



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:29 pm GMT

PDB ID : 2F9R  
Title : Crystal structure of the inactive state of the Smase I, a sphingomyelinase D from *Loxosceles laeta* venom  
Authors : Murakami, M.T.; Gabdoulkhakov, A.; Fernandes-Pedrosa, M.F.; Betzel, C.; Tambourgi, D.V.; Arni, R.K.  
Deposited on : 2005-12-06  
Resolution : 1.85 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

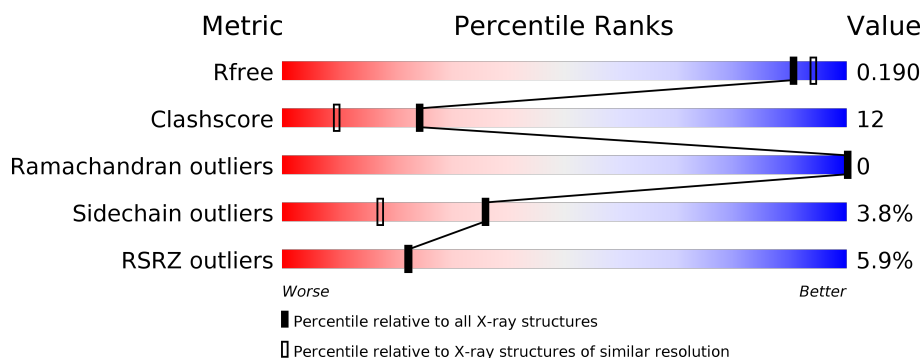
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	111664	2111 (1.86-1.86)
Clashscore	122126	2258 (1.86-1.86)
Ramachandran outliers	120053	2234 (1.86-1.86)
Sidechain outliers	120020	2234 (1.86-1.86)
RSRZ outliers	108989	2075 (1.86-1.86)

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  $\geq 3$ , 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	285	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	285	<div> <div>5%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	285	<div> <div>9%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	D	285	<div> <div>6%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9891 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 Sphingomyelinase D 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	12	0
			2346	1511	391	438	6			
1	B	285	Total	C	N	O	S	0	8	0
			2318	1488	386	438	6			
1	C	285	Total	C	N	O	S	0	11	0
			2339	1506	388	439	6			
1	D	285	Total	C	N	O	S	0	10	0
			2329	1497	389	437	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

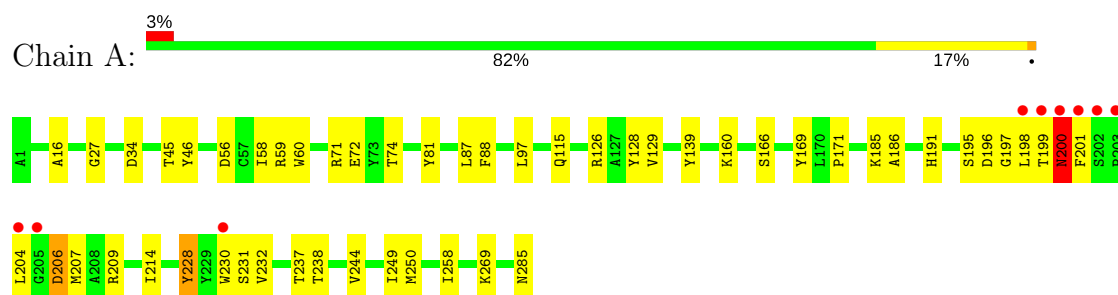
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total	O	0	2
			182	182		
4	B	162	Total	O	0	0
			162	162		
4	C	72	Total	O	0	0
			72	72		
4	D	93	Total	O	0	1
			94	94		

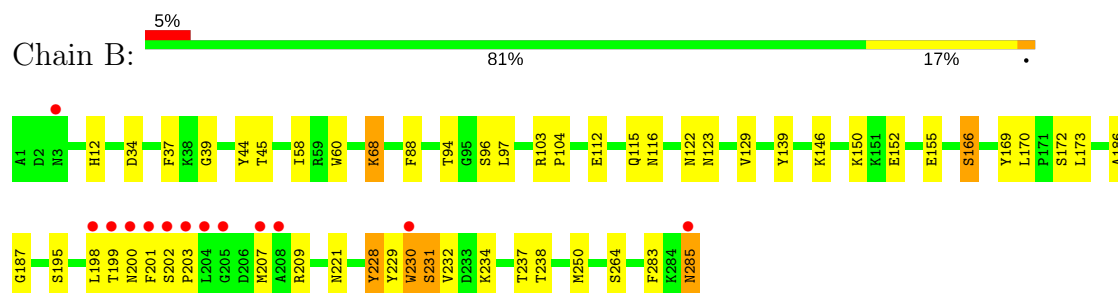
### 3 Residue-property plots [i](#)

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.

