



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 AM UTC

PDB ID : 5DCX / pdb_00005dcx
Title : Structural studies of AAV2 Rep68 reveal a partially structured linker and compact domain conformation
Authors : Musayev, F.N.; Zarate-Perez, F.
Deposited on : 2015-08-24
Resolution : 2.60 Å(reported)

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

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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
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

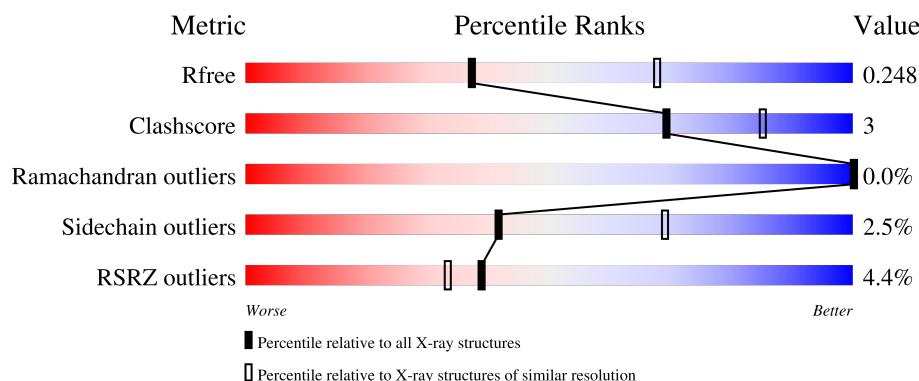
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	227	4% 82% 9% 8%
1	B	227	2% 79% 10% 10%
1	C	227	2% 80% 8% 11%
1	D	227	2% 79% 9% 11%
1	E	227	3% 78% 7% 14%

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Mol	Chain	Length	Quality of chain
1	F	227	 4% 75% 7% 17%
1	G	227	 4% 79% 10% 11%
1	H	227	 4% 81% 7% 11%
1	I	227	 5% 73% 9% 17%
1	J	227	 15% 69% 13% 19%
1	K	227	 15% 71% 11% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	301	-	-	-	X
2	MG	B	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17626 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 Rep68.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1698	1091	288	314	5			
1	B	205	Total	C	N	O	S	0	0	0
			1675	1076	284	310	5			
1	C	202	Total	C	N	O	S	0	0	0
			1622	1046	272	298	6			
1	D	202	Total	C	N	O	S	0	0	0
			1643	1057	276	305	5			
1	E	195	Total	C	N	O	S	0	0	0
			1594	1030	267	291	6			
1	F	188	Total	C	N	O	S	0	0	0
			1524	988	252	278	6			
1	G	203	Total	C	N	O	S	0	0	0
			1620	1044	276	295	5			
1	H	202	Total	C	N	O	S	0	0	0
			1609	1036	268	300	5			
1	I	189	Total	C	N	O	S	0	0	0
			1541	998	255	282	6			
1	J	185	Total	C	N	O	S	0	0	0
			1478	957	249	268	4			
1	K	189	Total	C	N	O	S	0	0	0
			1438	939	237	256	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P03132
A	-1	SER	-	expression tag	UNP P03132
A	0	HIS	-	expression tag	UNP P03132
A	151	SER	CYS	engineered mutation	UNP P03132
B	-2	GLY	-	expression tag	UNP P03132
B	-1	SER	-	expression tag	UNP P03132
B	0	HIS	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	151	SER	CYS	engineered mutation	UNP P03132
C	-2	GLY	-	expression tag	UNP P03132
C	-1	SER	-	expression tag	UNP P03132
C	0	HIS	-	expression tag	UNP P03132
C	151	SER	CYS	engineered mutation	UNP P03132
D	-2	GLY	-	expression tag	UNP P03132
D	-1	SER	-	expression tag	UNP P03132
D	0	HIS	-	expression tag	UNP P03132
D	151	SER	CYS	engineered mutation	UNP P03132
E	-2	GLY	-	expression tag	UNP P03132
E	-1	SER	-	expression tag	UNP P03132
E	0	HIS	-	expression tag	UNP P03132
E	151	SER	CYS	engineered mutation	UNP P03132
F	-2	GLY	-	expression tag	UNP P03132
F	-1	SER	-	expression tag	UNP P03132
F	0	HIS	-	expression tag	UNP P03132
F	151	SER	CYS	engineered mutation	UNP P03132
G	-2	GLY	-	expression tag	UNP P03132
G	-1	SER	-	expression tag	UNP P03132
G	0	HIS	-	expression tag	UNP P03132
G	151	SER	CYS	engineered mutation	UNP P03132
H	-2	GLY	-	expression tag	UNP P03132
H	-1	SER	-	expression tag	UNP P03132
H	0	HIS	-	expression tag	UNP P03132
H	151	SER	CYS	engineered mutation	UNP P03132
I	-2	GLY	-	expression tag	UNP P03132
I	-1	SER	-	expression tag	UNP P03132
I	0	HIS	-	expression tag	UNP P03132
I	151	SER	CYS	engineered mutation	UNP P03132
J	-2	GLY	-	expression tag	UNP P03132
J	-1	SER	-	expression tag	UNP P03132
J	0	HIS	-	expression tag	UNP P03132
J	151	SER	CYS	engineered mutation	UNP P03132
K	-2	GLY	-	expression tag	UNP P03132
K	-1	SER	-	expression tag	UNP P03132
K	0	HIS	-	expression tag	UNP P03132
K	151	SER	CYS	engineered mutation	UNP P03132

