



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2016 – 07:07 PM EDT

PDB ID : 5G0R  
Title : METHYL-COENZYME M REDUCTASE I FROM METHANOTHERMOBACTER MARBURGENSIS EXPOSED TO 3-NITROOXYPROPANOL  
Authors : Wagner, T.  
Deposited on : 2016-03-22  
Resolution : 1.25 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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) : rb-20027674

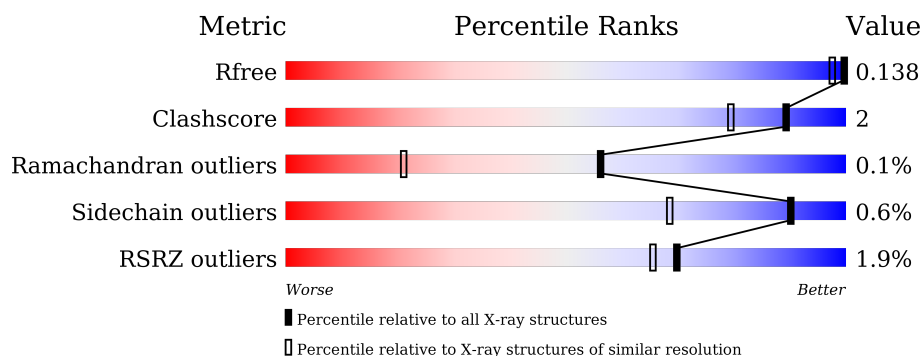
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.25 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	1442 (1.30-1.22)
Clashscore	102246	1530 (1.30-1.22)
Ramachandran outliers	100387	1467 (1.30-1.22)
Sidechain outliers	100360	1465 (1.30-1.22)
RSRZ outliers	91569	1442 (1.30-1.22)

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	550	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	D	550	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
2	B	443	<div> <div></div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
2	E	443	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
3	C	249	<div> <div>6%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
3	F	249	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>5%</div> </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
4	MG	A	562	-	-	-	X
4	MG	F	250	-	-	-	X
5	F43	A	554	X	-	-	-
5	F43	D	552	X	-	-	-
7	NA	D	558	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22540 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 METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	25	1
			4391	2790	724	857	20			
1	D	548	Total	C	N	O	S	0	24	0
			4394	2793	722	859	20			

- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	19	0
			3433	2185	563	664	21			
2	E	442	Total	C	N	O	S	0	17	0
			3409	2177	557	653	22			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE I SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	8	0
			2052	1271	360	410	11			
3	F	248	Total	C	N	O	S	0	8	0
			2061	1278	367	405	11			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

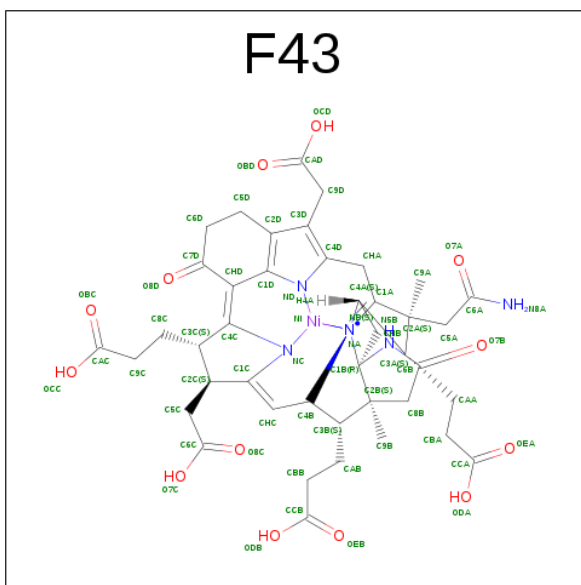
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Mg	0	0
			3	3		
4	E	4	Total	Mg	0	1
			4	4		
4	B	2	Total	Mg	0	1
			2	2		