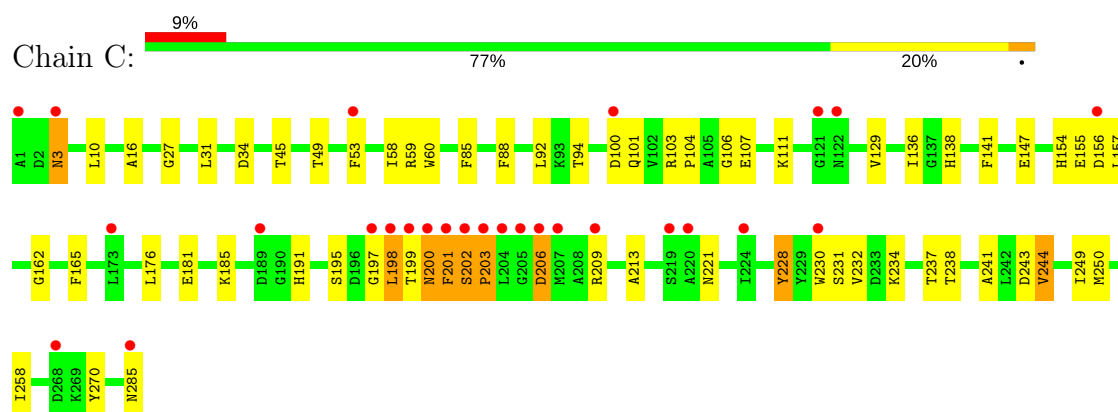
#### • Molecule 1: Spingomyelinase D 1



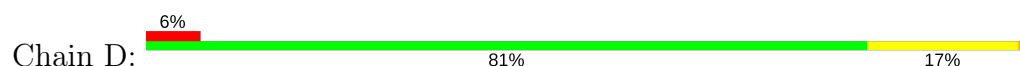
#### • Molecule 1: Spingomyelinase D 1

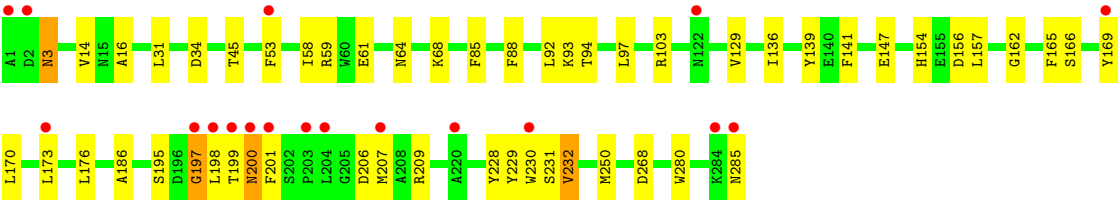


#### • Molecule 1: Spingomyelinase D 1



#### • Molecule 1: Spingomyelinase D 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.59Å 140.59Å 113.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.85 19.98 – 1.85	Depositor EDS
% Data completeness (in resolution range)	83.5 (20.00-1.85) 83.5 (19.98-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.187 , 0.234 0.189 , 0.190	Depositor DCC
$R_{free}$ test set	4507 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, EPE

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	0.62	0/2439	0.72	1/3312 (0.0%)
1	B	0.60	0/2398	0.71	0/3260
1	C	0.57	2/2429 (0.1%)	0.65	3/3298 (0.1%)
1	D	0.52	0/2415	0.67	1/3283 (0.0%)
All	All	0.58	2/9681 (0.0%)	0.68	5/13153 (0.0%)

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	B	0	1
1	C	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	SER	C-N	14.12	1.61	1.34
1	C	203	PRO	N-CD	-6.53	1.38	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	GLY	N-CA-C	10.86	140.25	113.10
1	A	200	ASN	N-CA-CB	-9.75	93.05	110.60
1	C	202	SER	O-C-N	6.84	134.10	121.10
1	C	202	SER	CA-C-N	-5.57	101.50	117.10
1	C	203	PRO	N-CA-CB	-5.27	96.80	102.60



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	44	TYR	Peptide
1	C	199	THR	Peptide
1	C	201	PHE	Mainchain

## 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	2346	0	2299	62	0
1	B	2318	0	2250	50	0
1	C	2339	0	2282	72	0
1	D	2329	0	2272	54	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
3	B	15	0	17	0	0
3	C	15	0	17	0	0
3	D	15	0	17	2	0
4	A	182	0	0	10	0
4	B	162	0	0	8	0
4	C	72	0	0	1	0
4	D	94	0	0	3	0
All	All	9891	0	9154	218	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 12.