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	35	Total O 35 35	0	0
3	C	16	Total O 16 16	0	0
3	D	18	Total O 18 18	0	0
3	E	19	Total O 19 19	0	0
3	F	18	Total O 18 18	0	0
3	G	15	Total O 15 15	0	0

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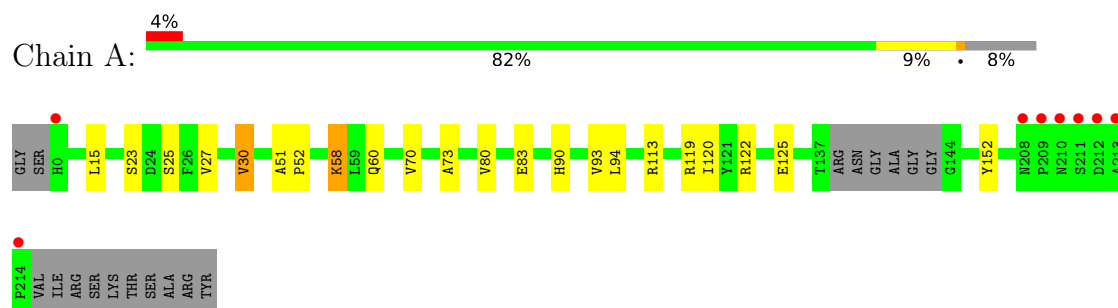
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	10	Total 10	O 10	0	0
3	I	6	Total 6	O 6	0	0
3	J	11	Total 11	O 11	0	0
3	K	3	Total 3	O 3	0	0

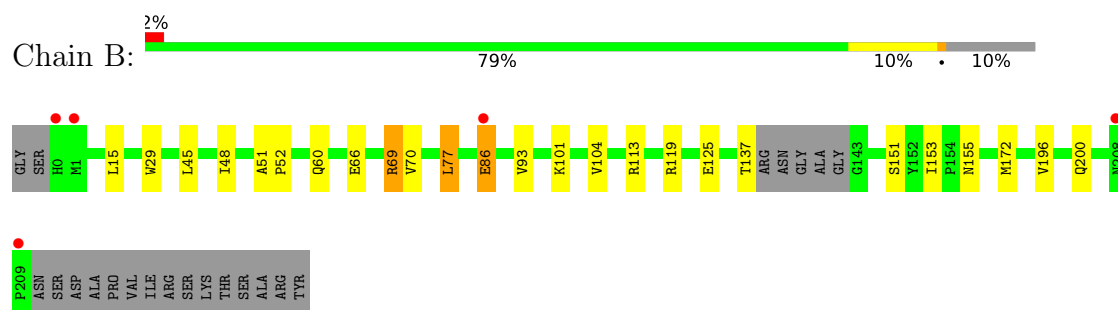
3 Residue-property plots [i](#)

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.

