



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:03 am GMT

PDB ID : 3WST
Title : Crystal structure of C.elegans PRMT7 in complex with SAH(P31)
Authors : Hasegawa, M.; Toma-fukai, S.; Shimizu, T.
Deposited on : 2014-03-21
Resolution : 2.39 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28972

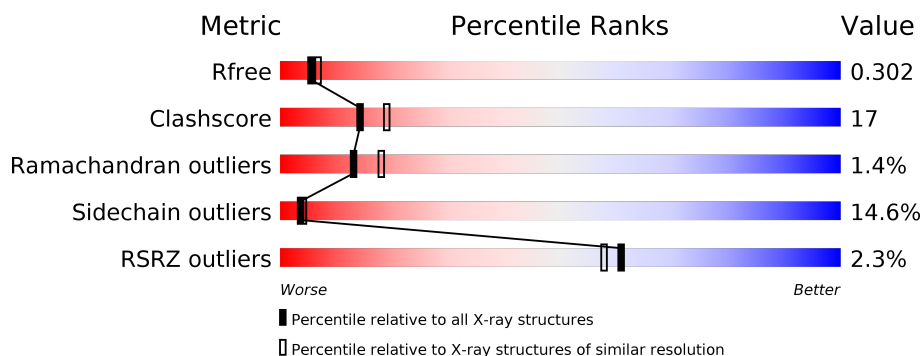
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	655	
1	B	655	
1	C	655	
1	D	655	
1	E	655	
1	F	655	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	655	
1	H	655	
1	I	655	
1	J	655	
1	K	655	
1	L	655	
1	M	655	
1	N	655	
1	O	655	
1	P	655	
1	Q	655	
1	R	655	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 92645 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 Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	D	637	Total	C	N	O	S	0	0	0
			5078	3231	852	968	27			
1	B	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	C	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	F	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	E	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	G	636	Total	C	N	O	S	0	0	0
			5070	3227	850	966	27			
1	H	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	I	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			
1	M	633	Total	C	N	O	S	0	0	0
			5049	3216	844	962	27			
1	N	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	O	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	P	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	Q	632	Total	C	N	O	S	0	0	0
			5039	3209	845	958	27			
1	R	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	J	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	L	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
A	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
A	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
A	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
A	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
D	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
D	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
D	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
D	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
D	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
D	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
D	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
D	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
B	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
B	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
B	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
B	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
B	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
B	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
B	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
B	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
C	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
C	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
C	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
C	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
C	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
C	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
C	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
C	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
F	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
F	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
F	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
F	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
F	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
F	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
F	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
E	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
E	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
E	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
E	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
E	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
E	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
E	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
E	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
G	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
G	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
G	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
G	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
G	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
G	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
G	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
G	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
H	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
H	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
H	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
H	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
H	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
H	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
H	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
H	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
I	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
I	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
I	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
I	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
I	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
I	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
I	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
I	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
M	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
M	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
M	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
M	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42

Continued on next page...

Continued from previous page...

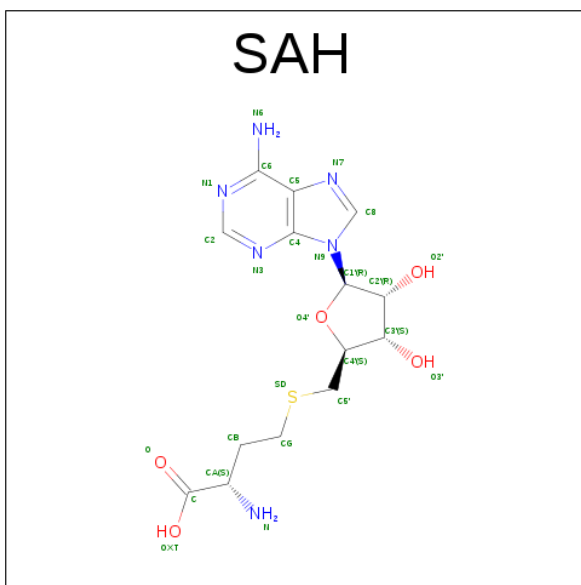
Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
M	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
M	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
M	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
N	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
N	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
N	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
N	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
N	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
N	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
N	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
N	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
O	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
O	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
O	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
O	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
O	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
O	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
O	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
O	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
P	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
P	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
P	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
P	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
P	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
P	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
P	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
P	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
Q	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
Q	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
Q	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
Q	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
Q	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
Q	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
Q	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
Q	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
R	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
R	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
R	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
R	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
R	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
R	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
R	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
J	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
J	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
J	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
J	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
J	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
J	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
J	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
J	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
K	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
K	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
K	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
K	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
K	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
K	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
K	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
K	0	PRO	-	EXPRESSION TAG	UNP Q9XW42
L	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
L	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
L	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
L	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
L	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
L	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
L	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
L	0	PRO	-	EXPRESSION TAG	UNP Q9XW42

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



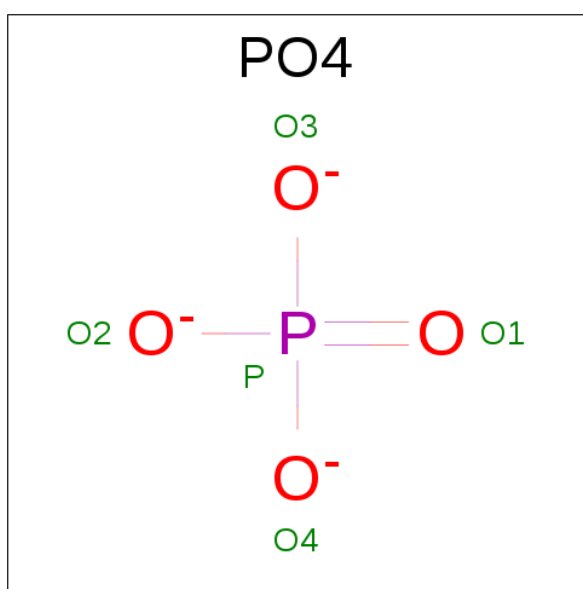
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	D	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	B	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	C	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	F	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	E	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	G	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	H	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	I	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	M	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	N	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	O	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	P	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	Q	1	Total 26	C 14	N 6	O 5	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	R	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	D	93	Total	O	0	0
			93	93		
4	B	26	Total	O	0	0
			26	26		
4	C	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		
4	E	41	Total	O	0	0
			41	41		
4	G	19	Total	O	0	0
			19	19		
4	H	59	Total	O	0	0
			59	59		

Continued on next page...

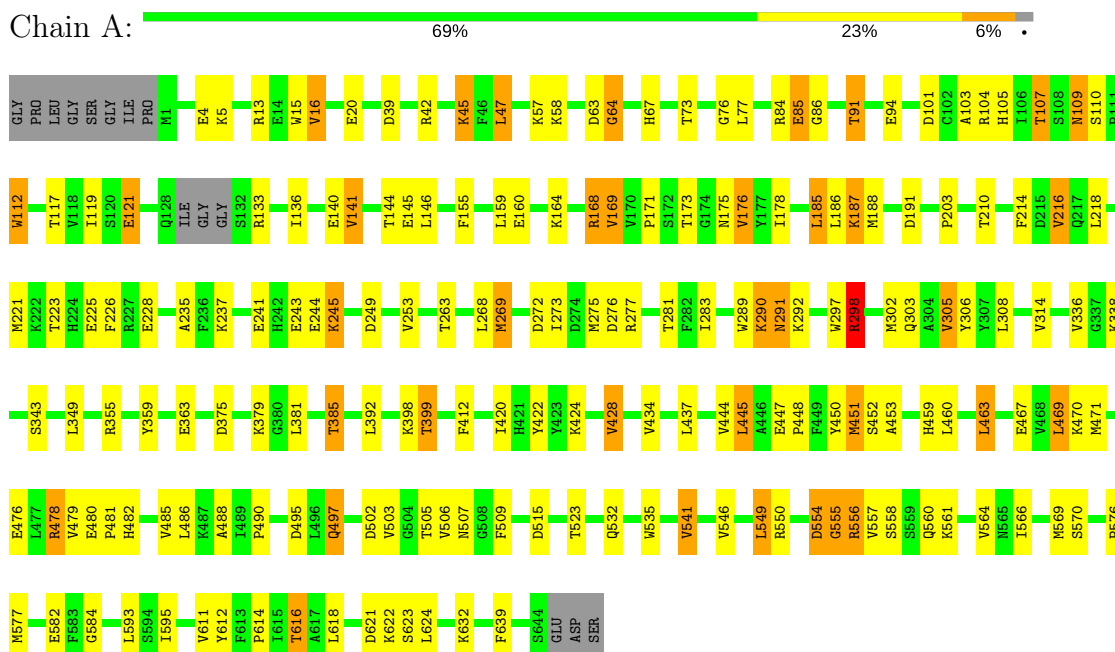
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	21	Total 21	O 21	0	0
4	M	2	Total 2	O 2	0	0
4	P	10	Total 10	O 10	0	0
4	Q	2	Total 2	O 2	0	0
4	R	2	Total 2	O 2	0	0
4	J	12	Total 12	O 12	0	0
4	K	6	Total 6	O 6	0	0
4	L	85	Total 85	O 85	0	0

