



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:49 pm BST

PDB ID : 6EC3
Title : Crystal Structure of EvdMO1
Authors : McCulloch, K.M.; Iverson, T.M.; Starbird, C.A.; Perry, N.A.; Chen, Q.;
Berndt, S.; Yamakawa, I.; Loukachevitch, L.V.
Deposited on : 2018-08-07
Resolution : 3.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

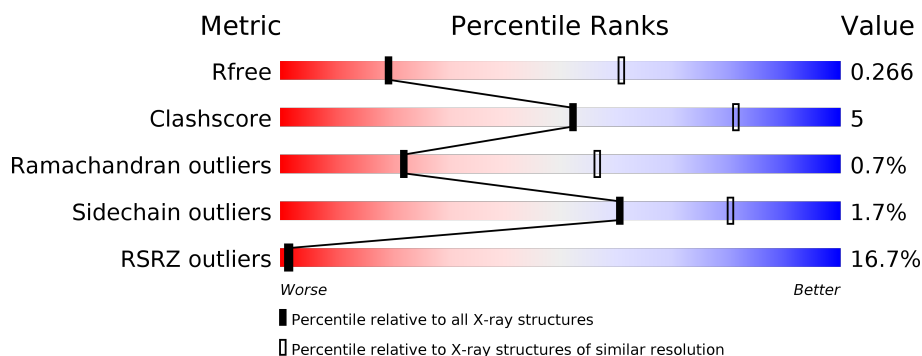
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 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	471	<div> <div>13%</div> <div>75%</div> <div>13%</div> <div>12%</div> </div>
1	B	471	<div> <div>15%</div> <div>75%</div> <div>12%</div> <div>12%</div> </div>
1	C	471	<div> <div>15%</div> <div>76%</div> <div>12%</div> <div>12%</div> </div>

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
3	BTB	C	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9743 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 Methyltransferase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3227	2036	581	603	7			
1	B	413	Total	C	N	O	S	0	0	0
			3223	2031	583	602	7			
1	C	416	Total	C	N	O	S	0	0	0
			3248	2047	586	608	7			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP A0A1C5AE13
A	-19	GLY	-	expression tag	UNP A0A1C5AE13
A	-18	SER	-	expression tag	UNP A0A1C5AE13
A	-17	SER	-	expression tag	UNP A0A1C5AE13
A	-16	HIS	-	expression tag	UNP A0A1C5AE13
A	-15	HIS	-	expression tag	UNP A0A1C5AE13
A	-14	HIS	-	expression tag	UNP A0A1C5AE13
A	-13	HIS	-	expression tag	UNP A0A1C5AE13
A	-12	HIS	-	expression tag	UNP A0A1C5AE13
A	-11	HIS	-	expression tag	UNP A0A1C5AE13
A	-10	SER	-	expression tag	UNP A0A1C5AE13
A	-9	SER	-	expression tag	UNP A0A1C5AE13
A	-8	GLY	-	expression tag	UNP A0A1C5AE13
A	-7	LEU	-	expression tag	UNP A0A1C5AE13
A	-6	VAL	-	expression tag	UNP A0A1C5AE13
A	-5	PRO	-	expression tag	UNP A0A1C5AE13
A	-4	ARG	-	expression tag	UNP A0A1C5AE13
A	-3	GLY	-	expression tag	UNP A0A1C5AE13
A	-2	SER	-	expression tag	UNP A0A1C5AE13
A	-1	HIS	-	expression tag	UNP A0A1C5AE13
A	0	MET	-	expression tag	UNP A0A1C5AE13
A	100	HIS	ASN	variant	UNP A0A1C5AE13
A	219	THR	LYS	variant	UNP A0A1C5AE13

