



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:09 PM BST

PDB ID : 6PC0  
Title : Crystal structure of Helicobacter pylori PPX/GppA  
Authors : Song, H.; Wang, C.; Shaw, G.X.; Ji, X.  
Deposited on : 2019-06-15  
Resolution : 1.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

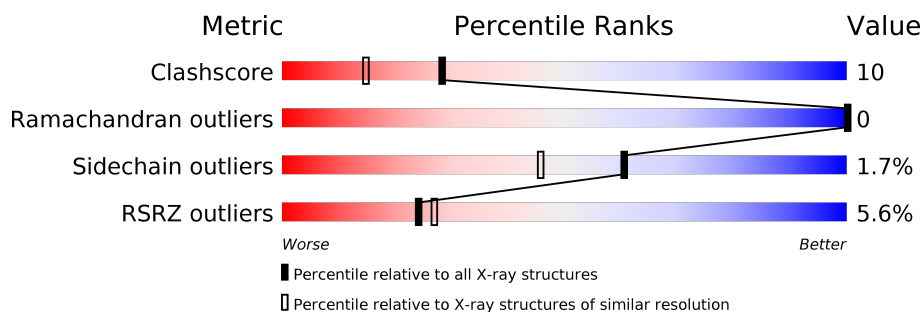
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	
1	B	495	

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
2	SO4	A	509	-	-	X	-
4	MLT	A	514	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MLT	A	515	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8756 atoms, of which 76 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.

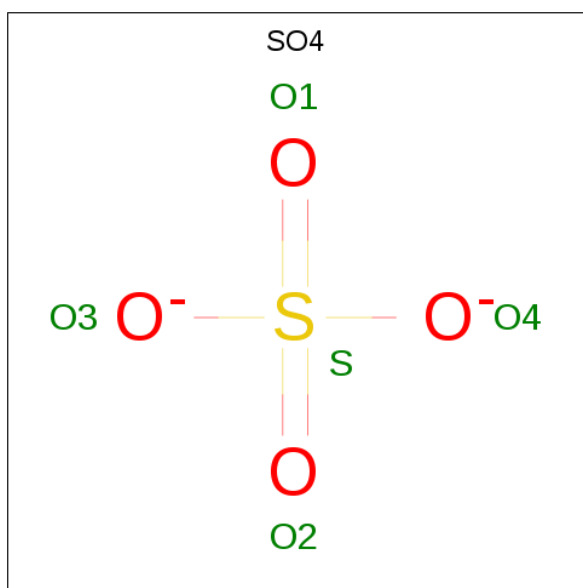
- Molecule 1 is a protein called Guanosine pentaphosphate phosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	14	0
			3860	2506	661	672	21			
1	B	484	Total	C	N	O	S	0	21	0
			3962	2562	676	700	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP B5ZA44
A	-9	ARG	-	expression tag	UNP B5ZA44
A	-8	GLY	-	expression tag	UNP B5ZA44
A	-7	SER	-	expression tag	UNP B5ZA44
A	-6	HIS	-	expression tag	UNP B5ZA44
A	-5	HIS	-	expression tag	UNP B5ZA44
A	-4	HIS	-	expression tag	UNP B5ZA44
A	-3	HIS	-	expression tag	UNP B5ZA44
A	-2	HIS	-	expression tag	UNP B5ZA44
A	-1	HIS	-	expression tag	UNP B5ZA44
A	0	GLY	-	expression tag	UNP B5ZA44
A	1	SER	-	expression tag	UNP B5ZA44
B	-10	MET	-	initiating methionine	UNP B5ZA44
B	-9	ARG	-	expression tag	UNP B5ZA44
B	-8	GLY	-	expression tag	UNP B5ZA44
B	-7	SER	-	expression tag	UNP B5ZA44
B	-6	HIS	-	expression tag	UNP B5ZA44
B	-5	HIS	-	expression tag	UNP B5ZA44
B	-4	HIS	-	expression tag	UNP B5ZA44
B	-3	HIS	-	expression tag	UNP B5ZA44
B	-2	HIS	-	expression tag	UNP B5ZA44
B	-1	HIS	-	expression tag	UNP B5ZA44
B	0	GLY	-	expression tag	UNP B5ZA44
B	1	SER	-	expression tag	UNP B5ZA44

