



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:20 PM GMT

PDB ID : 4C3E
Title : HRSV M2-1 mutant S58D S61D, P21 crystal
Authors : Tanner, S.J.; Ariza, A.; Richard, C.A.; Wu, W.; Trincao, J.; Hiscox, J.A.;
Carroll, M.W.; Silman, N.J.; Eleouet, J.F.; Edwards, T.A.; Barr, J.N.
Deposited on : 2013-08-22
Resolution : 2.40 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

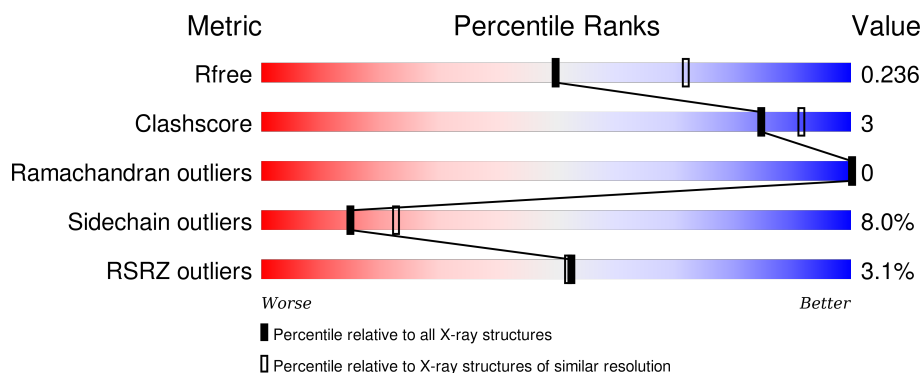
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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	199	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 75% 11% • 14% </div> </div>
1	B	199	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 4% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 72% 12% • 16% </div> </div>
1	C	199	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 9% • 14% </div> </div>
1	D	199	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 72% 11% • 16% </div> </div>
1	E	199	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 72% 8% • 20% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	199	<p>3% 70% 9% •• 20%</p>
1	G	199	<p>4% 71% 12% • 16%</p>
1	H	199	<p>2% 72% 9% • 18%</p>
1	I	199	<p>5% 71% 10% • 18%</p>
1	J	199	<p>4% 73% 9% • 17%</p>
1	K	199	<p>3% 70% 12% • 17%</p>
1	L	199	<p>3% 70% 9% •• 18%</p>
1	M	199	<p>1% 70% 7% • 22%</p>
1	N	199	<p>6% 74% 10% • 15%</p>
1	O	199	<p>3% 74% 10% • 16%</p>
1	P	199	<p>3% 70% 10% •• 20%</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21997 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 MATRIX M2-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	3	0
			1404	880	258	258	8			
1	B	168	Total	C	N	O	S	0	5	0
			1391	874	257	253	7			
1	C	171	Total	C	N	O	S	0	2	0
			1390	871	255	256	8			
1	D	167	Total	C	N	O	S	0	3	0
			1372	861	253	251	7			
1	E	160	Total	C	N	O	S	0	2	0
			1311	823	245	235	8			
1	F	160	Total	C	N	O	S	0	3	0
			1316	826	246	236	8			
1	G	167	Total	C	N	O	S	0	2	0
			1359	850	253	248	8			
1	H	163	Total	C	N	O	S	0	2	0
			1329	835	244	243	7			
1	I	164	Total	C	N	O	S	0	1	0
			1332	837	243	245	7			
1	J	166	Total	C	N	O	S	0	2	0
			1356	852	248	249	7			
1	K	165	Total	C	N	O	S	0	3	0
			1355	851	250	247	7			
1	L	163	Total	C	N	O	S	0	3	0
			1338	842	247	242	7			
1	M	155	Total	C	N	O	S	0	2	0
			1276	804	237	228	7			
1	N	170	Total	C	N	O	S	0	4	0
			1396	875	259	254	8			
1	O	168	Total	C	N	O	S	0	1	0
			1358	851	250	249	8			
1	P	160	Total	C	N	O	S	0	1	0
			1303	818	242	235	8			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P04545
A	-3	PRO	-	EXPRESSION TAG	UNP P04545
A	-2	LEU	-	EXPRESSION TAG	UNP P04545
A	-1	GLY	-	EXPRESSION TAG	UNP P04545
A	0	SER	-	EXPRESSION TAG	UNP P04545
A	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
A	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
B	-4	GLY	-	EXPRESSION TAG	UNP P04545
B	-3	PRO	-	EXPRESSION TAG	UNP P04545
B	-2	LEU	-	EXPRESSION TAG	UNP P04545
B	-1	GLY	-	EXPRESSION TAG	UNP P04545
B	0	SER	-	EXPRESSION TAG	UNP P04545
B	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
B	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
C	-4	GLY	-	EXPRESSION TAG	UNP P04545
C	-3	PRO	-	EXPRESSION TAG	UNP P04545
C	-2	LEU	-	EXPRESSION TAG	UNP P04545
C	-1	GLY	-	EXPRESSION TAG	UNP P04545
C	0	SER	-	EXPRESSION TAG	UNP P04545
C	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
C	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
D	-4	GLY	-	EXPRESSION TAG	UNP P04545
D	-3	PRO	-	EXPRESSION TAG	UNP P04545
D	-2	LEU	-	EXPRESSION TAG	UNP P04545
D	-1	GLY	-	EXPRESSION TAG	UNP P04545
D	0	SER	-	EXPRESSION TAG	UNP P04545
D	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
D	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
E	-4	GLY	-	EXPRESSION TAG	UNP P04545
E	-3	PRO	-	EXPRESSION TAG	UNP P04545
E	-2	LEU	-	EXPRESSION TAG	UNP P04545
E	-1	GLY	-	EXPRESSION TAG	UNP P04545
E	0	SER	-	EXPRESSION TAG	UNP P04545
E	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
E	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
F	-4	GLY	-	EXPRESSION TAG	UNP P04545
F	-3	PRO	-	EXPRESSION TAG	UNP P04545
F	-2	LEU	-	EXPRESSION TAG	UNP P04545
F	-1	GLY	-	EXPRESSION TAG	UNP P04545
F	0	SER	-	EXPRESSION TAG	UNP P04545
F	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
F	61	ASP	SER	ENGINEERED MUTATION	UNP P04545