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Chain	Residue	Modelled	Actual	Comment	Reference
A	232	ALA	THR	variant	UNP A0A1C5AE13
A	444	SER	ALA	variant	UNP A0A1C5AE13
B	-20	MET	-	expression tag	UNP A0A1C5AE13
B	-19	GLY	-	expression tag	UNP A0A1C5AE13
B	-18	SER	-	expression tag	UNP A0A1C5AE13
B	-17	SER	-	expression tag	UNP A0A1C5AE13
B	-16	HIS	-	expression tag	UNP A0A1C5AE13
B	-15	HIS	-	expression tag	UNP A0A1C5AE13
B	-14	HIS	-	expression tag	UNP A0A1C5AE13
B	-13	HIS	-	expression tag	UNP A0A1C5AE13
B	-12	HIS	-	expression tag	UNP A0A1C5AE13
B	-11	HIS	-	expression tag	UNP A0A1C5AE13
B	-10	SER	-	expression tag	UNP A0A1C5AE13
B	-9	SER	-	expression tag	UNP A0A1C5AE13
B	-8	GLY	-	expression tag	UNP A0A1C5AE13
B	-7	LEU	-	expression tag	UNP A0A1C5AE13
B	-6	VAL	-	expression tag	UNP A0A1C5AE13
B	-5	PRO	-	expression tag	UNP A0A1C5AE13
B	-4	ARG	-	expression tag	UNP A0A1C5AE13
B	-3	GLY	-	expression tag	UNP A0A1C5AE13
B	-2	SER	-	expression tag	UNP A0A1C5AE13
B	-1	HIS	-	expression tag	UNP A0A1C5AE13
B	0	MET	-	expression tag	UNP A0A1C5AE13
B	100	HIS	ASN	variant	UNP A0A1C5AE13
B	219	THR	LYS	variant	UNP A0A1C5AE13
B	232	ALA	THR	variant	UNP A0A1C5AE13
B	444	SER	ALA	variant	UNP A0A1C5AE13
C	-20	MET	-	expression tag	UNP A0A1C5AE13
C	-19	GLY	-	expression tag	UNP A0A1C5AE13
C	-18	SER	-	expression tag	UNP A0A1C5AE13
C	-17	SER	-	expression tag	UNP A0A1C5AE13
C	-16	HIS	-	expression tag	UNP A0A1C5AE13
C	-15	HIS	-	expression tag	UNP A0A1C5AE13
C	-14	HIS	-	expression tag	UNP A0A1C5AE13
C	-13	HIS	-	expression tag	UNP A0A1C5AE13
C	-12	HIS	-	expression tag	UNP A0A1C5AE13
C	-11	HIS	-	expression tag	UNP A0A1C5AE13
C	-10	SER	-	expression tag	UNP A0A1C5AE13
C	-9	SER	-	expression tag	UNP A0A1C5AE13
C	-8	GLY	-	expression tag	UNP A0A1C5AE13
C	-7	LEU	-	expression tag	UNP A0A1C5AE13
C	-6	VAL	-	expression tag	UNP A0A1C5AE13

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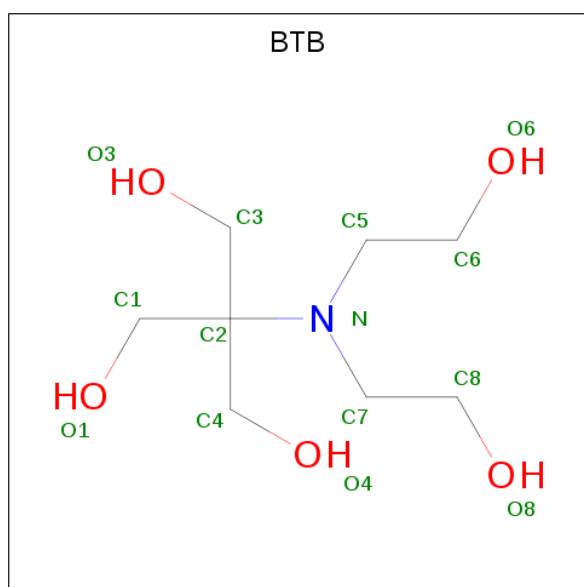
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	PRO	-	expression tag	UNP A0A1C5AE13
C	-4	ARG	-	expression tag	UNP A0A1C5AE13
C	-3	GLY	-	expression tag	UNP A0A1C5AE13
C	-2	SER	-	expression tag	UNP A0A1C5AE13
C	-1	HIS	-	expression tag	UNP A0A1C5AE13
C	0	MET	-	expression tag	UNP A0A1C5AE13
C	100	HIS	ASN	variant	UNP A0A1C5AE13
C	219	THR	LYS	variant	UNP A0A1C5AE13
C	232	ALA	THR	variant	UNP A0A1C5AE13
C	444	SER	ALA	variant	UNP A0A1C5AE13

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).