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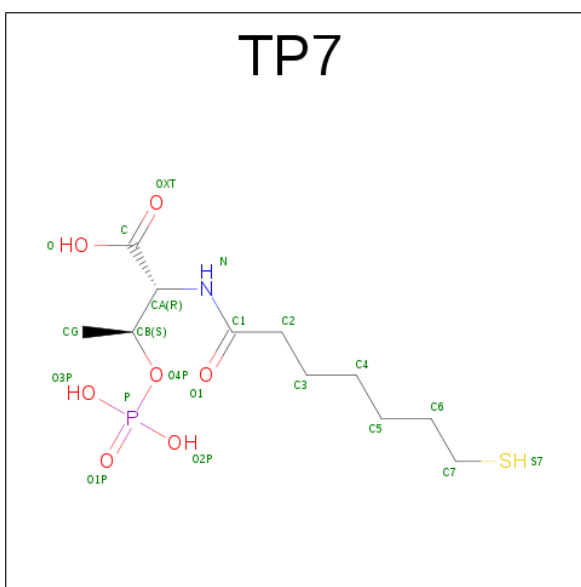
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total Mg 2 2	0	0
4	A	6	Total Mg 6 6	0	1
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula:  $\text{C}_{42}\text{H}_{49}\text{N}_6\text{NiO}_{13}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
5	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

- Molecule 6 is COENZYME B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
6	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Na 2 2	0	0
7	D	1	Total Na 1 1	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0
9	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Cl	0	0
			1	1		

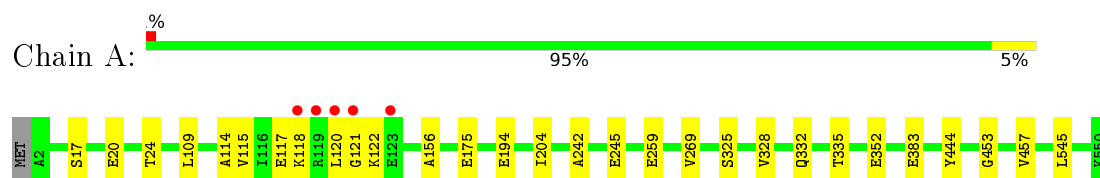
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	640	Total	O	0	0
			640	640		
10	B	511	Total	O	0	0
			511	511		
10	C	263	Total	O	0	2
			263	263		
10	D	542	Total	O	0	1
			542	542		
10	E	413	Total	O	0	0
			413	413		
10	F	240	Total	O	0	0
			240	240		

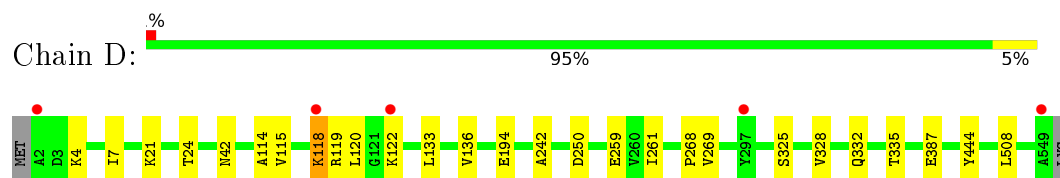
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

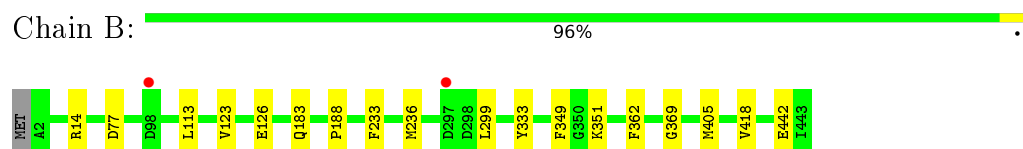
- Molecule 1: METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA



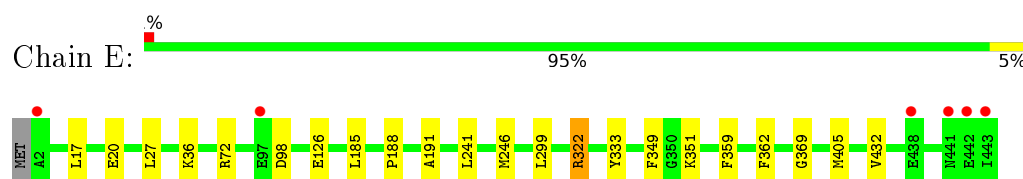
- Molecule 1: METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA



