



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EWJ  
Title : CRYSTAL STRUCTURE OF BLEOMYCIN-BINDING PROTEIN COM-  
PLEXED WITH BLEOMYCIN  
Authors : Maruyama, M.; Kumagai, T.; Matoba, Y.; Hata, Y.; Sugiyama, M.  
Deposited on : 2000-04-26  
Resolution : 2.50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

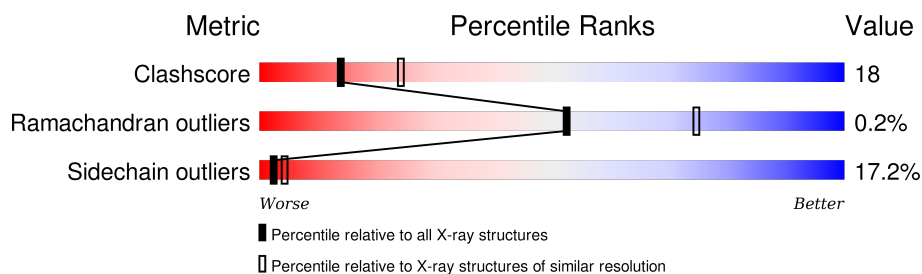
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

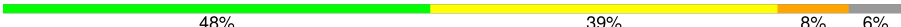
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	126	
1	B	126	
1	C	126	
1	D	126	
1	E	126	
1	F	126	
1	G	126	

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Mol	Chain	Length	Quality of chain
1	H	126	 A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: green (48%), yellow (39%), orange (8%), and grey (6%).

## 2 Entry composition

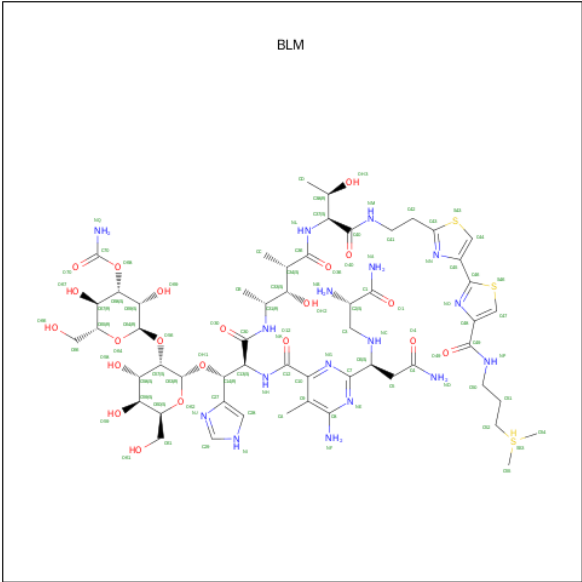
There are 3 unique types of molecules in this entry. The entry contains 8352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BLEOMYCIN RESISTANCE DETERMINANT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	B	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	C	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	D	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	E	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	F	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	G	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			
1	H	119	Total	C	N	O	S	0	0	0
			942	600	159	177	6			

- Molecule 2 is BLEOMYCIN A2 (three-letter code: BLM) (formula: C<sub>55</sub>H<sub>85</sub>N<sub>17</sub>O<sub>21</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	B	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	D	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	C	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	E	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	F	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	H	1	Total	C	N	O	S	0	0
			96	55	17	21	3		
2	G	1	Total	C	N	O	S	0	0
			96	55	17	21	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	6	Total	O	0	0
			6	6		
3	C	7	Total	O	0	0
			7	7		
3	D	5	Total	O	0	0
			5	5		

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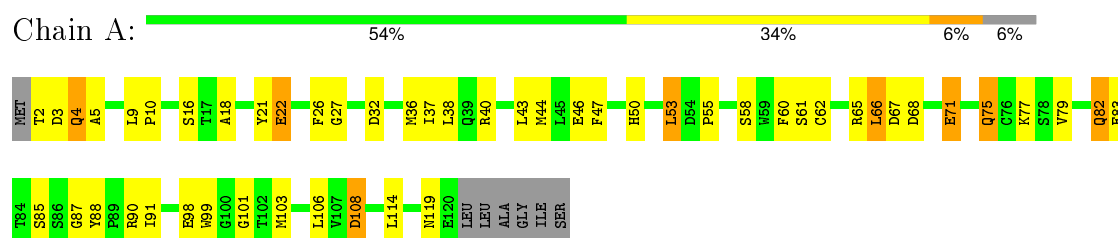
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	7	Total 7	O 7	0	0
3	F	5	Total 5	O 5	0	0
3	G	7	Total 7	O 7	0	0
3	H	5	Total 5	O 5	0	0

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

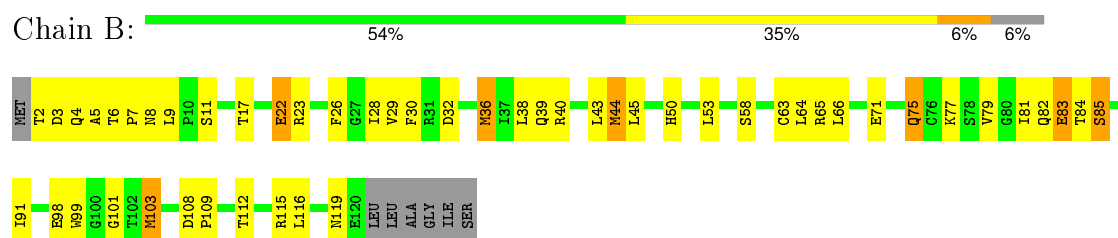
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

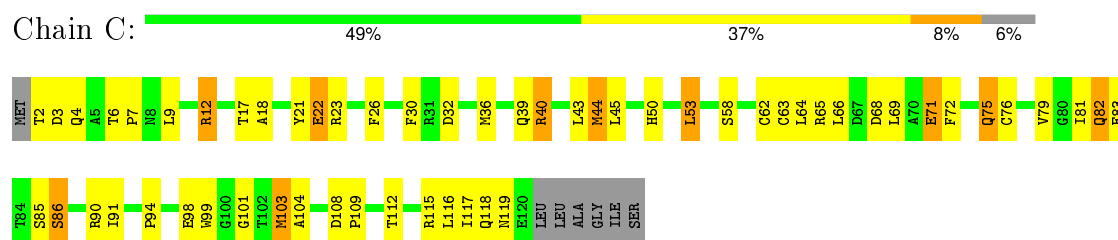
#### • Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT



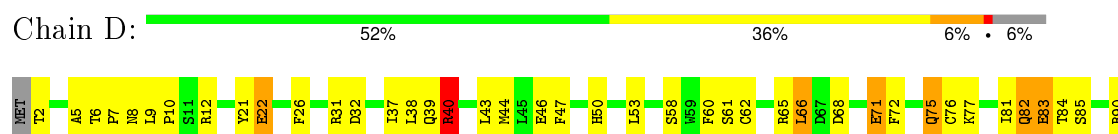
#### • Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT



#### • Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT



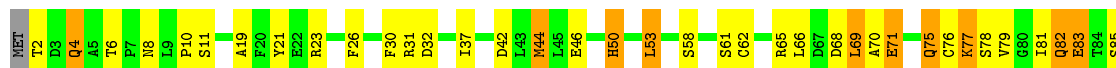
#### • Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT





• Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT

Chain E: 53% 33% 8% 6%



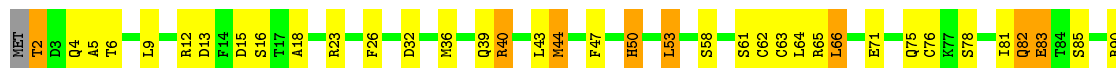
• Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT