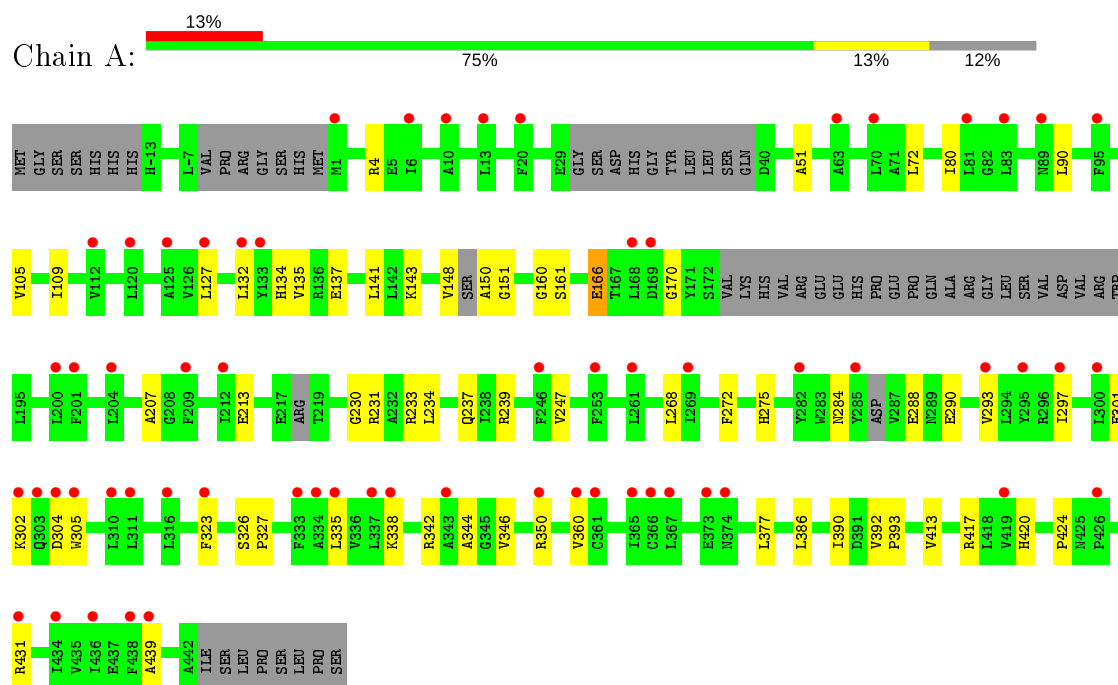


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

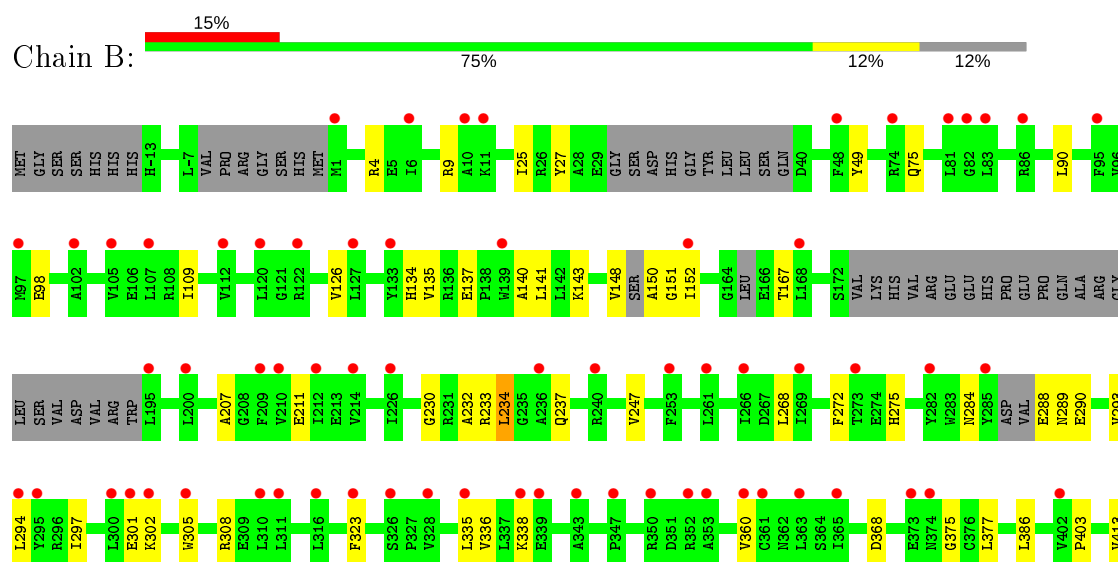
3 Residue-property plots [i](#)

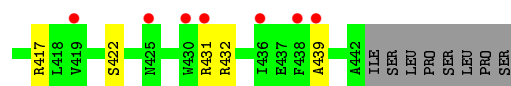
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