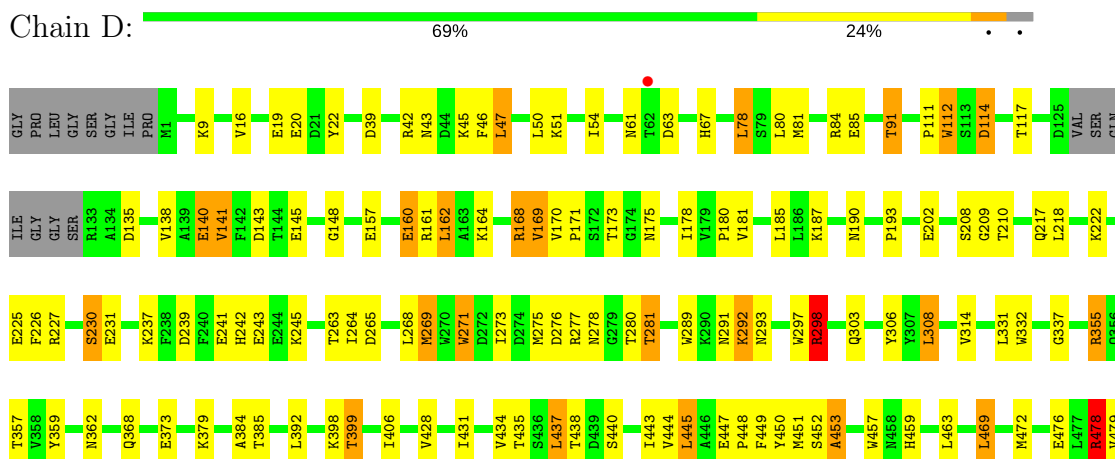
3 Residue-property plots

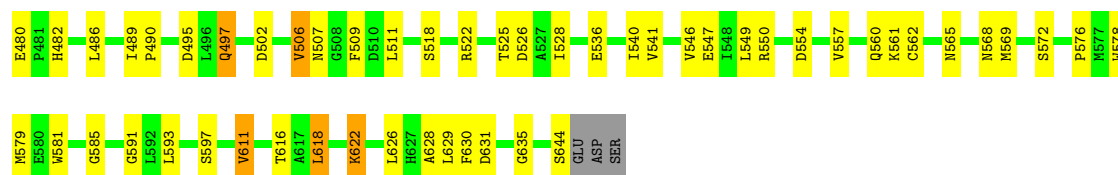
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein arginine N-methyltransferase 7