Chain F: 52% 38% 5% 6%



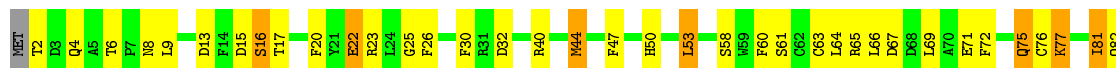
• Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT

Chain G: 57% 31% 6% 6%



• Molecule 1: BLEOMYCIN RESISTANCE DETERMINANT

Chain H: 48% 39% 8% 6%





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.27Å 117.00Å 79.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	71.0 (30.00-2.50)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.218 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 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: BLM

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	0.39	0/967	0.60	0/1313
1	B	0.37	0/967	0.57	0/1313
1	C	0.40	0/967	0.58	0/1313
1	D	0.40	0/967	0.58	0/1313
1	E	0.38	0/967	0.62	0/1313
1	F	0.39	0/967	0.57	0/1313
1	G	0.40	0/967	0.59	0/1313
1	H	0.39	0/967	0.57	0/1313
All	All	0.39	0/7736	0.59	0/10504

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 [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	942	0	896	29	0
1	B	942	0	896	34	0
1	C	942	0	896	47	0
1	D	942	0	896	42	0
1	E	942	0	896	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	942	0	896	38	0
1	G	942	0	896	29	0
1	H	942	0	896	43	0
2	A	96	0	85	4	0
2	B	96	0	85	2	0
2	C	96	0	85	7	0
2	D	96	0	85	3	0
2	E	96	0	85	4	0
2	F	96	0	85	6	0
2	G	96	0	85	5	0
2	H	96	0	85	6	0
3	A	6	0	0	1	0
3	B	6	0	0	1	0
3	C	7	0	0	5	0
3	D	5	0	0	1	0
3	E	7	0	0	2	0
3	F	5	0	0	1	0
3	G	7	0	0	1	0
3	H	5	0	0	1	0
All	All	8352	0	7848	297	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 18.