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



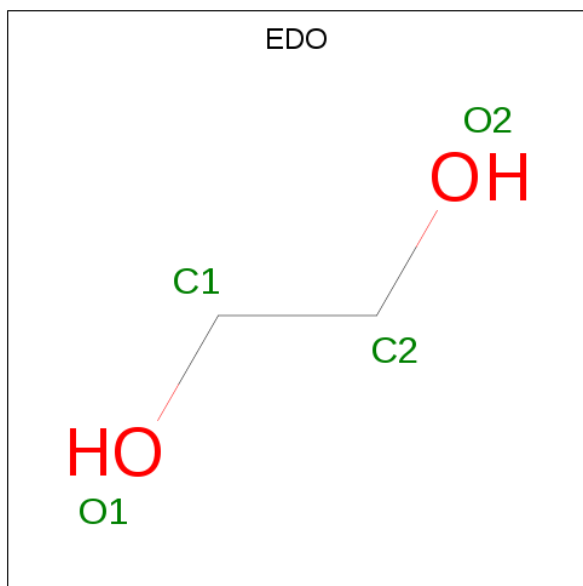
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



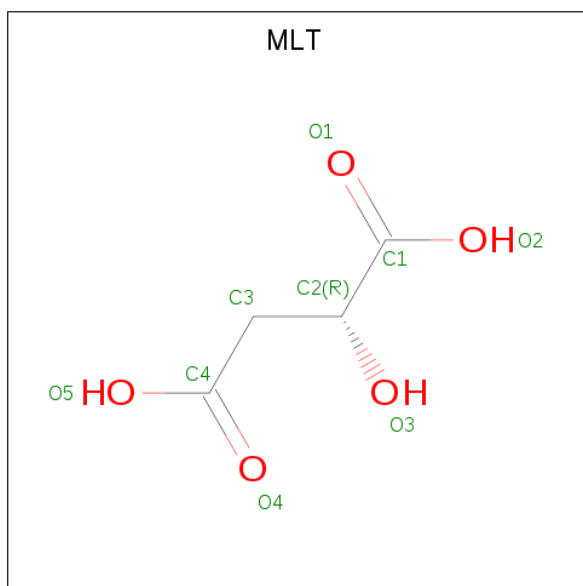
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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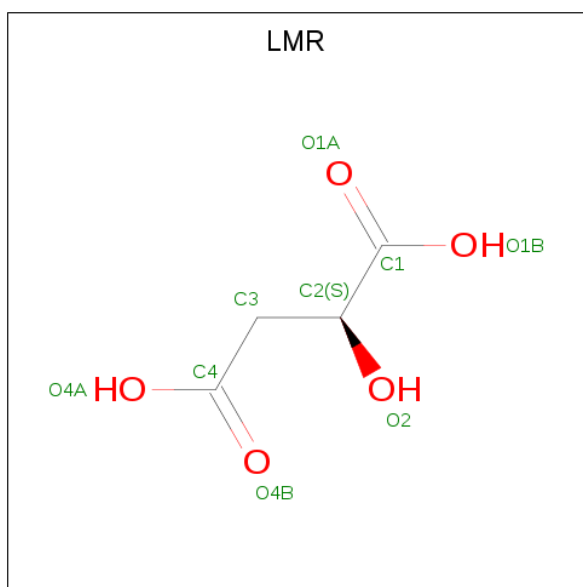
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	1
			20	4	12	4		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			13	4	4	5		
4	A	1	Total	C	H	O	0	0
			13	4	4	5		

- Molecule 5 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			13	4	4	5		
5	B	1	Total	C	H	O	0	0
			13	4	4	5		

- Molecule 6 is water.