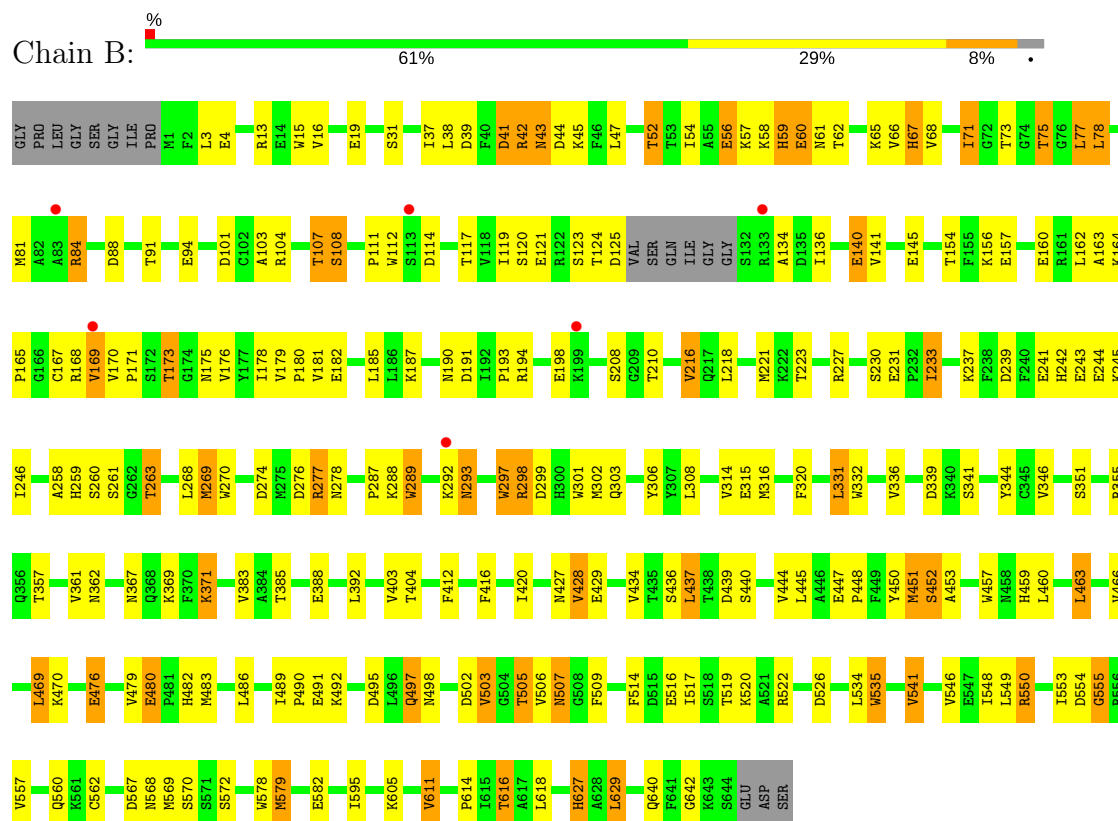


• Molecule 1: Protein arginine N-methyltransferase 7

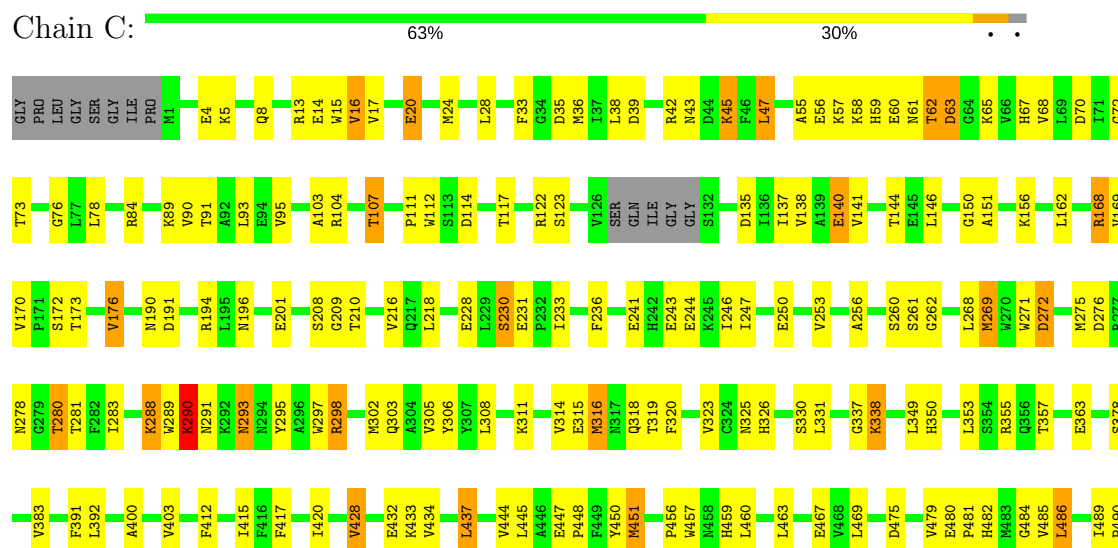




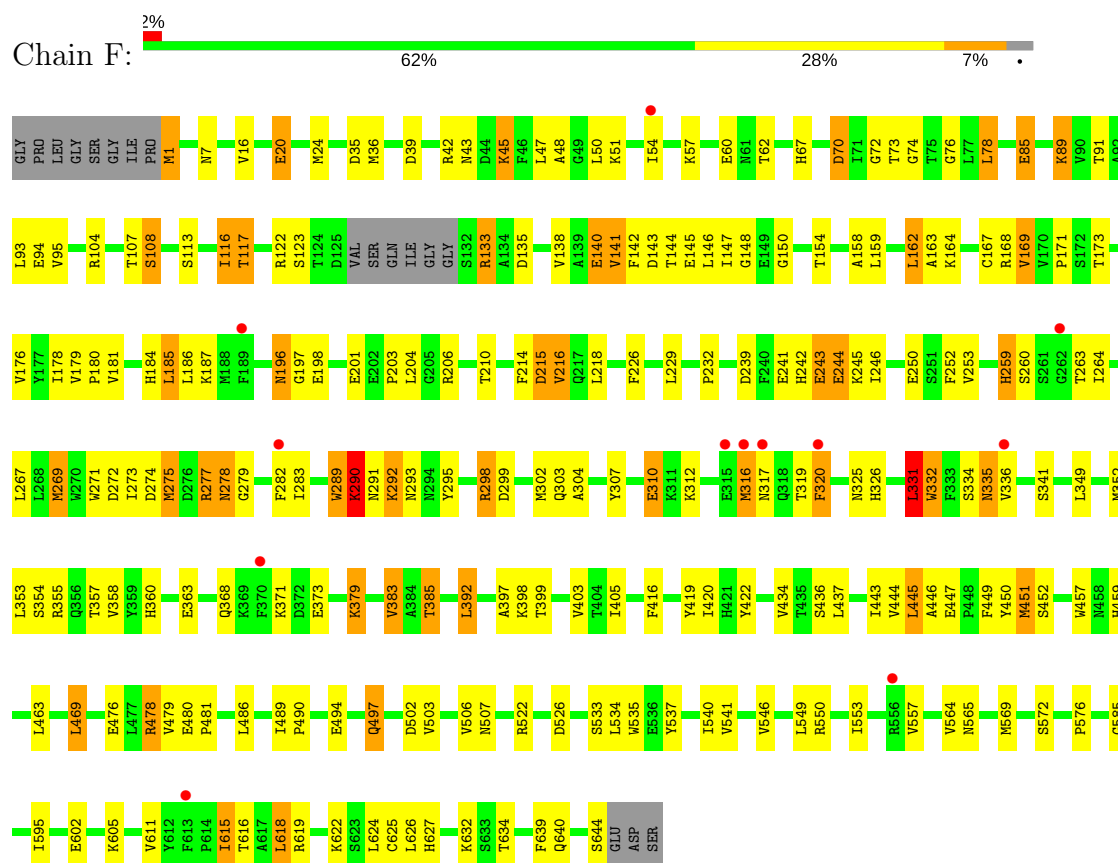
• Molecule 1: Protein arginine N-methyltransferase 7



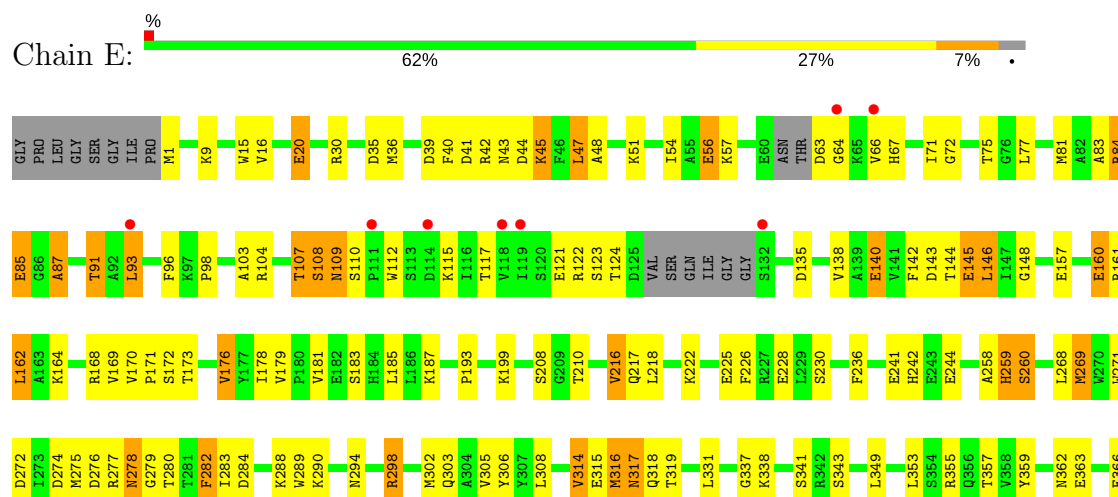
• Molecule 1: Protein arginine N-methyltransferase 7