All (297) 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:E:108:ASP:HB2	1:E:109:PRO:HD2	1.48	0.96
1:D:108:ASP:HB2	1:D:109:PRO:HD2	1.51	0.90
1:C:108:ASP:HB2	1:C:109:PRO:HD2	1.54	0.90
1:F:108:ASP:HB2	1:F:109:PRO:HD2	1.54	0.89
1:A:82:GLN:HG2	1:C:23:ARG:CZ	2.02	0.89
1:B:108:ASP:HB2	1:B:109:PRO:HD2	1.56	0.86
1:E:23:ARG:CZ	1:G:82:GLN:HG2	2.06	0.86
1:C:43:LEU:HA	3:C:844:HOH:O	1.75	0.84
1:F:81:ILE:HG21	1:F:91:ILE:HG23	1.62	0.81
1:D:39:GLN:HG2	1:D:40:ARG:H	1.45	0.81
1:D:77:LYS:HE2	1:D:83:GLU:HG3	1.62	0.80
1:H:108:ASP:HB2	1:H:109:PRO:HD2	1.64	0.80
1:H:64:LEU:HD11	1:H:114:LEU:HD23	1.64	0.78
1:D:91:ILE:HG22	1:D:106:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ARG:NH2	1:G:82:GLN:HG2	1.97	0.78
1:E:6:THR:HG21	1:E:44:MET:HG2	1.66	0.76
1:F:21:TYR:O	1:F:26:PHE:HB2	1.87	0.75
1:D:37:ILE:HG12	1:D:46:GLU:HG2	1.69	0.74
1:B:4:GLN:HG3	1:B:5:ALA:H	1.52	0.74
1:F:77:LYS:HE2	1:F:83:GLU:HG3	1.72	0.71
1:H:77:LYS:HE2	1:H:83:GLU:HG3	1.73	0.70
1:C:40:ARG:O	1:C:40:ARG:HG3	1.92	0.69
1:C:69:LEU:HD23	1:C:118:GLN:HB2	1.74	0.69
1:F:6:THR:HG21	1:F:44:MET:HE2	1.74	0.69
1:H:103:MET:HB2	1:H:117:ILE:HG12	1.75	0.69
1:D:91:ILE:CG2	1:D:106:LEU:HD12	2.25	0.67
1:B:4:GLN:HG3	1:B:5:ALA:N	2.10	0.67
1:G:43:LEU:HD22	1:G:64:LEU:HD22	1.78	0.66
1:D:26:PHE:HA	1:D:39:GLN:O	1.96	0.66
2:E:2001:BLM:H2E	3:E:1826:HOH:O	1.96	0.65
1:E:69:LEU:HD23	1:E:118:GLN:HB2	1.79	0.65
1:F:62:CYS:SG	1:F:114:LEU:HG	2.38	0.64
1:D:7:PRO:C	1:D:8:ASN:HD22	2.00	0.64
1:D:90:ARG:HH22	2:D:1003:BLM:H662	1.63	0.63
1:D:66:LEU:O	1:D:119:ASN:HB2	1.98	0.63
1:D:81:ILE:HG21	1:D:91:ILE:HG23	1.81	0.62
1:E:61:SER:O	1:F:8:ASN:HB2	1.99	0.62
2:F:2002:BLM:H2E	3:F:1816:HOH:O	1.98	0.62
1:G:66:LEU:O	1:G:119:ASN:HB2	2.00	0.61
1:F:67:ASP:HA	1:F:119:ASN:HB2	1.81	0.61
1:E:21:TYR:HB3	1:E:26:PHE:HB2	1.82	0.61
1:D:12:ARG:HB2	1:D:110:ASP:OD2	2.00	0.61
1:D:9:LEU:O	1:D:47:PHE:HA	2.00	0.61
1:E:8:ASN:HB2	1:F:61:SER:O	2.01	0.61
1:A:82:GLN:HG2	1:C:23:ARG:NH2	2.16	0.61
1:A:66:LEU:O	1:A:119:ASN:HB2	2.01	0.61
1:G:115:ARG:NH2	2:G:2004:BLM:O4	2.28	0.60
1:H:76:CYS:O	1:H:81:ILE:HG13	2.00	0.60
1:C:64:LEU:HD12	1:C:116:LEU:CD2	2.31	0.60
1:H:13:ASP:HB3	1:H:16:SER:OG	2.01	0.60
1:E:77:LYS:HE2	1:E:83:GLU:HG3	1.84	0.60
1:B:99:TRP:CZ3	1:B:101:GLY:HA3	2.36	0.60
1:C:6:THR:HG21	1:C:44:MET:HE3	1.83	0.60
1:D:39:GLN:HG2	1:D:40:ARG:N	2.15	0.60
1:C:65:ARG:HH12	1:C:117:ILE:HG21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:SER:O	1:H:8:ASN:HB2	2.02	0.60
1:B:39:GLN:HG3	1:B:40:ARG:N	2.15	0.59
1:B:108:ASP:HB2	1:B:109:PRO:CD	2.30	0.59
1:A:5:ALA:HB2	1:B:64:LEU:HD23	1.83	0.59
2:C:1004:BLM:H2E	3:D:846:HOH:O	2.02	0.59
1:H:108:ASP:CB	1:H:109:PRO:HD2	2.32	0.59
1:F:113:LEU:HB2	2:F:2002:BLM:HAC	1.84	0.58
1:H:99:TRP:CZ3	1:H:101:GLY:HA3	2.38	0.58
1:D:21:TYR:O	1:D:26:PHE:HB2	2.02	0.58
1:E:19:ALA:O	1:E:23:ARG:HG3	2.03	0.57
1:A:5:ALA:HA	1:B:63:CYS:O	2.05	0.56
1:G:2:THR:HA	1:H:67:ASP:OD2	2.04	0.56
1:D:82:GLN:HB3	1:D:84:THR:HG22	1.86	0.56
1:A:65:ARG:NH1	2:A:1001:BLM:HNP	2.03	0.56
1:E:37:ILE:HG12	1:E:46:GLU:HG2	1.87	0.56
1:E:68:ASP:OD1	1:E:71:GLU:HB3	2.05	0.56
1:C:4:GLN:HA	3:C:834:HOH:O	2.06	0.56
1:E:42:ASP:HB2	1:F:3:ASP:HB2	1.87	0.56
1:C:30:PHE:O	1:C:36:MET:HA	2.07	0.55
1:B:108:ASP:CB	1:B:109:PRO:HD2	2.32	0.55
1:B:11:SER:HG	1:B:17:THR:HG1	1.55	0.55
1:D:104:ALA:HB3	1:D:116:LEU:HB2	1.89	0.55
1:D:118:GLN:NE2	1:D:119:ASN:N	2.55	0.55
1:C:39:GLN:HG3	1:C:40:ARG:N	2.22	0.55
1:A:9:LEU:O	1:A:47:PHE:HA	2.08	0.54
1:H:115:ARG:NH1	2:H:2003:BLM:O40	2.40	0.54
1:A:67:ASP:N	1:B:3:ASP:OD1	2.37	0.54
1:D:113:LEU:HD21	1:D:115:ARG:HG3	1.88	0.54
1:H:67:ASP:HA	1:H:119:ASN:HB2	1.88	0.54
1:E:65:ARG:HG2	1:E:65:ARG:HH11	1.71	0.54
1:B:44:MET:HG3	1:B:44:MET:O	2.06	0.54
1:H:118:GLN:HE21	1:H:119:ASN:N	2.06	0.54
1:A:43:LEU:HD21	1:B:3:ASP:HB3	1.89	0.54
1:F:108:ASP:CB	1:F:109:PRO:HD2	2.33	0.53
1:C:99:TRP:CZ3	1:C:101:GLY:HA3	2.43	0.53
1:E:69:LEU:CD2	1:E:118:GLN:HB2	2.38	0.53
1:H:108:ASP:HB2	1:H:109:PRO:CD	2.38	0.53
1:D:6:THR:HG21	1:D:44:MET:HG2	1.91	0.53
1:H:81:ILE:HG21	1:H:91:ILE:HG23	1.91	0.53
1:E:65:ARG:HG2	1:E:65:ARG:NH1	2.25	0.52
1:D:72:PHE:HA	1:D:75:GLN:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:PRO:HB3	1:E:108:ASP:HA	1.91	0.52
1:G:43:LEU:HD11	1:G:66:LEU:CD2	2.39	0.52
1:F:22:GLU:HA	1:F:26:PHE:O	2.10	0.52
1:D:10:PRO:HG3	1:D:60:PHE:CD1	2.45	0.52
1:E:108:ASP:CB	1:E:109:PRO:HD2	2.28	0.52
1:F:68:ASP:CG	1:F:71:GLU:HB3	2.31	0.52