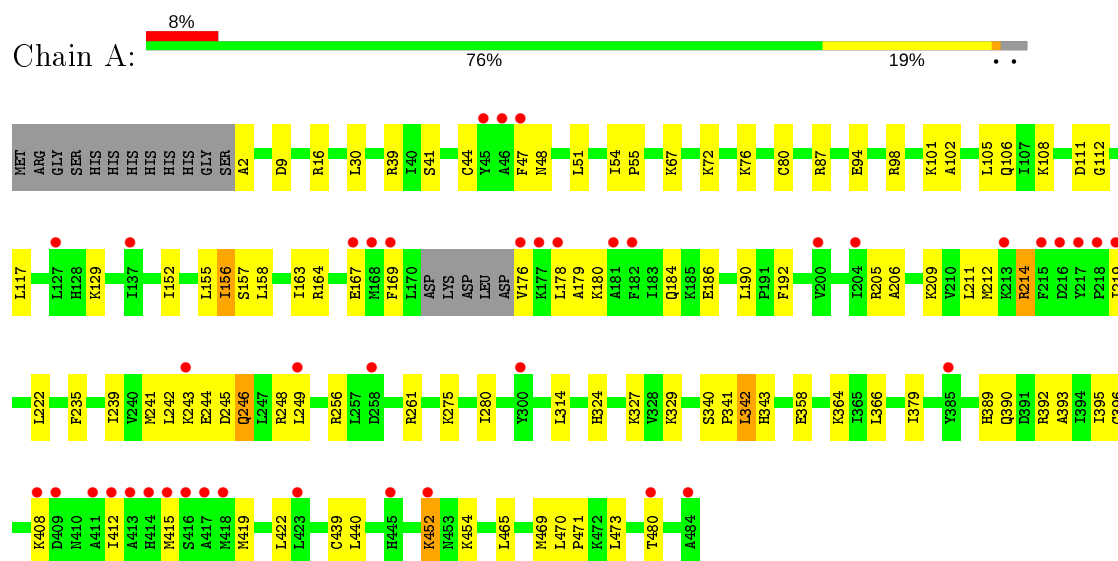
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	290	Total	O	0	1
			290	290		
6	B	382	Total	O	0	1
			382	382		



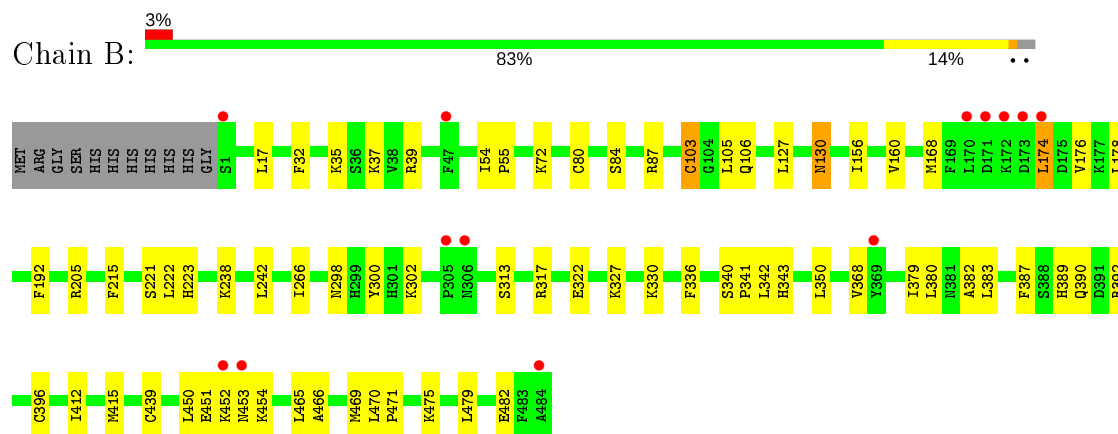
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Guanosine pentaphosphate phosphohydrolase



- Molecule 1: Guanosine pentaphosphate phosphohydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.36Å 129.46Å 166.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 1.70 39.68 – 1.69	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.11-1.70) 98.7 (39.68-1.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.70Å)	Xtriage
Refinement program	PHENIX (dev_3352: ???)	Depositor
R, $R_{free}$	0.189 , 0.212 0.189 , (Not available)	Depositor DCC
$R_{free}$ test set	1000 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, SO4, MLT, EDO