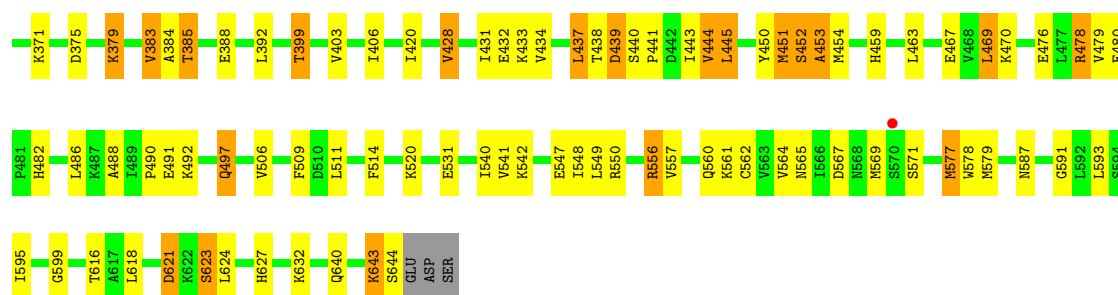


- Molecule 1: Protein arginine N-methyltransferase 7



- Molecule 1: Protein arginine N-methyltransferase 7

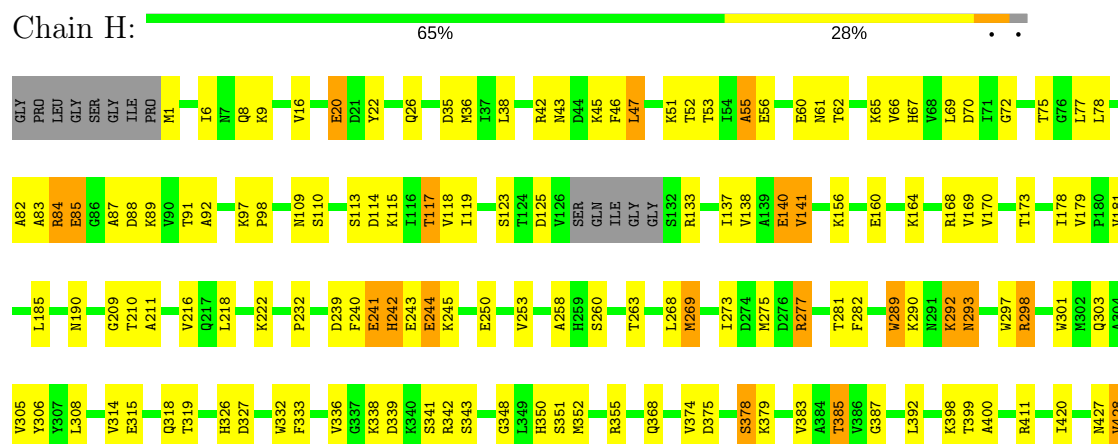




• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7

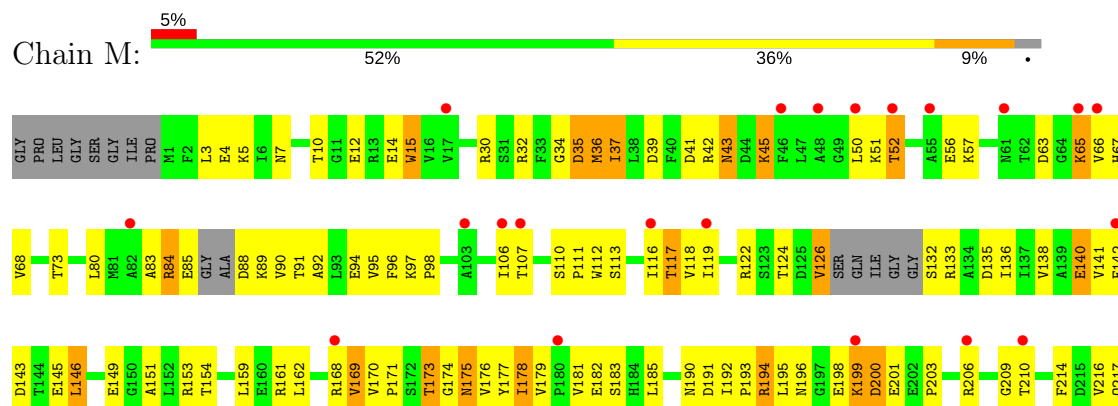