1:E:99:TRP:CZ3	1:E:101:GLY:HA3	2.45	0.52
1:C:81:ILE:HG21	1:C:91:ILE:HG23	1.92	0.51
1:G:5:ALA:HB2	1:H:64:LEU:HD23	1.92	0.51
1:H:30:PHE:CE2	1:H:32:ASP:HB2	2.46	0.51
1:H:20:PHE:HA	1:H:23:ARG:NH2	2.26	0.51
1:E:75:GLN:O	1:E:79:VAL:HG22	2.11	0.51
1:F:115:ARG:NH2	2:F:2002:BLM:O4	2.34	0.51
1:F:61:SER:HB2	1:F:113:LEU:O	2.11	0.51
1:C:44:MET:HE3	1:D:65:ARG:HD2	1.94	0.50
1:A:62:CYS:HA	1:B:8:ASN:ND2	2.27	0.50
1:F:99:TRP:CZ3	1:F:101:GLY:HA3	2.46	0.50
1:E:82:GLN:HG2	1:G:23:ARG:CZ	2.42	0.50
1:E:23:ARG:O	1:E:79:VAL:HG11	2.10	0.50
1:F:91:ILE:HG22	1:F:106:LEU:HD13	1.93	0.50
1:G:113:LEU:HB2	2:G:2004:BLM:HAC	1.94	0.50
1:A:27:GLY:O	1:A:38:LEU:HA	2.11	0.50
1:H:113:LEU:HD21	2:H:2003:BLM:HBC	1.93	0.50
1:B:30:PHE:CE2	1:B:32:ASP:HB2	2.47	0.50
1:G:90:ARG:HH22	2:G:2004:BLM:H662	1.77	0.50
1:D:68:ASP:OD1	1:D:71:GLU:HB3	2.12	0.50
1:B:84:THR:OG1	1:B:85:SER:N	2.45	0.49
1:E:108:ASP:HB2	1:E:109:PRO:CD	2.30	0.49
1:A:22:GLU:HA	1:A:26:PHE:O	2.13	0.49
1:B:81:ILE:HG21	1:B:91:ILE:HG23	1.93	0.49
1:C:30:PHE:CE2	1:C:32:ASP:HB2	2.47	0.49
1:B:83:GLU:HG2	1:B:91:ILE:HG13	1.95	0.49
2:G:2004:BLM:O12	2:G:2004:BLM:HAA	2.13	0.48
1:A:61:SER:O	1:A:62:CYS:HB3	2.13	0.48
1:G:18:ALA:HB2	1:G:36:MET:SD	2.53	0.48
2:A:1001:BLM:O12	2:A:1001:BLM:HAA	2.12	0.48
1:E:114:LEU:HD12	1:E:114:LEU:N	2.28	0.48
1:F:22:GLU:HG3	1:F:26:PHE:O	2.13	0.48
2:C:1004:BLM:O12	2:C:1004:BLM:HAA	2.12	0.48
1:H:60:PHE:HB2	3:H:1841:HOH:O	2.14	0.48
1:B:115:ARG:NH1	2:B:1002:BLM:O40	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:LEU:HD23	1:H:118:GLN:HB2	1.96	0.48
1:A:43:LEU:HA	3:A:824:HOH:O	2.14	0.48
1:C:115:ARG:NH2	2:C:1004:BLM:O4	2.46	0.47
1:F:68:ASP:OD1	1:F:71:GLU:HB3	2.14	0.47
1:G:99:TRP:CZ3	1:G:101:GLY:HA3	2.50	0.47
1:A:10:PRO:HG3	1:A:60:PHE:CD1	2.49	0.47
2:B:1002:BLM:HAA	2:B:1002:BLM:O12	2.14	0.47
1:B:9:LEU:HD22	1:B:112:THR:HG21	1.95	0.47
1:C:50:HIS:O	1:C:53:LEU:HB3	2.14	0.47
1:E:50:HIS:O	1:E:53:LEU:HB3	2.15	0.47
2:D:1003:BLM:O12	2:D:1003:BLM:HAA	2.12	0.47
1:C:64:LEU:HD12	1:C:116:LEU:HD22	1.97	0.47
1:E:4:GLN:HE22	1:E:44:MET:CE	2.28	0.47
2:F:2002:BLM:HAA	2:F:2002:BLM:O12	2.13	0.47
2:H:2003:BLM:HAA	2:H:2003:BLM:O12	2.15	0.47
1:G:12:ARG:HB2	1:G:110:ASP:OD2	2.15	0.47
1:E:31:ARG:HG3	1:E:32:ASP:N	2.29	0.47
1:H:8:ASN:O	1:H:9:LEU:HD23	2.15	0.47
1:E:30:PHE:CD2	1:E:30:PHE:C	2.88	0.47
1:F:73:TYR:CZ	1:F:93:ALA:HA	2.50	0.47
1:G:26:PHE:HA	1:G:40:ARG:HB2	1.97	0.47
1:E:104:ALA:HB3	1:E:116:LEU:HB2	1.96	0.46
1:D:22:GLU:HA	1:D:26:PHE:O	2.15	0.46
1:C:75:GLN:O	1:C:79:VAL:HG22	2.16	0.46
1:G:43:LEU:HD11	1:G:66:LEU:HD21	1.97	0.46
1:E:115:ARG:NH1	2:E:2001:BLM:O40	2.48	0.46
3:G:1836:HOH:O	2:H:2003:BLM:H2E	2.16	0.46
1:B:108:ASP:CB	1:B:109:PRO:CD	2.94	0.46
1:F:88:TYR:N	1:F:88:TYR:CD1	2.84	0.46
1:F:12:ARG:HB2	1:F:110:ASP:OD2	2.16	0.46
1:H:25:GLY:C	1:H:40:ARG:HG3	2.36	0.46
1:C:6:THR:HG21	1:C:44:MET:CE	2.45	0.46
1:C:115:ARG:NH1	2:C:1004:BLM:O40	2.49	0.46
1:G:6:THR:HG21	1:G:44:MET:HG2	1.97	0.46
1:D:81:ILE:CG2	1:D:91:ILE:HG23	2.46	0.45
1:G:26:PHE:HA	1:G:39:GLN:O	2.17	0.45
1:G:63:CYS:HB2	1:H:6:THR:OG1	2.16	0.45
1:D:22:GLU:HG3	1:D:26:PHE:O	2.16	0.45
1:F:69:LEU:O	1:F:69:LEU:HD12	2.16	0.45
1:D:76:CYS:O	1:D:81:ILE:HG13	2.16	0.45
1:B:23:ARG:O	1:B:79:VAL:HG11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASP:CB	1:C:109:PRO:HD2	2.32	0.45
1:E:10:PRO:HB2	1:E:53:LEU:HD22	1.99	0.45
1:H:65:ARG:HB3	1:H:119:ASN:OD1	2.16	0.45
1:B:7:PRO:HA	3:B:815:HOH:O	2.15	0.45
1:A:37:ILE:HG12	1:A:46:GLU:HG2	1.98	0.45
1:G:108:ASP:HB2	1:G:109:PRO:CD	2.47	0.45
1:H:72:PHE:HA	1:H:75:GLN:HG3	1.97	0.45
2:E:2001:BLM:HAA	2:E:2001:BLM:O12	2.16	0.45
1:C:63:CYS:O	1:D:5:ALA:HA	2.16	0.45
1:H:115:ARG:NH2	2:H:2003:BLM:O4	2.41	0.45
1:B:36:MET:SD	1:B:38:LEU:HD21	2.57	0.45
1:G:83:GLU:HA	1:G:91:ILE:O	2.16	0.45
1:G:50:HIS:O	1:G:53:LEU:HB3	2.16	0.45
1:F:77:LYS:HD3	1:F:91:ILE:HD11	1.99	0.45
1:B:43:LEU:HD22	1:B:64:LEU:HD22	1.99	0.45
1:F:61:SER:OG	2:F:2002:BLM:ND	2.50	0.45
1:H:108:ASP:CB	1:H:109:PRO:CD	2.94	0.44
1:D:8:ASN:N	1:D:8:ASN:HD22	2.15	0.44
3:C:834:HOH:O	1:D:43:LEU:HA	2.18	0.44
1:G:76:CYS:O	1:G:81:ILE:HG13	2.17	0.44
1:F:72:PHE:HA	1:F:75:GLN:HG3	2.00	0.44
1:C:7:PRO:HA	1:D:7:PRO:HB3	2.00	0.44
1:E:110:ASP:HB2	3:E:1812:HOH:O	2.18	0.44
1:E:90:ARG:HH22	2:E:2001:BLM:H662	1.83	0.44
1:A:50:HIS:O	1:A:53:LEU:HB3	2.17	0.44
1:F:82:GLN:HA	1:F:82:GLN:NE2	2.33	0.44
1:A:90:ARG:HH22	2:A:1001:BLM:H662	1.83	0.44