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	GLY	-	EXPRESSION TAG	UNP P04545
G	-3	PRO	-	EXPRESSION TAG	UNP P04545
G	-2	LEU	-	EXPRESSION TAG	UNP P04545
G	-1	GLY	-	EXPRESSION TAG	UNP P04545
G	0	SER	-	EXPRESSION TAG	UNP P04545
G	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
G	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
H	-4	GLY	-	EXPRESSION TAG	UNP P04545
H	-3	PRO	-	EXPRESSION TAG	UNP P04545
H	-2	LEU	-	EXPRESSION TAG	UNP P04545
H	-1	GLY	-	EXPRESSION TAG	UNP P04545
H	0	SER	-	EXPRESSION TAG	UNP P04545
H	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
H	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
I	-4	GLY	-	EXPRESSION TAG	UNP P04545
I	-3	PRO	-	EXPRESSION TAG	UNP P04545
I	-2	LEU	-	EXPRESSION TAG	UNP P04545
I	-1	GLY	-	EXPRESSION TAG	UNP P04545
I	0	SER	-	EXPRESSION TAG	UNP P04545
I	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
I	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
J	-4	GLY	-	EXPRESSION TAG	UNP P04545
J	-3	PRO	-	EXPRESSION TAG	UNP P04545
J	-2	LEU	-	EXPRESSION TAG	UNP P04545
J	-1	GLY	-	EXPRESSION TAG	UNP P04545
J	0	SER	-	EXPRESSION TAG	UNP P04545
J	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
J	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
K	-4	GLY	-	EXPRESSION TAG	UNP P04545
K	-3	PRO	-	EXPRESSION TAG	UNP P04545
K	-2	LEU	-	EXPRESSION TAG	UNP P04545
K	-1	GLY	-	EXPRESSION TAG	UNP P04545
K	0	SER	-	EXPRESSION TAG	UNP P04545
K	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
K	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
L	-4	GLY	-	EXPRESSION TAG	UNP P04545
L	-3	PRO	-	EXPRESSION TAG	UNP P04545
L	-2	LEU	-	EXPRESSION TAG	UNP P04545
L	-1	GLY	-	EXPRESSION TAG	UNP P04545
L	0	SER	-	EXPRESSION TAG	UNP P04545
L	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
L	61	ASP	SER	ENGINEERED MUTATION	UNP P04545