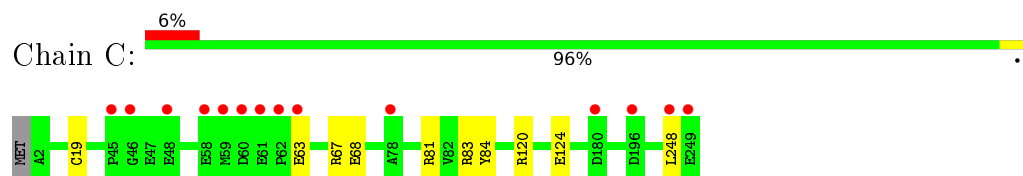
- Molecule 2: METHYL-COENZYME M REDUCTASE I SUBUNIT BETA



- Molecule 2: METHYL-COENZYME M REDUCTASE I SUBUNIT BETA



- Molecule 3: METHYL-COENZYME M REDUCTASE I SUBUNIT GAMMA



- Molecule 3: METHYL-COENZYME M REDUCTASE I SUBUNIT GAMMA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.20 Å 118.10 Å 122.64 Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	38.80 – 1.25 38.79 – 1.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.80-1.25) 98.5 (38.79-1.25)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 1.25 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.105 , 0.124 0.121 , 0.138	Depositor DCC
$R_{free}$ test set	31719 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.0	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.007 for -h,-l,-k 0.013 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	22540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, AGM, F43, MGN, TP7, DYA, GL3, SMC, MHS

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	0.56	0/4498	0.72	0/6106
1	D	0.55	2/4495 (0.0%)	0.74	0/6101
2	B	0.50	0/3532	0.70	0/4777
2	E	0.49	0/3514	0.70	3/4752 (0.1%)
3	C	0.57	1/2110 (0.0%)	0.79	1/2841 (0.0%)
3	F	0.53	1/2118 (0.0%)	0.77	2/2849 (0.1%)
All	All	0.53	4/20267 (0.0%)	0.73	6/27426 (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
2	B	0	1
2	E	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	19	CYS	CB-SG	-7.84	1.69	1.82
3	F	19	CYS	CB-SG	-6.87	1.70	1.82
1	D	269	VAL	CA-CB	5.16	1.65	1.54
1	D	259	GLU	CD-OE1	5.01	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	ARG	NE-CZ-NH2	-7.32	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	120	ARG	NE-CZ-NH2	-6.21	117.20	120.30
2	E	322[A]	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	E	322[B]	ARG	NE-CZ-NH1	5.95	123.28	120.30
3	F	120	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	E	359	PHE	CB-CG-CD2	-5.04	117.27	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	333	TYR	Sidechain
2	E	333	TYR	Sidechain
2	E	72	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4391	0	4234	25	0
1	D	4394	0	4227	24	0
2	B	3433	0	3466	22	0
2	E	3409	0	3469	19	0
3	C	2052	0	1987	9	0
3	F	2061	0	2015	10	0
4	A	6	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	4	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	1	0
6	A	21	0	19	0	0
6	D	21	0	19	0	0
7	A	2	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
10	A	640	0	0	14	1
10	B	511	0	0	6	0
10	C	263	0	0	1	0
10	D	542	0	0	9	1
10	E	413	0	0	2	0
10	F	240	0	0	2	0
All	All	22540	0	19522	93	1

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 2.

