



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:34 am GMT

PDB ID : 1KXG  
Title : The 2.0 Ang Resolution Structure of BLyS, B Lymphocyte Stimulator.  
Authors : Oren, D.A.; Li, Y.; Volovik, Y.; Morris, T.S.; Dharia, C.; Das, K.; Galperina, O.; Gentz, R.; Arnold, E.  
Deposited on : 2002-01-31  
Resolution : 2.00 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

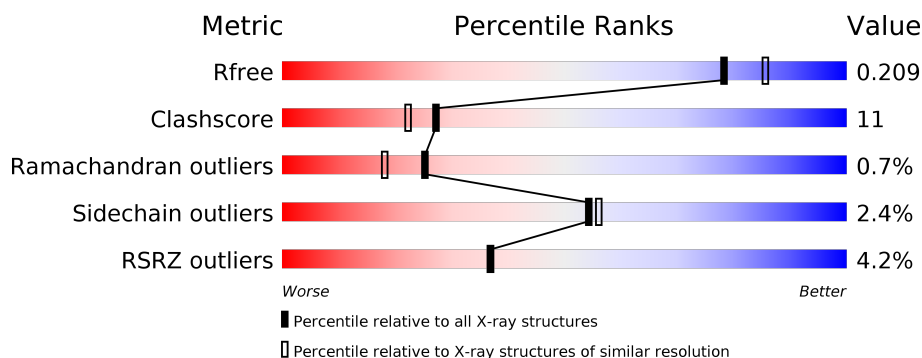
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	152	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	152	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	C	152	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	D	152	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	E	152	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	F	152	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>9%</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
3	CIT	A	889	-	-	-	X
3	CIT	F	888	-	-	-	X
4	DIO	A	1002	-	-	-	X
4	DIO	A	1015	-	-	-	X
4	DIO	A	1017	-	-	-	X
4	DIO	B	1018	-	-	-	X
4	DIO	C	1003	-	-	-	X
4	DIO	C	1006	-	-	X	X
4	DIO	C	1008	-	-	-	X
4	DIO	D	1012	-	-	-	X
4	DIO	E	1010	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7473 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.

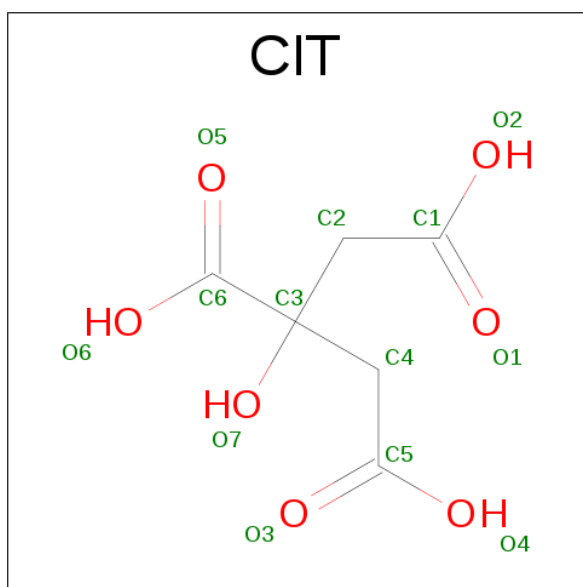
- Molecule 1 is a protein called B lymphocyte stimulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	B	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	C	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	D	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	E	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	F	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

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

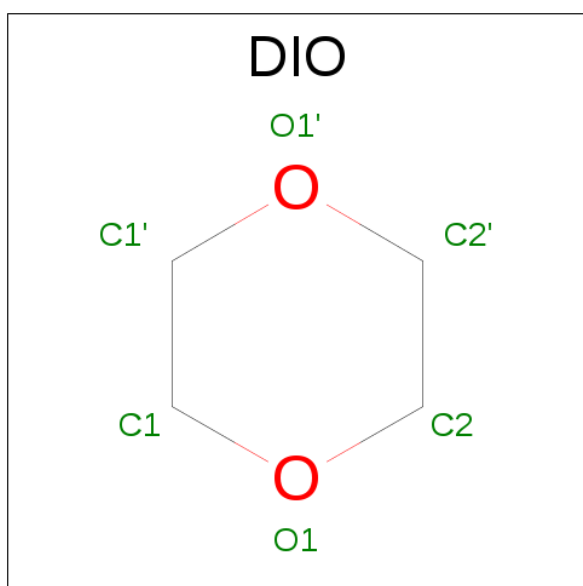
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	3	Total	Mg	0	0
			3	3		
2	D	2	Total	Mg	0	0
			2	2		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula:  $C_4H_8O_2$ ).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 4 2	0	0
4	A	1	Total C O 6 4 2	0	0
4	B	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	D	1	Total C O 6 4 2	0	0
4	E	1	Total C O 6 4 2	0	0
4	E	1	Total C O 6 4 2	0	0
4	D	1	Total C O 6 4 2	0	0
4	F	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	A	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	A	1	Total C O 6 4 2	0	0
4	B	1	Total C O 6 4 2	0	0
4	E	1	Total C O 6 4 2	0	0
4	F	1	Total C O 6 4 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0