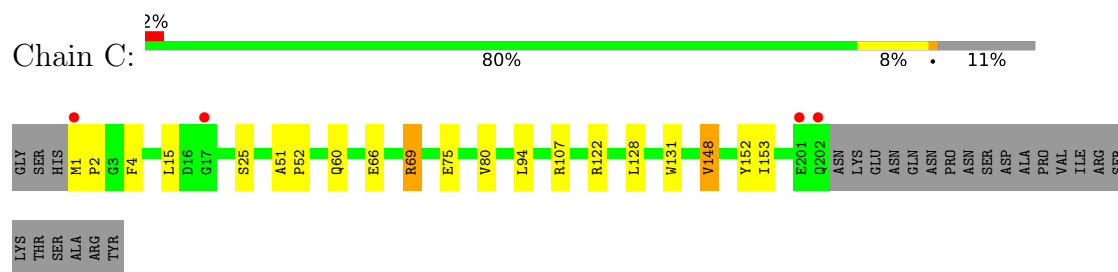
• Molecule 1: Protein Rep68



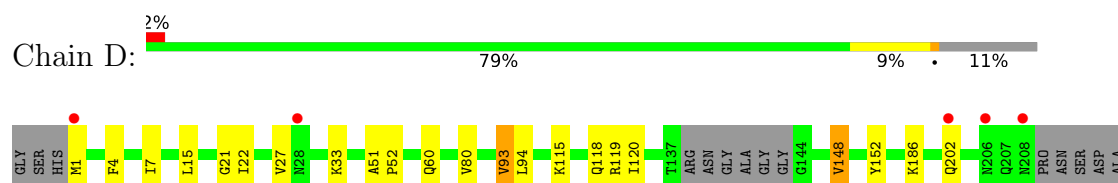
• Molecule 1: Protein Rep68



• Molecule 1: Protein Rep68

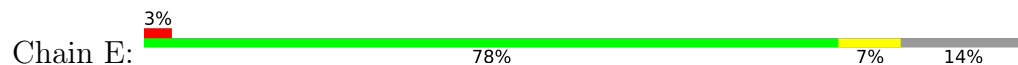


• Molecule 1: Protein Rep68



PRO VAL ILE ARG SER LYS THR SER ALA ARG TYR

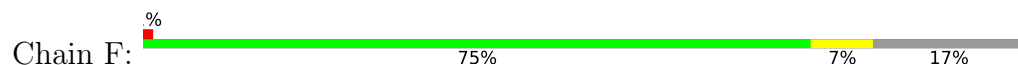
• Molecule 1: Protein Rep68



GLY SER SER HIS M1 L15 V27 A51 P52 L59 Q60 V80 R113 E114 I120 Y121 E125 R138 ASN GLY ALA GLY GLY G144 V147 T194 H195 Q198 T199 Q200 GLU GLN ASN LYS GLU ASN GLN ASN PRO ASN ASP ALA PRO VAL ILE ARG LYS

THR SER SER ARG TYR

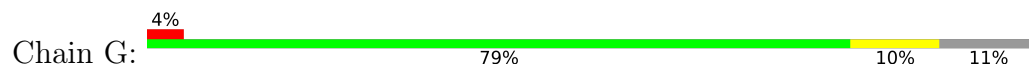
• Molecule 1: Protein Rep68



GLY SER SER HIS M1 G17 H13 W35 P38 A51 P52 E57 E66 R69 L94 Q111 K115 T127 L128 W131 V134 T137 ARG ASN GLY ALA GLY G143 V147 Y152 Q191 H192 L193 THR HIS VAL SER GLN THR GLN GLN LYS

GLU ASN GLN ASN PRO SER ALA PRO VAL ILE ARG SER LYS THR SER ALA ARG TYR

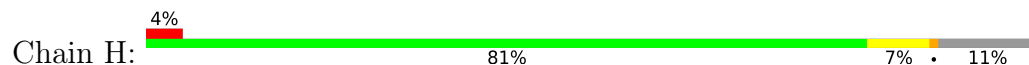
• Molecule 1: Protein Rep68



GLY SER SER HIS M1 P2 G3 F4 D14 L15 D16 G17 E24 S25 F26 V27 D44 A51 P52 Q60 K72 E75 A76 L77 V80 E86 V93 L94 P95 E96 K101 R122 V147 V148 Y152 Q162 E173 L176 K186 R203 GLU

ASN GLN ASN PRO ASN SER ASP ALA PRO VAL ILE ARG SER LYS THR SER ALA ARG TYR

• Molecule 1: Protein Rep68



GLY SER SER HIS M1 P2 G17 E32 A51 P52 K58 L59 Q60 L77 V80 I120 L128 W131 V134 T135 K136 T137 R138 ASN GLY ALA GLY GLY G144 V147 E150 M172 E173 Q174 T183 K186 Q202 Q207 ASN PRO ASN SER ASP ALA

PRO VAL ILE ARG SER LYS THR SER ALA ARG TYR

• Molecule 1: Protein Rep68



GLY SER SER HIS M1 G17 D40 A51 P52 K58 D62 R68 P74 L77 L94 I120 Y121 I124 E125 T137 ARG ASN GLY ALA GLY GLY G144 V147 E150 S161 Y162 I163 P163 Q166 T170 M171 M172 E173 Q174 Y175 L176 H195 VAL

SER
GLN
THR
GLN
GLU
GLN
ASN
LYS
GLU
ASN
GLN
ASN
PRO
ASN
SER
ASP
ALA
PRO
VAL
TLE
ARG
SER
LYS
THR
SER
ALA
ARG
TYR

● Molecule 1: Protein Rep68



GLY
SER
HIS
MET
PRO
G3
K10
L15
G21
V27
P38
P39
D40
E49
Q50
A51
P52
A73
A76
L77
V80
F89
H90
M91
H92
V93
L94
V95
E96
T97
T98
M103
R107
R119
L128
P129
R138
ASN
GLY
ALA
GLY
GLY
G144
V147