All (93) 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:A:259[B]:GLU:OE2	10:A:2215:HOH:O	1.64	1.13
10:A:2548:HOH:O	2:B:351[A]:LYS:NZ	1.78	1.13
10:B:2434:HOH:O	3:C:67[A]:ARG:NH2	1.84	1.11
10:D:2478:HOH:O	2:E:351[B]:LYS:NZ	1.81	1.11
2:B:442[A]:GLU:OE1	10:B:2508:HOH:O	1.83	0.94
1:D:42[B]:ASN:OD1	10:D:2130:HOH:O	1.98	0.81
1:D:114:ALA:O	1:D:118:LYS:HG2	1.83	0.78
2:B:405[A]:MET:SD	1:D:115:VAL:HG22	2.25	0.76
2:E:322[B]:ARG:NH2	3:F:67[B]:ARG:HG3	2.05	0.71
2:B:14[A]:ARG:CZ	3:C:63:GLU:OE2	2.43	0.67
2:B:299:LEU:HD21	2:B:349[A]:PHE:CE1	2.30	0.66
1:A:269[B]:VAL:HG12	10:A:2407:HOH:O	1.95	0.65
2:E:17:LEU:HD21	2:E:20:GLU:HG3	1.77	0.65
2:B:77:ASP:OD1	10:B:2123:HOH:O	2.13	0.65
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.39	0.62
3:F:243[A]:GLN:OE1	10:F:2233:HOH:O	2.17	0.60
1:A:118:LYS:O	3:F:81[B]:ARG:NH1	2.35	0.59
1:D:114:ALA:HB1	1:D:118:LYS:HE2	1.83	0.59
1:D:42[B]:ASN:ND2	10:D:2122:HOH:O	2.37	0.57
3:C:63:GLU:HG3	3:C:68:GLU:OE2	2.04	0.56
2:E:299:LEU:HD21	2:E:349[B]:PHE:CE1	2.41	0.56
2:B:113[B]:LEU:HD23	2:B:418:VAL:HG13	1.88	0.56
3:F:178:ASN:OD1	3:F:180:ASP:N	2.39	0.55
2:E:246[B]:MET:HE2	2:E:432:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67[B]:ARG:HG2	3:F:67[B]:ARG:HH11	1.71	0.55
1:D:4[A]:LYS:NZ	10:D:2012:HOH:O	2.37	0.55
2:E:299:LEU:HD21	2:E:349[B]:PHE:HE1	1.71	0.54
1:A:115:VAL:HG22	2:E:405:MET:SD	2.46	0.54
1:A:121:GLY:HA3	10:A:2232:HOH:O	2.06	0.54
10:B:2287:HOH:O	2:E:188:PRO:HD3	2.08	0.54
2:E:322[B]:ARG:CZ	3:F:67[B]:ARG:HG3	2.39	0.53
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.44	0.52
1:A:242:ALA:HB3	1:A:245[A]:GLU:OE2	2.09	0.52
2:E:98:ASP:OD2	10:E:2179:HOH:O	2.18	0.52
2:B:14[A]:ARG:NH1	3:C:63:GLU:OE2	2.42	0.52
1:D:114:ALA:O	1:D:118:LYS:CG	2.55	0.52
2:E:246[B]:MET:CE	2:E:432:VAL:HG11	2.40	0.52
2:B:405[A]:MET:SD	1:D:115:VAL:CG2	2.99	0.51
2:B:188:PRO:HD3	10:E:2231:HOH:O	2.10	0.51
1:D:114:ALA:CB	1:D:118:LYS:HE2	2.42	0.50
1:A:114:ALA:HB1	1:A:118:LYS:HD3	1.95	0.49
1:D:122:LYS:HE2	10:D:2223:HOH:O	2.13	0.49
1:A:194[A]:GLU:HG2	10:A:2335:HOH:O	2.12	0.49
2:B:299:LEU:HD21	2:B:349[A]:PHE:HE1	1.76	0.48
1:D:122:LYS:HG3	10:D:2225:HOH:O	2.13	0.48
