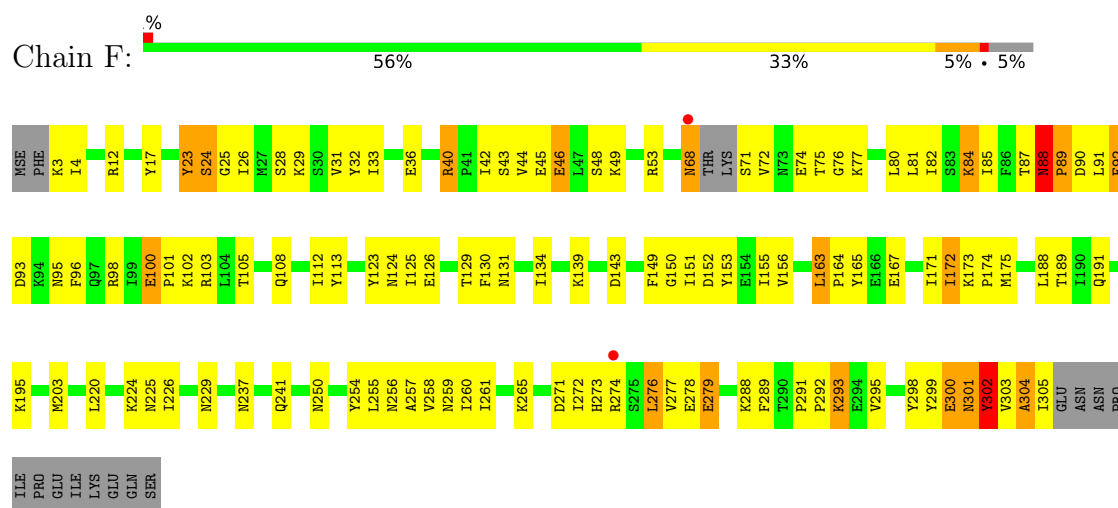
• Molecule 1: PrgX



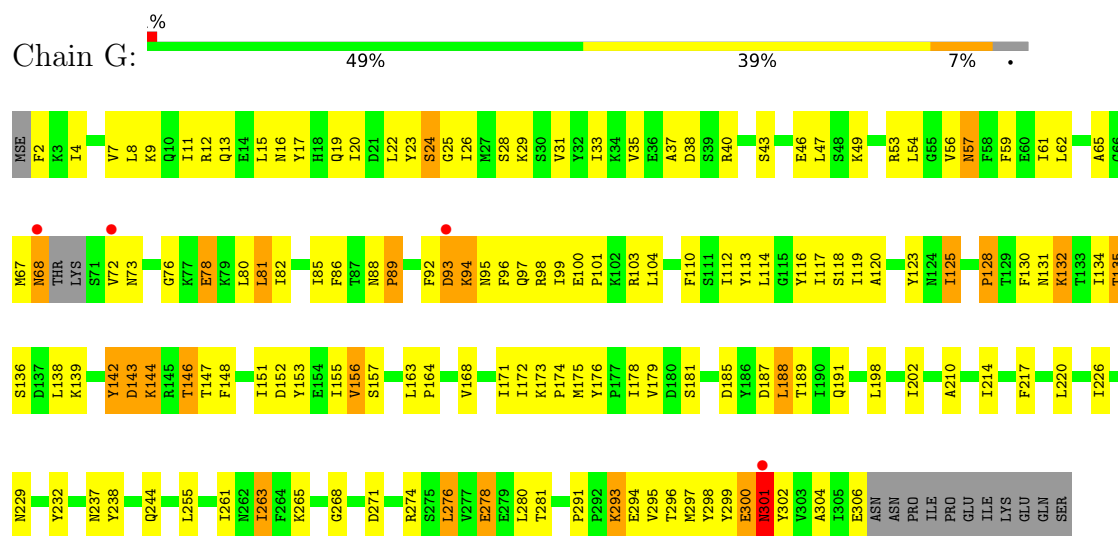
• Molecule 1: PrgX



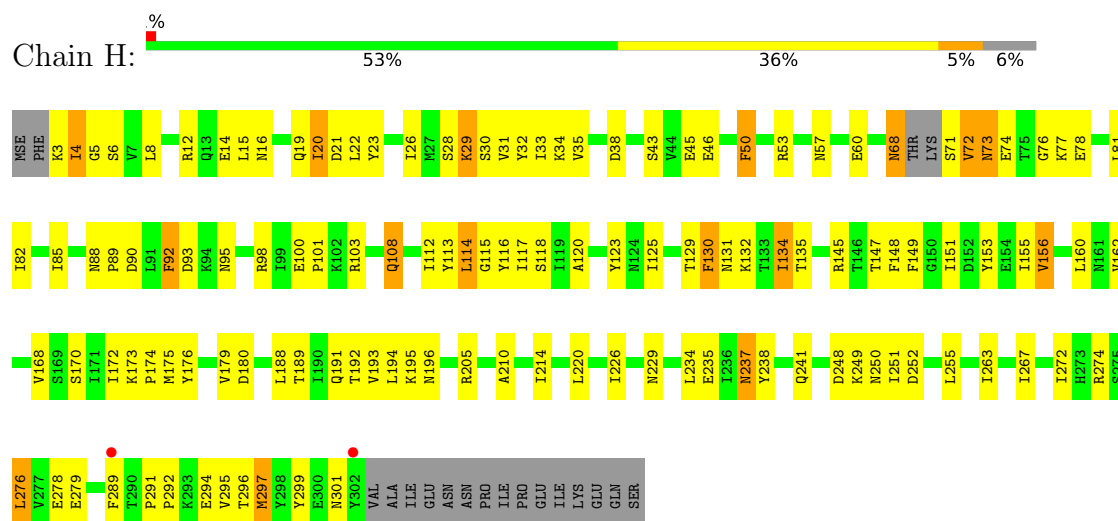
• Molecule 1: PrgX



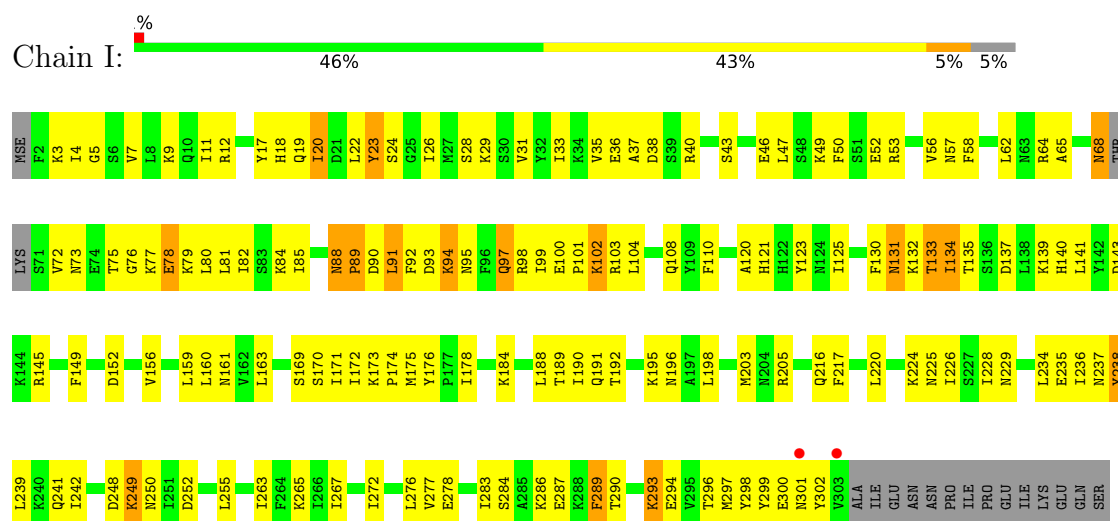
• Molecule 1: PrgX



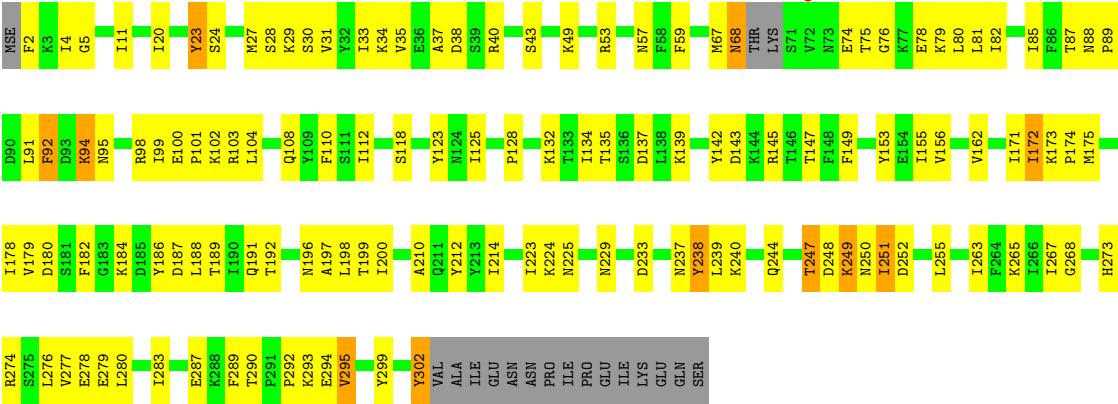
• Molecule 1: PrgX



• Molecule 1: PrgX



Chain L: 53% 38% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.65Å 134.72Å 195.93Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.90) 99.1 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.266 0.197 , 0.223	Depositor DCC
R_{free} test set	10564 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.1	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	0.94	EDS