Y152
Y153
P154
L158
E173
Q174
S177
A178
R185
L188
V189
A190
Q191
H192
LEU
THR
HIS
VAL
SER
GLN
THR
GLN
GLU
GLN
ASN
LYS
GLU
ASN
GLN
ASN
PRO
ASN
SER
ASP
ALA
PRO
VAL
TLE
ARG
SER
LYS
THR
SER
ALA
ARG
TYR

● Molecule 1: Protein Rep68



GLY
SER
HIS
M1
P2
L15
D16
G17
H18
W35
P39
D40
S41
D42
M43
D44
L45
M46
L47
I48
D62
T65
Q81
F82
E83
L94
I117
T124
E125
P126
T127
L128
W131
T137
ARG
ASN
GLY
ALA
GLY
GLY
G144
N145
K146
D149
Y152
I153
P154

W155
Y156
L157
L158
P159
K160
T161
Q162
P163
E164
Q174
S177
A178
C179
L180
M181
L182
T183
E184
R185
L188
V189
A190
Q191
H192
L193
T194
H195
VAL
SER
GLN
THR
GLN
GLU
GLN
ASN
LYS
GLU
ASN
GLN
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ASN
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SER
ASP
ALA
PRO
VAL
ILE
ARG
SER
LYS
THR
SER
ALA
ARG
TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.64Å 178.71Å 130.36Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	29.81 – 2.60 29.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.81-2.60) 98.6 (29.81-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.237 0.207 , 0.248	Depositor DCC
R_{free} test set	5239 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17626	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: MG

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	0.29	0/1743	0.73	2/2372 (0.1%)
1	B	0.30	0/1719	0.73	2/2337 (0.1%)
1	C	0.28	0/1665	0.74	2/2266 (0.1%)
1	D	0.30	0/1685	0.72	0/2291
1	E	0.28	0/1635	0.74	0/2222
1	F	0.30	0/1565	0.75	0/2129
1	G	0.32	0/1663	0.75	0/2264
1	H	0.29	0/1651	0.70	0/2253
1	I	0.28	0/1583	0.77	4/2154 (0.2%)
1	J	0.29	0/1518	0.76	1/2069 (0.0%)
1	K	0.32	0/1478	0.86	2/2025 (0.1%)
All	All	0.30	0/17905	0.75	13/24382 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	125	GLU	CA-C-N	7.54	127.59	119.90
1	K	125	GLU	C-N-CA	7.54	127.59	119.90
1	I	125	GLU	CA-C-N	5.54	126.77	119.84
1	I	125	GLU	C-N-CA	5.54	126.77	119.84
1	I	153	ILE	CA-C-N	-5.27	114.32	119.64
1	I	153	ILE	C-N-CA	-5.27	114.32	119.64
1	B	153	ILE	CA-C-N	-5.23	114.39	120.04
1	B	153	ILE	C-N-CA	-5.23	114.39	120.04
1	A	73	ALA	CA-C-N	5.08	124.69	119.05
1	A	73	ALA	C-N-CA	5.08	124.69	119.05
1	J	38	PRO	O-C-N	5.05	123.53	121.15
1	C	153	ILE	CA-C-N	-5.05	114.54	119.64
1	C	153	ILE	C-N-CA	-5.05	114.54	119.64

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	1698	0	1660	13	0
1	B	1675	0	1645	15	0
1	C	1622	0	1594	11	0
1	D	1643	0	1608	10	0
1	E	1594	0	1584	9	0
1	F	1524	0	1499	9	0
1	G	1620	0	1585	11	0
1	H	1609	0	1539	8	0
1	I	1541	0	1514	12	0
1	J	1478	0	1420	15	0
1	K	1438	0	1345	16	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
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	22	0	0	1	0
3	B	35	0	0	1	0
3	C	16	0	0	1	0
3	D	18	0	0	0	0
3	E	19	0	0	0	0
3	F	18	0	0	0	0
3	G	15	0	0	1	0
3	H	10	0	0	0	0
3	I	6	0	0	0	0
3	J	11	0	0	0	0
3	K	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17626	0	16993	120	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.