All (218) 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:201:PHE:CG	1:D:58:ILE:HD11	1.76	1.19
1:C:230[B]:TRP:HB3	1:C:250[B]:MET:HB3	1.25	1.09
1:D:198:LEU:HD21	4:D:756[B]:HOH:O	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:PHE:CB	1:D:58:ILE:HD11	1.86	1.04
1:D:197:GLY:HA3	1:D:230[B]:TRP:O	1.62	0.97
1:C:198:LEU:H	1:C:230[A]:TRP:HE1	1.16	0.93
1:A:200:ASN:HD22	1:A:200:ASN:H	1.15	0.92
1:A:200:ASN:HD22	1:A:200:ASN:N	1.72	0.87
1:C:230[B]:TRP:HB3	1:C:250[B]:MET:CB	2.06	0.84
1:A:269:LYS:HE3	4:A:724:HOH:O	1.77	0.84
1:D:200:ASN:HA	1:D:206:ASP:OD2	1.78	0.84
1:B:230[B]:TRP:HE3	1:B:250[B]:MET:SD	2.01	0.83
1:C:230[A]:TRP:HE3	1:C:250[A]:MET:HE2	1.42	0.82
1:D:197:GLY:C	1:D:230[A]:TRP:O	2.18	0.81
1:C:200:ASN:ND2	1:C:200:ASN:N	2.30	0.80
1:A:166:SER:HB2	4:A:765:HOH:O	1.82	0.79
1:A:115[A]:GLN:HG3	4:A:732:HOH:O	1.82	0.78
1:C:201:PHE:CG	1:D:58:ILE:CD1	2.63	0.78
1:D:197:GLY:CA	1:D:230[B]:TRP:O	2.31	0.77
1:C:53[B]:PHE:CZ	1:D:53:PHE:HB2	2.21	0.76
1:D:197:GLY:C	1:D:230[B]:TRP:O	2.23	0.76
1:A:228[A]:TYR:CE1	1:A:230[A]:TRP:HZ2	2.05	0.75
1:C:200:ASN:HD22	1:C:200:ASN:N	1.85	0.74
1:B:199:THR:HB	1:B:201:PHE:HD1	1.53	0.73
1:A:200:ASN:H	1:A:200:ASN:ND2	1.87	0.72
1:A:228[A]:TYR:CE1	1:A:230[A]:TRP:CZ2	2.79	0.71
1:C:58:ILE:HD11	1:D:201:PHE:HB3	1.73	0.70
1:C:230[B]:TRP:CB	1:C:250[B]:MET:HB3	2.14	0.70
1:A:46:TYR:CE1	1:B:170:LEU:HD21	2.26	0.69
1:C:198:LEU:N	1:C:230[A]:TRP:HE1	1.91	0.69
1:C:234:LYS:HB2	1:C:237[B]:THR:HG22	1.74	0.68
1:C:198:LEU:HB2	1:C:230[A]:TRP:HE1	1.58	0.68
1:C:237[B]:THR:HG21	4:C:711:HOH:O	1.92	0.68
1:B:198:LEU:N	1:B:230[A]:TRP:HE1	1.91	0.67
1:C:200:ASN:ND2	1:C:200:ASN:H	1.92	0.67
1:B:234:LYS:HB2	1:B:237[B]:THR:HG22	1.76	0.66
1:C:201:PHE:CB	1:D:58:ILE:CD1	2.70	0.66
1:B:198:LEU:CA	1:B:230[A]:TRP:HE1	2.08	0.66
1:B:150:LYS:HG2	1:B:155:GLU:HB2	1.79	0.65
1:C:230[A]:TRP:HB2	1:C:231[A]:SER:OG	1.96	0.65
1:C:198:LEU:N	1:C:230[A]:TRP:CD1	2.65	0.65
1:C:201:PHE:CD1	1:D:58:ILE:CD1	2.80	0.65
1:B:200:ASN:O	1:B:203:PRO:HD3	1.96	0.64
1:A:201:PHE:HB3	1:B:58:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASP:O	1:C:209:ARG:HB3	1.97	0.63
1:C:31[B]:LEU:HD13	1:C:85:PHE:CZ	2.33	0.63
1:A:195:SER:HB2	1:A:230[B]:TRP:CD1	2.34	0.63
1:B:230[B]:TRP:HB3	1:B:250[B]:MET:HB3	1.81	0.63
1:A:169:TYR:CE2	1:A:199:THR:HG22	2.33	0.63
1:C:198:LEU:N	1:C:230[A]:TRP:NE1	2.44	0.63
1:C:230[A]:TRP:CE3	1:C:250[A]:MET:HE2	2.29	0.62
1:D:173[A]:LEU:HD11	1:D:201:PHE:HE1	1.64	0.62
1:D:31[B]:LEU:HD13	1:D:85:PHE:CZ	2.34	0.62
1:A:232[B]:VAL:CG2	1:A:249:ILE:HG23	2.29	0.62
1:A:46:TYR:CD1	1:B:170:LEU:HD21	2.34	0.62
1:C:230[A]:TRP:HB3	1:C:250[A]:MET:HB3	1.83	0.61
1:D:173[B]:LEU:HD22	1:D:209:ARG:HE	1.66	0.60