1:D:61:SER:HA	1:D:113:LEU:O	2.18	0.44
1:G:13:ASP:OD1	1:G:15:ASP:HB2	2.18	0.44
1:E:65:ARG:HH12	1:E:117:ILE:HG21	1.83	0.43
1:H:6:THR:HG21	1:H:44:MET:HE3	2.00	0.43
1:H:87:GLY:O	1:H:90:ARG:HG2	2.18	0.43
1:C:18:ALA:O	1:C:22:GLU:HB2	2.18	0.43
1:B:22:GLU:HA	1:B:26:PHE:O	2.18	0.43
1:C:109:PRO:HG2	3:C:832:HOH:O	2.18	0.43
1:H:30:PHE:C	1:H:30:PHE:CD2	2.92	0.43
1:C:17:THR:O	1:C:21:TYR:HD1	2.02	0.43
1:C:90:ARG:HH22	2:C:1004:BLM:H662	1.84	0.43
1:C:69:LEU:CD2	1:C:118:GLN:HB2	2.46	0.43
1:E:106:LEU:HD23	1:E:114:LEU:HD22	2.00	0.43
1:D:39:GLN:O	1:D:40:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:TRP:CZ3	1:A:101:GLY:HA3	2.53	0.43
1:F:81:ILE:CG2	1:F:91:ILE:HG23	2.43	0.43
1:A:3:ASP:O	1:A:4:GLN:HB3	2.18	0.43
1:C:94:PRO:HA	1:C:103:MET:O	2.18	0.43
1:H:69:LEU:HD22	1:H:118:GLN:N	2.33	0.42
1:E:68:ASP:OD2	1:E:70:ALA:HB3	2.19	0.42
1:F:10:PRO:HG3	1:F:60:PHE:CD1	2.54	0.42
1:H:53:LEU:HD21	1:H:110:ASP:HB3	2.00	0.42
1:F:90:ARG:HH22	2:F:2002:BLM:H662	1.83	0.42
1:E:62:CYS:SG	1:E:114:LEU:HG	2.59	0.42
1:E:50:HIS:CD2	1:E:53:LEU:HB2	2.54	0.42
1:H:106:LEU:HB2	1:H:116:LEU:HD11	2.01	0.42
1:E:108:ASP:CB	1:E:109:PRO:CD	2.96	0.42
2:C:1004:BLM:NH	2:C:1004:BLM:NJ	2.66	0.42
1:C:94:PRO:HG3	1:C:104:ALA:HB2	2.01	0.42
1:A:75:GLN:O	1:A:79:VAL:HG22	2.20	0.42
1:H:22:GLU:HA	1:H:26:PHE:O	2.20	0.42
2:A:1001:BLM:NH	2:A:1001:BLM:NJ	2.66	0.42
1:C:72:PHE:HA	1:C:75:GLN:HG3	2.02	0.42
1:H:84:THR:OG1	1:H:85:SER:N	2.53	0.42
1:F:30:PHE:CE2	1:F:32:ASP:HB2	2.55	0.42
1:C:86:SER:HA	2:C:1004:BLM:O66	2.19	0.42
1:H:118:GLN:NE2	1:H:119:ASN:N	2.68	0.42
1:D:21:TYR:HB2	1:D:38:LEU:HD13	2.02	0.42
1:C:53:LEU:HD11	1:C:58:SER:HB2	2.02	0.42
1:C:9:LEU:HD22	1:C:112:THR:HG21	2.01	0.42
1:E:76:CYS:O	1:E:81:ILE:HG13	2.20	0.42
1:A:18:ALA:HB2	1:A:36:MET:SD	2.60	0.42
1:G:5:ALA:HA	1:H:63:CYS:O	2.20	0.41
1:B:29:VAL:HG23	1:B:39:GLN:HB3	2.01	0.41
1:C:7:PRO:HG2	1:C:45:LEU:HD23	2.02	0.41
1:G:65:ARG:HH12	2:G:2004:BLM:HNP	1.67	0.41
1:A:87:GLY:O	1:A:90:ARG:NH2	2.48	0.41
1:F:2:THR:HG22	1:F:3:ASP:N	2.36	0.41
1:A:26:PHE:CD1	1:A:40:ARG:HB2	2.55	0.41
1:B:28:ILE:HG12	1:B:38:LEU:CD2	2.50	0.41
1:C:64:LEU:HD23	1:D:5:ALA:HB2	2.03	0.41
1:A:91:ILE:CG2	1:A:106:LEU:HD13	2.50	0.41
1:A:21:TYR:O	1:A:26:PHE:HB2	2.20	0.41
1:F:55:PRO:HB3	1:F:111:GLY:HA3	2.03	0.41
1:C:82:GLN:HA	1:C:82:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:HB3	1:C:119:ASN:OD1	2.21	0.41
1:A:68:ASP:OD1	1:A:71:GLU:HB3	2.21	0.41
1:F:97:GLN:HB3	1:F:99:TRP:NE1	2.36	0.41
1:C:44:MET:CE	1:D:65:ARG:HD2	2.50	0.41
1:H:9:LEU:O	1:H:47:PHE:HA	2.21	0.41
1:B:75:GLN:O	1:B:79:VAL:HG22	2.21	0.41
1:C:62:CYS:HA	1:D:8:ASN:ND2	2.35	0.41
1:E:77:LYS:HE2	1:E:83:GLU:OE2	2.20	0.41
1:D:71:GLU:HG2	1:D:75:GLN:HE21	1.85	0.41
1:B:30:PHE:HE2	1:B:32:ASP:HB2	1.86	0.41
3:C:836:HOH:O	2:D:1003:BLM:H2E	2.20	0.41
1:E:65:ARG:NH1	1:E:117:ILE:HG21	2.36	0.41
1:E:11:SER:HA	1:E:110:ASP:OD1	2.20	0.41
1:B:103:MET:HA	1:B:116:LEU:O	2.21	0.41
1:B:44:MET:CG	1:B:44:MET:O	2.68	0.40
1:A:55:PRO:HB2	1:A:88:TYR:CZ	2.56	0.40
1:D:76:CYS:SG	1:D:106:LEU:HD13	2.61	0.40
1:C:26:PHE:CD2	1:C:40:ARG:HB3	2.55	0.40
1:C:21:TYR:HB3	1:C:26:PHE:HB2	2.01	0.40
1:H:113:LEU:HB2	2:H:2003:BLM:HAC	2.03	0.40
1:D:68:ASP:CG	1:D:71:GLU:HB3	2.41	0.40
1:C:12:ARG:HB2	1:C:12:ARG:HE	1.69	0.40
1:B:65:ARG:HB3	1:B:119:ASN:OD1	2.22	0.40
1:E:68:ASP:CG	1:E:71:GLU:HB3	2.42	0.40
1:B:6:THR:HG21	1:B:44:MET:HG2	2.03	0.40
1:C:76:CYS:O	1:C:81:ILE:HG13	2.21	0.40
1:F:30:PHE:CD2	1:F:30:PHE:C	2.95	0.40
1:G:9:LEU:O	1:G:47:PHE:HA	2.22	0.40
1:C:68:ASP:OD1	1:C:71:GLU:HB3	2.22	0.40
1:F:35:TRP:CZ3	1:F:48:PHE:HB3	2.56	0.40
1:F:108:ASP:HB2	1:F:109:PRO:CD	2.39	0.40
1:D:118:GLN:HE21	1:D:119:ASN:N	2.20	0.40
1:H:91:ILE:HA	1:H:105:ALA:O	2.22	0.40
1:H:13:ASP:OD2	1:H:15:ASP:HB2	2.21	0.40
1:H:61:SER:HB2	1:H:113:LEU:O	2.21	0.40
1:A:21:TYR:OH	1:A:108:ASP:CB	2.69	0.40
1:G:81:ILE:HG21	1:G:91:ILE:HG23	2.01	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	117/126 (93%)	108 (92%)	9 (8%)	0	100	100
1	B	117/126 (93%)	110 (94%)	7 (6%)	0	100	100
1	C	117/126 (93%)	109 (93%)	8 (7%)	0	100	100
1	D	117/126 (93%)	109 (93%)	7 (6%)	1 (1%)	21	37
1	E	117/126 (93%)	105 (90%)	12 (10%)	0	100	100
1	F	117/126 (93%)	107 (92%)	10 (8%)	0	100	100
1	G	117/126 (93%)	106 (91%)	11 (9%)	0	100	100
1	H	117/126 (93%)	107 (92%)	9 (8%)	1 (1%)	21	37
All	All	936/1008 (93%)	861 (92%)	73 (8%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	ARG
1	H	17	THR