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	GLY	-	EXPRESSION TAG	UNP P04545
M	-3	PRO	-	EXPRESSION TAG	UNP P04545
M	-2	LEU	-	EXPRESSION TAG	UNP P04545
M	-1	GLY	-	EXPRESSION TAG	UNP P04545
M	0	SER	-	EXPRESSION TAG	UNP P04545
M	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
M	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
N	-4	GLY	-	EXPRESSION TAG	UNP P04545
N	-3	PRO	-	EXPRESSION TAG	UNP P04545
N	-2	LEU	-	EXPRESSION TAG	UNP P04545
N	-1	GLY	-	EXPRESSION TAG	UNP P04545
N	0	SER	-	EXPRESSION TAG	UNP P04545
N	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
N	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
O	-4	GLY	-	EXPRESSION TAG	UNP P04545
O	-3	PRO	-	EXPRESSION TAG	UNP P04545
O	-2	LEU	-	EXPRESSION TAG	UNP P04545
O	-1	GLY	-	EXPRESSION TAG	UNP P04545
O	0	SER	-	EXPRESSION TAG	UNP P04545
O	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
O	61	ASP	SER	ENGINEERED MUTATION	UNP P04545
P	-4	GLY	-	EXPRESSION TAG	UNP P04545
P	-3	PRO	-	EXPRESSION TAG	UNP P04545
P	-2	LEU	-	EXPRESSION TAG	UNP P04545
P	-1	GLY	-	EXPRESSION TAG	UNP P04545
P	0	SER	-	EXPRESSION TAG	UNP P04545
P	58	ASP	SER	ENGINEERED MUTATION	UNP P04545
P	61	ASP	SER	ENGINEERED MUTATION	UNP P04545

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	N	1	Total 1	Zn 1	0	0
2	O	1	Total 1	Zn 1	0	0
2	L	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0
2	M	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

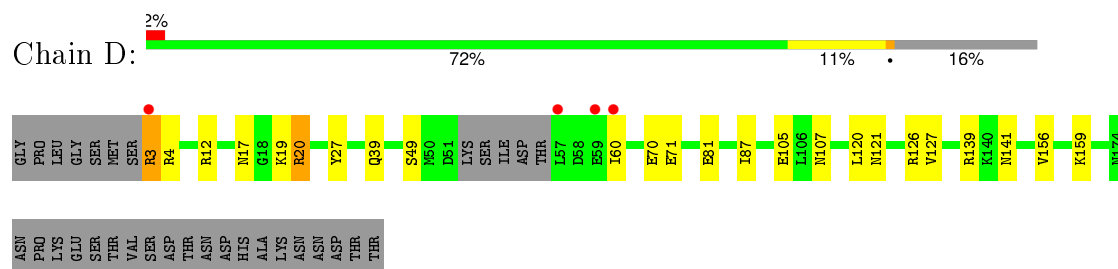
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	39	Total 39	O 39	0	0
3	C	27	Total 27	O 27	0	0
3	D	49	Total 49	O 49	0	0
3	E	29	Total 29	O 29	0	0
3	F	8	Total 8	O 8	0	0
3	G	28	Total 28	O 28	0	0
3	H	24	Total 24	O 24	0	0

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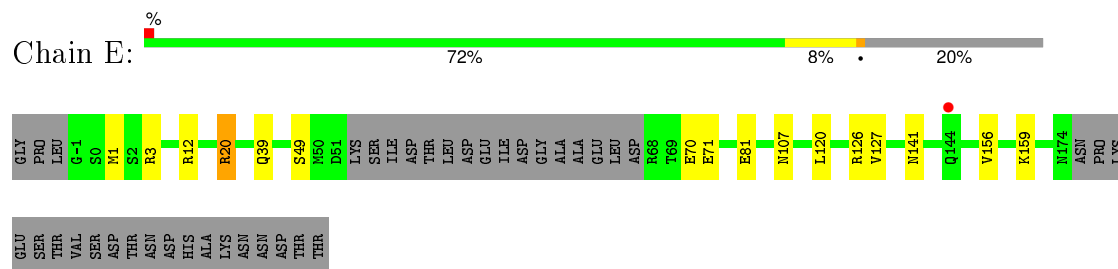
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	24	Total 24	O 24	0	0
3	J	30	Total 30	O 30	0	0
3	K	27	Total 27	O 27	0	0
3	L	15	Total 15	O 15	0	0
3	M	19	Total 19	O 19	0	0
3	N	21	Total 21	O 21	0	0
3	O	18	Total 18	O 18	0	0
3	P	12	Total 12	O 12	0	0