All (120) 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:I:173:GLU:HA	1:I:176:LEU:HG	1.63	0.80
1:A:119:ARG:NH1	1:D:21:GLY:O	2.26	0.68
1:B:66:GLU:OE2	1:B:69:ARG:NH2	2.29	0.66
1:C:66:GLU:OE2	1:C:69:ARG:NH1	2.30	0.64
1:A:25:SER:OG	1:A:122:ARG:NH2	2.31	0.63
1:D:119:ARG:NH2	1:F:38:PRO:O	2.31	0.63
1:A:15:LEU:HD21	1:A:27:VAL:HG22	1.83	0.61
1:H:150:GLU:OE2	1:H:174:GLN:NE2	2.34	0.60
1:G:94:LEU:HD11	1:G:152:TYR:HD2	1.66	0.59
1:G:25:SER:OG	1:G:122:ARG:NH1	2.35	0.58
1:I:58:LYS:HG2	1:I:120:ILE:HD12	1.85	0.58
1:E:198:GLN:OE1	1:E:199:THR:OG1	2.21	0.57
1:G:15:LEU:HD13	1:G:27:VAL:HG22	1.86	0.56
1:I:150:GLU:OE1	1:I:174:GLN:NE2	2.39	0.56
1:A:113:ARG:NH2	1:A:125:GLU:OE1	2.40	0.55
1:F:35:TRP:HH2	1:F:57:GLU:HG3	1.70	0.55
1:I:77:LEU:HD22	1:I:172:MET:HG2	1.89	0.55
1:B:29:TRP:HA	1:J:129:PRO:HG3	1.90	0.54
1:H:58:LYS:HD3	1:H:120:ILE:HG13	1.90	0.54
1:K:154:PRO:HA	1:K:158:LEU:HB2	1.90	0.54
1:J:76:ALA:HB1	1:J:96:GLU:HG2	1.91	0.53
1:C:75:GLU:CD	1:J:119:ARG:HH12	2.17	0.53
1:I:94:LEU:HD11	1:I:152:TYR:HD2	1.74	0.53
1:C:94:LEU:HD11	1:C:152:TYR:HD2	1.74	0.52
1:H:134:VAL:HG13	1:H:136:LYS:HE2	1.92	0.52
1:K:18:HIS:CG	1:K:128:LEU:HD21	2.44	0.51
1:I:68:ARG:HD3	1:I:74:PRO:HA	1.92	0.51
1:C:4:PHE:HB2	1:C:148:VAL:HG22	1.93	0.51
1:E:59:LEU:HD23	1:E:120:ILE:HD12	1.93	0.51
1:J:178:ALA:HB2	1:J:188:LEU:HD12	1.94	0.50
1:D:80:VAL:HG22	1:D:93:VAL:HB	1.94	0.50
1:C:25:SER:OG	1:C:122:ARG:NH1	2.45	0.50
1:I:94:LEU:HD11	1:I:152:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:NH2	1:B:125:GLU:OE1	2.45	0.49
1:D:7:ILE:O	1:D:93:VAL:HG13	2.12	0.49
1:J:154:PRO:HA	1:J:158:LEU:HD12	1.94	0.49
1:J:185:ARG:O	1:J:189:VAL:HG23	2.12	0.49
1:K:94:LEU:HD11	1:K:152:TYR:CD2	2.48	0.49
1:B:104:VAL:HG12	1:E:15:LEU:HD22	1.94	0.49
1:D:94:LEU:HD11	1:D:152:TYR:HD2	1.77	0.48
1:A:30:VAL:HG13	1:A:51:ALA:HB1	1.95	0.48
1:D:4:PHE:HB2	1:D:148:VAL:HG22	1.95	0.48
1:E:15:LEU:HD21	1:E:27:VAL:HG22	1.94	0.48
1:G:4:PHE:HB2	1:G:148:VAL:HG22	1.95	0.48
1:I:51:ALA:HB3	1:I:52:PRO:HD3	1.95	0.48
1:B:77:LEU:HG	1:B:172:MET:HG2	1.94	0.48
1:J:51:ALA:HB3	1:J:52:PRO:HD3	1.94	0.48
1:D:15:LEU:HD13	1:D:27:VAL:HG22	1.96	0.48
1:I:163:PRO:O	1:I:166:GLN:NE2	2.44	0.48
1:A:60:GLN:NE2	3:A:403:HOH:O	2.46	0.47
1:B:60:GLN:NE2	3:B:401:HOH:O	2.33	0.46
1:H:51:ALA:HB3	1:H:52:PRO:HD3	1.97	0.46
1:D:51:ALA:HB3	1:D:52:PRO:HD3	1.98	0.46
1:F:66:GLU:OE2	1:F:115:LYS:HD2	2.15	0.46
1:I:121:TYR:HB3	1:I:124:ILE:O	2.15	0.46
1:B:101:LYS:HD3	1:E:51:ALA:HB2	1.98	0.46
1:K:94:LEU:HD11	1:K:152:TYR:HD2	1.81	0.46
1:G:44:ASP:H	1:G:162:GLN:HE22	1.63	0.46
1:H:128:LEU:HB2	1:H:131:TRP:HB3	1.98	0.46
1:B:151:SER:O	1:B:155:ASN:HB2	2.16	0.46