1:C:232:VAL:HG11	1:C:238:THR:HA	1.83	0.60
1:A:195:SER:HB2	1:A:230[B]:TRP:NE1	2.16	0.60
1:B:173:LEU:HD13	1:B:209:ARG:CZ	2.31	0.60
1:B:103:ARG:HB3	1:B:104:PRO:HD3	1.84	0.59
1:A:198:LEU:HG	1:A:230[B]:TRP:HB2	1.84	0.59
1:B:198:LEU:CG	1:B:230[A]:TRP:HE1	2.15	0.59
1:B:115:GLN:HG2	4:B:823:HOH:O	2.01	0.59
1:C:201:PHE:HB3	1:D:58:ILE:CD1	2.33	0.59
1:C:230[A]:TRP:HE3	1:C:250[A]:MET:CE	2.15	0.59
1:A:60:TRP:CD1	1:B:170:LEU:HD22	2.38	0.59
1:B:198:LEU:HG	1:B:230[A]:TRP:NE1	2.16	0.59
1:B:237[B]:THR:HG21	4:B:702:HOH:O	2.04	0.58
1:B:198:LEU:CG	1:B:230[A]:TRP:NE1	2.56	0.57
1:A:195:SER:HB3	1:A:230[B]:TRP:HE1	1.68	0.57
1:A:195:SER:CB	1:A:230[B]:TRP:HE1	2.18	0.57
1:D:198:LEU:O	1:D:200:ASN:OD1	2.22	0.57
1:A:72:GLU:HG2	4:A:745:HOH:O	2.04	0.57
1:C:197:GLY:O	1:C:198:LEU:C	2.42	0.57
1:B:199:THR:CB	1:B:201:PHE:HD1	2.16	0.56
1:D:3:ASN:OD1	1:D:3:ASN:N	2.33	0.56
1:C:58:ILE:HD11	1:D:201:PHE:CG	2.40	0.56
1:B:152:GLU:HA	1:B:152:GLU:OE1	2.06	0.55
1:B:230[A]:TRP:HB3	1:B:250[A]:MET:HB3	1.89	0.55
1:B:96:SER:HB3	4:B:749:HOH:O	2.07	0.54
1:D:200:ASN:OD1	1:D:200:ASN:N	2.41	0.54
1:A:97:LEU:HD21	4:B:749:HOH:O	2.06	0.54
1:A:56:ASP:HB3	4:A:739:HOH:O	2.08	0.53
1:B:88:PHE:CZ	1:B:129:VAL:HG22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:VAL:HG13	1:C:237[B]:THR:HG23	1.89	0.53
1:B:283:PHE:CE2	1:B:285:ASN:HA	2.44	0.53
1:C:195:SER:HB3	1:C:228:TYR:CZ	2.44	0.53
1:A:97:LEU:CD2	4:B:749:HOH:O	2.57	0.53
1:B:229:TYR:HD2	1:B:232:VAL:HG23	1.73	0.53
1:C:103:ARG:HB3	1:C:104:PRO:HD3	1.90	0.53
1:D:197:GLY:HA3	1:D:230[A]:TRP:O	2.08	0.53
1:A:195:SER:CB	1:A:230[B]:TRP:NE1	2.73	0.52
1:A:88:PHE:CZ	1:A:129[A]:VAL:HG22	2.44	0.51
1:C:154:HIS:HB3	1:C:157:LEU:HD12	1.93	0.51
1:C:58:ILE:HD11	1:D:201:PHE:CB	2.39	0.51
1:C:230[A]:TRP:CE3	1:C:250[A]:MET:CE	2.92	0.51
1:B:166:SER:HB3	4:B:805:HOH:O	2.10	0.51
1:B:232:VAL:HG11	1:B:238:THR:HA	1.93	0.51
1:C:94:THR:O	1:C:138:HIS:HE1	1.93	0.51
1:A:139:TYR:HB2	1:A:186:ALA:HB2	1.92	0.51
1:B:230[B]:TRP:HB2	1:B:231[B]:SER:OG	2.10	0.51
1:D:173[A]:LEU:HD11	1:D:201:PHE:CE1	2.44	0.50
1:A:244:VAL:HG13	4:A:648:HOH:O	2.11	0.50
1:C:3:ASN:N	1:C:3:ASN:OD1	2.44	0.50
1:B:199:THR:HG1	1:B:201:PHE:HE1	1.56	0.50
1:A:228[B]:TYR:CE1	1:A:230[B]:TRP:NE1	2.80	0.50
1:A:71:ARG:HD3	4:A:658:HOH:O	2.10	0.50
1:B:94:THR:HB	1:B:97:LEU:HD12	1.93	0.50
1:D:92:LEU:HD13	1:D:141:PHE:CZ	2.47	0.50
1:C:58:ILE:HG21	1:D:169:TYR:HD1	1.77	0.50
1:B:198:LEU:N	1:B:230[A]:TRP:NE1	2.59	0.49
1:C:60:TRP:CD1	1:D:170:LEU:HD22	2.47	0.49
1:B:112[A]:GLU:OE1	1:B:116:ASN:ND2	2.43	0.49
1:B:198:LEU:CB	1:B:230[A]:TRP:HE1	2.24	0.49
1:C:88:PHE:CZ	1:C:129:VAL:HG22	2.47	0.49
1:A:232[B]:VAL:HG22	1:A:249:ILE:HG23	1.95	0.49
1:B:34:ASP:O	1:B:45:THR:HA	2.12	0.49