*Continued on next page...*

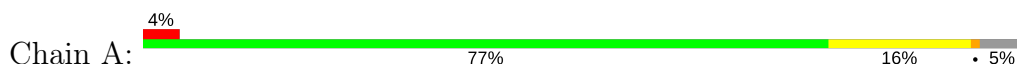
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	65	Total 65	O 65	0	0
5	C	72	Total 72	O 72	0	0
5	D	86	Total 86	O 86	0	0
5	E	73	Total 73	O 73	0	0
5	F	97	Total 97	O 97	0	0

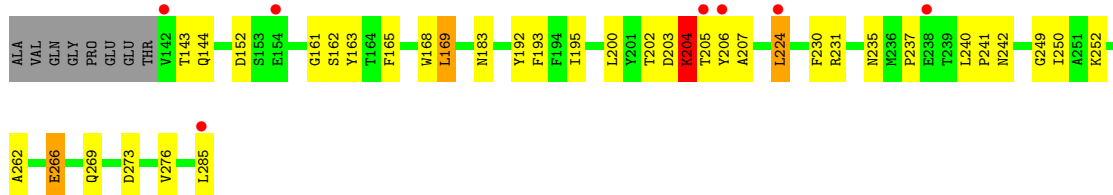
### 3 Residue-property plots [i](#)

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

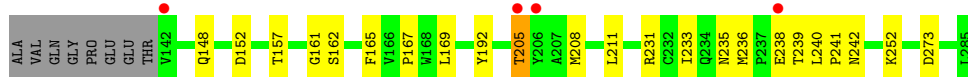
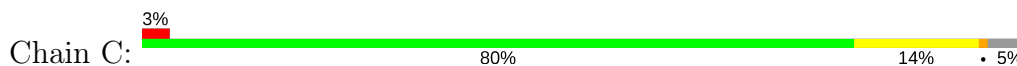
#### • Molecule 1: B lymphocyte stimulator



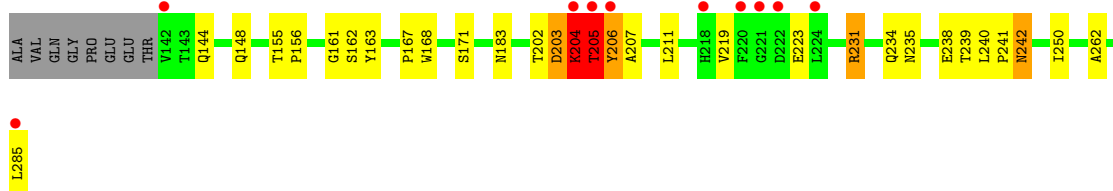
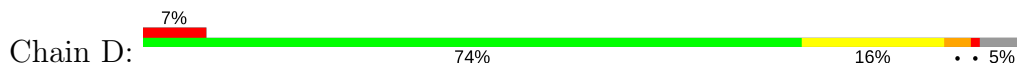
#### • Molecule 1: B lymphocyte stimulator



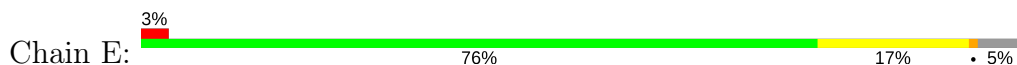
#### • Molecule 1: B lymphocyte stimulator



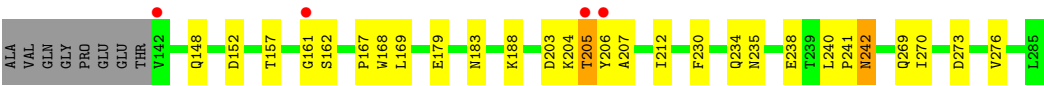
#### • Molecule 1: B lymphocyte stimulator