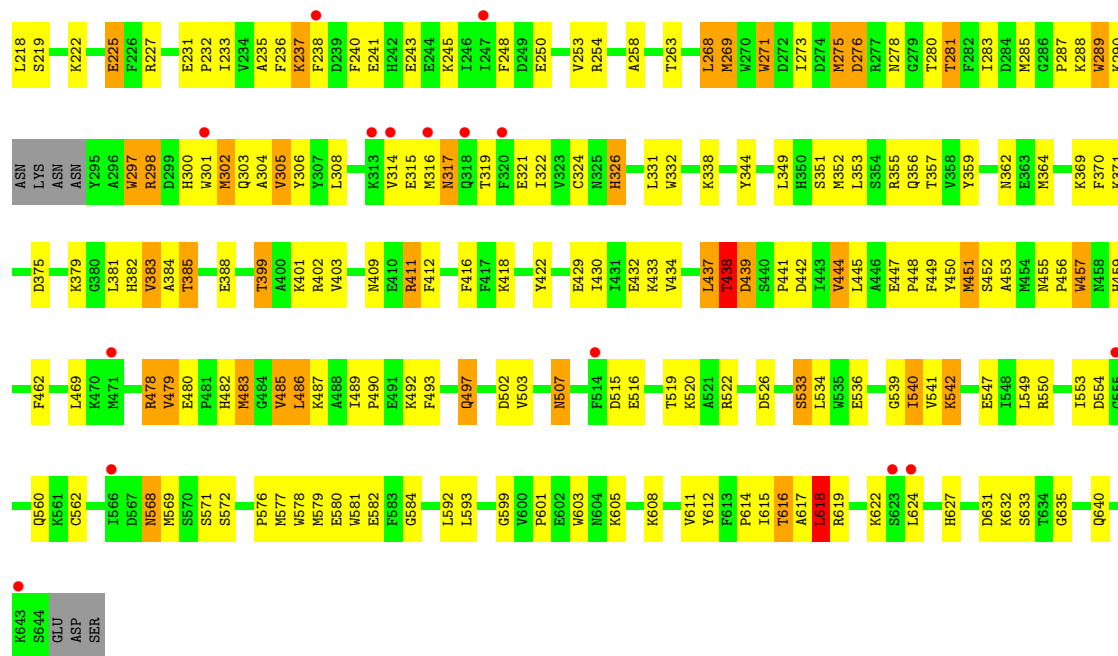


• Molecule 1: Protein arginine N-methyltransferase 7

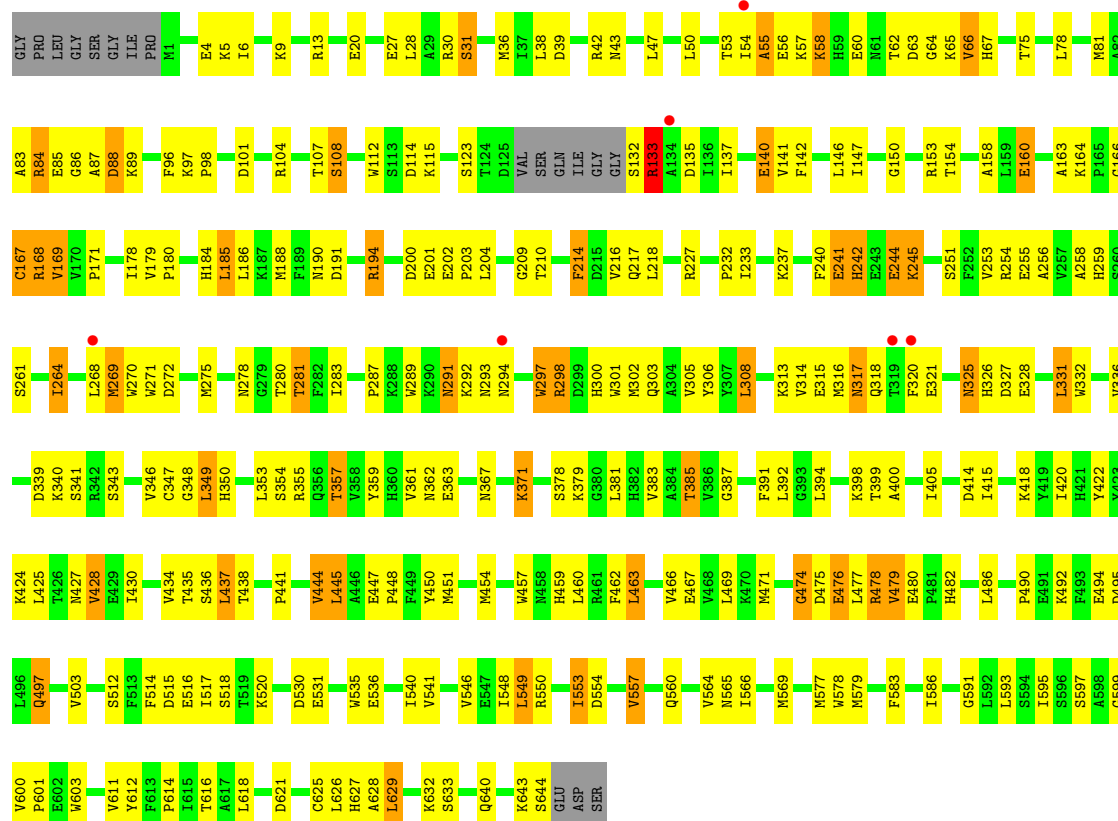


• Molecule 1: Protein arginine N-methyltransferase 7

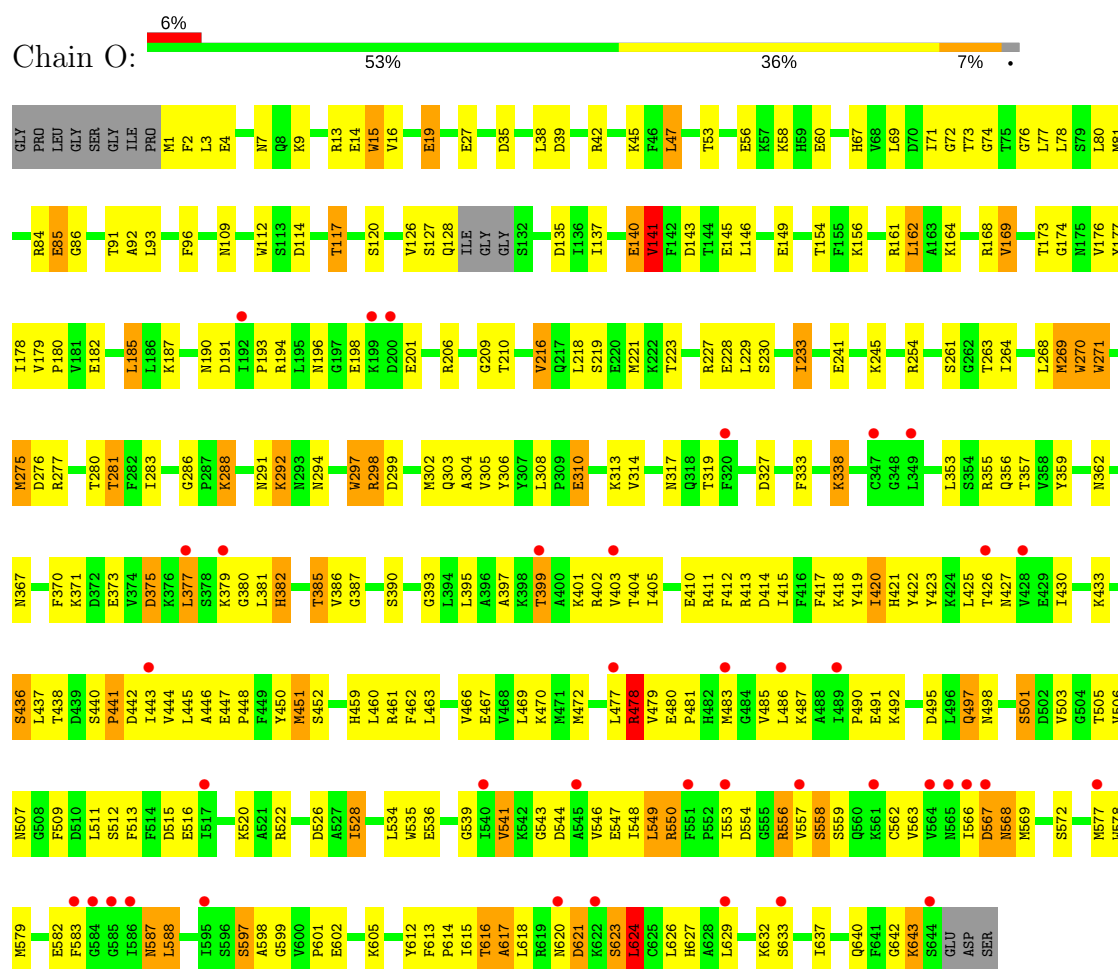




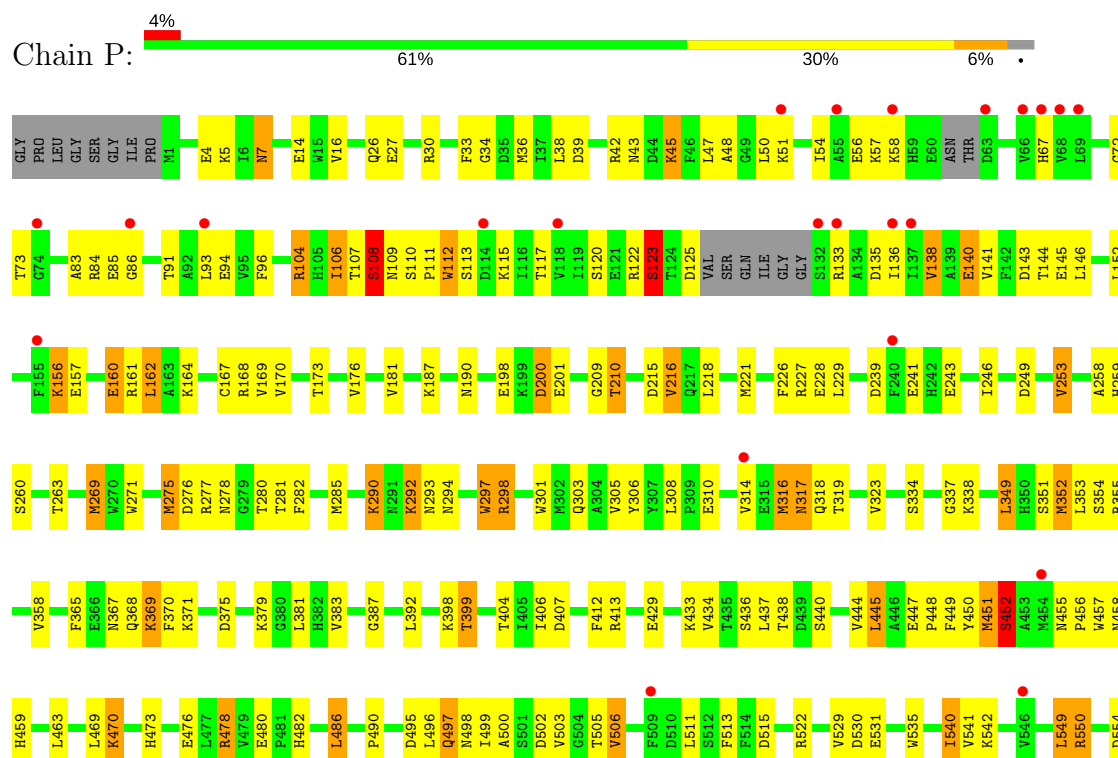
• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7