1:A:197:GLY:HA3	1:A:230[B]:TRP:O	2.13	0.48
1:C:243:ASP:HA	1:C:270:TYR:OH	2.13	0.48
1:A:34:ASP:O	1:A:45:THR:HA	2.12	0.48
1:A:58:ILE:HG12	4:A:739:HOH:O	2.13	0.48
1:A:195:SER:HB3	1:A:228[B]:TYR:CZ	2.48	0.48
1:C:181:GLU:O	1:C:185:LYS:HG3	2.14	0.48
1:C:202:SER:O	1:C:206:ASP:N	2.46	0.47
1:A:214:ILE:HD13	1:A:244:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230[A]:TRP:CB	1:B:250[A]:MET:HB3	2.44	0.47
1:D:197:GLY:CA	1:D:230[A]:TRP:O	2.62	0.47
1:A:232[A]:VAL:HG11	1:A:238:THR:HA	1.96	0.47
1:C:198:LEU:HB2	1:C:230[A]:TRP:NE1	2.26	0.47
1:B:68:LYS:HD2	1:B:68:LYS:C	2.34	0.47
1:A:230[A]:TRP:CH2	1:A:250[A]:MET:HE3	2.50	0.47
1:D:154:HIS:HB3	1:D:157:LEU:HD12	1.97	0.47
1:C:206:ASP:O	1:C:209:ARG:CB	2.61	0.47
1:C:230[B]:TRP:HA	1:C:231[B]:SER:HA	1.52	0.47
1:C:198:LEU:CB	1:C:230[A]:TRP:HE1	2.25	0.47
1:C:202:SER:O	1:C:206:ASP:HB2	2.14	0.47
1:A:139:TYR:CZ	1:A:185:LYS:HD3	2.50	0.46
1:A:198:LEU:HD11	1:A:230[B]:TRP:CE3	2.50	0.46
1:D:14:VAL:HB	1:D:31[B]:LEU:HG	1.96	0.46
1:B:139:TYR:HB2	1:B:186:ALA:HB2	1.96	0.46
1:A:171:PRO:HA	1:B:60:TRP:CZ2	2.50	0.46
1:D:195:SER:CB	1:D:230[B]:TRP:HE1	2.29	0.46
1:D:34:ASP:HB3	1:D:93:LYS:HE3	1.97	0.46
1:C:201:PHE:HB2	1:D:58:ILE:HD11	1.88	0.46
1:A:198:LEU:HG	1:A:230[B]:TRP:CB	2.45	0.46
1:C:107:GLU:HB3	1:C:111:LYS:HZ3	1.81	0.46
1:A:74:THR:O	1:A:126:ARG:HG2	2.16	0.45
1:D:136:ILE:HG22	1:D:165:PHE:HB3	1.96	0.45
1:D:162:GLY:HA3	1:D:280:TRP:CH2	2.50	0.45
1:D:268:ASP:HB2	4:D:755:HOH:O	2.16	0.45
1:A:195:SER:HB3	1:A:228[B]:TYR:CE2	2.52	0.45
1:A:27:GLY:HA3	1:A:258:ILE:HG13	1.98	0.45
1:B:195:SER:HB3	1:B:228:TYR:CZ	2.51	0.45
1:A:200:ASN:ND2	1:A:200:ASN:N	2.37	0.45
1:D:61:GLU:OE2	3:D:704:EPE:H72	2.16	0.45
1:D:230[B]:TRP:CZ3	1:D:250[B]:MET:SD	3.10	0.45
1:D:230[B]:TRP:CE3	1:D:250[B]:MET:SD	3.10	0.45
1:B:230[B]:TRP:HE3	1:B:250[B]:MET:CE	2.30	0.44
1:A:285:ASN:HB3	4:A:781:HOH:O	2.18	0.44
1:A:160:LYS:HA	1:A:160:LYS:HD2	1.76	0.44
1:C:176:LEU:HD11	1:C:213:ALA:HA	2.00	0.44
1:C:100[B]:ASP:OD1	1:C:101:GLN:HG3	2.17	0.44
1:C:136:ILE:HG22	1:C:165:PHE:HB3	1.98	0.44
1:B:37:PHE:HB3	1:B:39:GLY:O	2.18	0.44
1:C:34:ASP:O	1:C:45:THR:HA	2.16	0.44
1:C:232:VAL:HB	1:C:249:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PHE:CZ	1:D:129[A]:VAL:HG22	2.53	0.44
1:A:81:TYR:OH	1:A:126:ARG:CZ	2.66	0.43
1:C:103:ARG:NH2	1:C:147:GLU:OE1	2.49	0.43
1:B:200:ASN:C	1:B:202:SER:N	2.72	0.43
1:B:231[A]:SER:HB2	4:B:861:HOH:O	2.17	0.43
1:C:241:ALA:O	1:C:244:VAL:HG12	2.19	0.43
1:D:16:ALA:HB2	1:D:59:ARG:HB3	2.00	0.43
1:D:103[B]:ARG:HH22	1:D:147:GLU:CD	2.22	0.43
1:A:230[A]:TRP:CZ3	1:A:250[A]:MET:HE3	2.53	0.43
1:D:34:ASP:O	1:D:45:THR:HA	2.18	0.43
1:A:166:SER:O	1:A:166:SER:OG	2.36	0.43
1:B:230[B]:TRP:CE3	1:B:250[B]:MET:CE	3.02	0.43