### 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	99/104 (95%)	80 (81%)	19 (19%)	2	3
1	B	99/104 (95%)	82 (83%)	17 (17%)	2	4
1	C	99/104 (95%)	83 (84%)	16 (16%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	99/104 (95%)	82 (83%)	17 (17%)	2	4
1	E	99/104 (95%)	83 (84%)	16 (16%)	3	5
1	F	99/104 (95%)	84 (85%)	15 (15%)	3	6
1	G	99/104 (95%)	81 (82%)	18 (18%)	2	3
1	H	99/104 (95%)	81 (82%)	18 (18%)	2	3
All	All	792/832 (95%)	656 (83%)	136 (17%)	2	4

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	GLN
1	A	16	SER
1	A	22	GLU
1	A	32	ASP
1	A	44	MET
1	A	53	LEU
1	A	58	SER
1	A	66	LEU
1	A	71	GLU
1	A	75	GLN
1	A	77	LYS
1	A	82	GLN
1	A	83	GLU
1	A	85	SER
1	A	98	GLU
1	A	103	MET
1	A	108	ASP
1	A	114	LEU
1	B	2	THR
1	B	22	GLU
1	B	36	MET
1	B	44	MET
1	B	45	LEU
1	B	50	HIS
1	B	53	LEU
1	B	58	SER
1	B	66	LEU
1	B	71	GLU
1	B	75	GLN

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Mol	Chain	Res	Type
1	B	77	LYS
1	B	82	GLN
1	B	83	GLU
1	B	85	SER
1	B	98	GLU
1	B	103	MET
1	C	2	THR
1	C	3	ASP
1	C	12	ARG
1	C	22	GLU
1	C	40	ARG
1	C	44	MET
1	C	53	LEU
1	C	66	LEU
1	C	71	GLU
1	C	75	GLN
1	C	82	GLN
1	C	83	GLU
1	C	85	SER
1	C	86	SER
1	C	98	GLU
1	C	103	MET
1	D	2	THR
1	D	22	GLU
1	D	31	ARG
1	D	32	ASP
1	D	40	ARG
1	D	50	HIS
1	D	53	LEU
1	D	58	SER
1	D	62	CYS
1	D	66	LEU
1	D	71	GLU
1	D	75	GLN
1	D	82	GLN
1	D	83	GLU
1	D	85	SER
1	D	98	GLU
1	D	113	LEU
1	E	2	THR
1	E	4	GLN
1	E	44	MET