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	0.37	0/3955	0.55	0/5312
1	B	0.40	0/4048	0.61	0/5436
All	All	0.38	0/8003	0.58	0/10748

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3860	0	4094	97	0
1	B	3962	0	4177	65	0
2	A	55	0	0	2	0
2	B	55	0	0	2	0
3	A	8	12	12	4	0
3	B	32	48	48	8	0
4	A	18	8	8	9	0
5	B	18	8	8	2	0
6	A	290	0	0	12	0
6	B	382	0	0	12	0
All	All	8680	76	8347	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 10.

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:256:ARG:HH22	4:A:515:MLT:H2	1.14	1.11
1:B:342:LEU:HD13	1:B:450:LEU:HD21	1.40	1.02
1:A:256:ARG:HH22	4:A:515:MLT:C2	1.79	0.95
1:A:256:ARG:NH2	4:A:515:MLT:H2	1.92	0.85
1:A:212:MET:HE1	1:A:222:LEU:HD13	1.63	0.81
1:B:168[B]:MET:SD	6:B:978:HOH:O	2.40	0.78
1:B:342:LEU:CD1	1:B:450:LEU:HD21	2.14	0.78
1:B:238:LYS:HE2	1:B:242:LEU:HD21	1.65	0.78
1:B:223:HIS:H	5:B:520:LMR:H3A	1.49	0.76
1:A:156:ILE:HG21	1:A:190:LEU:HD23	1.69	0.73
2:A:509:SO4:S	6:A:602:HOH:O	2.47	0.72
1:A:156:ILE:HD13	1:A:157:SER:N	2.05	0.71
1:A:212:MET:CE	1:A:222:LEU:HD13	2.20	0.71
1:B:452:LYS:HG3	1:B:453:ASN:H	1.56	0.69
1:A:156:ILE:CD1	1:A:158:LEU:HD23	2.22	0.68
1:A:241:MET:HB2	6:A:667:HOH:O	1.91	0.68
1:B:470:LEU:HB3	1:B:471:PRO:HD3	1.76	0.68
1:B:390:GLN:HA	1:B:415[B]:MET:HE1	1.75	0.66
1:B:452:LYS:HG3	1:B:453:ASN:N	2.10	0.66
1:A:156:ILE:HG21	1:A:190:LEU:CD2	2.27	0.64
1:A:44[B]:CYS:SG	1:A:51:LEU:HD23	2.38	0.64
1:A:209:LYS:HG2	1:A:222:LEU:HD11	1.79	0.64
1:A:275:LYS:HE3	6:A:803:HOH:O	1.99	0.63
1:B:313[B]:SER:O	1:B:317[B]:ARG:HG3	1.99	0.62
1:A:470:LEU:HB3	1:A:471:PRO:HD3	1.82	0.62
1:B:205:ARG:HG3	1:B:222:LEU:HD13	1.82	0.62
1:B:466:ALA:HA	1:B:469:MET:HE2	1.81	0.61
1:B:35:LYS:HE3	2:B:509:SO4:O3	2.00	0.61
1:A:156:ILE:HD11	1:A:158:LEU:HD23	1.84	0.60
1:B:452:LYS:CG	1:B:453:ASN:H	2.14	0.60
1:A:80[B]:CYS:SG	1:A:105[B]:LEU:HG	2.43	0.59
1:A:39:ARG:NH1	6:A:611:HOH:O	2.35	0.59
1:B:342:LEU:HD13	1:B:450:LEU:CD2	2.26	0.59
1:A:205:ARG:O	1:A:209:LYS:HG3	2.03	0.59
1:A:245:ASP:O	1:A:249:LEU:HG	2.02	0.59
1:B:454:LYS:HD2	1:B:482:GLU:CD	2.24	0.58
1:B:390:GLN:HA	1:B:415[B]:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.68	0.58
1:A:219:ILE:HD12	1:A:389:HIS:HB3	1.86	0.58
1:A:340:SER:OG	1:A:341:PRO:HD3	2.03	0.57