1:B:169:TYR:CZ	1:B:173:LEU:HD21	2.53	0.43
1:C:92:LEU:HD13	1:C:141:PHE:CZ	2.54	0.43
1:A:169:TYR:N	1:A:169:TYR:CD1	2.87	0.42
1:A:230[A]:TRP:HA	1:A:231[A]:SER:HA	1.70	0.42
1:D:229:TYR:HD2	1:D:232:VAL:HG22	1.84	0.42
1:C:49:THR:HB	1:D:198:LEU:HD22	2.02	0.42
1:C:162:GLY:HA2	1:C:191:HIS:HB3	2.02	0.42
1:D:139:TYR:HB2	1:D:186:ALA:HB2	2.02	0.42
1:D:230[B]:TRP:HA	1:D:231[B]:SER:OG	2.20	0.42
1:A:195:SER:HB3	1:A:228[A]:TYR:CE2	2.55	0.42
1:A:198:LEU:HG	1:A:230[A]:TRP:HB2	2.01	0.42
1:A:232[B]:VAL:HG23	1:A:249:ILE:HG23	2.00	0.42
1:D:195:SER:HB2	1:D:230[B]:TRP:NE1	2.34	0.42
3:D:704:EPE:H32	3:D:704:EPE:H81	1.64	0.42
1:D:64:ASN:O	1:D:68:LYS:HG3	2.20	0.42
1:C:101:GLN:C	1:C:104:PRO:HD2	2.40	0.41
1:A:87:LEU:HA	1:A:128:TYR:O	2.20	0.41
1:D:198:LEU:HD11	4:D:756[B]:HOH:O	2.20	0.41
1:A:191:HIS:CD2	1:A:191:HIS:N	2.89	0.41
1:C:221:ASN:N	1:C:221:ASN:OD1	2.49	0.41
1:A:200:ASN:HA	1:A:206:ASP:OD1	2.20	0.41
1:D:176:LEU:HA	1:D:176:LEU:HD12	1.93	0.41
1:A:232[A]:VAL:HG13	1:A:237:THR:OG1	2.20	0.41
1:B:169:TYR:CE2	1:B:173:LEU:HD21	2.56	0.41
1:C:106:GLY:HA3	1:C:141:PHE:O	2.20	0.41
1:C:16:ALA:HB2	1:C:59:ARG:HB3	2.03	0.41
1:C:202:SER:HA	1:C:203:PRO:HD2	1.77	0.41
1:B:122:ASN:ND2	4:B:776:HOH:O	2.53	0.41
1:A:196:ASP:OD1	4:A:757:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PHE:CE1	1:C:129:VAL:HG13	2.56	0.41
1:A:16:ALA:HB2	1:A:59:ARG:HB3	2.01	0.40
1:B:146:LYS:NZ	1:B:187:GLY:O	2.54	0.40
1:C:198:LEU:CB	1:C:230[A]:TRP:NE1	2.84	0.40
1:A:228[A]:TYR:CZ	1:A:230[A]:TRP:HZ2	2.39	0.40
1:B:12:HIS:HB2	1:B:250[B]:MET:HG2	2.04	0.40
1:C:201:PHE:CD1	1:D:58:ILE:HD13	2.57	0.40
1:C:27:GLY:HA3	1:C:258:ILE:HG13	2.02	0.40
1:D:94:THR:HB	1:D:97:LEU:HD12	2.03	0.40
1:C:58:ILE:HD11	1:D:201:PHE:CD1	2.57	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	295/285 (104%)	290 (98%)	5 (2%)	0	100	100
1	B	291/285 (102%)	284 (98%)	7 (2%)	0	100	100
1	C	294/285 (103%)	285 (97%)	9 (3%)	0	100	100
1	D	293/285 (103%)	284 (97%)	9 (3%)	0	100	100
All	All	1173/1140 (103%)	1143 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	252/240 (105%)	245 (97%)	7 (3%)	47	29
1	B	248/240 (103%)	234 (94%)	14 (6%)	23	8
1	C	251/240 (105%)	241 (96%)	10 (4%)	34	16
1	D	250/240 (104%)	241 (96%)	9 (4%)	38	19
All	All	1001/960 (104%)	961 (96%)	40 (4%)	36	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	204	LEU
1	A	206	ASP
1	A	207	MET
1	A	209	ARG
1	A	228[A]	TYR
1	A	228[B]	TYR
1	B	68	LYS
1	B	123[A]	ASN
1	B	123[B]	ASN
1	B	166	SER
1	B	172	SER
1	B	207	MET
1	B	221	ASN
1	B	228	TYR
1	B	230[A]	TRP
1	B	230[B]	TRP
1	B	231[A]	SER
1	B	231[B]	SER
1	B	264	SER
1	B	285	ASN
1	C	3	ASN
1	C	10	LEU
1	C	155	GLU
1	C	156	ASP
1	C	198	LEU
1	C	200	ASN
1	C	206	ASP
1	C	228	TYR
1	C	244	VAL