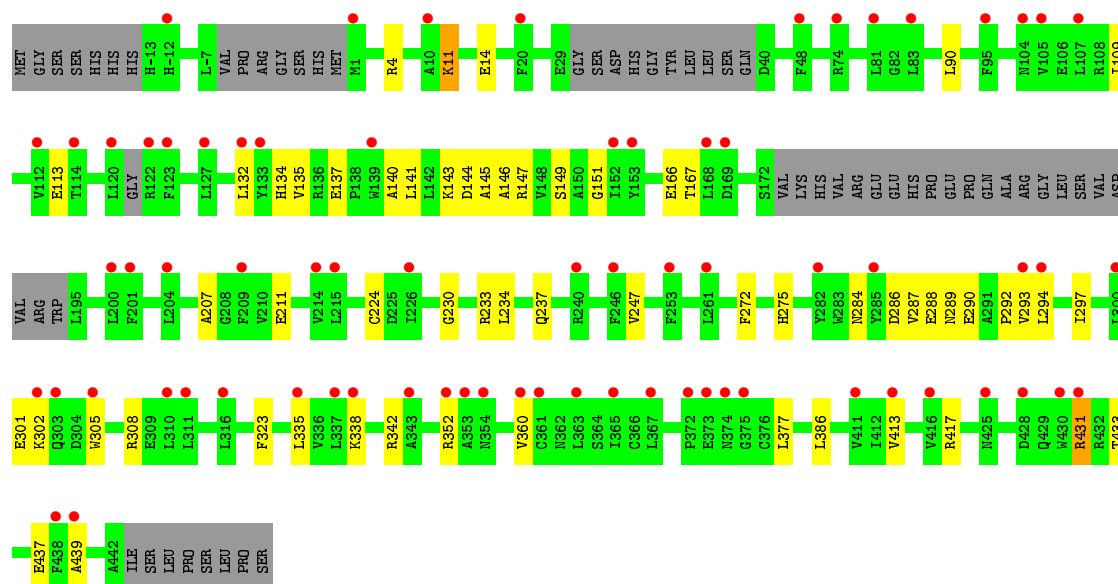
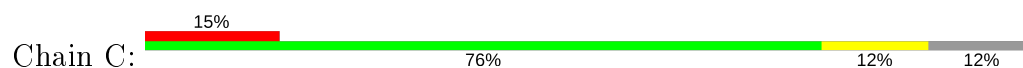


- Molecule 1: Methyltransferase domain-containing protein





• Molecule 1: Methyltransferase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	191.63Å 191.63Å 269.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 3.35 45.80 – 3.35	Depositor EDS
% Data completeness (in resolution range)	95.9 (45.64-3.35) 94.8 (45.80-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.266 0.221 , 0.266	Depositor DCC
R_{free} test set	1815 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	121.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 104.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.377 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.390 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9743	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: NI, BTB

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	0.24	0/3298	0.44	0/4480
1	B	0.25	0/3294	0.44	0/4473
1	C	0.24	0/3321	0.43	0/4514
All	All	0.24	0/9913	0.44	0/13467

There are no bond length outliers.

There are no bond angle outliers.

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	3227	0	3137	36	0
1	B	3223	0	3130	38	0
1	C	3248	0	3158	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	14	0	19	5	0
3	B	14	0	19	3	0
3	C	14	0	19	2	0
All	All	9743	0	9482	105	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 5.