1:G:72:LYS:NZ	3:G:401:HOH:O	2.48	0.46
1:K:125:GLU:HA	1:K:126:PRO:HD3	1.72	0.46
1:F:128:LEU:HB2	1:F:131:TRP:HB3	1.97	0.45
1:G:51:ALA:HB3	1:G:52:PRO:HD3	1.98	0.45
1:C:51:ALA:HB3	1:C:52:PRO:HD3	1.97	0.45
1:K:45:LEU:HA	1:K:48:ILE:HD12	1.99	0.45
1:D:60:GLN:HG3	1:D:80:VAL:HG11	1.97	0.45
1:C:107:ARG:NH2	1:D:22:ILE:O	2.40	0.45
1:E:51:ALA:HB3	1:E:52:PRO:HD3	1.99	0.45
1:K:137:THR:HG23	1:K:146:LYS:HB2	1.99	0.45
1:B:51:ALA:HB3	1:B:52:PRO:HD3	1.99	0.45
1:F:51:ALA:HB3	1:F:52:PRO:HD3	1.97	0.45
1:B:119:ARG:HG2	1:J:21:GLY:HA3	1.99	0.44
1:E:60:GLN:HG3	1:E:80:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:117:ILE:HD13	1:K:125:GLU:HB2	1.99	0.44
1:H:60:GLN:HG3	1:H:80:VAL:HG11	1.99	0.44
1:K:81:GLN:NE2	1:K:83:GLU:OE1	2.48	0.44
1:B:196:VAL:O	1:B:200:GLN:HG3	2.18	0.44
1:F:18:HIS:HA	1:F:127:THR:HB	1.99	0.44
1:K:43:MET:HG3	1:K:180:LEU:O	2.18	0.44
1:C:1:MET:HA	1:C:2:PRO:HD3	1.86	0.44
1:A:25:SER:HG	1:A:122:ARG:NH2	2.15	0.44
1:J:94:LEU:HD11	1:J:152:TYR:CD1	2.53	0.43
1:I:170:THR:HG23	1:I:176:LEU:HD23	2.00	0.43
1:F:94:LEU:HD11	1:F:152:TYR:HD2	1.83	0.43
1:J:10:LYS:NZ	1:J:129:PRO:O	2.39	0.43
1:J:15:LEU:HD13	1:J:27:VAL:HG22	2.01	0.43
1:K:1:MET:HG3	1:K:2:PRO:HD2	2.01	0.43
1:K:185:ARG:O	1:K:189:VAL:HG23	2.18	0.43
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.89	0.42
1:G:60:GLN:HG3	1:G:80:VAL:HG11	2.01	0.42
1:A:23:SER:O	1:A:27:VAL:HG23	2.18	0.42
1:C:60:GLN:NE2	3:C:401:HOH:O	2.52	0.42
1:J:49:GLU:HG3	1:J:89:PHE:HZ	1.83	0.42
1:A:51:ALA:HB3	1:A:52:PRO:HD3	2.00	0.42
1:A:83:GLU:OE2	1:A:90:HIS:NE2	2.53	0.42
1:C:128:LEU:HB2	1:C:131:TRP:HB3	2.02	0.42
1:K:154:PRO:HA	1:K:158:LEU:HD22	2.02	0.42
1:G:173:GLU:HA	1:G:176:LEU:HG	2.01	0.42
1:H:77:LEU:HD22	1:H:172:MET:HG2	2.02	0.42
1:B:137:THR:O	1:B:137:THR:OG1	2.33	0.42
1:E:59:LEU:HD11	1:E:121:TYR:OH	2.20	0.42
1:G:77:LEU:H	1:G:96:GLU:CD	2.27	0.42
1:K:128:LEU:HB2	1:K:131:TRP:HB3	2.02	0.42
1:F:111:GLN:O	1:F:115:LYS:HG3	2.20	0.41
1:A:58:LYS:HD3	1:A:120:ILE:HG12	2.02	0.41
1:A:94:LEU:HD11	1:A:152:TYR:HD2	1.85	0.41
1:K:62:ASP:HA	1:K:65:THR:HG22	2.02	0.41
1:K:43:MET:HE2	1:K:162:GLN:HE21	1.84	0.41
1:B:45:LEU:HA	1:B:48:ILE:HD12	2.01	0.41
1:F:94:LEU:HD11	1:F:152:TYR:CD2	2.55	0.41
1:E:113:ARG:NH2	1:E:125:GLU:OE2	2.54	0.41
1:J:128:LEU:HA	1:J:129:PRO:HD3	1.90	0.41
1:G:101:LYS:HE2	1:J:50:GLN:HB2	2.01	0.40
1:I:58:LYS:NZ	1:I:62:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HG13	1:A:93:VAL:HG22	2.04	0.40
1:B:86:GLU:CD	1:B:86:GLU:H	2.25	0.40
1:C:60:GLN:HG3	1:C:80:VAL:HG11	2.03	0.40
1:H:186:LYS:HB2	1:H:186:LYS:HE3	1.78	0.40
1:J:80:VAL:HG22	1:J:93:VAL:HG13	2.04	0.40