Total number of atoms	30147	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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

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	0.35	0/2554	0.87	6/3442 (0.2%)
1	B	0.34	0/2533	0.88	6/3414 (0.2%)
1	C	0.32	0/2521	0.84	1/3398 (0.0%)
1	D	0.34	0/2514	0.89	7/3388 (0.2%)
1	E	0.34	0/2526	0.88	9/3405 (0.3%)
1	F	0.32	0/2534	0.91	7/3416 (0.2%)
1	G	0.48	3/2555 (0.1%)	0.91	6/3444 (0.2%)
1	H	0.34	0/2514	0.89	2/3388 (0.1%)
1	I	0.32	0/2533	0.84	5/3414 (0.1%)
1	J	0.34	0/2492	0.87	3/3359 (0.1%)
1	K	0.34	0/2517	0.87	6/3394 (0.2%)
1	L	0.33	0/2526	0.88	5/3404 (0.1%)
All	All	0.35	3/30319 (0.0%)	0.88	63/40866 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	301	ASN	CA-C	-8.63	1.41	1.52
1	G	300	GLU	N-CA	-6.78	1.38	1.46
1	G	300	GLU	C-O	6.13	1.31	1.24

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	ALA	N-CA-C	-9.84	101.45	112.57
1	G	300	GLU	N-CA-C	-9.54	99.38	111.02
1	H	6	SER	N-CA-C	-9.35	100.97	111.82
1	F	172	ILE	N-CA-C	8.46	118.48	110.53
1	C	4	ILE	N-CA-C	8.38	119.17	110.62

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	2507	0	2543	93	0
1	B	2486	0	2515	112	0
1	C	2475	0	2506	126	0
1	D	2468	0	2497	94	0
1	E	2480	0	2511	101	0
1	F	2488	0	2522	129	0
1	G	2508	0	2537	159	0
1	H	2468	0	2497	135	0
1	I	2486	0	2515	153	0
1	J	2447	0	2475	122	0
1	K	2471	0	2498	102	0
1	L	2479	0	2506	117	0
2	A	37	0	0	11	0
2	B	45	0	0	6	0
2	C	25	0	0	11	0
2	D	29	0	0	6	0
2	E	33	0	0	6	0
2	F	42	0	0	6	0
2	G	28	0	0	19	0
2	H	36	0	0	5	0
2	I	23	0	0	10	0
2	J	28	0	0	5	0
2	K	28	0	0	12	0
2	L	30	0	0	6	0
All	All	30147	0	30122	1380	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 23.