1:B:223:HIS:H	5:B:520:LMR:C3	2.18	0.57
1:A:214:ARG:NH2	6:A:616:HOH:O	2.37	0.57
1:B:465:LEU:O	1:B:469:MET:HG3	2.05	0.57
1:B:160[A]:VAL:HG22	1:B:266:ILE:CD1	2.35	0.57
1:A:340:SER:HA	1:A:343:HIS:CE1	2.40	0.57
1:B:205:ARG:HD3	6:B:643:HOH:O	2.05	0.56
1:A:169:PHE:HE1	1:A:178:LEU:HG	1.72	0.55
1:A:324[B]:HIS:CE1	1:B:72:LYS:HG2	2.41	0.55
1:A:102:ALA:HB2	3:A:513:EDO:H11	1.89	0.55
1:A:16:ARG:HD3	4:A:515:MLT:O2	2.07	0.55
1:A:180:LYS:O	1:A:184:GLN:HG3	2.08	0.54
1:A:393:ALA:HB1	1:A:412:ILE:CG2	2.37	0.54
1:A:2:ALA:HB1	1:A:76:LYS:HB2	1.89	0.54
1:A:379:ILE:HG22	1:A:396[B]:CYS:SG	2.48	0.54
1:A:156:ILE:HD12	1:A:158:LEU:CD2	2.38	0.54
1:B:215:PHE:HB3	3:B:517:EDO:H12	1.90	0.54
1:B:340:SER:HA	1:B:343:HIS:CE1	2.44	0.53
1:B:54:ILE:HB	1:B:55:PRO:HD3	1.90	0.53
1:B:380:LEU:HB2	1:B:396[B]:CYS:SG	2.49	0.53
1:A:47:PHE:O	1:A:48:ASN:HB2	2.09	0.52
1:A:206:ALA:HB2	1:A:256:ARG:CD	2.40	0.52
1:B:327:LYS:HG3	1:B:439:CYS:SG	2.50	0.52
1:A:9:ASP:OD1	1:A:16:ARG:HB2	2.10	0.52
1:B:176:VAL:HG23	6:B:776:HOH:O	2.09	0.52
1:B:466:ALA:HA	1:B:469:MET:CE	2.40	0.51
1:A:256:ARG:HG3	1:A:256:ARG:NH1	2.26	0.51
1:A:106[A]:GLN:HG3	6:A:617:HOH:O	2.11	0.51
1:A:211:LEU:HD21	1:A:235:PHE:HD2	1.74	0.51
1:A:324[B]:HIS:HD2	4:A:514:MLT:C3	2.25	0.50
1:B:300:TYR:HB2	6:B:698:HOH:O	2.11	0.50
1:A:261:ARG:HB2	6:A:625:HOH:O	2.10	0.50
1:A:244:GLU:O	1:A:248:ARG:HG3	2.12	0.50
1:A:206:ALA:HB2	1:A:256:ARG:HD2	1.94	0.49
1:A:324[A]:HIS:HB3	4:A:514:MLT:H31	1.93	0.49
1:B:379:ILE:HG22	1:B:396[B]:CYS:SG	2.53	0.49
1:B:383:LEU:HG	1:B:387:PHE:CD2	2.48	0.49
1:A:390:GLN:HG3	1:A:419:MET:SD	2.53	0.49
1:A:41:SER:O	1:A:44[B]:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HB3	1:B:178:LEU:HD12	1.95	0.48
1:B:80[B]:CYS:SG	1:B:105:LEU:HD22	2.54	0.48
1:A:452:LYS:HB2	1:A:452:LYS:HE3	1.39	0.48
1:A:245:ASP:HA	1:A:248:ARG:NH1	2.29	0.48
1:A:465:LEU:O	1:A:469:MET:HG3	2.14	0.48
1:A:48:ASN:HB3	6:A:687:HOH:O	2.13	0.48
1:A:72[A]:LYS:HD3	6:B:681:HOH:O	2.12	0.47
1:B:451:GLU:O	1:B:452:LYS:HG2	2.14	0.47
1:B:106:GLN:NE2	6:B:623:HOH:O	2.47	0.47
1:A:169:PHE:CG	1:A:179:ALA:HB2	2.49	0.47
1:A:364:LYS:HD2	4:A:514:MLT:O2	2.15	0.47
1:B:392:ARG:NH2	6:B:608:HOH:O	2.40	0.47
1:A:379:ILE:HD13	1:A:395:ILE:HG22	1.95	0.47