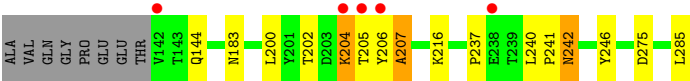
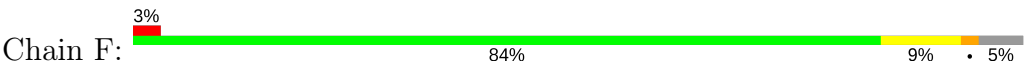
#### • Molecule 1: B lymphocyte stimulator







● Molecule 1: B lymphocyte stimulator



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.58Å 123.58Å 161.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.64 – 2.00 29.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.64-2.00) 99.3 (29.72-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.189 , 0.209 0.188 , 0.209	Depositor DCC
$R_{free}$ test set	1849 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7473	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DIO, CIT

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	0.36	0/1165	0.61	0/1574
1	B	0.35	0/1165	0.62	1/1574 (0.1%)
1	C	0.34	0/1165	0.60	0/1574
1	D	0.37	0/1165	0.65	1/1574 (0.1%)
1	E	0.36	0/1165	0.67	0/1574
1	F	0.37	0/1165	0.65	0/1574
All	All	0.36	0/6990	0.63	2/9444 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	LYS	N-CA-C	5.67	126.31	111.00
1	B	204	LYS	C-N-CA	5.04	134.29	121.70

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	1143	0	1145	38	0
1	B	1143	0	1145	43	0
1	C	1143	0	1145	26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1143	0	1145	30	0
1	E	1143	0	1145	33	0
1	F	1143	0	1145	18	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	F	1	0	0	0	0
3	A	13	0	5	0	0
3	F	13	0	5	0	0
4	A	30	0	40	8	0
4	B	12	0	16	3	0
4	C	36	0	48	8	0
4	D	12	0	16	2	0
4	E	18	0	24	3	0
4	F	12	0	16	2	0
5	A	69	0	0	0	0
5	B	65	0	0	0	0
5	C	72	0	0	3	0
5	D	86	0	0	0	0
5	E	73	0	0	0	0
5	F	97	0	0	2	0
All	All	7473	0	7040	160	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 11.