The worst 5 of 1380 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:B:156:VAL:HG21	1:B:175:MSE:HE1	1.21	1.19
1:I:93:ASP:HB3	1:I:97:GLN:HE22	1.21	1.03
1:H:4:ILE:HG21	1:H:38:ASP:HA	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ILE:HG13	1:D:263:ILE:HG13	1.42	1.01
1:B:20:ILE:HD12	1:B:20:ILE:H	1.24	0.99

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	299/317 (94%)	273 (91%)	23 (8%)	3 (1%)	12	39
1	B	296/317 (93%)	279 (94%)	15 (5%)	2 (1%)	18	48
1	C	295/317 (93%)	251 (85%)	32 (11%)	12 (4%)	2	9
1	D	294/317 (93%)	275 (94%)	14 (5%)	5 (2%)	7	26
1	E	296/317 (93%)	271 (92%)	20 (7%)	5 (2%)	7	26
1	F	297/317 (94%)	266 (90%)	23 (8%)	8 (3%)	4	16
1	G	299/317 (94%)	257 (86%)	32 (11%)	10 (3%)	3	13
1	H	294/317 (93%)	268 (91%)	18 (6%)	8 (3%)	4	16
1	I	296/317 (93%)	257 (87%)	33 (11%)	6 (2%)	6	22
1	J	292/317 (92%)	259 (89%)	30 (10%)	3 (1%)	12	39
1	K	295/317 (93%)	274 (93%)	17 (6%)	4 (1%)	9	30
1	L	295/317 (93%)	269 (91%)	24 (8%)	2 (1%)	18	48
All	All	3548/3804 (93%)	3199 (90%)	281 (8%)	68 (2%)	6	23

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	C	72	VAL
1	C	88	ASN

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Mol	Chain	Res	Type
1	C	249	LYS
1	D	88	ASN

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	285/294 (97%)	270 (95%)	15 (5%)	20	52
1	B	283/294 (96%)	271 (96%)	12 (4%)	26	60
1	C	282/294 (96%)	266 (94%)	16 (6%)	18	49
1	D	281/294 (96%)	271 (96%)	10 (4%)	31	65
1	E	282/294 (96%)	266 (94%)	16 (6%)	18	49
1	F	283/294 (96%)	271 (96%)	12 (4%)	26	60
1	G	285/294 (97%)	265 (93%)	20 (7%)	14	40
1	H	281/294 (96%)	267 (95%)	14 (5%)	22	53
1	I	283/294 (96%)	270 (95%)	13 (5%)	24	57
1	J	279/294 (95%)	264 (95%)	15 (5%)	20	51
1	K	281/294 (96%)	272 (97%)	9 (3%)	34	68
1	L	282/294 (96%)	270 (96%)	12 (4%)	26	60
All	All	3387/3528 (96%)	3223 (95%)	164 (5%)	23	55

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	20	ILE
1	K	68	ASN
1	I	94	LYS
1	J	93	ASP
1	K	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	97	GLN
1	K	158	ASN
1	I	211	GLN
1	J	131	ASN
1	K	259	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](#)

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	298/317 (94%)	-0.58	1 (0%) 90 87	19, 42, 99, 133	0
1	B	296/317 (93%)	-0.55	1 (0%) 90 87	15, 42, 95, 193	0
1	C	295/317 (93%)	-0.26	3 (1%) 79 73	19, 60, 121, 160	0
1	D	294/317 (92%)	-0.44	2 (0%) 84 79	19, 56, 110, 189	0
1	E	296/317 (93%)	-0.53	2 (0%) 84 79	16, 47, 98, 132	0
1	F	297/317 (93%)	-0.36	2 (0%) 84 79	18, 53, 116, 167	0
1	G	299/317 (94%)	-0.28	4 (1%) 75 67	23, 57, 121, 159	0
1	H	294/317 (92%)	-0.41	2 (0%) 84 79	18, 52, 111, 169	0
1	I	296/317 (93%)	-0.27	2 (0%) 84 79	28, 66, 134, 169	0
1	J	292/317 (92%)	-0.42	3 (1%) 79 73	24, 56, 119, 171	0
1	K	295/317 (93%)	-0.36	1 (0%) 90 87	17, 51, 112, 169	0
1	L	295/317 (93%)	-0.46	1 (0%) 90 87	16, 52, 103, 149	0
All	All	3547/3804 (93%)	-0.41	24 (0%) 84 79	15, 53, 114, 193	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	VAL	3.1
1	G	301	ASN	2.9
1	J	289	PHE	2.8
1	G	72	VAL	2.8
1	E	304	ALA	2.7

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.