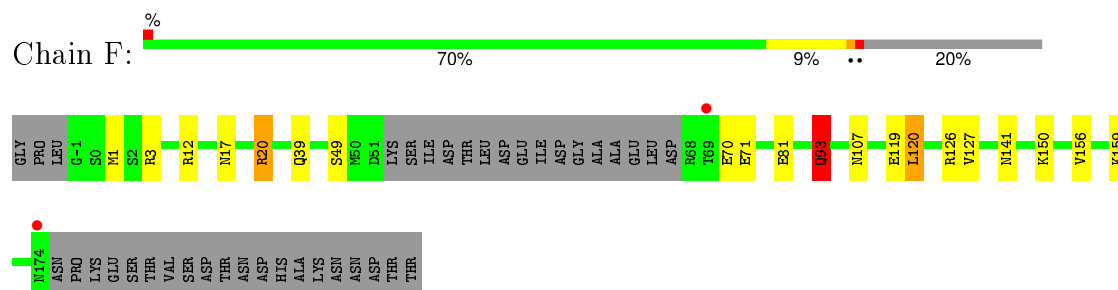
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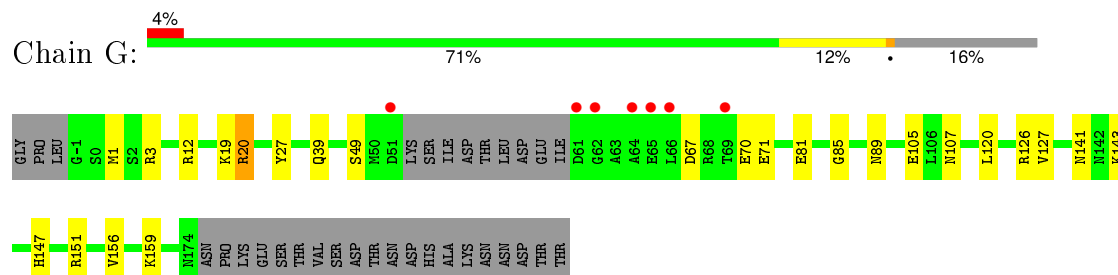
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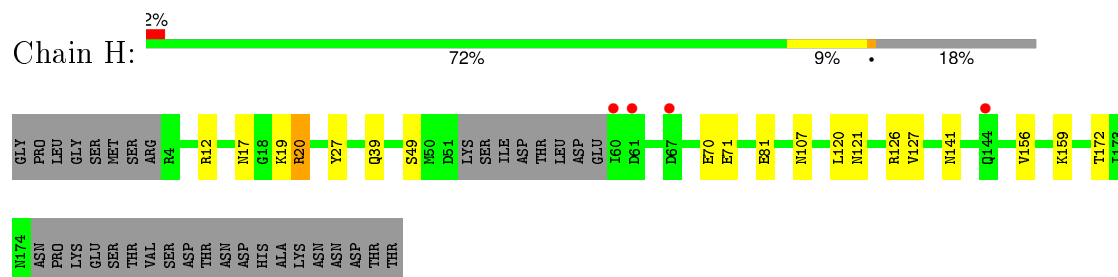
- Molecule 1: MATRIX M2-1