All (160) 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:235:ASN:HD21	1:B:242:ASN:H	1.06	1.03
1:D:206:TYR:HD1	1:D:207:ALA:H	0.99	0.97
1:B:235:ASN:HD21	1:C:242:ASN:H	1.12	0.96
1:E:235:ASN:HD21	1:F:242:ASN:H	1.11	0.95
1:A:242:ASN:HD22	1:C:233:ILE:HD13	1.34	0.92
1:D:235:ASN:HD21	1:E:242:ASN:H	1.16	0.92
1:E:168:TRP:H	1:E:183:ASN:HD21	1.18	0.91
1:A:242:ASN:H	1:C:235:ASN:HD21	1.13	0.90
1:B:168:TRP:H	1:B:183:ASN:HD21	1.21	0.89
1:D:206:TYR:HD1	1:D:207:ALA:N	1.71	0.87
1:E:269:GLN:HA	4:E:1019:DIO:H11	1.55	0.87
1:D:168:TRP:H	1:D:183:ASN:HD21	1.25	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:THR:HG22	1:D:238:GLU:HG2	1.62	0.82
1:B:266:GLU:H	1:B:266:GLU:CD	1.84	0.81
1:B:204:LYS:H	1:B:204:LYS:HD2	1.45	0.80
1:A:168:TRP:H	1:A:183:ASN:HD21	1.29	0.80
1:F:183:ASN:HD22	4:F:1013:DIO:H11	1.46	0.79
1:B:224:LEU:H	1:B:224:LEU:HD12	1.48	0.78
1:C:205:THR:HG21	1:C:208:MET:SD	2.27	0.75
1:A:235:ASN:ND2	1:B:242:ASN:H	1.83	0.75
1:E:270:ILE:H	4:E:1019:DIO:H12	1.52	0.74
1:C:238:GLU:HG2	5:C:1020:HOH:O	1.87	0.72
1:E:235:ASN:ND2	1:F:242:ASN:H	1.86	0.71
1:D:250:ILE:H	1:E:148:GLN:HE22	1.37	0.71
4:D:1012:DIO:H22	1:F:246:TYR:H	1.56	0.71
1:D:204:LYS:HG2	1:D:241:PRO:HG2	1.73	0.70
1:F:204:LYS:HB2	1:F:237:PRO:O	1.91	0.69
1:B:235:ASN:ND2	1:C:242:ASN:H	1.90	0.69
1:B:204:LYS:HB2	1:B:237:PRO:O	1.92	0.69
1:A:144:GLN:NE2	1:B:144:GLN:HE22	1.91	0.68
4:A:1004:DIO:H1'1	5:C:1020:HOH:O	1.93	0.67
1:A:204:LYS:NZ	1:A:241:PRO:HD3	2.10	0.66
1:A:204:LYS:HD2	1:A:238:GLU:O	1.96	0.66
1:A:242:ASN:H	1:C:235:ASN:ND2	1.88	0.66
1:B:204:LYS:HG2	1:B:205:THR:HG23	1.78	0.66
1:D:206:TYR:CD1	1:D:207:ALA:N	2.58	0.66
1:C:231:ARG:HD2	4:C:1006:DIO:H22	1.79	0.65
1:B:204:LYS:HE3	1:B:241:PRO:HG3	1.79	0.64
1:D:235:ASN:ND2	1:E:242:ASN:H	1.93	0.64
1:E:204:LYS:HD2	1:E:238:GLU:O	1.97	0.64
1:C:239:THR:HG22	5:C:1021:HOH:O	1.98	0.63
1:E:204:LYS:HG3	1:E:205:THR:HG23	1.80	0.63
1:E:235:ASN:HD21	1:F:242:ASN:N	1.89	0.63
1:B:250:ILE:H	1:C:148:GLN:HE22	1.46	0.63
1:A:242:ASN:N	1:C:235:ASN:HD21	1.92	0.63
1:A:269:GLN:HA	4:A:1015:DIO:H1'1	1.79	0.62
1:C:205:THR:O	1:C:236:MET:HB2	2.00	0.62
1:D:144:GLN:HE21	1:F:285:LEU:H	1.48	0.61
1:A:204:LYS:HD2	1:A:238:GLU:C	2.20	0.61
1:A:235:ASN:HD21	1:B:242:ASN:N	1.89	0.61
1:E:270:ILE:H	4:E:1019:DIO:C1	2.12	0.61
1:B:224:LEU:N	1:B:224:LEU:HD12	2.16	0.60
1:A:203:ASP:CG	1:A:265:ARG:HH12	2.04	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:H	1:B:144:GLN:HE21	1.48	0.60
1:B:204:LYS:H	1:B:204:LYS:CD	2.13	0.59
1:A:204:LYS:HD2	1:A:238:GLU:HA	1.82	0.59
1:C:165:PHE:CD2	4:C:1007:DIO:H12	2.38	0.58