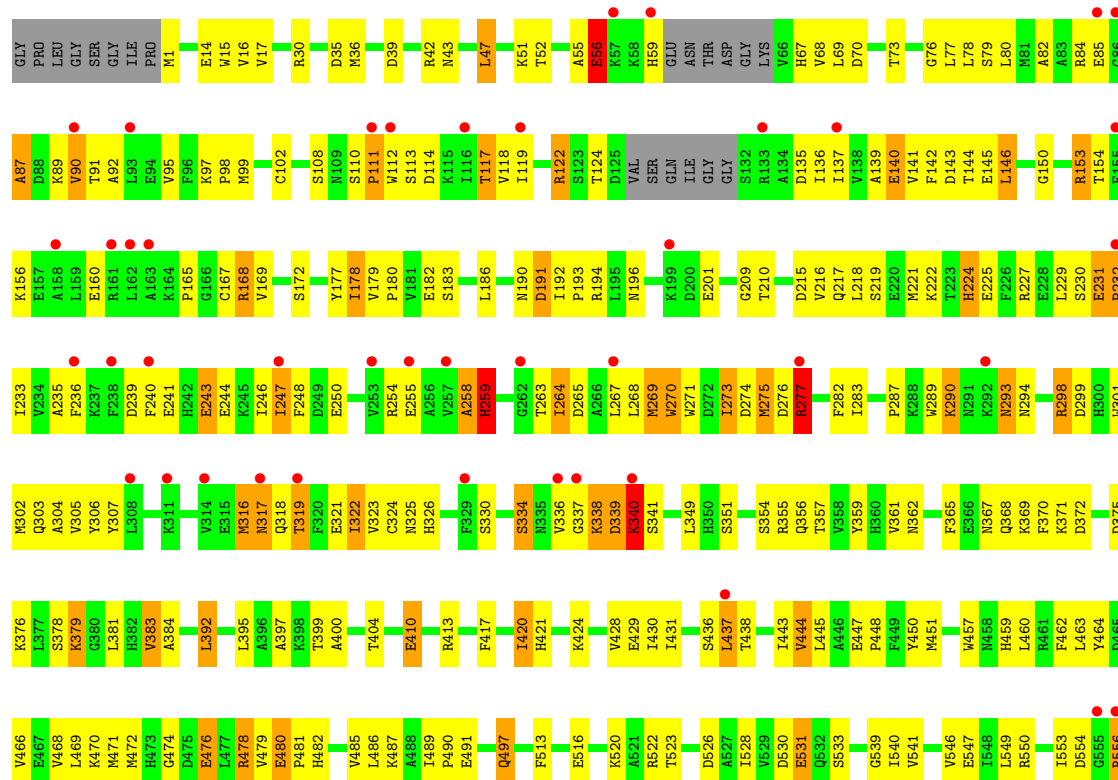


• Molecule 1: Protein arginine N-methyltransferase 7

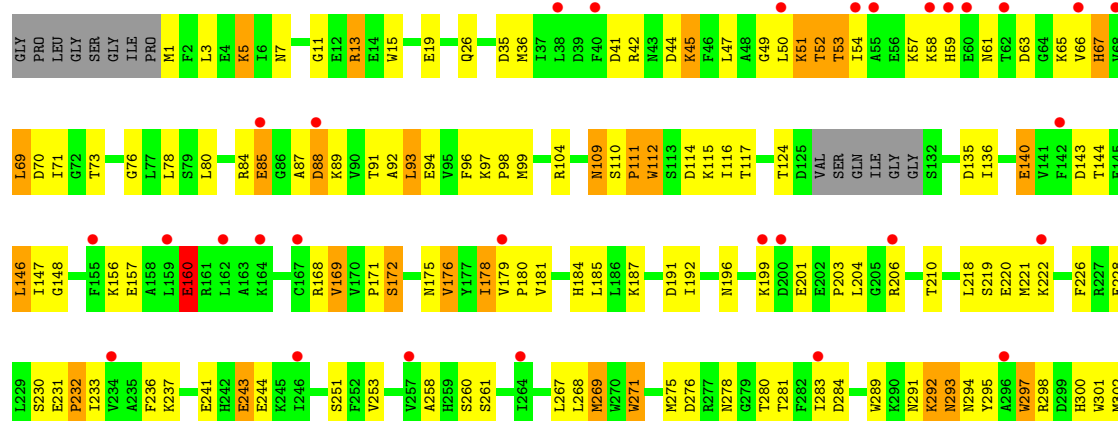




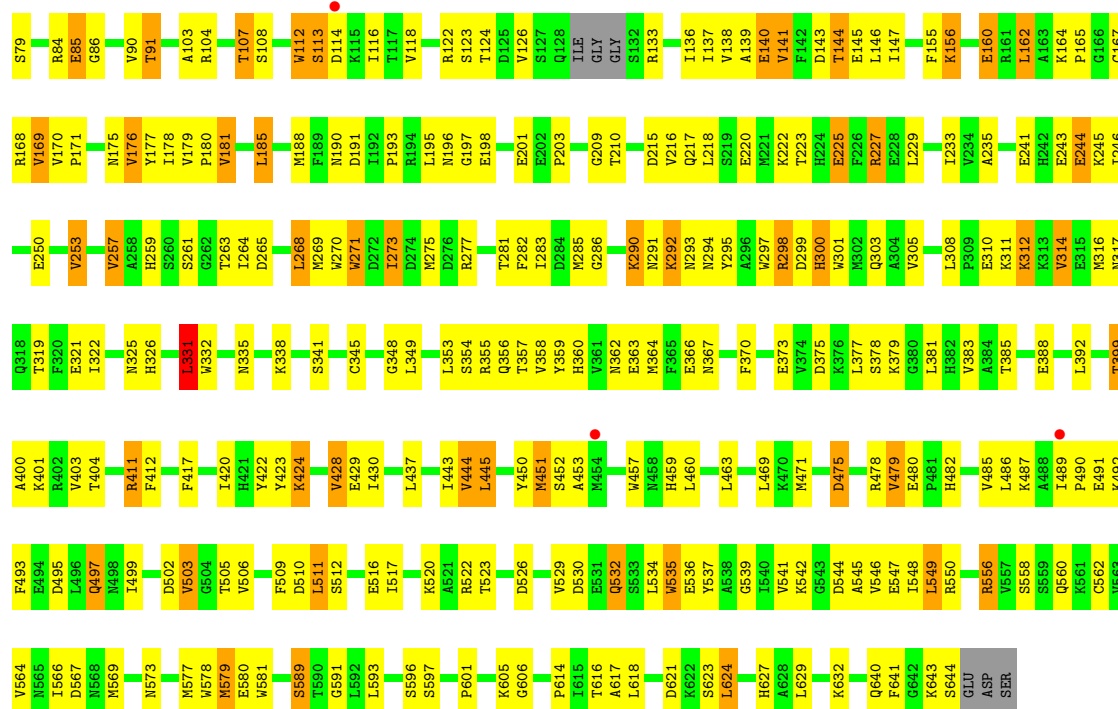
• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7

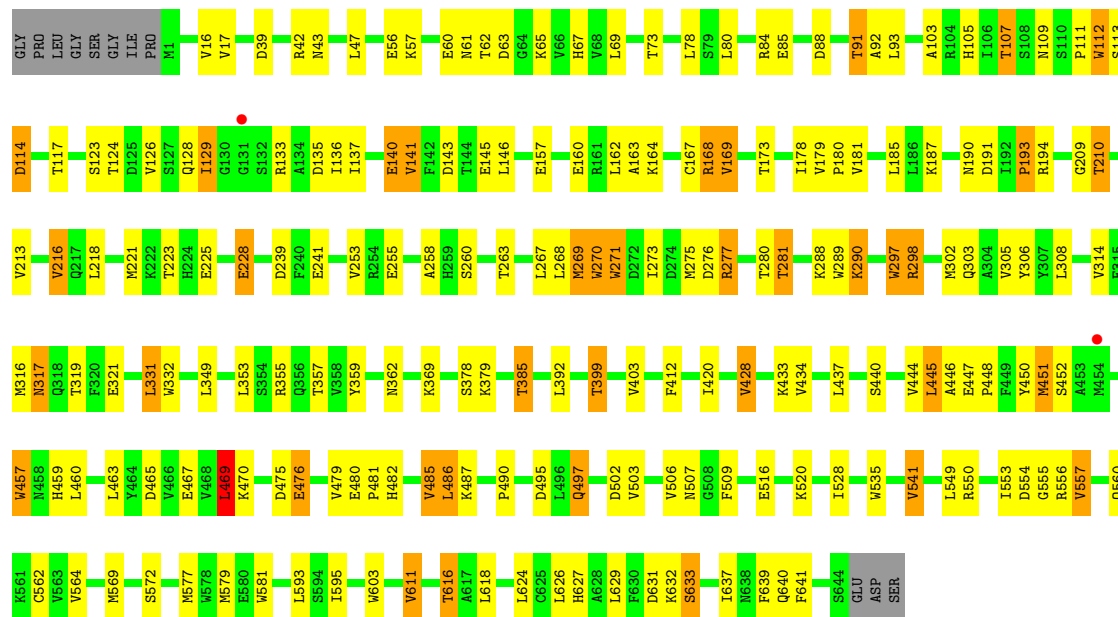






Molecule 1: Protein arginine N-methyltransferase 7

Chain L: 68% 25% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	190.70Å 190.70Å 373.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.41 – 2.39 47.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.41-2.39) 98.9 (47.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.303 0.233 , 0.302	Depositor DCC
R_{free} test set	29764 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 15.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.069 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	92645	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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: PO4, SAH

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	0.85	4/5217 (0.1%)	0.95	5/7044 (0.1%)
1	B	0.79	7/5195 (0.1%)	0.88	0/7014
1	C	0.77	2/5202 (0.0%)	0.88	3/7024 (0.0%)
1	D	0.81	6/5189 (0.1%)	0.96	8/7006 (0.1%)
1	E	0.79	2/5179 (0.0%)	0.94	3/6990 (0.0%)
1	F	0.73	4/5195 (0.1%)	0.88	7/7014 (0.1%)
1	G	0.77	6/5180 (0.1%)	0.90	5/6993 (0.1%)
1	H	0.81	5/5202 (0.1%)	0.92	3/7024 (0.0%)
1	I	0.76	4/5234 (0.1%)	0.86	3/7068 (0.0%)
1	J	0.74	2/5234 (0.0%)	0.88	6/7068 (0.1%)
1	K	0.73	4/5217 (0.1%)	0.85	5/7044 (0.1%)
1	L	0.86	9/5234 (0.2%)	0.99	8/7068 (0.1%)
1	M	0.70	7/5158 (0.1%)	0.81	3/6962 (0.0%)
1	N	0.70	4/5195 (0.1%)	0.84	4/7014 (0.1%)
1	O	0.66	5/5217 (0.1%)	0.78	3/7044 (0.0%)
1	P	0.74	7/5179 (0.1%)	0.85	4/6990 (0.1%)
1	Q	0.68	5/5149 (0.1%)	0.81	1/6951 (0.0%)
1	R	0.65	8/5195 (0.2%)	0.77	0/7014
All	All	0.76	91/93571 (0.1%)	0.88	71/126332 (0.1%)

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
1	E	0	2
1	H	0	1
1	J	0	2
All	All	0	6

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	332	TRP	CD2-CE2	7.16	1.50	1.41
1	M	271	TRP	CD2-CE2	6.90	1.49	1.41
1	L	297	TRP	CD2-CE2	6.63	1.49	1.41
1	D	332	TRP	CD2-CE2	6.55	1.49	1.41
1	A	289	TRP	CD2-CE2	6.37	1.49	1.41

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	277	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	F	331	LEU	CA-CB-CG	9.32	136.75	115.30
1	L	611	VAL	CB-CA-C	-8.32	95.60	111.40
1	L	277	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	D	611	VAL	CB-CA-C	-7.93	96.34	111.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLU	Peptide
1	E	282	PHE	Peptide
1	E	316	MET	Peptide
1	H	282	PHE	Peptide
1	J	291	ASN	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	5106	0	4989	129	0
1	B	5084	0	4967	174	0
1	C	5091	0	4976	158	1
1	D	5078	0	4962	138	1
1	E	5069	0	4953	160	0
1	F	5084	0	4967	153	0
1	G	5070	0	4955	145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	5091	0	4976	136	0
1	I	5122	0	5007	173	0
1	J	5122	0	5007	184	0
1	K	5106	0	4989	212	0
1	L	5122	0	5007	136	0
1	M	5049	0	4935	270	0
1	N	5084	0	4967	225	1
1	O	5106	0	4989	214	0
1	P	5069	0	4953	158	1
1	Q	5039	0	4927	233	0
1	R	5084	0	4967	202	0
2	A	26	0	19	0	0
2	B	26	0	19	2	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
2	E	26	0	19	3	0
2	F	26	0	19	2	0
2	G	26	0	19	2	0
2	H	26	0	19	1	0
2	I	26	0	19	1	0
2	J	26	0	19	0	0
2	K	26	0	19	3	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
2	N	26	0	19	1	0
2	O	26	0	19	0	0
2	P	26	0	19	3	0
2	Q	26	0	19	1	0
2	R	26	0	19	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	1	0
3	R	5	0	0	0	0
4	A	105	0	0	0	0
4	B	26	0	0	0	0
4	C	16	0	0	1	0
4	D	93	0	0	3	0
4	E	41	0	0	0	0
4	F	12	0	0	1	0
4	G	19	0	0	1	0
4	H	59	0	0	1	0
4	I	21	0	0	3	0
4	J	12	0	0	1	0
4	K	6	0	0	0	0
4	L	85	0	0	4	0
4	M	2	0	0	2	0
4	P	10	0	0	2	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
All	All	92645	0	89835	3158	2