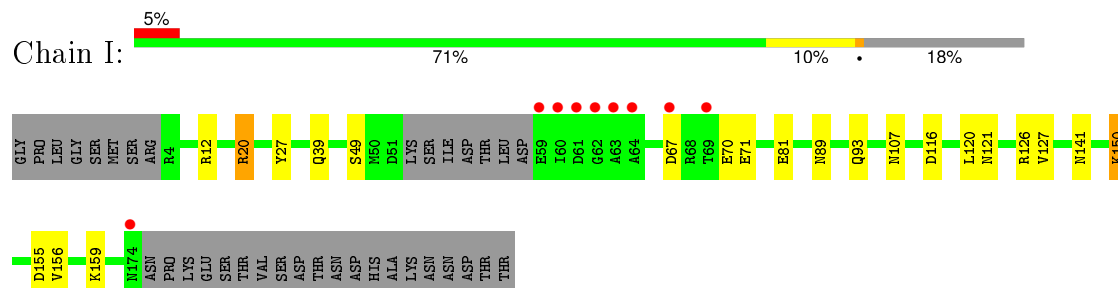
- Molecule 1: MATRIX M2-1



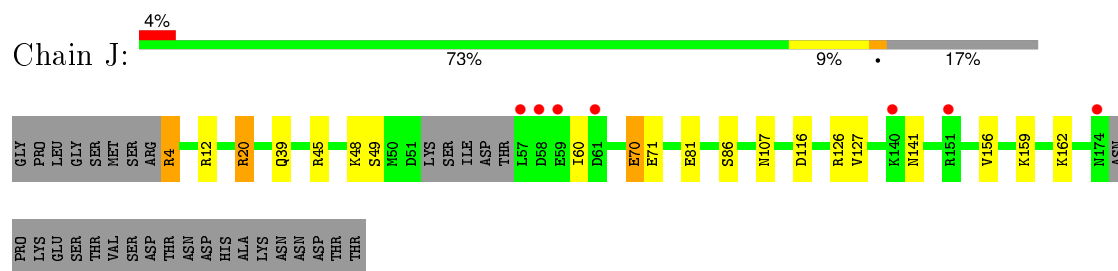
- Molecule 1: MATRIX M2-1



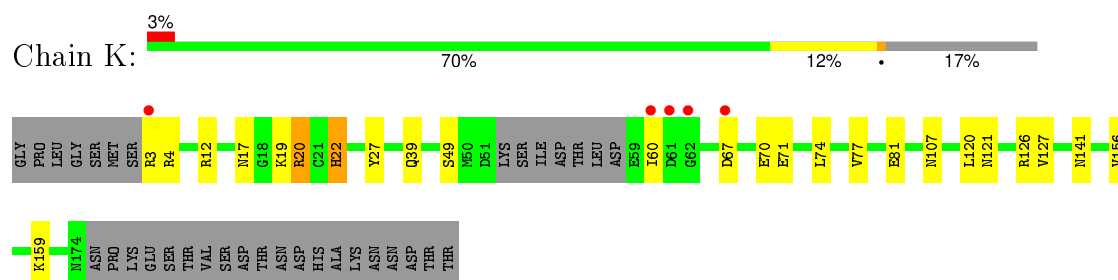
- Molecule 1: MATRIX M2-1



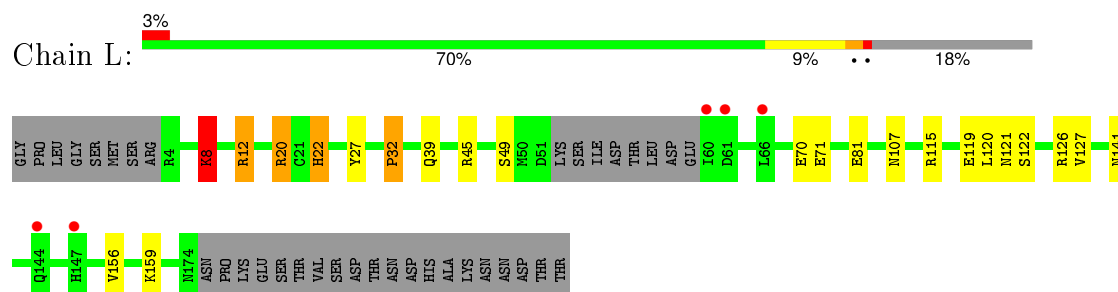
- Molecule 1: MATRIX M2-1



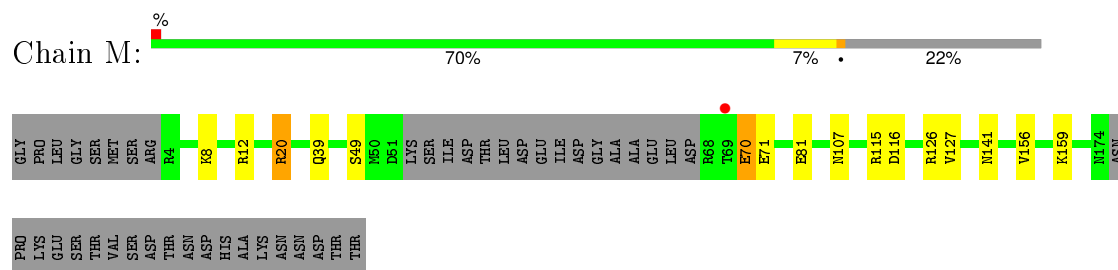
- Molecule 1: MATRIX M2-1



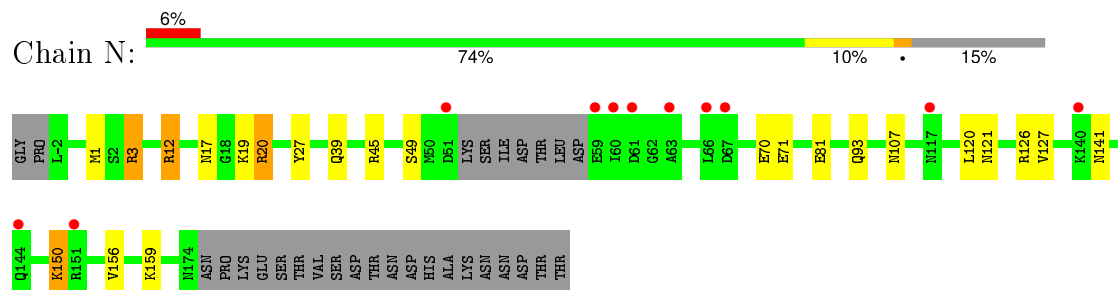
- Molecule 1: MATRIX M2-1



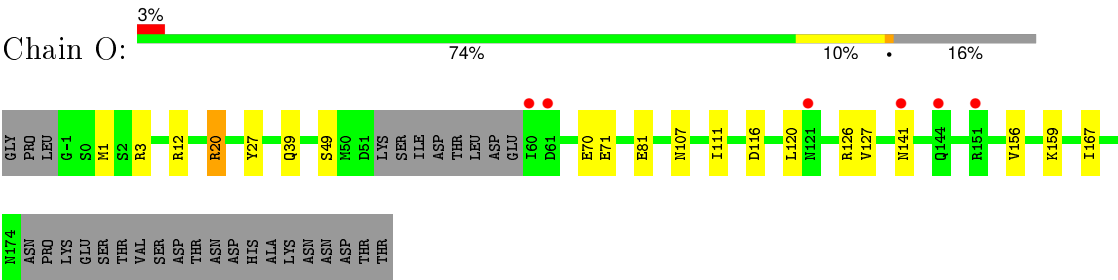
- Molecule 1: MATRIX M2-1



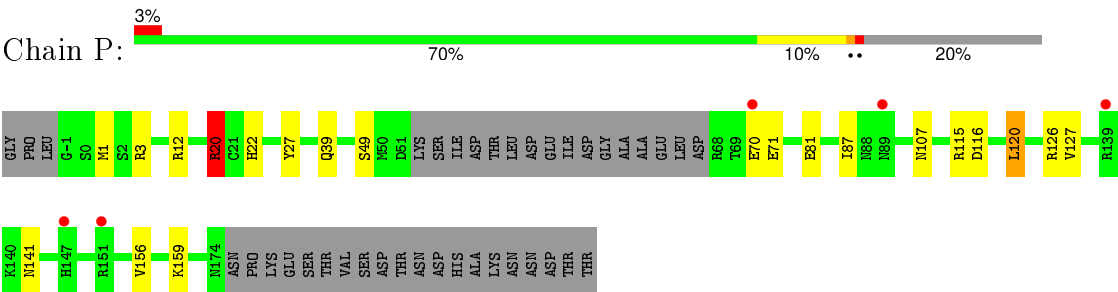
- Molecule 1: MATRIX M2-1



● Molecule 1: MATRIX M2-1



● Molecule 1: MATRIX M2-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.68Å 141.60Å 142.16Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	78.24 – 2.40 78.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.24-2.40) 100.0 (78.12-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.203 , 0.238 0.205 , 0.236	Depositor DCC
R_{free} test set	6851 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 138114 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21997	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 6.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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:
ZN

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	2/1434 (0.1%)	0.84	2/1928 (0.1%)
1	B	0.79	1/1428 (0.1%)	0.88	4/1920 (0.2%)
1	C	0.80	2/1418 (0.1%)	0.87	6/1907 (0.3%)
1	D	0.76	1/1402 (0.1%)	0.82	2/1886 (0.1%)
1	E	0.78	0/1338	0.80	2/1797 (0.1%)
1	F	0.79	0/1346	0.84	3/1808 (0.2%)
1	G	0.78	1/1385 (0.1%)	0.79	2/1860 (0.1%)
1	H	0.77	1/1355 (0.1%)	0.77	1/1823 (0.1%)
1	I	0.77	1/1356 (0.1%)	0.78	2/1825 (0.1%)
1	J	0.74	0/1383	0.78	1/1861 (0.1%)
1	K	0.76	1/1386 (0.1%)	0.83	3/1865 (0.2%)
1	L	0.78	2/1369 (0.1%)	0.84	4/1842 (0.2%)
1	M	0.75	0/1303	0.78	1/1752 (0.1%)
1	N	0.76	1/1429 (0.1%)	0.81	3/1920 (0.2%)
1	O	0.74	1/1382 (0.1%)	0.79	2/1858 (0.1%)
1	P	0.75	1/1327 (0.1%)	0.79	3/1783 (0.2%)
All	All	0.77	15/22041 (0.1%)	0.82	41/29635 (0.1%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	TYR	CE1-CZ	-7.89	1.28	1.38
1	H	27	TYR	CE1-CZ	-6.96	1.29	1.38
1	L	27	TYR	CE1-CZ	-6.84	1.29	1.38
1	N	27	TYR	CE1-CZ	-6.71	1.29	1.38
1	G	27	TYR	CE1-CZ	-6.30	1.30	1.38