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Mol	Chain	Res	Type
1	C	285	ASN
1	D	3	ASN
1	D	156	ASP
1	D	166	SER
1	D	199	THR
1	D	200	ASN
1	D	207	MET
1	D	228	TYR
1	D	232	VAL
1	D	285	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	200	ASN
1	B	99	ASN
1	B	122	ASN
1	B	221	ASN
1	C	99	ASN
1	C	120	ASN
1	C	123	ASN
1	C	154	HIS
1	C	200	ASN
1	D	123	ASN
1	D	154	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 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	EPE	B	701	-	15,15,15	0.63	0	18,20,20	1.55	2 (11%)
3	EPE	C	703	-	15,15,15	0.58	0	18,20,20	1.86	4 (22%)
3	EPE	D	704	-	15,15,15	0.53	0	18,20,20	2.36	6 (33%)

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	EPE	B	701	-	-	0/9/19/19	0/1/1/1
3	EPE	C	703	-	-	0/9/19/19	0/1/1/1
3	EPE	D	704	-	-	0/9/19/19	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	EPE	C9-N1-C6	-2.38	105.03	111.24
3	D	704	EPE	C6-N1-C2	2.04	113.39	108.87
3	C	703	EPE	O2S-S-C10	2.18	109.53	106.92
3	D	704	EPE	C6-C5-N4	2.41	115.38	110.64
3	D	704	EPE	C7-N4-C3	2.77	118.48	111.24
3	C	703	EPE	O3S-S-C10	2.85	110.37	105.77
3	B	701	EPE	C7-N4-C3	3.02	119.11	111.24
3	D	704	EPE	C2-C3-N4	3.07	116.69	110.64
3	B	701	EPE	C5-N4-C3	3.94	117.58	108.87
3	D	704	EPE	O2S-S-C10	4.60	112.45	106.92
3	C	703	EPE	C5-N4-C3	4.85	119.60	108.87
3	D	704	EPE	C5-N4-C3	6.09	122.34	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	704	EPE	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	202:SER	C	203:PRO	N	1.61