1:D:235:ASN:HD21	1:E:242:ASN:N	1.96	0.58
1:A:204:LYS:HZ3	1:A:241:PRO:HD3	1.68	0.57
4:F:1020:DIO:H1'1	5:F:423:HOH:O	2.04	0.57
1:C:231:ARG:NH1	4:C:1006:DIO:H22	2.20	0.57
1:D:206:TYR:CZ	1:E:240:LEU:HD13	2.40	0.57
1:D:206:TYR:CE2	1:E:240:LEU:HD13	2.40	0.56
1:E:273:ASP:HB3	1:E:276:VAL:HG12	1.88	0.56
1:D:144:GLN:HE22	1:F:144:GLN:NE2	2.03	0.56
1:A:205:THR:OG1	1:A:265:ARG:NH1	2.39	0.56
1:D:219:VAL:HG13	1:D:223:GLU:HB2	1.89	0.55
1:A:161:GLY:O	1:A:162:SER:HB3	2.05	0.55
1:E:168:TRP:H	1:E:183:ASN:ND2	1.98	0.55
1:A:231:ARG:HH11	1:A:231:ARG:HG3	1.72	0.54
1:A:269:GLN:HA	4:A:1015:DIO:C1'	2.38	0.54
1:E:203:ASP:HB3	1:E:269:GLN:HB2	1.89	0.54
1:A:205:THR:O	1:A:236:MET:HB2	2.08	0.53
1:B:224:LEU:H	1:B:224:LEU:CD1	2.18	0.53
1:B:165:PHE:CD2	4:B:1005:DIO:H1'2	2.43	0.53
1:B:231:ARG:HD2	4:B:1018:DIO:H22	1.90	0.53
1:C:252:LYS:NZ	4:C:1008:DIO:H1'1	2.23	0.53
1:A:203:ASP:CG	1:A:265:ARG:NH1	2.62	0.53
1:B:192:TYR:OH	1:B:252:LYS:HE2	2.09	0.53
1:D:203:ASP:N	1:D:203:ASP:OD1	2.40	0.52
1:B:240:LEU:N	1:B:240:LEU:HD22	2.24	0.52
1:C:240:LEU:N	1:C:241:PRO:HD3	2.24	0.52
1:D:202:THR:HG22	1:D:242:ASN:ND2	2.25	0.52
1:A:204:LYS:HD2	1:A:238:GLU:CA	2.40	0.52
1:D:144:GLN:N	1:F:285:LEU:OXT	2.38	0.51
1:A:144:GLN:NE2	1:B:144:GLN:NE2	2.59	0.51
1:A:143:THR:HG22	1:A:144:GLN:N	2.26	0.51
1:F:204:LYS:HD3	1:F:204:LYS:H	1.76	0.51
1:E:161:GLY:O	1:E:162:SER:HB2	2.11	0.50
1:C:231:ARG:HH11	4:C:1006:DIO:H22	1.75	0.50
1:D:156:PRO:O	1:D:167:PRO:HG2	2.11	0.50
1:B:203:ASP:HB2	1:B:269:GLN:HB2	1.92	0.50
1:F:200:LEU:HD11	1:F:242:ASN:ND2	2.26	0.50
1:C:205:THR:CG2	1:C:208:MET:SD	2.99	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:LEU:N	1:E:241:PRO:HD3	2.26	0.50
1:E:205:THR:HG22	1:E:238:GLU:CD	2.33	0.49
1:A:205:THR:OG1	1:A:265:ARG:CZ	2.60	0.49
1:B:161:GLY:O	1:B:162:SER:HB3	2.13	0.49
1:B:273:ASP:HB2	1:B:276:VAL:HG12	1.94	0.49
1:A:168:TRP:H	1:A:183:ASN:ND2	2.05	0.49
1:C:231:ARG:HD2	4:C:1006:DIO:C2	2.42	0.48
1:B:168:TRP:H	1:B:183:ASN:ND2	2.00	0.48
1:B:144:GLN:HG2	1:B:285:LEU:HG	1.94	0.47
1:B:231:ARG:CG	4:B:1018:DIO:H22	2.45	0.47
1:D:239:THR:HG22	1:D:240:LEU:HG	1.96	0.47
1:E:179:GLU:OE2	1:E:188:LYS:HE3	2.14	0.47
1:B:193:PHE:O	1:B:195:ILE:HD12	2.15	0.47
1:E:188:LYS:HB3	1:E:188:LYS:NZ	2.30	0.47
1:B:195:ILE:N	1:B:195:ILE:HD12	2.30	0.47
1:D:168:TRP:H	1:D:183:ASN:ND2	2.04	0.47
1:A:144:GLN:HE22	1:B:144:GLN:HE22	1.61	0.46
1:D:211:LEU:HD23	1:D:231:ARG:HB2	1.96	0.46
1:E:152:ASP:HB2	1:E:169:LEU:HG	1.97	0.46
1:E:204:LYS:HB3	1:E:241:PRO:CG	2.45	0.46
1:A:270:ILE:H	4:A:1015:DIO:H1'2	1.79	0.46