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Mol	Chain	Res	Type
1	E	50	HIS
1	E	53	LEU
1	E	58	SER
1	E	66	LEU
1	E	69	LEU
1	E	71	GLU
1	E	75	GLN
1	E	77	LYS
1	E	78	SER
1	E	82	GLN
1	E	83	GLU
1	E	85	SER
1	E	98	GLU
1	F	4	GLN
1	F	22	GLU
1	F	40	ARG
1	F	50	HIS
1	F	53	LEU
1	F	58	SER
1	F	66	LEU
1	F	71	GLU
1	F	77	LYS
1	F	81	ILE
1	F	82	GLN
1	F	83	GLU
1	F	85	SER
1	F	98	GLU
1	F	103	MET
1	G	2	THR
1	G	4	GLN
1	G	16	SER
1	G	32	ASP
1	G	40	ARG
1	G	44	MET
1	G	50	HIS
1	G	53	LEU
1	G	58	SER
1	G	62	CYS
1	G	66	LEU
1	G	71	GLU
1	G	75	GLN
1	G	78	SER

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Mol	Chain	Res	Type
1	G	82	GLN
1	G	83	GLU
1	G	85	SER
1	G	98	GLU
1	H	2	THR
1	H	4	GLN
1	H	16	SER
1	H	22	GLU
1	H	44	MET
1	H	50	HIS
1	H	53	LEU
1	H	58	SER
1	H	66	LEU
1	H	71	GLU
1	H	75	GLN
1	H	77	LYS
1	H	81	ILE
1	H	82	GLN
1	H	83	GLU
1	H	85	SER
1	H	98	GLU
1	H	103	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	B	8	ASN
1	C	4	GLN
1	C	8	ASN
1	C	82	GLN
1	C	92	HIS
1	D	8	ASN
1	D	82	GLN
1	D	92	HIS
1	E	4	GLN
1	E	8	ASN
1	F	4	GLN
1	F	8	ASN
1	F	82	GLN
1	G	8	ASN
1	H	8	ASN

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Mol	Chain	Res	Type
1	H	118	GLN

### 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 ⓘ

8 ligands 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	$\# Z  > 2$
2	BLM	A	1001	-	89,101,101	1.87	8 (8%)	102,143,143	1.77	23 (22%)
2	BLM	B	1002	-	89,101,101	1.84	9 (10%)	102,143,143	1.75	21 (20%)
2	BLM	C	1004	-	89,101,101	1.88	7 (7%)	102,143,143	1.74	22 (21%)
2	BLM	D	1003	-	89,101,101	1.88	9 (10%)	102,143,143	1.70	21 (20%)
2	BLM	E	2001	-	89,101,101	1.85	9 (10%)	102,143,143	1.79	21 (20%)
2	BLM	F	2002	-	89,101,101	1.87	8 (8%)	102,143,143	1.73	22 (21%)
2	BLM	G	2004	-	89,101,101	1.86	7 (7%)	102,143,143	1.78	23 (22%)
2	BLM	H	2003	-	89,101,101	1.86	10 (11%)	102,143,143	1.75	22 (21%)

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
2	BLM	A	1001	-	-	0/85/142/142	0/6/6/6
2	BLM	B	1002	-	-	0/85/142/142	0/6/6/6
2	BLM	C	1004	-	-	0/85/142/142	0/6/6/6
2	BLM	D	1003	-	-	0/85/142/142	0/6/6/6
2	BLM	E	2001	-	-	0/85/142/142	0/6/6/6
2	BLM	F	2002	-	-	0/85/142/142	0/6/6/6
2	BLM	G	2004	-	-	0/85/142/142	0/6/6/6
2	BLM	H	2003	-	-	0/85/142/142	0/6/6/6

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2003	BLM	C7-NE	-6.81	1.22	1.34
2	D	1003	BLM	C7-NE	-6.80	1.22	1.34
2	G	2004	BLM	C7-NE	-6.72	1.22	1.34
2	F	2002	BLM	C7-NE	-6.67	1.22	1.34
2	C	1004	BLM	C10-C9	-6.65	1.30	1.40
2	C	1004	BLM	C7-NE	-6.59	1.22	1.34
2	E	2001	BLM	C7-NE	-6.58	1.22	1.34
2	D	1003	BLM	C10-C9	-6.56	1.30	1.40
2	A	1001	BLM	C10-C9	-6.56	1.30	1.40
2	B	1002	BLM	C7-NE	-6.54	1.22	1.34
2	F	2002	BLM	C10-C9	-6.54	1.30	1.40
2	A	1001	BLM	C7-NE	-6.53	1.22	1.34
2	G	2004	BLM	C10-C9	-6.39	1.30	1.40
2	H	2003	BLM	C10-C9	-6.35	1.30	1.40
2	B	1002	BLM	C10-C9	-6.32	1.30	1.40
2	E	2001	BLM	C10-C9	-6.10	1.31	1.40
2	C	1004	BLM	C10-C12	-4.62	1.43	1.50
2	A	1001	BLM	C10-C12	-4.42	1.43	1.50
2	H	2003	BLM	C10-C12	-4.41	1.43	1.50
2	D	1003	BLM	C10-C12	-4.38	1.43	1.50
2	G	2004	BLM	C10-C12	-4.37	1.43	1.50
2	B	1002	BLM	C10-C12	-4.26	1.43	1.50
2	E	2001	BLM	C10-C12	-4.13	1.43	1.50
2	F	2002	BLM	C10-C12	-4.12	1.43	1.50
2	E	2001	BLM	C45-C46	-4.02	1.41	1.49
2	A	1001	BLM	C45-C46	-4.00	1.41	1.49
2	B	1002	BLM	C45-C46	-3.88	1.41	1.49
2	H	2003	BLM	C45-C46	-3.78	1.42	1.49
2	C	1004	BLM	C45-C46	-3.75	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2002	BLM	C45-C46	-3.71	1.42	1.49
2	G	2004	BLM	C45-C46	-3.63	1.42	1.49
2	D	1003	BLM	C45-C46	-3.53	1.42	1.49
2	H	2003	BLM	O68-C68	-2.62	1.40	1.44
2	A	1001	BLM	O68-C68	-2.09	1.41	1.44
2	D	1003	BLM	O68-C68	-2.02	1.41	1.44
2	B	1002	BLM	C12-NH	2.00	1.38	1.34
2	B	1002	BLM	C47-S46	2.16	1.74	1.70
2	E	2001	BLM	C47-S46	2.19	1.74	1.70
2	E	2001	BLM	C12-NH	2.20	1.39	1.34
2	D	1003	BLM	C47-S46	2.21	1.74	1.70
2	H	2003	BLM	C12-NH	2.21	1.39	1.34
2	F	2002	BLM	C47-S46	2.24	1.74	1.70
2	H	2003	BLM	C47-S46	2.35	1.74	1.70
2	F	2002	BLM	C1-NA	2.74	1.38	1.32
2	C	1004	BLM	C1-NA	2.93	1.38	1.32
2	G	2004	BLM	C1-NA	2.94	1.38	1.32
2	B	1002	BLM	C1-NA	2.98	1.38	1.32
2	A	1001	BLM	C1-NA	3.03	1.38	1.32
2	H	2003	BLM	C1-NA	3.05	1.38	1.32
2	D	1003	BLM	C1-NA	3.07	1.39	1.32
2	E	2001	BLM	C1-NA	3.12	1.39	1.32
2	D	1003	BLM	C8-NE	7.02	1.45	1.35
2	F	2002	BLM	C8-NE	7.08	1.46	1.35
2	B	1002	BLM	C8-NE	7.11	1.46	1.35
2	H	2003	BLM	C8-NE	7.12	1.46	1.35
2	E	2001	BLM	C8-NE	7.18	1.46	1.35
2	G	2004	BLM	C8-NE	7.20	1.46	1.35
2	A	1001	BLM	C8-NE	7.43	1.46	1.35
2	C	1004	BLM	C8-NE	7.47	1.46	1.35
2	H	2003	BLM	C10-NG	8.96	1.49	1.34
2	C	1004	BLM	C10-NG	8.99	1.49	1.34
2	B	1002	BLM	C10-NG	9.12	1.49	1.34
2	A	1001	BLM	C10-NG	9.19	1.49	1.34
2	E	2001	BLM	C10-NG	9.21	1.49	1.34
2	D	1003	BLM	C10-NG	9.23	1.49	1.34
2	F	2002	BLM	C10-NG	9.40	1.50	1.34
2	G	2004	BLM	C10-NG	9.40	1.50	1.34