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 3158 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:L:490:PRO:HB3	1:L:569:MET:CE	1.55	1.36
1:G:490:PRO:HB3	1:G:569:MET:CE	1.58	1.32
1:F:490:PRO:HB3	1:F:569:MET:CE	1.60	1.28
1:M:569:MET:HG3	1:M:624:LEU:CD1	1.67	1.23
1:B:490:PRO:HB3	1:B:569:MET:CE	1.71	1.20

All (2) 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)
1:D:554:ASP:OD1	1:C:550:ARG:NH2[3_554]	2.01	0.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:554:ASP:OD1	1:P:550:ARG:NH2[3_654]	2.09	0.11

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	637/655 (97%)	600 (94%)	34 (5%)	3 (0%)	32	46
1	B	634/655 (97%)	561 (88%)	62 (10%)	11 (2%)	11	13
1	C	635/655 (97%)	578 (91%)	47 (7%)	10 (2%)	11	15
1	D	633/655 (97%)	595 (94%)	34 (5%)	4 (1%)	28	41
1	E	630/655 (96%)	569 (90%)	53 (8%)	8 (1%)	14	19
1	F	634/655 (97%)	563 (89%)	62 (10%)	9 (1%)	13	18
1	G	630/655 (96%)	575 (91%)	50 (8%)	5 (1%)	22	33
1	H	635/655 (97%)	590 (93%)	39 (6%)	6 (1%)	20	29
1	I	642/655 (98%)	572 (89%)	58 (9%)	12 (2%)	9	11
1	J	642/655 (98%)	578 (90%)	54 (8%)	10 (2%)	11	15
1	K	637/655 (97%)	570 (90%)	53 (8%)	14 (2%)	8	9
1	L	642/655 (98%)	607 (94%)	34 (5%)	1 (0%)	51	67
1	M	625/655 (95%)	551 (88%)	65 (10%)	9 (1%)	13	18
1	N	634/655 (97%)	558 (88%)	67 (11%)	9 (1%)	13	18
1	O	637/655 (97%)	567 (89%)	61 (10%)	9 (1%)	13	18
1	P	630/655 (96%)	576 (91%)	48 (8%)	6 (1%)	18	26
1	Q	626/655 (96%)	526 (84%)	81 (13%)	19 (3%)	5	4
1	R	634/655 (97%)	567 (89%)	52 (8%)	15 (2%)	7	7
All	All	11417/11790 (97%)	10303 (90%)	954 (8%)	160 (1%)	13	18

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	ASP
1	B	59	HIS
1	B	60	GLU
1	B	278	ASN
1	F	290	LYS

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	556/569 (98%)	479 (86%)	77 (14%)	4	5
1	B	553/569 (97%)	474 (86%)	79 (14%)	4	4
1	C	554/569 (97%)	484 (87%)	70 (13%)	5	6
1	D	552/569 (97%)	488 (88%)	64 (12%)	6	8
1	E	551/569 (97%)	459 (83%)	92 (17%)	2	3
1	F	553/569 (97%)	471 (85%)	82 (15%)	3	4
1	G	552/569 (97%)	473 (86%)	79 (14%)	4	4
1	H	554/569 (97%)	481 (87%)	73 (13%)	5	5
1	I	557/569 (98%)	476 (86%)	81 (14%)	4	4
1	J	557/569 (98%)	481 (86%)	76 (14%)	4	5
1	K	556/569 (98%)	465 (84%)	91 (16%)	2	3
1	L	557/569 (98%)	483 (87%)	74 (13%)	4	5
1	M	550/569 (97%)	470 (86%)	80 (14%)	4	4
1	N	553/569 (97%)	455 (82%)	98 (18%)	2	2
1	O	556/569 (98%)	472 (85%)	84 (15%)	3	4
1	P	551/569 (97%)	469 (85%)	82 (15%)	3	4
1	Q	548/569 (96%)	465 (85%)	83 (15%)	3	4
1	R	553/569 (97%)	467 (84%)	86 (16%)	3	3
All	All	9963/10242 (97%)	8512 (85%)	1451 (15%)	3	4

5 of 1451 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	331	LEU
1	N	259	HIS
1	K	385	THR
1	I	476	GLU
1	M	319	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	300	HIS
1	N	259	HIS
1	K	482	HIS
1	I	459	HIS
1	M	190	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

36 ligands 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
2	SAH	A	701	-	20,28,28	1.36	2 (10%)	20,40,40	2.10	7 (35%)
3	PO4	A	702	-	4,4,4	0.54	0	6,6,6	1.15	1 (16%)
2	SAH	B	701	-	20,28,28	1.05	1 (5%)	20,40,40	2.03	5 (25%)
3	PO4	B	702	-	4,4,4	0.78	0	6,6,6	0.94	0
2	SAH	C	701	-	20,28,28	1.22	2 (10%)	20,40,40	1.87	4 (20%)
3	PO4	C	702	-	4,4,4	0.66	0	6,6,6	1.00	0
2	SAH	D	701	-	20,28,28	1.31	2 (10%)	20,40,40	1.88	5 (25%)
3	PO4	D	702	-	4,4,4	0.95	0	6,6,6	1.46	2 (33%)
2	SAH	E	701	-	20,28,28	1.20	1 (5%)	20,40,40	2.10	6 (30%)
3	PO4	E	702	-	4,4,4	0.62	0	6,6,6	0.80	0
2	SAH	F	701	-	20,28,28	1.08	2 (10%)	20,40,40	2.08	6 (30%)
3	PO4	F	702	-	4,4,4	0.93	0	6,6,6	1.21	0
2	SAH	G	701	-	20,28,28	1.34	2 (10%)	20,40,40	2.06	4 (20%)
3	PO4	G	702	-	4,4,4	0.85	0	6,6,6	0.84	0
2	SAH	H	701	-	20,28,28	1.45	4 (20%)	20,40,40	2.32	5 (25%)
3	PO4	H	702	-	4,4,4	0.66	0	6,6,6	1.28	1 (16%)
2	SAH	I	701	-	20,28,28	1.27	3 (15%)	20,40,40	2.75	9 (45%)
3	PO4	I	702	-	4,4,4	0.92	0	6,6,6	1.26	0
2	SAH	J	701	-	20,28,28	1.03	1 (5%)	20,40,40	1.88	6 (30%)
3	PO4	J	702	-	4,4,4	0.84	0	6,6,6	0.67	0
2	SAH	K	701	-	20,28,28	1.31	4 (20%)	20,40,40	2.03	5 (25%)
3	PO4	K	702	-	4,4,4	0.85	0	6,6,6	0.53	0
2	SAH	L	701	-	20,28,28	1.43	3 (15%)	20,40,40	2.42	6 (30%)
3	PO4	L	702	-	4,4,4	0.87	0	6,6,6	0.77	0
2	SAH	M	701	-	20,28,28	1.63	5 (25%)	20,40,40	2.35	4 (20%)
3	PO4	M	702	-	4,4,4	0.66	0	6,6,6	0.70	0
2	SAH	N	701	-	20,28,28	1.29	3 (15%)	20,40,40	2.35	5 (25%)
3	PO4	N	702	-	4,4,4	0.89	0	6,6,6	0.63	0
2	SAH	O	701	-	20,28,28	1.19	2 (10%)	20,40,40	2.25	6 (30%)
3	PO4	O	702	-	4,4,4	0.82	0	6,6,6	0.35	0
2	SAH	P	701	-	20,28,28	1.27	1 (5%)	20,40,40	2.23	8 (40%)
3	PO4	P	702	-	4,4,4	0.68	0	6,6,6	0.85	0
2	SAH	Q	701	-	20,28,28	1.08	1 (5%)	20,40,40	2.13	4 (20%)
3	PO4	Q	702	-	4,4,4	0.81	0	6,6,6	0.49	0
2	SAH	R	701	-	20,28,28	1.11	1 (5%)	20,40,40	2.03	4 (20%)
3	PO4	R	702	-	4,4,4	0.64	0	6,6,6	0.69	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
2	SAH	A	701	-	-	0/7/31/31	0/3/3/3
3	PO4	A	702	-	-	0/0/0/0	0/0/0/0
2	SAH	B	701	-	-	0/7/31/31	0/3/3/3
3	PO4	B	702	-	-	0/0/0/0	0/0/0/0
2	SAH	C	701	-	-	0/7/31/31	0/3/3/3
3	PO4	C	702	-	-	0/0/0/0	0/0/0/0
2	SAH	D	701	-	-	0/7/31/31	0/3/3/3
3	PO4	D	702	-	-	0/0/0/0	0/0/0/0
2	SAH	E	701	-	-	0/7/31/31	0/3/3/3
3	PO4	E	702	-	-	0/0/0/0	0/0/0/0
2	SAH	F	701	-	-	0/7/31/31	0/3/3/3
3	PO4	F	702	-	-	0/0/0/0	0/0/0/0
2	SAH	G	701	-	-	0/7/31/31	0/3/3/3
3	PO4	G	702	-	-	0/0/0/0	0/0/0/0
2	SAH	H	701	-	-	0/7/31/31	0/3/3/3
3	PO4	H	702	-	-	0/0/0/0	0/0/0/0
2	SAH	I	701	-	-	0/7/31/31	0/3/3/3
3	PO4	I	702	-	-	0/0/0/0	0/0/0/0
2	SAH	J	701	-	-	0/7/31/31	0/3/3/3
3	PO4	J	702	-	-	0/0/0/0	0/0/0/0
2	SAH	K	701	-	-	0/7/31/31	0/3/3/3
3	PO4	K	702	-	-	0/0/0/0	0/0/0/0
2	SAH	L	701	-	-	0/7/31/31	0/3/3/3
3	PO4	L	702	-	-	0/0/0/0	0/0/0/0
2	SAH	M	701	-	-	0/7/31/31	0/3/3/3
3	PO4	M	702	-	-	0/0/0/0	0/0/0/0
2	SAH	N	701	-	-	0/7/31/31	0/3/3/3
3	PO4	N	702	-	-	0/0/0/0	0/0/0/0
2	SAH	O	701	-	-	0/7/31/31	0/3/3/3
3	PO4	O	702	-	-	0/0/0/0	0/0/0/0
2	SAH	P	701	-	-	0/7/31/31	0/3/3/3
3	PO4	P	702	-	-	0/0/0/0	0/0/0/0
2	SAH	Q	701	-	-	0/7/31/31	0/3/3/3
3	PO4	Q	702	-	-	0/0/0/0	0/0/0/0
2	SAH	R	701	-	-	0/7/31/31	0/3/3/3
3	PO4	R	702	-	-	0/0/0/0	0/0/0/0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	701	SAH	C2'-C1'	-3.17	1.48	1.53
2	I	701	SAH	C2'-C1'	-2.57	1.49	1.53
2	H	701	SAH	C2'-C1'	-2.29	1.50	1.53
2	K	701	SAH	C5'-SD	-2.24	1.75	1.81
2	A	701	SAH	C2'-C1'	-2.20	1.50	1.53