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	LYS	CB-CG-CD	12.62	144.42	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ARG	CA-CB-CG	9.86	135.09	113.40
1	L	8	LYS	CD-CE-NZ	8.28	130.75	111.70
1	N	3	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	I	150	LYS	CA-CB-CG	6.60	127.92	113.40

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	1404	0	1442	14	0
1	B	1391	0	1431	12	0
1	C	1390	0	1419	5	0
1	D	1372	0	1406	15	0
1	E	1311	0	1355	4	0
1	F	1316	0	1361	16	0
1	G	1359	0	1399	20	0
1	H	1329	0	1365	9	0
1	I	1332	0	1359	14	0
1	J	1356	0	1387	13	0
1	K	1355	0	1385	14	0
1	L	1338	0	1373	17	0
1	M	1276	0	1317	9	0
1	N	1396	0	1440	18	0
1	O	1358	0	1391	6	0
1	P	1303	0	1342	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	25	0	0	0	0
3	B	39	0	0	3	0
3	C	27	0	0	0	0
3	D	49	0	0	1	0
3	E	29	0	0	0	0
3	F	8	0	0	0	0
3	G	28	0	0	1	0
3	H	24	0	0	0	0
3	I	24	0	0	1	0
3	J	30	0	0	2	0
3	K	27	0	0	1	0
3	L	15	0	0	1	0
3	M	19	0	0	1	0
3	N	21	0	0	0	0
3	O	18	0	0	0	0
3	P	12	0	0	2	0
All	All	21997	0	22172	128	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 128 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:G:20[B]:ARG:CB	1:G:20[B]:ARG:HH11	1.39	1.35
1:G:20[B]:ARG:HB3	1:G:20[B]:ARG:NH1	1.62	1.15
1:F:120:LEU:HD22	1:L:119:GLU:HB2	1.27	1.08
1:G:20[B]:ARG:HB3	1:G:20[B]:ARG:HH11	0.89	1.05
1:F:120:LEU:CD2	1:L:119:GLU:HB2	1.89	1.00

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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	171/199 (86%)	164 (96%)	7 (4%)	0	100	100
1	B	169/199 (85%)	163 (96%)	6 (4%)	0	100	100
1	C	169/199 (85%)	162 (96%)	7 (4%)	0	100	100
1	D	166/199 (83%)	159 (96%)	7 (4%)	0	100	100
1	E	158/199 (79%)	153 (97%)	5 (3%)	0	100	100
1	F	159/199 (80%)	152 (96%)	7 (4%)	0	100	100
1	G	165/199 (83%)	158 (96%)	7 (4%)	0	100	100
1	H	161/199 (81%)	154 (96%)	7 (4%)	0	100	100
1	I	161/199 (81%)	154 (96%)	7 (4%)	0	100	100
1	J	164/199 (82%)	156 (95%)	8 (5%)	0	100	100
1	K	164/199 (82%)	157 (96%)	7 (4%)	0	100	100
1	L	162/199 (81%)	155 (96%)	7 (4%)	0	100	100
1	M	153/199 (77%)	146 (95%)	7 (5%)	0	100	100
1	N	170/199 (85%)	164 (96%)	6 (4%)	0	100	100
1	O	165/199 (83%)	158 (96%)	7 (4%)	0	100	100
1	P	157/199 (79%)	150 (96%)	7 (4%)	0	100	100
All	All	2614/3184 (82%)	2505 (96%)	109 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	161/183 (88%)	146 (91%)	15 (9%)	11	16
1	B	160/183 (87%)	145 (91%)	15 (9%)	11	16
1	C	159/183 (87%)	144 (91%)	15 (9%)	11	16
1	D	157/183 (86%)	144 (92%)	13 (8%)	14	21
1	E	151/183 (82%)	139 (92%)	12 (8%)	15	23
1	F	152/183 (83%)	138 (91%)	14 (9%)	11	16
1	G	155/183 (85%)	141 (91%)	14 (9%)	12	17
1	H	152/183 (83%)	141 (93%)	11 (7%)	18	28
1	I	152/183 (83%)	142 (93%)	10 (7%)	21	32
1	J	155/183 (85%)	143 (92%)	12 (8%)	16	24
1	K	155/183 (85%)	141 (91%)	14 (9%)	12	17
1	L	153/183 (84%)	139 (91%)	14 (9%)	11	16
1	M	147/183 (80%)	137 (93%)	10 (7%)	20	31
1	N	160/183 (87%)	147 (92%)	13 (8%)	15	22
1	O	155/183 (85%)	143 (92%)	12 (8%)	16	24
1	P	150/183 (82%)	138 (92%)	12 (8%)	15	23
All	All	2474/2928 (84%)	2268 (92%)	206 (8%)	15	21