All (105) 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:C:338:LYS:HB2	1:C:431:ARG:HB3	1.66	0.77
1:A:338:LYS:HB2	1:A:431:ARG:HB3	1.68	0.75
1:B:375:GLY:O	1:B:431:ARG:NH2	2.24	0.70
1:A:51:ALA:O	1:A:231:ARG:NH2	2.23	0.69
1:A:377:LEU:HD13	3:A:501:BTB:H82	1.77	0.66
1:A:431:ARG:NH1	3:A:501:BTB:O4	2.32	0.62
1:C:143:LYS:HG2	1:C:207:ALA:HA	1.81	0.62
1:A:170:GLY:HA2	1:B:211:GLU:CD	2.20	0.61
1:B:284:ASN:HA	1:B:293:VAL:O	2.01	0.60
1:B:338:LYS:HG3	1:B:431:ARG:NH2	2.16	0.60
1:C:386:LEU:O	1:C:417:ARG:NH2	2.35	0.59
1:B:143:LYS:HG2	1:B:207:ALA:HA	1.83	0.59
1:A:213:GLU:OE2	1:A:231:ARG:NH1	2.36	0.58
1:A:420:HIS:HD2	3:A:501:BTB:H52	1.67	0.58
1:B:25:ILE:HB	1:B:27:TYR:HE1	1.68	0.57
1:A:237:GLN:HB3	1:A:247:VAL:HG11	1.86	0.57
1:A:284:ASN:HA	1:A:293:VAL:O	2.04	0.57
1:A:90:LEU:HD22	1:A:109:ILE:HB	1.87	0.56
1:C:377:LEU:HB2	3:C:501:BTB:H82	1.86	0.56
1:B:137:GLU:OE1	1:B:137:GLU:N	2.39	0.56
1:C:237:GLN:HB3	1:C:247:VAL:HG11	1.88	0.56
1:B:167:THR:HG21	1:C:211:GLU:HG3	1.87	0.55
1:C:137:GLU:OE1	1:C:137:GLU:N	2.40	0.55
1:C:90:LEU:HD22	1:C:109:ILE:HB	1.88	0.55
1:A:137:GLU:N	1:A:137:GLU:OE1	2.41	0.54
1:A:323:PHE:CE1	1:A:413:VAL:HG11	2.43	0.53
1:B:90:LEU:HD22	1:B:109:ILE:HB	1.89	0.53
1:A:386:LEU:O	1:A:417:ARG:NH2	2.41	0.53
1:C:352:ARG:NH1	1:C:437:GLU:OE2	2.38	0.53
1:B:377:LEU:O	1:B:403:PRO:HA	2.09	0.53
3:A:501:BTB:O4	3:A:501:BTB:O1	2.12	0.52
1:C:145:ALA:O	1:C:149:SER:HB3	2.09	0.52
1:B:237:GLN:HB3	1:B:247:VAL:HG11	1.91	0.52
1:C:294:LEU:HD21	1:C:297:ILE:HD11	1.90	0.52
1:A:166:GLU:N	1:A:166:GLU:OE1	2.42	0.52
1:A:301:GLU:OE2	1:A:302:LYS:NZ	2.42	0.52
1:B:301:GLU:OE2	1:B:302:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:HG21	1:B:141:LEU:HD22	1.92	0.52
1:B:386:LEU:O	1:B:417:ARG:NH2	2.38	0.51
1:A:326:SER:OG	1:A:327:PRO:HD3	2.11	0.51
1:C:132:LEU:HD12	1:C:141:LEU:HD23	1.93	0.51
1:C:377:LEU:HB2	3:C:501:BTB:C8	2.41	0.51
1:C:301:GLU:OE2	1:C:302:LYS:NZ	2.43	0.51
1:B:288:GLU:O	1:B:290:GLU:N	2.44	0.50
1:C:144:ASP:HA	1:C:147:ARG:HG3	1.92	0.50
1:A:346:VAL:HG21	3:A:501:BTB:H12	1.94	0.50
1:A:135:VAL:HG21	1:A:141:LEU:HD22	1.94	0.49
1:B:151:GLY:HA2	1:B:230:GLY:O	2.12	0.49
1:B:338:LYS:HB2	1:B:431:ARG:HB3	1.94	0.49
1:A:143:LYS:HG2	1:A:207:ALA:HA	1.95	0.49
1:C:288:GLU:O	1:C:290:GLU:N	2.45	0.49
1:C:233:ARG:O	1:C:234:LEU:HB3	2.14	0.48