3:F:10:LYS:NZ	10:F:2017:HOH:O	2.42	0.48
1:A:328:VAL:HB	5:D:552:F43:H9A1	1.94	0.48
1:A:156:ALA:O	10:A:2277:HOH:O	2.20	0.48
1:D:119:ARG:NH1	1:D:250:ASP:OD2	2.47	0.48
1:D:24[B]:THR:HG23	10:D:2092:HOH:O	2.13	0.47
10:A:2232:HOH:O	3:F:81[A]:ARG:HD3	2.15	0.47
2:B:405[A]:MET:CE	1:D:115:VAL:HG22	2.43	0.47
1:A:259[A]:GLU:CG	10:A:2217:HOH:O	2.63	0.46
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.15	0.45
2:E:185[B]:LEU:HD21	2:E:191:ALA:HA	1.98	0.45
1:D:21:LYS:HE2	10:D:2446:HOH:O	2.16	0.45
1:A:383[A]:GLU:HG3	10:A:2501:HOH:O	2.16	0.45
1:D:4[A]:LYS:HB2	1:D:7:ILE:HG12	1.99	0.45
1:A:115:VAL:HG22	2:E:405:MET:CE	2.47	0.45
2:E:241:LEU:HD11	2:E:246[B]:MET:HE3	1.98	0.44
1:D:261[B]:ILE:CD1	1:D:508:LEU:HD12	2.48	0.44
1:D:194[A]:GLU:HG2	10:D:2302:HOH:O	2.16	0.44
3:F:181:THR:HB	3:F:183[A]:ARG:HG3	2.00	0.42
5:A:554:F43:H9A1	1:D:328:VAL:HB	2.02	0.42
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:185[B]:LEU:CD2	2:E:191:ALA:HA	2.49	0.42
1:A:117:GLU:HG2	1:A:122:LYS:O	2.19	0.42
1:A:109:LEU:HB2	1:A:204[B]:ILE:HG23	2.02	0.42
1:A:24[B]:THR:HG23	10:A:2085:HOH:O	2.19	0.42
2:B:113[B]:LEU:HD23	2:B:418:VAL:CG1	2.50	0.42
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.54	0.42
1:D:332:GLN:HA	1:D:335:THR:OG1	2.20	0.42
1:A:117:GLU:HA	1:A:122:LYS:O	2.20	0.41
2:B:362:PHE:O	2:B:369:GLY:HA3	2.20	0.41
3:C:81:ARG:NH1	3:C:83:ARG:NH2	2.68	0.41
2:B:233[B]:PHE:HD1	2:B:236[B]:MET:HE3	1.84	0.41
1:A:175:GLU:HG2	10:A:2295:HOH:O	2.21	0.41
1:A:453:GLY:O	1:A:457:VAL:HG23	2.20	0.41
1:A:545[B]:LEU:CD1	10:A:2278:HOH:O	2.68	0.41
1:A:545[B]:LEU:HD12	10:A:2278:HOH:O	2.19	0.41
1:A:332:GLN:HA	1:A:335:THR:OG1	2.18	0.41
3:C:124:GLU:HG3	10:C:2147:HOH:O	2.20	0.41
10:B:2319:HOH:O	1:D:268:PRO:HB3	2.19	0.41
2:B:14[A]:ARG:NH1	3:C:63:GLU:HG2	2.36	0.41
2:E:362:PHE:O	2:E:369:GLY:HA3	2.19	0.41
10:A:2547:HOH:O	2:B:351[B]:LYS:NZ	1.88	0.41
2:B:14[A]:ARG:NH2	3:C:63:GLU:OE2	2.54	0.41
2:B:183:GLN:HG2	10:B:2319:HOH:O	2.20	0.40
1:D:133:LEU:HA	1:D:136:VAL:HG12	2.03	0.40
1:A:115:VAL:CG2	2:E:405:MET:SD	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2630:HOH:O	10:D:2436:HOH:O[2_644]	2.15	0.05