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	127	VAL
1	I	127	VAL
1	O	127	VAL
1	G	151	ARG
1	H	126	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	141	ASN
1	I	117	ASN
1	O	117	ASN
1	H	141	ASN
1	I	141	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](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	172/199 (86%)	0.03	2 (1%) 81 81	17, 41, 80, 98	0
1	B	168/199 (84%)	0.14	8 (4%) 34 35	18, 41, 84, 139	0
1	C	171/199 (85%)	0.10	6 (3%) 48 48	16, 44, 88, 127	0
1	D	167/199 (83%)	0.06	4 (2%) 62 61	20, 43, 87, 119	0
1	E	160/199 (80%)	-0.04	1 (0%) 90 90	19, 43, 80, 115	0
1	F	160/199 (80%)	-0.03	2 (1%) 79 79	19, 41, 81, 123	0
1	G	167/199 (83%)	0.11	7 (4%) 40 41	22, 43, 84, 106	0
1	H	163/199 (81%)	0.06	4 (2%) 61 60	17, 44, 84, 101	0
1	I	164/199 (82%)	0.14	9 (5%) 29 29	20, 42, 94, 124	0
1	J	166/199 (83%)	0.16	7 (4%) 40 41	18, 44, 93, 122	0
1	K	165/199 (82%)	0.10	5 (3%) 54 53	19, 44, 95, 138	0
1	L	163/199 (81%)	0.21	5 (3%) 52 52	19, 46, 92, 115	0
1	M	155/199 (77%)	-0.02	1 (0%) 90 90	19, 46, 85, 110	0
1	N	170/199 (85%)	0.24	11 (6%) 22 22	20, 51, 97, 131	0
1	O	168/199 (84%)	0.22	6 (3%) 46 47	20, 51, 88, 127	0
1	P	160/199 (80%)	0.15	5 (3%) 52 52	20, 55, 114, 137	0
All	All	2639/3184 (82%)	0.10	83 (3%) 52 52	16, 45, 93, 139	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	59	GLU	6.3
1	D	3	ARG	6.1
1	O	121	ASN	5.8
1	K	3	ARG	5.7
1	B	2	SER	4.9

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	ZN	P	201	1/1	1.00	0.14	0.91	26,26,26,26	0
2	ZN	I	201	1/1	0.99	0.15	0.66	27,27,27,27	0
2	ZN	C	201	1/1	0.99	0.14	0.32	22,22,22,22	0
2	ZN	O	201	1/1	0.99	0.14	0.01	28,28,28,28	0
2	ZN	N	201	1/1	0.99	0.14	-0.03	25,25,25,25	0
2	ZN	G	201	1/1	1.00	0.14	-0.09	33,33,33,33	0
2	ZN	L	201	1/1	1.00	0.13	-0.11	27,27,27,27	0
2	ZN	A	201	1/1	1.00	0.13	-0.13	26,26,26,26	0
2	ZN	H	201	1/1	0.99	0.14	-0.27	25,25,25,25	0
2	ZN	J	201	1/1	1.00	0.12	-0.44	27,27,27,27	0
2	ZN	F	201	1/1	1.00	0.13	-0.49	28,28,28,28	0
2	ZN	D	201	1/1	0.99	0.13	-0.61	27,27,27,27	0
2	ZN	M	201	1/1	1.00	0.12	-0.85	27,27,27,27	0
2	ZN	B	201	1/1	0.99	0.13	-0.91	28,28,28,28	0
2	ZN	K	201	1/1	1.00	0.14	-0.95	30,30,30,30	0
2	ZN	E	201	1/1	0.99	0.11	-2.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.