1:A:233:ARG:O	1:A:234:LEU:HB3	2.13	0.48
1:B:294:LEU:HD21	1:B:297:ILE:HD11	1.95	0.48
1:C:11:LYS:HA	1:C:14:GLU:HG3	1.95	0.48
1:B:135:VAL:HG12	1:B:137:GLU:H	1.79	0.47
1:C:431:ARG:NH2	1:C:433:THR:OG1	2.47	0.47
1:A:148:VAL:O	1:A:150:ALA:N	2.48	0.47
1:C:151:GLY:HA2	1:C:230:GLY:O	2.14	0.47
1:C:293:VAL:HG12	1:C:342:ARG:CZ	2.45	0.47
1:C:135:VAL:HG21	1:C:141:LEU:HD22	1.96	0.47
1:B:305:TRP:HB2	1:B:308:ARG:HB3	1.97	0.46
1:B:336:VAL:HG21	3:B:501:BTB:H11	1.97	0.46
1:C:286:ASP:HB3	1:C:292:PRO:HB3	1.98	0.46
1:A:151:GLY:HA2	1:A:230:GLY:O	2.15	0.46
1:A:239:ARG:NH2	1:C:167:THR:O	2.48	0.46
1:A:350:ARG:HD2	1:A:390:ILE:HD11	1.97	0.46
1:A:360:VAL:HG13	1:A:439:ALA:HB2	1.99	0.45
1:C:305:TRP:HB2	1:C:308:ARG:HB3	1.98	0.45
1:C:290:GLU:HB3	1:C:342:ARG:HH11	1.81	0.45
1:B:375:GLY:O	1:B:422:SER:OG	2.32	0.44
1:B:9:ARG:NH1	1:B:98:GLU:OE1	2.48	0.44
1:A:268:LEU:HD11	1:A:305:TRP:HE1	1.82	0.44
1:B:268:LEU:HD11	1:B:305:TRP:HE1	1.83	0.44
1:B:49:TYR:CZ	1:B:75:GLN:HG3	2.53	0.44
1:C:284:ASN:HA	1:C:293:VAL:O	2.17	0.44
1:B:368:ASP:OD2	1:B:432:ARG:NH1	2.51	0.44
3:B:501:BTB:H71	3:B:501:BTB:H12	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD12	1:A:141:LEU:HD23	2.00	0.43
1:A:297:ILE:HB	1:A:335:LEU:HB3	1.99	0.43
1:B:148:VAL:O	1:B:150:ALA:N	2.51	0.43
1:C:146:ALA:HA	1:C:149:SER:OG	2.17	0.43
1:B:232:ALA:O	1:B:234:LEU:N	2.50	0.43
1:B:137:GLU:HG2	1:B:140:ALA:HB3	2.00	0.43
1:B:323:PHE:CE1	1:B:413:VAL:HG11	2.53	0.43
1:A:268:LEU:CD1	1:A:305:TRP:HE1	2.31	0.42
1:B:360:VAL:HG13	1:B:439:ALA:HB2	2.00	0.42
1:B:431:ARG:HH22	3:B:501:BTB:C4	2.33	0.42
1:A:135:VAL:HG12	1:A:137:GLU:H	1.85	0.42
1:C:297:ILE:HB	1:C:335:LEU:HB3	2.01	0.42
1:C:360:VAL:HG13	1:C:439:ALA:HB2	2.01	0.42
1:C:137:GLU:HG2	1:C:140:ALA:HB3	2.01	0.42
1:A:392:VAL:N	1:A:393:PRO:HD2	2.35	0.41
1:B:297:ILE:HB	1:B:335:LEU:HB3	2.02	0.41
1:A:72:LEU:HD11	1:A:127:LEU:HD22	2.03	0.41
1:A:290:GLU:OE1	1:A:342:ARG:HD3	2.20	0.41
1:A:344:ALA:HA	1:A:424:PRO:HB3	2.02	0.41
1:B:268:LEU:CD1	1:B:305:TRP:HE1	2.34	0.41
1:B:305:TRP:CB	1:B:308:ARG:HB3	2.50	0.41
1:C:323:PHE:CE1	1:C:413:VAL:HG11	2.56	0.41
1:A:80:ILE:HB	1:A:105:VAL:HG22	2.03	0.41
1:B:126:VAL:O	1:B:152:ILE:HA	2.20	0.41
1:B:237:GLN:O	1:B:247:VAL:HG21	2.21	0.41
1:B:338:LYS:HE3	1:B:431:ARG:NH2	2.36	0.41
1:A:288:GLU:O	1:A:290:GLU:N	2.54	0.41