## 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	566/550 (103%)	548 (97%)	17 (3%)	1 (0%)	52	20
1	D	564/550 (102%)	544 (96%)	19 (3%)	1 (0%)	52	20
2	B	460/443 (104%)	453 (98%)	7 (2%)	0	100	100
2	E	458/443 (103%)	451 (98%)	7 (2%)	0	100	100
3	C	254/249 (102%)	249 (98%)	5 (2%)	0	100	100
3	F	254/249 (102%)	248 (98%)	6 (2%)	0	100	100
All	All	2556/2484 (103%)	2493 (98%)	61 (2%)	2 (0%)	56	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	D	325	SER

### 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	457/434 (105%)	453 (99%)	4 (1%)	84	56
1	D	456/434 (105%)	453 (99%)	3 (1%)	88	65
2	B	361/342 (106%)	360 (100%)	1 (0%)	94	79
2	E	359/342 (105%)	358 (100%)	1 (0%)	94	79
3	C	224/217 (103%)	223 (100%)	1 (0%)	93	77
3	F	224/217 (103%)	221 (99%)	3 (1%)	76	40
All	All	2081/1986 (105%)	2068 (99%)	13 (1%)	90	68

All (13) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	120	LEU
1	A	352[A]	GLU
1	A	352[B]	GLU
1	A	444	TYR
2	B	126	GLU
3	C	248	LEU
1	D	118	LYS
1	D	120	LEU
1	D	444	TYR
2	E	126	GLU
3	F	61	GLU
3	F	148[A]	SER
3	F	148[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	111	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MHS	A	257	1	7,11,12	1.15	0	7,14,16	1.06	1 (14%)
1	AGM	A	271	1	6,11,12	0.70	0	5,13,15	1.16	0
1	MGN	A	400	1	7,9,10	0.55	0	4,12,14	0.50	0
1	GL3	A	445	1	3,3,4	2.90	1 (33%)	2,2,4	1.70	1 (50%)
1	DYA	A	450	1	4,7,8	1.80	1 (25%)	1,8,10	3.36	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SMC	A	452	1	4,6,7	0.59	0	2,6,8	1.42	0
1	MHS	D	257	1	7,11,12	1.47	2 (28%)	7,14,16	1.13	1 (14%)
1	AGM	D	271	1	6,11,12	0.73	0	5,13,15	1.21	1 (20%)
1	MGN	D	400	1	7,9,10	0.69	0	4,12,14	0.40	0
1	GL3	D	445	1	3,3,4	2.24	1 (33%)	2,2,4	1.24	0
1	DYA	D	450	1	4,7,8	1.41	1 (25%)	1,8,10	2.57	1 (100%)
1	SMC	D	452	1	4,6,7	0.88	0	2,6,8	1.31	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
1	MHS	A	257	1	-	0/4/6/8	0/1/1/1
1	AGM	A	271	1	-	0/7/11/13	0/0/0/0
1	MGN	A	400	1	-	0/7/9/12	0/0/0/0
1	GL3	A	445	1	-	0/1/1/2	0/0/0/0
1	DYA	A	450	1	-	0/1/6/8	0/0/0/0
1	SMC	A	452	1	-	0/3/5/7	0/0/0/0
1	MHS	D	257	1	-	0/4/6/8	0/1/1/1
1	AGM	D	271	1	-	0/7/11/13	0/0/0/0
1	MGN	D	400	1	-	0/7/9/12	0/0/0/0
1	GL3	D	445	1	-	0/1/1/2	0/0/0/0
1	DYA	D	450	1	-	0/1/6/8	0/0/0/0
1	SMC	D	452	1	-	0/3/5/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GL3	C-S	-5.02	1.63	1.80
1	D	445	GL3	C-S	-3.87	1.67	1.80
1	D	257	MHS	CB-CG	-2.31	1.46	1.50
1	D	257	MHS	CM-ND1	-2.13	1.42	1.47
1	D	450	DYA	CA-N	2.27	1.40	1.35
1	A	450	DYA	CA-N	2.73	1.41	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	DYA	O-C-CA	-3.36	120.90	125.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	450	DYA	O-C-CA	-2.57	122.00	125.59
1	D	271	AGM	CE2-CD-NE1	-2.09	108.21	112.02
1	D	257	MHS	CD2-CG-ND1	-2.01	104.67	108.07
1	A	257	MHS	CM-ND1-CG	2.06	127.18	124.44
1	A	445	GL3	CA-C-S	2.37	119.35	113.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 25 are monoatomic - leaving 4 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	$\# Z  > 2$
5	F43	A	554	1,10	42,71,71	3.17	6 (14%)	39,118,118	2.69	6 (15%)
6	TP7	A	557	-	15,20,20	0.50	0	19,26,26	0.96	1 (5%)
5	F43	D	552	1,10	42,71,71	3.06	6 (14%)	39,118,118	2.81	5 (12%)
6	TP7	D	556	-	15,20,20	0.63	0	19,26,26	0.89	1 (5%)