All (175) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2001	BLM	C9-C10-NG	-5.86	117.93	123.25
2	F	2002	BLM	C9-C10-NG	-5.76	118.01	123.25
2	H	2003	BLM	C9-C10-NG	-5.62	118.14	123.25
2	G	2004	BLM	C9-C10-NG	-5.59	118.17	123.25
2	A	1001	BLM	C9-C10-NG	-5.55	118.21	123.25
2	C	1004	BLM	C9-C10-NG	-5.54	118.22	123.25
2	D	1003	BLM	C9-C10-NG	-5.43	118.31	123.25
2	B	1002	BLM	C9-C10-NG	-5.28	118.45	123.25
2	A	1001	BLM	O1-C1-NA	-4.17	116.90	123.08
2	H	2003	BLM	O1-C1-NA	-4.09	117.01	123.08
2	G	2004	BLM	O1-C1-NA	-3.99	117.17	123.08
2	B	1002	BLM	O1-C1-NA	-3.86	117.36	123.08
2	C	1004	BLM	O1-C1-NA	-3.79	117.45	123.08
2	F	2002	BLM	O1-C1-NA	-3.69	117.61	123.08
2	B	1002	BLM	C12-C10-NG	-3.51	108.68	115.31
2	E	2001	BLM	O1-C1-NA	-3.51	117.87	123.08
2	H	2003	BLM	C12-C10-NG	-3.39	108.92	115.31
2	D	1003	BLM	O1-C1-NA	-3.37	118.09	123.08
2	E	2001	BLM	C12-C10-NG	-3.30	109.09	115.31
2	C	1004	BLM	C12-C10-NG	-3.29	109.09	115.31
2	D	1003	BLM	C12-C10-NG	-3.20	109.28	115.31
2	C	1004	BLM	O70-C70-NQ	-3.18	119.24	125.34
2	G	2004	BLM	C12-C10-NG	-3.18	109.31	115.31
2	G	2004	BLM	O70-C70-NQ	-3.08	119.44	125.34
2	F	2002	BLM	C12-C10-NG	-3.07	109.52	115.31
2	D	1003	BLM	O70-C70-NQ	-3.06	119.48	125.34
2	E	2001	BLM	O70-C70-NQ	-3.05	119.50	125.34
2	A	1001	BLM	C12-C10-NG	-2.99	109.67	115.31
2	B	1002	BLM	O70-C70-NQ	-2.94	119.71	125.34
2	A	1001	BLM	O70-C70-NQ	-2.92	119.74	125.34
2	F	2002	BLM	O70-C70-NQ	-2.88	119.82	125.34
2	A	1001	BLM	C45-C44-S43	-2.66	108.52	111.79
2	A	1001	BLM	C3-C2-NB	-2.64	105.39	109.56
2	E	2001	BLM	CA-C9-C8	-2.60	117.38	120.05
2	E	2001	BLM	C45-C44-S43	-2.58	108.62	111.79
2	H	2003	BLM	C3-C2-NB	-2.58	105.49	109.56
2	H	2003	BLM	O70-C70-NQ	-2.53	120.50	125.34
2	B	1002	BLM	C3-C2-NB	-2.48	105.65	109.56
2	A	1001	BLM	CA-C9-C8	-2.47	117.51	120.05
2	C	1004	BLM	C45-C44-S43	-2.45	108.78	111.79
2	H	2003	BLM	CA-C9-C8	-2.44	117.55	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2004	BLM	C45-C44-S43	-2.42	108.81	111.79
2	H	2003	BLM	C45-C44-S43	-2.38	108.87	111.79
2	B	1002	BLM	C45-C44-S43	-2.38	108.87	111.79
2	F	2002	BLM	C45-C44-S43	-2.31	108.95	111.79
2	G	2004	BLM	C3-C2-NB	-2.30	105.93	109.56
2	D	1003	BLM	C45-C44-S43	-2.29	108.98	111.79
2	G	2004	BLM	CA-C9-C8	-2.28	117.71	120.05
2	B	1002	BLM	C27-C28-NI	-2.23	104.54	108.56
2	C	1004	BLM	C3-C2-NB	-2.22	106.05	109.56
2	F	2002	BLM	C27-C28-NI	-2.19	104.60	108.56
2	E	2001	BLM	C3-C2-NB	-2.17	106.13	109.56
2	H	2003	BLM	C27-C28-NI	-2.17	104.64	108.56
2	D	1003	BLM	C3-C2-NB	-2.15	106.17	109.56
2	F	2002	BLM	CA-C9-C8	-2.09	117.90	120.05
2	C	1004	BLM	C27-C28-NI	-2.07	104.82	108.56
2	A	1001	BLM	C27-C28-NI	-2.06	104.84	108.56
2	D	1003	BLM	C27-C28-NI	-2.06	104.85	108.56
2	G	2004	BLM	C27-C28-NI	-2.04	104.88	108.56
2	F	2002	BLM	C3-C2-NB	-2.03	106.35	109.56
2	G	2004	BLM	O64-C65-C67	2.10	113.62	109.68
2	C	1004	BLM	C5-C4-ND	2.12	120.76	116.08
2	C	1004	BLM	C7-NE-C8	2.13	122.42	118.23
2	F	2002	BLM	C5-C4-ND	2.17	120.86	116.08
2	H	2003	BLM	C5-C4-ND	2.17	120.87	116.08
2	B	1002	BLM	C5-C4-ND	2.19	120.91	116.08
2	A	1001	BLM	C7-NE-C8	2.19	122.55	118.23
2	F	2002	BLM	C55-S53-C52	2.24	105.89	101.73
2	E	2001	BLM	C7-NE-C8	2.29	122.74	118.23
2	A	1001	BLM	C63-OH1-C14	2.30	119.96	115.80
2	G	2004	BLM	C28-NI-C29	2.32	109.36	105.71
2	A	1001	BLM	C5-C4-ND	2.32	121.19	116.08
2	F	2002	BLM	C7-NE-C8	2.33	122.81	118.23
2	H	2003	BLM	C7-NE-C8	2.33	122.81	118.23
2	D	1003	BLM	C7-NE-C8	2.34	122.84	118.23
2	A	1001	BLM	C28-NI-C29	2.36	109.43	105.71
2	E	2001	BLM	C63-OH1-C14	2.37	120.08	115.80
2	G	2004	BLM	C7-NE-C8	2.37	122.90	118.23
2	C	1004	BLM	C28-NI-C29	2.37	109.45	105.71
2	D	1003	BLM	C63-OH1-C14	2.39	120.11	115.80
2	D	1003	BLM	O56-C57-C58	2.39	113.34	107.17
2	E	2001	BLM	C28-NI-C29	2.40	109.50	105.71
2	H	2003	BLM	O56-C57-C58	2.43	113.43	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1003	BLM	C28-NI-C29	2.44	109.56	105.71
2	D	1003	BLM	O1-C1-C2	2.45	123.66	120.33
2	C	1004	BLM	C55-S53-C52	2.46	106.29	101.73
2	A	1001	BLM	O56-C57-C58	2.47	113.55	107.17
2	H	2003	BLM	C28-NI-C29	2.48	109.63	105.71
2	G	2004	BLM	O56-C57-C58	2.50	113.61	107.17
2	B	1002	BLM	C7-NE-C8	2.50	123.15	118.23
2	C	1004	BLM	C63-OH1-C14	2.51	120.33	115.80
2	G	2004	BLM	C5-C4-ND	2.51	121.61	116.08
2	E	2001	BLM	O1-C1-C2	2.52	123.76	120.33
2	B	1002	BLM	C28-NI-C29	2.52	109.69	105.71
2	C	1004	BLM	O56-C57-C58	2.53	113.71	107.17
2	E	2001	BLM	O56-C57-C58	2.58	113.82	107.17
2	F	2002	BLM	C28-NI-C29	2.58	109.78	105.71
2	B	1002	BLM	O56-C57-C58	2.60	113.87	107.17
2	E	2001	BLM	C55-S53-C52	2.63	106.61	101.73
2	D	1003	BLM	NF-C8-NE	2.64	120.78	116.95
2	D	1003	BLM	C55-S53-C52	2.64	106.64	101.73
2	A	1001	BLM	C55-S53-C52	2.65	106.65	101.73
2	G	2004	BLM	NF-C8-NE	2.66	120.80	116.95
2	H	2003	BLM	C54-S53-C52	2.66	106.66	101.73
2	B	1002	BLM	NF-C8-NE	2.66	120.81	116.95
2	B	1002	BLM	C55-S53-C52	2.67	106.69	101.73
2	D	1003	BLM	C64-O64-C65	2.68	118.94	113.75
2	D	1003	BLM	C54-S53-C52	2.69	106.71	101.73
2	A	1001	BLM	O1-C1-C2	2.69	123.99	120.33
2	G	2004	BLM	C55-S53-C52	2.71	106.75	101.73
2	C	1004	BLM	NF-C8-NE	2.71	120.87	116.95
2	F	2002	BLM	NF-C8-NE	2.71	120.88	116.95
2	A	1001	BLM	C54-S53-C52	2.73	106.79	101.73
2	E	2001	BLM	NF-C8-NE	2.73	120.90	116.95
2	F	2002	BLM	O1-C1-C2	2.73	124.05	120.33
2	B	1002	BLM	C54-S53-C52	2.75	106.83	101.73
2	G	2004	BLM	C54-S53-C52	2.77	106.87	101.73
2	H	2003	BLM	NF-C8-NE	2.78	120.97	116.95
2	F	2002	BLM	C54-S53-C52	2.78	106.89	101.73
2	H	2003	BLM	O1-C1-C2	2.79	124.12	120.33
2	E	2001	BLM	C54-S53-C52	2.81	106.94	101.73
2	B	1002	BLM	O1-C1-C2	2.81	124.16	120.33
2	C	1004	BLM	C54-S53-C52	2.81	106.94	101.73
2	F	2002	BLM	O56-C57-C58	2.85	114.53	107.17
2	E	2001	BLM	C63-O62-C60	2.87	119.31	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1004	BLM	O1-C1-C2	2.97	124.38	120.33
2	G	2004	BLM	O1-C1-C2	2.99	124.40	120.33
2	C	1004	BLM	C63-O62-C60	3.00	119.56	113.75
2	H	2003	BLM	C55-S53-C52	3.03	107.35	101.73
2	A	1001	BLM	C63-O62-C60	3.11	119.79	113.75
2	H	2003	BLM	C64-O64-C65	3.17	119.89	113.75
2	B	1002	BLM	C64-O64-C65	3.24	120.03	113.75
2	E	2001	BLM	C64-O64-C65	3.32	120.19	113.75
2	F	2002	BLM	C64-O64-C65	3.32	120.20	113.75
2	A	1001	BLM	NF-C8-NE	3.33	121.77	116.95
2	G	2004	BLM	C63-O62-C60	3.34	120.23	113.75
2	A	1001	BLM	C64-O64-C65	3.46	120.45	113.75
2	B	1002	BLM	C63-O62-C60	3.46	120.47	113.75
2	C	1004	BLM	C64-O64-C65	3.54	120.62	113.75
2	D	1003	BLM	C63-O62-C60	3.62	120.77	113.75
2	F	2002	BLM	C63-O62-C60	3.67	120.87	113.75
2	G	2004	BLM	C6-C5-C4	3.80	120.34	112.48
2	H	2003	BLM	C63-O62-C60	3.82	121.16	113.75
2	G	2004	BLM	C64-O64-C65	3.88	121.28	113.75
2	F	2002	BLM	O68-C68-C69	3.93	116.49	107.76
2	H	2003	BLM	C6-C5-C4	3.95	120.65	112.48
2	A	1001	BLM	C6-C5-C4	3.97	120.70	112.48
2	C	1004	BLM	C6-C5-C4	4.06	120.89	112.48
2	A	1001	BLM	O68-C68-C69	4.09	116.83	107.76
2	D	1003	BLM	O68-C68-C69	4.17	117.01	107.76
2	F	2002	BLM	C6-C5-C4	4.23	121.24	112.48
2	H	2003	BLM	O68-C68-C69	4.24	117.18	107.76
2	G	2004	BLM	O68-C68-C69	4.31	117.34	107.76
2	B	1002	BLM	C10-C9-C8	4.34	119.40	115.69
2	B	1002	BLM	C6-C5-C4	4.38	121.55	112.48
2	D	1003	BLM	C6-C5-C4	4.42	121.64	112.48
2	D	1003	BLM	C10-C9-C8	4.44	119.48	115.69
2	C	1004	BLM	O68-C68-C69	4.48	117.72	107.76
2	G	2004	BLM	C10-C9-C8	4.51	119.55	115.69
2	B	1002	BLM	O68-C68-C69	4.53	117.83	107.76
2	C	1004	BLM	C10-C9-C8	4.55	119.58	115.69
2	H	2003	BLM	C10-C9-C8	4.59	119.61	115.69
2	F	2002	BLM	C10-C9-C8	4.60	119.63	115.69
2	E	2001	BLM	C10-C9-C8	4.68	119.69	115.69
2	A	1001	BLM	C10-C9-C8	4.69	119.70	115.69
2	E	2001	BLM	O68-C68-C69	4.75	118.31	107.76
2	E	2001	BLM	C6-C5-C4	5.08	123.00	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2003	BLM	C68-O68-C70	5.66	125.20	117.03
2	F	2002	BLM	C68-O68-C70	5.71	125.28	117.03
2	D	1003	BLM	C68-O68-C70	6.09	125.82	117.03
2	C	1004	BLM	C68-O68-C70	6.19	125.97	117.03
2	A	1001	BLM	C68-O68-C70	6.37	126.22	117.03
2	E	2001	BLM	C68-O68-C70	6.38	126.23	117.03
2	B	1002	BLM	C68-O68-C70	6.38	126.24	117.03
2	G	2004	BLM	C68-O68-C70	6.55	126.49	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	BLM	4	0
2	B	1002	BLM	2	0
2	C	1004	BLM	7	0
2	D	1003	BLM	3	0
2	E	2001	BLM	4	0
2	F	2002	BLM	6	0
2	G	2004	BLM	5	0
2	H	2003	BLM	6	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.