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/285 (100%)	-0.23	9 (3%) 47 46	12, 18, 30, 39	10 (3%)
1	B	285/285 (100%)	-0.16	13 (4%) 32 31	12, 19, 32, 46	11 (3%)
1	C	285/285 (100%)	0.52	27 (9%) 8 8	15, 30, 41, 46	27 (9%)
1	D	285/285 (100%)	0.12	18 (6%) 20 19	15, 26, 37, 42	22 (7%)
All	All	1140/1140 (100%)	0.06	67 (5%) 22 22	12, 22, 39, 46	70 (6%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	LEU	14.9
1	B	201	PHE	14.0
1	C	201	PHE	13.8
1	C	1	ALA	13.2
1	C	203	PRO	12.1
1	D	198	LEU	10.8
1	C	200	ASN	10.7
1	D	1	ALA	9.6
1	A	201	PHE	9.1
1	C	204	LEU	8.3
1	C	202	SER	8.3
1	C	199	THR	8.2
1	C	206	ASP	8.1
1	A	204	LEU	7.6
1	A	198	LEU	6.8
1	B	204	LEU	6.7
1	D	201	PHE	6.2
1	C	205	GLY	6.1
1	B	205	GLY	6.0
1	C	285	ASN	5.9
1	B	198	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	5.4
1	D	204	LEU	5.4
1	B	200	ASN	4.6
1	D	285	ASN	4.6
1	D	199	THR	4.6
1	A	200	ASN	4.5
1	B	202	SER	4.1
1	D	220	ALA	4.1
1	A	205	GLY	4.0
1	A	203	PRO	3.9
1	D	203	PRO	3.8
1	C	230[A]	TRP	3.7
1	B	230[A]	TRP	3.7
1	A	199	THR	3.6
1	C	220	ALA	3.6
1	D	284	LYS	3.3
1	C	53[A]	PHE	3.3
1	B	199	THR	3.3
1	C	207	MET	3.2
1	C	3	ASN	3.1
1	B	207	MET	3.1
1	C	209	ARG	3.1
1	A	230[A]	TRP	2.9
1	B	203	PRO	2.9
1	D	200	ASN	2.8
1	B	285	ASN	2.7
1	A	202	SER	2.5
1	C	156	ASP	2.5
1	D	230[A]	TRP	2.4
1	D	207	MET	2.4
1	C	189	ASP	2.4
1	D	169	TYR	2.4
1	C	197	GLY	2.3
1	B	208	ALA	2.3
1	C	224	ILE	2.2
1	D	53	PHE	2.2
1	C	173	LEU	2.2
1	D	122	ASN	2.1
1	C	100[A]	ASP	2.1
1	D	173[A]	LEU	2.1
1	C	121	GLY	2.1
1	D	2	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	122	ASN	2.0
1	C	268[A]	ASP	2.0
1	B	3	ASN	2.0
1	C	219	SER	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MG	C	603	1/1	0.97	0.13	25,25,25,25	1
3	EPE	D	704	15/15	0.98	0.08	22,25,27,30	0
3	EPE	C	703	15/15	0.98	0.08	23,28,30,32	0
2	MG	A	601	1/1	0.98	0.09	18,18,18,18	1
3	EPE	B	701	15/15	0.99	0.06	15,17,19,19	0
2	MG	B	602	1/1	0.99	0.03	19,19,19,19	0
2	MG	D	604	1/1	0.99	0.06	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.