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	400/471 (85%)	365 (91%)	32 (8%)	3 (1%)	19	53
1	B	399/471 (85%)	364 (91%)	32 (8%)	3 (1%)	19	53
1	C	406/471 (86%)	367 (90%)	36 (9%)	3 (1%)	22	56
All	All	1205/1413 (85%)	1096 (91%)	100 (8%)	9 (1%)	22	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	LEU
1	A	160	GLY
1	B	233	ARG
1	C	166	GLU
1	A	161	SER
1	C	287	VAL
1	A	166	GLU
1	B	289	ASN
1	C	289	ASN

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/383 (87%)	327 (98%)	5 (2%)	65	82
1	B	331/383 (86%)	327 (99%)	4 (1%)	71	85
1	C	335/383 (88%)	327 (98%)	8 (2%)	49	74
All	All	998/1149 (87%)	981 (98%)	17 (2%)	60	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	134	HIS
1	A	272	PHE
1	A	275	HIS

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Mol	Chain	Res	Type
1	A	304	ASP
1	B	4	ARG
1	B	134	HIS
1	B	272	PHE
1	B	275	HIS
1	C	4	ARG
1	C	11	LYS
1	C	113	GLU
1	C	134	HIS
1	C	224	CYS
1	C	272	PHE
1	C	275	HIS
1	C	431	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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
3	BTB	B	501	-	13,13,13	0.60	0	7,16,16	0.62	0
3	BTB	A	501	-	13,13,13	0.70	0	7,16,16	0.65	0
3	BTB	C	501	-	13,13,13	0.73	0	7,16,16	0.51	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
3	BTB	B	501	-	-	10/21/21/21	-
3	BTB	A	501	-	-	9/21/21/21	-
3	BTB	C	501	-	-	7/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	BTB	O1-C1-C2-C3
3	C	501	BTB	O1-C1-C2-C4
3	C	501	BTB	O1-C1-C2-N
3	C	501	BTB	C1-C2-C4-O4
3	C	501	BTB	C3-C2-C4-O4
3	C	501	BTB	N-C2-C4-O4
3	B	501	BTB	C1-C2-C4-O4
3	B	501	BTB	C3-C2-C4-O4
3	B	501	BTB	N-C2-C4-O4
3	B	501	BTB	C1-C2-N-C5
3	B	501	BTB	C3-C2-N-C5
3	B	501	BTB	C4-C2-N-C5
3	B	501	BTB	C6-C5-N-C7
3	A	501	BTB	O1-C1-C2-N
3	A	501	BTB	C1-C2-C4-O4
3	A	501	BTB	C3-C2-C4-O4
3	A	501	BTB	N-C2-C4-O4
3	A	501	BTB	C6-C5-N-C7
3	B	501	BTB	N-C5-C6-O6
3	C	501	BTB	N-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	501	BTB	N-C5-C6-O6
3	A	501	BTB	O1-C1-C2-C3
3	B	501	BTB	C1-C2-N-C7
3	B	501	BTB	C4-C2-N-C7
3	A	501	BTB	N-C7-C8-O8
3	A	501	BTB	O1-C1-C2-C4

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	BTB	3	0
3	A	501	BTB	5	0
3	C	501	BTB	2	0