1:C:192:TYR:HE2	4:C:1008:DIO:H1'2	1.80	0.45
1:D:163:TYR:HD2	1:D:262:ALA:HB1	1.81	0.45
1:C:157:THR:HA	1:C:167:PRO:HD3	1.98	0.45
1:B:163:TYR:HD2	1:B:262:ALA:HB1	1.82	0.45
1:E:212:ILE:HD12	1:E:230:PHE:CE1	2.51	0.45
1:A:204:LYS:HZ1	1:A:241:PRO:HD3	1.82	0.45
1:B:143:THR:O	1:B:285:LEU:HD21	2.17	0.44
1:B:230:PHE:CE2	1:B:249:GLY:HA3	2.53	0.44
1:E:207:ALA:HA	1:E:234:GLN:O	2.17	0.44
1:A:173:LYS:HE3	1:A:179:GLU:HG2	1.99	0.44
1:D:183:ASN:OD1	4:D:1009:DIO:H1'1	2.16	0.44
1:D:144:GLN:HG2	1:D:285:LEU:HG	1.99	0.44
1:E:242:ASN:HA	1:E:242:ASN:HD22	1.56	0.44
1:F:200:LEU:HD11	1:F:242:ASN:HD22	1.82	0.44
1:D:204:LYS:HB2	1:D:204:LYS:HE3	1.79	0.44
1:B:235:ASN:HD21	1:C:242:ASN:N	1.95	0.44
1:F:202:THR:O	1:F:241:PRO:HG2	2.16	0.44
1:A:258:GLU:OE1	4:A:1017:DIO:H22	2.18	0.44
1:C:152:ASP:HB2	1:C:169:LEU:HG	1.99	0.44
1:A:215:LYS:HB3	4:A:1017:DIO:H21	1.99	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASP:CB	1:B:169:LEU:HD12	2.48	0.43
1:C:211:LEU:HD21	4:C:1006:DIO:H21	2.00	0.43
1:B:202:THR:O	1:B:241:PRO:HG2	2.19	0.43
1:B:230:PHE:CZ	1:B:249:GLY:HA3	2.54	0.42
1:E:157:THR:HA	1:E:167:PRO:HD3	2.00	0.42
1:A:246:TYR:H	4:A:1002:DIO:C1	2.32	0.42
1:F:204:LYS:HD3	5:F:379:HOH:O	2.18	0.42
1:B:192:TYR:CZ	1:B:252:LYS:HE2	2.54	0.42
1:B:204:LYS:CD	1:B:204:LYS:N	2.82	0.42
1:A:217:VAL:HA	4:A:1017:DIO:H1'1	2.00	0.42
1:B:200:LEU:HB2	1:B:276:VAL:CG2	2.50	0.42
1:F:206:TYR:CD2	1:F:207:ALA:N	2.81	0.42
1:F:216:LYS:HB3	1:F:216:LYS:HE3	1.93	0.42
1:A:201:TYR:OH	1:A:210:HIS:HB3	2.20	0.42
1:D:161:GLY:O	1:D:162:SER:HB3	2.19	0.41
1:B:152:ASP:HB2	1:B:169:LEU:HD12	2.02	0.41
1:A:242:ASN:ND2	1:C:233:ILE:HD13	2.16	0.41
1:D:207:ALA:HA	1:D:234:GLN:O	2.20	0.41
1:D:148:GLN:O	1:D:171:SER:HB3	2.21	0.41
1:C:161:GLY:O	1:C:162:SER:HB2	2.20	0.41
1:E:206:TYR:CD2	1:E:207:ALA:N	2.80	0.41
1:E:230:PHE:HA	1:F:275:ASP:O	2.20	0.41
1:E:206:TYR:OH	1:F:240:LEU:HB3	2.21	0.41
1:D:205:THR:CG2	1:D:238:GLU:HG2	2.39	0.40
1:E:204:LYS:HB3	1:E:241:PRO:HG2	2.02	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	142/152 (93%)	139 (98%)	3 (2%)	0	100 100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	142/152 (93%)	138 (97%)	3 (2%)	1 (1%)	25	18
1	C	142/152 (93%)	138 (97%)	3 (2%)	1 (1%)	25	18
1	D	142/152 (93%)	139 (98%)	2 (1%)	1 (1%)	25	18
1	E	142/152 (93%)	137 (96%)	4 (3%)	1 (1%)	25	18
1	F	142/152 (93%)	137 (96%)	3 (2%)	2 (1%)	13	6
All	All	852/912 (93%)	828 (97%)	18 (2%)	6 (1%)	25	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	205	THR
1	F	205	THR
1	E	205	THR
1	B	207	ALA
1	C	205	THR
1	F	207	ALA