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	701	SAH	N3-C2-N1	-8.05	121.85	128.86
2	I	701	SAH	N3-C2-N1	-7.99	121.90	128.86
2	L	701	SAH	N3-C2-N1	-7.46	122.36	128.86
2	O	701	SAH	N3-C2-N1	-7.39	122.42	128.86
2	M	701	SAH	N3-C2-N1	-7.13	122.64	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	SAH	2	0
2	C	701	SAH	1	0
2	E	701	SAH	3	0
2	F	701	SAH	2	0
2	G	701	SAH	2	0
2	H	701	SAH	1	0
2	I	701	SAH	1	0
3	I	702	PO4	1	0
2	K	701	SAH	3	0
2	M	701	SAH	2	0
2	N	701	SAH	1	0
2	P	701	SAH	3	0
2	Q	701	SAH	1	0
3	Q	702	PO4	1	0
2	R	701	SAH	1	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 ⓘ

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	641/655 (97%)	-0.01	0 100 100	16, 33, 57, 83	0
1	B	638/655 (97%)	0.10	6 (0%) 84 82	24, 43, 74, 103	0
1	C	639/655 (97%)	0.03	0 100 100	26, 44, 68, 100	0
1	D	637/655 (97%)	-0.02	1 (0%) 94 94	19, 34, 56, 101	0
1	E	636/655 (97%)	0.15	9 (1%) 75 74	21, 41, 80, 124	0
1	F	638/655 (97%)	0.15	12 (1%) 67 64	27, 48, 75, 120	0
1	G	636/655 (97%)	0.10	10 (1%) 72 70	23, 43, 81, 129	0
1	H	639/655 (97%)	-0.02	1 (0%) 94 94	18, 38, 60, 91	0
1	I	644/655 (98%)	-0.00	4 (0%) 89 87	28, 44, 68, 94	0
1	J	644/655 (98%)	0.09	5 (0%) 86 84	29, 47, 69, 92	0
1	K	641/655 (97%)	0.13	4 (0%) 89 87	26, 52, 77, 99	0
1	L	644/655 (98%)	-0.03	2 (0%) 93 93	19, 33, 55, 78	0
1	M	633/655 (96%)	0.40	36 (5%) 24 23	38, 61, 84, 110	0
1	N	638/655 (97%)	0.15	6 (0%) 84 82	36, 55, 75, 93	0
1	O	641/655 (97%)	0.43	39 (6%) 22 20	39, 64, 96, 127	0
1	P	636/655 (97%)	0.19	28 (4%) 35 33	30, 51, 82, 105	0
1	Q	632/655 (96%)	0.46	43 (6%) 18 16	37, 62, 99, 124	0
1	R	638/655 (97%)	0.59	59 (9%) 10 8	44, 69, 99, 131	0
All	All	11495/11790 (97%)	0.16	265 (2%) 61 58	16, 48, 82, 131	0

The worst 5 of 265 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	586	ILE	8.7
1	E	64	GLY	6.6
1	E	119	ILE	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	644	SER	5.4
1	Q	116	ILE	5.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SAH	D	701	26/26	0.95	0.15	0.83	32,37,45,46	0
2	SAH	R	701	26/26	0.91	0.17	0.28	47,56,92,99	0
2	SAH	M	701	26/26	0.89	0.16	-0.03	36,61,74,79	0
3	PO4	M	702	5/5	0.91	0.13	-0.05	70,71,74,78	0
2	SAH	C	701	26/26	0.95	0.14	-0.12	36,48,57,59	0
2	SAH	F	701	26/26	0.95	0.14	-0.23	35,46,61,64	0
2	SAH	A	701	26/26	0.96	0.13	-0.33	27,33,38,38	0
2	SAH	G	701	26/26	0.93	0.14	-0.42	46,63,72,72	0
2	SAH	Q	701	26/26	0.92	0.14	-0.43	48,64,75,76	0
2	SAH	E	701	26/26	0.95	0.13	-0.51	43,53,63,65	0
2	SAH	B	701	26/26	0.96	0.12	-0.61	36,43,57,58	0
2	SAH	N	701	26/26	0.90	0.12	-0.63	40,53,58,58	0
2	SAH	K	701	26/26	0.94	0.13	-0.71	37,41,47,51	0
2	SAH	H	701	26/26	0.96	0.12	-0.75	24,29,33,34	0
2	SAH	I	701	26/26	0.96	0.12	-0.89	35,38,45,47	0
2	SAH	P	701	26/26	0.93	0.11	-0.98	43,53,63,65	0
2	SAH	J	701	26/26	0.96	0.11	-1.10	34,38,44,46	0
2	SAH	L	701	26/26	0.97	0.12	-1.23	27,33,36,39	0
3	PO4	E	702	5/5	0.98	0.10	-1.30	36,40,43,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SAH	O	701	26/26	0.95	0.10	-1.42	37,41,47,52	0
3	PO4	O	702	5/5	0.97	0.07	-1.69	57,58,70,72	0
3	PO4	K	702	5/5	0.98	0.09	-2.54	43,45,46,51	0
3	PO4	A	702	5/5	0.99	0.12	-	31,32,37,39	0
3	PO4	N	702	5/5	0.97	0.09	-	52,57,62,66	0
3	PO4	G	702	5/5	0.99	0.11	-	42,42,49,50	0
3	PO4	H	702	5/5	0.98	0.09	-	28,34,36,37	0
3	PO4	L	702	5/5	0.99	0.12	-	32,32,35,37	0
3	PO4	D	702	5/5	0.99	0.12	-	31,35,36,37	0
3	PO4	J	702	5/5	0.98	0.11	-	45,46,49,51	0
3	PO4	Q	702	5/5	0.96	0.12	-	59,63,72,72	0
3	PO4	F	702	5/5	0.98	0.08	-	38,42,49,56	0
3	PO4	P	702	5/5	0.98	0.12	-	43,43,45,47	0
3	PO4	R	702	5/5	0.96	0.09	-	52,55,59,61	0
3	PO4	I	702	5/5	0.97	0.14	-	36,37,44,49	0
3	PO4	C	702	5/5	0.98	0.09	-	37,41,44,44	0
3	PO4	B	702	5/5	0.98	0.13	-	36,39,45,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.