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	414/471 (87%)	1.02	63 (15%)	2 2	88, 135, 206, 247	0
1	B	413/471 (87%)	1.05	73 (17%)	1 1	96, 134, 200, 240	0
1	C	416/471 (88%)	1.03	72 (17%)	1 1	86, 132, 199, 262	0
All	All	1243/1413 (87%)	1.03	208 (16%)	1 2	86, 134, 201, 262	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	LYS	6.3
1	A	361	CYS	6.0
1	C	431	ARG	5.9
1	C	168	LEU	5.7
1	C	305	TRP	5.3
1	C	338	LYS	5.2
1	C	303	GLN	5.2
1	A	360	VAL	5.1
1	A	338	LYS	5.0
1	A	439	ALA	5.0
1	B	360	VAL	5.0
1	B	310	LEU	4.6
1	A	285	TYR	4.5
1	B	209	PHE	4.5
1	C	209	PHE	4.4
1	C	361	CYS	4.4
1	B	10	ALA	4.4
1	A	438	PHE	4.3
1	B	139	TRP	4.3
1	C	169	ASP	4.3
1	B	316	LEU	4.3
1	C	360	VAL	4.3
1	B	431	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	361	CYS	4.2
1	A	300	LEU	4.1
1	B	300	LEU	4.0
1	B	168	LEU	3.9
1	A	311	LEU	3.8
1	C	285	TYR	3.7
1	B	107	LEU	3.7
1	C	311	LEU	3.7
1	A	305	TRP	3.7
1	C	438	PHE	3.7
1	B	212	ILE	3.7
1	B	311	LEU	3.6
1	C	367	LEU	3.6
1	C	439	ALA	3.6
1	B	353	ALA	3.6
1	A	334	ALA	3.5
1	C	282	TYR	3.5
1	B	285	TYR	3.5
1	A	269	ILE	3.5
1	C	374	ASN	3.4
1	A	316	LEU	3.4
1	A	112	VAL	3.4
1	B	438	PHE	3.4
1	B	326	SER	3.4
1	C	120	LEU	3.3
1	A	419	VAL	3.3
1	C	105	VAL	3.3
1	A	310	LEU	3.3
1	A	1	MET	3.3
1	C	425	ASN	3.2
1	A	333	PHE	3.2
1	C	300	LEU	3.2
1	C	112	VAL	3.2
1	B	95	PHE	3.1
1	A	261	LEU	3.1
1	A	295	TYR	3.1
1	B	1	MET	3.1
1	B	425	ASN	3.1
1	B	439	ALA	3.0
1	B	365	ILE	3.0
1	A	431	ARG	3.0
1	C	261	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	104	ASN	3.0
1	C	83	LEU	3.0
1	B	301	GLU	3.0
1	B	430	TRP	3.0
1	B	133	TYR	2.9
1	B	305	TRP	2.9
1	A	169	ASP	2.9
1	A	297	ILE	2.9
1	B	122	ARG	2.9
1	B	112	VAL	2.9
1	A	6	ILE	2.9
1	B	374	ASN	2.8
1	A	373	GLU	2.8
1	C	316	LEU	2.8
1	C	302	LYS	2.8
1	A	168	LEU	2.8
1	C	20	PHE	2.8
1	B	83	LEU	2.8
1	C	352	ARG	2.8
1	B	214	VAL	2.8
1	C	293	VAL	2.8
1	A	426	PRO	2.8
1	B	200	LEU	2.8
1	C	428	ASP	2.8
1	C	294	LEU	2.8
1	B	302	LYS	2.8
1	C	430	TRP	2.7
1	B	102	ALA	2.7
1	C	375	GLY	2.7
1	B	350	ARG	2.7
1	C	127	LEU	2.7
1	B	120	LEU	2.7
1	A	63	ALA	2.7
1	C	310	LEU	2.7
1	C	416	VAL	2.7
1	B	352	ARG	2.7
1	A	365	ILE	2.7
1	A	303	GLN	2.6
1	C	132	LEU	2.6
1	C	343	ALA	2.6
1	C	200	LEU	2.6
1	B	253	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	293	VAL	2.5
1	A	366	CYS	2.5
1	A	127	LEU	2.5
1	C	95	PHE	2.5
1	B	328	VAL	2.5
1	C	122	ARG	2.5
1	C	-12	HIS	2.5
1	A	13	LEU	2.5
1	B	97	MET	2.5
1	A	204	LEU	2.5
1	B	236	ALA	2.4
1	B	6	ILE	2.4
1	A	10	ALA	2.4
1	C	107	LEU	2.4
1	A	209	PHE	2.4
1	B	86	ARG	2.4
1	C	139	TRP	2.4
1	B	335	LEU	2.4
1	C	411	VAL	2.4
1	A	302	LYS	2.4
1	A	253	PHE	2.4
1	B	240	ARG	2.4
1	B	195	LEU	2.4
1	B	82	GLY	2.4
1	B	48	PHE	2.4
1	B	347	PRO	2.4
1	B	74	ARG	2.3
1	C	373	GLU	2.3
1	C	354	ASN	2.3
1	B	226	ILE	2.3
1	C	363	LEU	2.3
1	C	365	ILE	2.3
1	C	335	LEU	2.3
1	A	304	ASP	2.3
1	A	132	LEU	2.3
1	B	210	VAL	2.3
1	B	323	PHE	2.3
1	C	1	MET	2.3
1	A	81	LEU	2.3
1	A	212	ILE	2.3
1	C	240	ARG	2.3
1	C	81	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	PHE	2.3
1	A	343	ALA	2.3
1	B	127	LEU	2.3
1	A	89	ASN	2.3
1	B	105	VAL	2.3
1	C	201	PHE	2.3
1	B	269	ILE	2.3
1	A	282	TYR	2.3
1	C	253	PHE	2.3
1	A	367	LEU	2.3
1	B	294	LEU	2.3
1	A	200	LEU	2.3
1	C	337	LEU	2.3
1	C	246	PHE	2.2
1	B	339	GLU	2.2
1	C	204	LEU	2.2
1	A	350	ARG	2.2
1	A	246	PHE	2.2
1	A	337	LEU	2.2
1	C	372	PRO	2.2
1	C	123	PHE	2.2
1	B	152	ILE	2.2
1	B	11	LYS	2.2
1	A	201	PHE	2.2
1	B	261	LEU	2.2
1	C	48	PHE	2.1
1	B	81	LEU	2.1
1	C	353	ALA	2.1
1	A	20	PHE	2.1
1	C	152	ILE	2.1
1	A	83	LEU	2.1
1	B	282	TYR	2.1
1	B	343	ALA	2.1
1	C	10	ALA	2.1
1	C	133	TYR	2.1
1	B	402	VAL	2.1
1	A	125	ALA	2.1
1	A	436	ILE	2.1
1	C	226	ILE	2.1
1	C	413	VAL	2.1
1	B	436	ILE	2.1
1	C	114	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	2.1
1	A	70	LEU	2.1
1	A	374	ASN	2.1
1	A	323	PHE	2.1
1	B	266	ILE	2.1
1	A	335	LEU	2.1
1	B	363	LEU	2.1
1	C	215	LEU	2.1
1	B	419	VAL	2.0
1	B	373	GLU	2.0
1	C	153	TYR	2.0
1	C	74	ARG	2.0
1	C	214	VAL	2.0
1	A	434	ILE	2.0
1	A	133	TYR	2.0
1	B	273	THR	2.0
1	B	295	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
3	BTB	C	501	14/14	0.76	0.59	151,159,172,173	0
3	BTB	B	501	14/14	0.82	0.38	157,167,179,182	0
3	BTB	A	501	14/14	0.85	0.38	178,189,199,204	0
2	NI	A	500	1/1	0.97	0.36	110,110,110,110	0
2	NI	B	500	1/1	0.97	0.32	105,105,105,105	0
2	NI	C	500	1/1	0.98	0.34	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.