1:A:239:ILE:HA	1:A:242:LEU:HG	1.97	0.47
1:A:163:ILE:O	1:A:167:GLU:HG2	2.14	0.47
1:A:256:ARG:HH22	4:A:515:MLT:C1	2.28	0.47
1:B:451:GLU:O	1:B:452:LYS:CG	2.63	0.47
1:A:30:LEU:O	1:B:368:VAL:HG13	2.15	0.47
1:B:37:LYS:HE3	1:B:39:ARG:NH2	2.29	0.47
1:A:54:ILE:HB	1:A:55:PRO:HD3	1.96	0.46
3:B:517:EDO:O1	6:B:601:HOH:O	2.20	0.46
1:A:80[B]:CYS:SG	1:A:105[B]:LEU:CG	3.04	0.46
1:B:302:LYS:HG3	6:B:812:HOH:O	2.15	0.46
1:A:72[A]:LYS:HE2	1:B:439:CYS:O	2.16	0.46
1:A:87:ARG:CD	1:A:111:ASP:HA	2.46	0.46
1:A:156:ILE:CD1	1:A:158:LEU:CD2	2.90	0.46
1:A:112:GLY:HA3	3:A:512:EDO:H12	1.96	0.46
1:A:454:LYS:HG3	1:A:480:THR:HG22	1.98	0.46
1:B:336:PHE:CD1	1:B:350[B]:LEU:HD21	2.51	0.45
1:A:108:LYS:HE2	1:A:108:LYS:HB2	1.69	0.45
1:A:117:LEU:HD12	1:A:152:ILE:HD13	1.98	0.45
1:B:174:LEU:CD1	1:B:174:LEU:N	2.79	0.45
1:A:327:LYS:HG3	1:A:439:CYS:SG	2.57	0.45
1:A:67:LYS:HD3	1:A:105[A]:LEU:CD2	2.47	0.45
1:B:103[B]:CYS:HA	6:B:928:HOH:O	2.16	0.45
1:B:412:ILE:HD13	6:B:897:HOH:O	2.17	0.45
1:A:212:MET:HE2	1:A:212:MET:HB2	1.75	0.44
1:A:243:LYS:O	1:A:246:GLN:HG3	2.17	0.44
1:A:329:LYS:HD3	1:A:358:GLU:HG3	1.98	0.44
1:A:366:LEU:CD1	1:B:382:ALA:HB2	2.48	0.44
1:B:205:ARG:CG	1:B:222:LEU:HD13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:OE1	6:A:601:HOH:O	2.21	0.44
1:B:383:LEU:O	1:B:392:ARG:HD3	2.17	0.44
1:A:152:ILE:HG21	1:A:155:LEU:HD21	2.00	0.44
1:A:169:PHE:CB	1:A:179:ALA:HB2	2.48	0.43
1:B:452:LYS:HE2	1:B:453:ASN:HB3	2.01	0.43
1:A:440:LEU:HD11	1:B:32:PHE:HZ	1.83	0.43
1:B:174:LEU:HD21	3:B:518:EDO:H12	1.98	0.43
1:A:342:LEU:HA	1:A:342:LEU:HD12	1.77	0.43
1:A:106[A]:GLN:NE2	6:A:617:HOH:O	2.37	0.43
1:A:129:LYS:HD2	1:A:280:ILE:HD11	2.00	0.43
1:A:98[A]:ARG:HG2	3:A:513:EDO:H12	2.00	0.43
1:A:180:LYS:HG2	1:A:184:GLN:OE1	2.19	0.42
1:A:101:LYS:HB3	3:A:513:EDO:O1	2.18	0.42
1:B:127:LEU:HD23	1:B:223:HIS:CE1	2.54	0.42
1:B:174:LEU:HD23	3:B:518:EDO:H11	1.99	0.42
1:A:94:GLU:O	1:A:98[B]:ARG:HG3	2.19	0.42
3:B:517:EDO:O2	6:B:602:HOH:O	2.22	0.42
1:B:17:LEU:C	1:B:17:LEU:HD23	2.40	0.42
1:A:169:PHE:CE1	1:A:179:ALA:HA	2.55	0.42
1:A:408:LYS:HG2	1:A:422:LEU:CD2	2.50	0.42
1:B:84:SER:HA	1:B:87:ARG:HG2	2.01	0.42
1:A:156:ILE:HD13	1:A:157:SER:C	2.40	0.42
1:B:340:SER:OG	1:B:341:PRO:HD3	2.20	0.41