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
5	F43	A	554	1,10	1/1/25/27	0/18/165/165	0/0/10/10
6	TP7	A	557	-	-	0/20/24/24	0/0/0/0
5	F43	D	552	1,10	1/1/25/27	0/18/165/165	0/0/10/10
6	TP7	D	556	-	-	0/20/24/24	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	554	F43	C4B-NB	-14.28	1.27	1.49
5	D	552	F43	C4B-NB	-12.59	1.30	1.49
5	D	552	F43	NI-ND	2.18	2.04	1.91
5	A	554	F43	NI-ND	2.74	2.07	1.91
5	D	552	F43	C1D-C2D	4.32	1.52	1.40
5	A	554	F43	C1D-C2D	4.49	1.52	1.40
5	A	554	F43	NI-NC	4.66	2.04	1.89
5	A	554	F43	C3D-C2D	4.88	1.51	1.39
5	D	552	F43	C3D-C2D	5.45	1.53	1.39
5	D	552	F43	NI-NC	5.46	2.07	1.89
5	D	552	F43	C4D-C3D	11.50	1.54	1.38
5	A	554	F43	C4D-C3D	11.57	1.54	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	552	F43	CHA-C4D-C3D	-14.38	112.33	129.68
5	A	554	F43	CHA-C4D-C3D	-12.99	114.01	129.68
5	A	554	F43	C9D-C3D-C4D	-7.92	112.28	127.13
5	D	552	F43	C9D-C3D-C4D	-7.11	113.80	127.13
5	D	552	F43	O8D-C7D-C6D	-3.14	114.82	120.78
5	A	554	F43	O8D-C7D-C6D	-3.03	115.03	120.78
5	A	554	F43	O7B-C6B-C8B	-2.88	122.32	126.54
6	A	557	TP7	C-CA-N	-2.56	108.49	113.40
5	A	554	F43	C2C-C1C-CHC	-2.34	120.47	123.82
6	D	556	TP7	C-CA-N	-2.30	108.97	113.40
5	D	552	F43	CAB-C3B-C4B	-2.18	108.95	115.01
5	A	554	F43	C6D-C7D-CHD	2.05	120.48	116.83
5	D	552	F43	C6D-C7D-CHD	2.29	120.91	116.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	554	F43	C4B
5	D	552	F43	C4B

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	554	F43	1	0
5	D	552	F43	1	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, 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	543/550 (98%)	-0.47	5 (0%)	85 84	5, 10, 23, 67	3 (0%)
1	D	542/550 (98%)	-0.49	5 (0%)	85 84	5, 10, 22, 69	0
2	B	442/443 (99%)	-0.53	2 (0%)	91 90	6, 12, 22, 51	0
2	E	442/443 (99%)	-0.43	6 (1%)	78 74	6, 13, 26, 52	0
3	C	248/249 (99%)	-0.18	14 (5%)	28 22	9, 16, 43, 73	0
3	F	248/249 (99%)	-0.21	14 (5%)	28 22	8, 16, 43, 89	0
All	All	2465/2484 (99%)	-0.42	46 (1%)	70 65	5, 12, 28, 89	3 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	LYS	5.4
3	F	60	ASP	5.3
3	C	45	PRO	5.2
3	C	60	ASP	4.5
3	F	248	LEU	4.4
3	F	45	PRO	4.3
3	F	62	PRO	4.2
1	D	549	ALA	4.0
3	C	61	GLU	3.9
3	F	46	GLY	3.8
2	E	441	ASN	3.8
1	D	2	ALA	3.7
3	C	248	LEU	3.6
3	C	196	ASP	3.5
3	C	62	PRO	3.4
2	E	443	ILE	3.3
3	F	180	ASP	3.2
3	F	63	GLU	3.2
1	A	121	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	249	GLU	3.1
1	A	123	GLU	3.0
1	D	297[A]	TYR	2.9
1	A	119	ARG	2.8
3	C	59	MET	2.8
1	A	118	LYS	2.7
2	E	442	GLU	2.6
3	C	46	GLY	2.6
2	E	2	ALA	2.6
2	E	438	GLU	2.5
3	F	59	MET	2.5
3	C	48	GLU	2.5
3	C	63	GLU	2.5
1	D	118	LYS	2.4
3	C	58	GLU	2.4
3	F	2	ALA	2.3
3	F	179	LYS	2.3
2	B	98	ASP	2.3
3	C	180	ASP	2.3
3	C	78	ALA	2.2
3	F	181	THR	2.2
2	E	97	GLU	2.2
3	C	249	GLU	2.2
3	F	196	ASP	2.2
3	F	48	GLU	2.1
2	B	297	ASP	2.1
1	A	120	LEU	2.0