### 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	126/132 (96%)	124 (98%)	2 (2%)	68	72
1	B	126/132 (96%)	121 (96%)	5 (4%)	36	32
1	C	126/132 (96%)	125 (99%)	1 (1%)	85	88
1	D	126/132 (96%)	119 (94%)	7 (6%)	25	19
1	E	126/132 (96%)	125 (99%)	1 (1%)	85	88
1	F	126/132 (96%)	124 (98%)	2 (2%)	68	72
All	All	756/792 (96%)	738 (98%)	18 (2%)	54	56

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	GLU
1	A	242	ASN
1	B	169	LEU
1	B	204	LYS
1	B	206	TYR
1	B	224	LEU
1	B	266	GLU
1	C	273	ASP
1	D	155	THR
1	D	203	ASP
1	D	204	LYS
1	D	205	THR
1	D	206	TYR
1	D	231	ARG
1	D	242	ASN
1	E	242	ASN
1	F	204	LYS
1	F	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	183	ASN
1	A	235	ASN
1	A	242	ASN
1	B	144	GLN
1	B	183	ASN
1	B	235	ASN
1	C	148	GLN
1	C	235	ASN
1	C	260	GLN
1	D	144	GLN
1	D	183	ASN
1	D	235	ASN
1	D	242	ASN
1	E	148	GLN
1	E	183	ASN
1	E	235	ASN
1	E	242	ASN
1	F	144	GLN
1	F	210	HIS
1	F	242	ASN