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	205/227 (90%)	203 (99%)	2 (1%)	0	100	100
1	B	201/227 (88%)	200 (100%)	1 (0%)	0	100	100
1	C	200/227 (88%)	197 (98%)	3 (2%)	0	100	100
1	D	198/227 (87%)	196 (99%)	2 (1%)	0	100	100
1	E	191/227 (84%)	189 (99%)	2 (1%)	0	100	100
1	F	184/227 (81%)	184 (100%)	0	0	100	100
1	G	201/227 (88%)	198 (98%)	3 (2%)	0	100	100
1	H	198/227 (87%)	196 (99%)	2 (1%)	0	100	100
1	I	185/227 (82%)	182 (98%)	3 (2%)	0	100	100
1	J	181/227 (80%)	175 (97%)	6 (3%)	0	100	100
1	K	185/227 (82%)	179 (97%)	5 (3%)	1 (0%)	24	46
All	All	2129/2497 (85%)	2099 (99%)	29 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	194	THR

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	186/203 (92%)	183 (98%)	3 (2%)	55	79
1	B	185/203 (91%)	180 (97%)	5 (3%)	39	67
1	C	176/203 (87%)	173 (98%)	3 (2%)	53	78
1	D	180/203 (89%)	171 (95%)	9 (5%)	22	46
1	E	176/203 (87%)	172 (98%)	4 (2%)	44	71
1	F	166/203 (82%)	163 (98%)	3 (2%)	51	76
1	G	173/203 (85%)	169 (98%)	4 (2%)	44	71
1	H	172/203 (85%)	168 (98%)	4 (2%)	44	71
1	I	169/203 (83%)	164 (97%)	5 (3%)	36	64
1	J	155/203 (76%)	151 (97%)	4 (3%)	40	68
1	K	142/203 (70%)	139 (98%)	3 (2%)	47	73
All	All	1880/2233 (84%)	1833 (98%)	47 (2%)	42	69

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	58	LYS
1	A	70	VAL
1	B	69	ARG
1	B	70	VAL
1	B	77	LEU
1	B	86	GLU
1	B	93	VAL
1	C	15	LEU
1	C	69	ARG
1	C	148	VAL
1	D	1	MET
1	D	33	LYS
1	D	93	VAL
1	D	115	LYS

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Mol	Chain	Res	Type
1	D	118	GLN
1	D	120	ILE
1	D	148	VAL
1	D	186	LYS
1	D	202	GLN
1	E	1	MET
1	E	114	GLU
1	E	138	ARG
1	E	147	VAL
1	F	134	VAL
1	F	147	VAL
1	F	191	GLN
1	G	75	GLU
1	G	93	VAL
1	G	147	VAL
1	G	148	VAL
1	H	120	ILE
1	H	134	VAL
1	H	147	VAL
1	H	183	THR
1	I	40	ASP
1	I	58	LYS
1	I	120	ILE
1	I	147	VAL
1	I	173	GLU
1	J	40	ASP
1	J	91	MET
1	J	107	ARG
1	J	147	VAL
1	K	125	GLU
1	K	182	LEU
1	K	194	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	B	145	ASN
1	B	155	ASN
1	D	145	ASN
1	D	200	GLN
1	D	202	GLN

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Mol	Chain	Res	Type
1	G	118	GLN
1	G	155	ASN
1	G	191	GLN
1	G	195	HIS
1	H	28	ASN
1	H	145	ASN
1	H	192	HIS
1	K	46	ASN
1	K	145	ASN
1	K	162	GLN

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](#)

Of 11 ligands modelled in this entry, 11 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 ⓘ