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

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	AGM	A	271	12/13	0.99	0.05	-	5,6,6,7	0
1	AGM	D	271	12/13	0.99	0.06	-	5,5,6,6	0
1	DYA	A	450	8/9	0.99	0.06	-	6,8,9,9	0
1	GL3	A	445	4/5	1.00	0.06	-	6,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MGN	D	400	10/11	0.98	0.07	-	6,7,8,8	0
1	MGN	A	400	10/11	0.98	0.07	-	7,8,9,9	0
1	MHS	D	257	11/12	0.99	0.03	-	8,9,12,13	0
1	GL3	D	445	4/5	1.00	0.06	-	6,6,7,7	0
1	SMC	D	452	7/8	0.99	0.07	-	7,8,10,10	0
1	SMC	A	452	7/8	0.99	0.07	-	7,8,9,10	0
1	DYA	D	450	8/9	0.99	0.06	-	6,8,9,9	0
1	MHS	A	257	11/12	0.97	0.05	-	8,9,12,13	0

## 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	F	250	1/1	0.99	0.09	7.47	18,18,18,18	0
7	NA	D	558	1/1	1.00	0.10	6.24	13,13,13,13	0
4	MG	A	562	1/1	0.99	0.23	3.19	20,20,20,20	0
7	NA	A	1502	1/1	1.00	0.06	1.38	16,16,16,16	0
4	MG	E	1500	1/1	0.99	0.09	1.11	19,19,19,19	1
4	MG	C	250	1/1	0.99	0.07	0.91	18,18,18,18	0
4	MG	D	557	1/1	0.99	0.10	0.57	22,22,22,22	0
5	F43	D	552	62/62	0.99	0.06	0.13	6,8,10,14	0
4	MG	A	563	1/1	0.99	0.10	-0.19	26,26,26,26	0
5	F43	A	554	62/62	0.99	0.06	-0.44	5,7,10,12	0
6	TP7	A	557	21/21	0.99	0.05	-0.52	6,6,7,7	0
9	CL	B	1444	1/1	1.00	0.04	-0.85	16,16,16,16	0
9	CL	E	1444	1/1	1.00	0.03	-0.94	20,20,20,20	0
9	CL	A	1551	1/1	1.00	0.04	-1.09	18,18,18,18	0
6	TP7	D	556	21/21	0.99	0.05	-1.09	5,6,6,7	0
7	NA	A	564	1/1	1.00	0.03	-1.40	14,14,14,14	0
8	K	A	1550	1/1	1.00	0.02	-3.62	8,8,8,8	0
4	MG	D	551	1/1	0.98	0.06	-	13,13,13,13	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	444	1/1	0.98	0.25	-	31,31,31,31	0
4	MG	A	1501	1/1	0.94	0.23	-	24,24,24,24	1
4	MG	E	446	1/1	0.96	0.07	-	25,25,25,25	1
4	MG	E	445[A]	1/1	0.97	0.30	-	16,16,16,16	1
4	MG	B	445[B]	1/1	0.94	0.16	-	20,20,20,20	1
4	MG	A	551	1/1	0.90	0.30	-	33,33,33,33	0
4	MG	E	444	1/1	0.98	0.14	-	18,18,18,18	1
4	MG	A	553[A]	1/1	0.98	0.17	-	14,14,14,14	1
4	MG	C	251	1/1	0.99	0.05	-	11,11,11,11	1
4	MG	D	1500	1/1	0.98	0.20	-	22,22,22,22	1
4	MG	A	1500	1/1	0.93	0.06	-	23,23,23,23	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.