### 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 29 ligands modelled in this entry, 7 are monoatomic - leaving 22 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	$\# Z  > 2$
4	DIO	A	1001	-	6,6,6	0.90	0	6,6,6	0.88	0
4	DIO	A	1002	-	6,6,6	0.86	0	6,6,6	0.91	0
4	DIO	A	1004	-	6,6,6	0.74	0	6,6,6	0.96	0
4	DIO	A	1015	-	6,6,6	0.82	0	6,6,6	0.93	0
4	DIO	A	1017	-	6,6,6	0.84	0	6,6,6	0.91	0
3	CIT	A	889	2	3,12,12	2.22	1 (33%)	3,17,17	1.89	1 (33%)
4	DIO	B	1005	-	6,6,6	0.84	0	6,6,6	0.89	0
4	DIO	B	1018	-	6,6,6	0.85	0	6,6,6	0.91	0
4	DIO	C	1003	-	6,6,6	0.81	0	6,6,6	0.93	0
4	DIO	C	1006	-	6,6,6	0.85	0	6,6,6	0.89	0
4	DIO	C	1007	-	6,6,6	0.84	0	6,6,6	0.87	0
4	DIO	C	1008	-	6,6,6	0.82	0	6,6,6	0.92	0
4	DIO	C	1014	-	6,6,6	0.84	0	6,6,6	0.93	0
4	DIO	C	1016	-	6,6,6	0.82	0	6,6,6	0.95	0
4	DIO	D	1009	-	6,6,6	0.89	0	6,6,6	0.87	0
4	DIO	D	1012	-	6,6,6	0.86	0	6,6,6	0.91	0
4	DIO	E	1010	-	6,6,6	0.80	0	6,6,6	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DIO	E	1011	-	6,6,6	0.86	0	6,6,6	0.92	0
4	DIO	E	1019	-	6,6,6	0.83	0	6,6,6	0.90	0
4	DIO	F	1013	-	6,6,6	0.90	0	6,6,6	0.84	0
4	DIO	F	1020	-	6,6,6	0.81	0	6,6,6	0.96	0
3	CIT	F	888	2	3,12,12	1.84	1 (33%)	3,17,17	1.73	1 (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
4	DIO	A	1001	-	-	0/0/6/6	0/1/1/1
4	DIO	A	1002	-	-	0/0/6/6	0/1/1/1
4	DIO	A	1004	-	-	0/0/6/6	0/1/1/1
4	DIO	A	1015	-	-	0/0/6/6	0/1/1/1
4	DIO	A	1017	-	-	0/0/6/6	0/1/1/1
3	CIT	A	889	2	-	0/6/16/16	0/0/0/0
4	DIO	B	1005	-	-	0/0/6/6	0/1/1/1
4	DIO	B	1018	-	-	0/0/6/6	0/1/1/1
4	DIO	C	1003	-	-	0/0/6/6	0/1/1/1
4	DIO	C	1006	-	-	0/0/6/6	0/1/1/1
4	DIO	C	1007	-	-	0/0/6/6	0/1/1/1
4	DIO	C	1008	-	-	0/0/6/6	0/1/1/1
4	DIO	C	1014	-	-	0/0/6/6	0/1/1/1
4	DIO	C	1016	-	-	0/0/6/6	0/1/1/1
4	DIO	D	1009	-	-	0/0/6/6	0/1/1/1
4	DIO	D	1012	-	-	0/0/6/6	0/1/1/1
4	DIO	E	1010	-	-	0/0/6/6	0/1/1/1
4	DIO	E	1011	-	-	0/0/6/6	0/1/1/1
4	DIO	E	1019	-	-	0/0/6/6	0/1/1/1
4	DIO	F	1013	-	-	0/0/6/6	0/1/1/1
4	DIO	F	1020	-	-	0/0/6/6	0/1/1/1
3	CIT	F	888	2	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	888	CIT	O7-C3	3.08	1.47	1.43
3	A	889	CIT	O7-C3	3.33	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	888	CIT	C3-C2-C1	2.98	119.61	114.95
3	A	889	CIT	C3-C2-C1	3.09	119.78	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	DIO	1	0
4	A	1004	DIO	1	0
4	A	1015	DIO	3	0
4	A	1017	DIO	3	0
4	B	1005	DIO	1	0
4	B	1018	DIO	2	0
4	C	1006	DIO	5	0
4	C	1007	DIO	1	0
4	C	1008	DIO	2	0
4	D	1009	DIO	1	0
4	D	1012	DIO	1	0
4	E	1019	DIO	3	0
4	F	1013	DIO	1	0
4	F	1020	DIO	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(Å²)	Q<0.9
1	A	144/152 (94%)	-0.14	6 (4%)	37	37	17, 25, 47, 58	0
1	B	144/152 (94%)	0.03	7 (4%)	30	30	18, 31, 49, 63	0
1	C	144/152 (94%)	-0.24	4 (2%)	53	53	17, 28, 48, 58	0
1	D	144/152 (94%)	-0.07	10 (6%)	18	18	16, 27, 56, 69	0
1	E	144/152 (94%)	-0.17	4 (2%)	53	53	16, 28, 49, 62	0
1	F	144/152 (94%)	-0.23	5 (3%)	44	45	16, 24, 43, 61	0
All	All	864/912 (94%)	-0.14	36 (4%)	37	37	16, 27, 49, 69	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	206	TYR	7.7
1	F	205	THR	6.8
1	B	206	TYR	6.1
1	B	205	THR	6.1
1	E	206	TYR	6.0
1	A	206	TYR	5.9
1	E	205	THR	5.8
1	C	206	TYR	5.7
1	F	206	TYR	5.4
1	D	205	THR	5.1
1	C	142	VAL	4.3
1	D	142	VAL	4.0
1	B	142	VAL	3.9
1	A	142	VAL	3.6
1	E	161	GLY	3.5
1	D	218	HIS	3.3
1	C	205	THR	3.2
1	D	221	GLY	3.2
1	D	220	PHE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	222	ASP	3.1
1	B	238	GLU	3.0
1	F	204	LYS	2.9
1	B	285	LEU	2.8
1	E	142	VAL	2.7
1	D	285	LEU	2.7
1	F	238	GLU	2.6
1	F	142	VAL	2.4
1	D	204	LYS	2.3
1	D	224	LEU	2.3
1	A	205	THR	2.2
1	A	238	GLU	2.2
1	B	224	LEU	2.1
1	A	154	GLU	2.1
1	B	154	GLU	2.1
1	C	238	GLU	2.0
1	A	161	GLY	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. 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
4	DIO	A	1017	6/6	0.85	0.26	9.17	57,58,58,59	0
4	DIO	D	1012	6/6	0.88	0.41	8.07	56,57,57,57	0
4	DIO	A	1002	6/6	0.84	0.37	6.50	54,54,55,55	0
4	DIO	A	1015	6/6	0.79	0.29	5.96	63,64,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DIO	E	1010	6/6	0.87	0.29	5.13	52,52,53,54	0
4	DIO	C	1008	6/6	0.82	0.15	4.58	65,66,67,67	0
4	DIO	C	1006	6/6	0.89	0.20	4.21	59,59,59,59	0
4	DIO	B	1018	6/6	0.81	0.20	4.07	66,66,67,67	0
4	DIO	C	1003	6/6	0.96	0.21	3.32	44,44,45,46	0
3	CIT	A	889	13/13	0.88	0.13	3.23	29,33,37,38	0
3	CIT	F	888	13/13	0.85	0.14	3.18	33,37,40,41	0
4	DIO	A	1001	6/6	0.93	0.15	0.77	35,36,36,37	0
4	DIO	F	1020	6/6	0.88	0.21	0.50	61,61,62,62	0
2	MG	D	801	1/1	0.99	0.09	0.39	29,29,29,29	0
4	DIO	F	1013	6/6	0.91	0.11	0.10	29,32,33,34	0
4	DIO	D	1009	6/6	0.91	0.10	-0.03	34,36,36,39	0
4	DIO	C	1007	6/6	0.92	0.11	-0.05	40,41,41,42	0
4	DIO	B	1005	6/6	0.94	0.07	-0.96	47,47,48,48	0
4	DIO	E	1011	6/6	0.94	0.07	-1.05	38,40,40,40	0
2	MG	B	702	1/1	0.98	0.05	-4.86	31,31,31,31	0
2	MG	D	802	1/1	0.99	0.06	-5.92	28,28,28,28	0
2	MG	A	701	1/1	0.99	0.05	-12.86	27,27,27,27	0
2	MG	A	903	1/1	0.99	0.08	-	41,41,41,41	0
4	DIO	E	1019	6/6	0.85	0.23	-	60,61,61,62	0
2	MG	A	901	1/1	0.93	0.20	-	47,47,47,47	0
4	DIO	A	1004	6/6	0.85	0.31	-	64,64,64,65	0
4	DIO	C	1016	6/6	0.70	0.31	-	68,68,69,70	0
2	MG	F	902	1/1	0.98	0.08	-	43,43,43,43	0
4	DIO	C	1014	6/6	0.79	0.21	-	65,65,66,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.