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(Å²)	Q<0.9
1	A	209/227 (92%)	-0.12	8 (3%)	44	38	28, 46, 82, 166	0
1	B	205/227 (90%)	-0.21	5 (2%)	59	54	27, 43, 70, 112	0
1	C	202/227 (88%)	-0.25	4 (1%)	65	60	28, 45, 76, 118	0
1	D	202/227 (88%)	-0.28	5 (2%)	58	52	29, 43, 78, 114	0
1	E	195/227 (85%)	-0.15	6 (3%)	51	45	32, 48, 93, 176	0
1	F	188/227 (82%)	-0.13	3 (1%)	70	66	28, 49, 82, 96	0
1	G	203/227 (89%)	0.06	8 (3%)	43	38	36, 57, 90, 125	0
1	H	202/227 (88%)	0.47	8 (3%)	42	37	49, 73, 102, 123	0
1	I	189/227 (83%)	0.14	3 (1%)	70	66	42, 67, 97, 133	0
1	J	185/227 (81%)	0.37	11 (5%)	28	23	33, 69, 111, 138	0
1	K	189/227 (83%)	0.98	34 (17%)	3	3	41, 82, 138, 188	0
All	All	2169/2497 (86%)	0.07	95 (4%)	39	33	27, 55, 104, 188	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	ALA	6.8
1	A	212	ASP	5.9
1	A	211	SER	5.7
1	J	177	SER	4.8
1	K	192	HIS	4.6
1	K	177	SER	4.6
1	E	200	GLN	4.4
1	K	194	THR	4.4
1	C	202	GLN	4.2
1	G	1	MET	4.1
1	K	40	ASP	4.1
1	K	193	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	173	GLU	3.9
1	A	210	ASN	3.8
1	A	214	PRO	3.7
1	G	24	ASP	3.7
1	B	208	ASN	3.6
1	A	209	PRO	3.5
1	K	182	LEU	3.5
1	E	198	GLN	3.5
1	K	195	HIS	3.5
1	K	16	ASP	3.5
1	I	195	HIS	3.4
1	K	15	LEU	3.4
1	H	1	MET	3.4
1	H	173	GLU	3.3
1	K	42	ASP	3.3
1	C	17	GLY	3.2
1	E	199	THR	3.2
1	K	183	THR	3.2
1	G	17	GLY	3.2
1	K	185	ARG	3.2
1	B	1	MET	3.2
1	K	137	THR	3.2
1	H	32	GLU	3.1
1	J	98	THR	3.1
1	D	208	ASN	3.1
1	D	206	ASN	3.1
1	K	161	THR	3.1
1	K	188	LEU	3.0
1	G	14	ASP	3.0
1	E	138	ARG	2.8
1	H	17	GLY	2.8
1	C	1	MET	2.8
1	K	124	ILE	2.7
1	B	0	HIS	2.7
1	F	17	GLY	2.7
1	K	1	MET	2.7
1	J	76	ALA	2.7
1	A	208	ASN	2.7
1	K	46	ASN	2.7
1	K	39	PRO	2.7
1	B	209	PRO	2.7
1	K	43	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	203	ASN	2.6
1	K	174	GLN	2.6
1	J	174	GLN	2.5
1	K	162	GLN	2.5
1	E	194	THR	2.5
1	K	44	ASP	2.5
1	H	2	PRO	2.5
1	K	163	PRO	2.5
1	G	86	GLU	2.4
1	H	202	GLN	2.4
1	H	138	ARG	2.4
1	A	0	HIS	2.4
1	J	190	ALA	2.4
1	I	40	ASP	2.4
1	K	164	GLU	2.4
1	J	3	GLY	2.4
1	H	207	GLN	2.4
1	G	2	PRO	2.4
1	I	17	GLY	2.4
1	E	195	HIS	2.3
1	K	181	ASN	2.3
1	J	103	MET	2.3
1	J	138	ARG	2.3
1	G	186	LYS	2.3
1	K	35	TRP	2.3
1	F	192	HIS	2.3
1	D	202	GLN	2.2
1	K	191	GLN	2.2
1	K	17	GLY	2.2
1	D	1	MET	2.2
1	J	77	LEU	2.2
1	K	178	ALA	2.1
1	K	184	GLU	2.1
1	B	86	GLU	2.1
1	C	201	GLU	2.1
1	F	69	ARG	2.1
1	K	156	TYR	2.1
1	J	73	ALA	2.0
1	K	159	PRO	2.0
1	D	28	ASN	2.0
1	K	149	ASP	2.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	301	1/1	0.17	0.66	443,443,443,443	0
2	MG	A	301	1/1	0.62	0.53	95,95,95,95	0
2	MG	H	301	1/1	0.92	0.17	46,46,46,46	0
2	MG	D	301	1/1	0.93	0.21	32,32,32,32	0
2	MG	I	301	1/1	0.93	0.18	57,57,57,57	0
2	MG	F	301	1/1	0.94	0.16	39,39,39,39	0
2	MG	G	301	1/1	0.95	0.15	36,36,36,36	0
2	MG	K	301	1/1	0.95	0.12	63,63,63,63	0
2	MG	J	301	1/1	0.96	0.13	48,48,48,48	0
2	MG	C	301	1/1	0.97	0.12	34,34,34,34	0
2	MG	E	301	1/1	0.98	0.10	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.