1:A:324[B]:HIS:HB2	4:A:514:MLT:H31	2.01	0.41
1:A:392:ARG:NH2	6:A:641:HOH:O	2.53	0.41
1:A:324[B]:HIS:NE2	1:B:72:LYS:HG2	2.36	0.41
1:B:130:ASN:C	1:B:130:ASN:HD22	2.23	0.41
1:B:221:SER:O	1:B:389:HIS:CE1	2.74	0.41
1:B:475:LYS:HZ1	3:B:512:EDO:H21	1.86	0.41
1:B:453:ASN:O	1:B:479:LEU:HD12	2.20	0.41
1:B:453:ASN:HB2	3:B:515:EDO:O2	2.20	0.41
1:A:389:HIS:HB3	1:A:415:MET:HE1	2.03	0.41
2:A:509:SO4:O4	6:A:602:HOH:O	2.21	0.41
1:A:393:ALA:HB1	1:A:412:ILE:HG22	2.03	0.41
1:A:454:LYS:HG3	1:A:480:THR:CG2	2.51	0.41
1:B:156:ILE:HG23	3:B:513:EDO:H12	2.03	0.41
1:B:330:LYS:NZ	2:B:508:SO4:O1	2.32	0.40
1:A:156:ILE:C	1:A:156:ILE:HD13	2.42	0.40
1:A:87:ARG:HD3	1:A:111:ASP:HA	2.03	0.40
1:A:164[B]:ARG:HD2	1:A:164[B]:ARG:HA	1.84	0.40
1:A:470:LEU:HD12	1:A:473:LEU:HD12	2.04	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	488/495 (99%)	476 (98%)	12 (2%)	0	100	100
1	B	504/495 (102%)	494 (98%)	10 (2%)	0	100	100
All	All	992/990 (100%)	970 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/430 (100%)	421 (98%)	8 (2%)	57	41
1	B	442/430 (103%)	435 (98%)	7 (2%)	62	48
All	All	871/860 (101%)	856 (98%)	15 (2%)	60	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ILE
1	A	176	VAL
1	A	192	PHE
1	A	214	ARG
1	A	246	GLN

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Mol	Chain	Res	Type
1	A	314	LEU
1	A	342	LEU
1	A	452	LYS
1	B	103[A]	CYS
1	B	103[B]	CYS
1	B	130	ASN
1	B	174	LEU
1	B	192	PHE
1	B	298	ASN
1	B	322	GLU

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

Mol	Chain	Res	Type
1	B	130	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

36 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	SO4	B	504	-	4,4,4	0.16	0	6,6,6	0.12	0
4	MLT	A	514	-	2,8,8	0.45	0	3,10,10	1.44	1 (33%)
2	SO4	B	509	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	507	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	A	508	-	4,4,4	0.17	0	6,6,6	0.10	0
5	LMR	B	519	-	2,8,8	0.29	0	3,10,10	0.88	0
3	EDO	B	515	-	3,3,3	0.45	0	2,2,2	0.37	0
2	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	B	506	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	510	-	4,4,4	0.19	0	6,6,6	0.36	0
2	SO4	B	505	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	B	514	-	3,3,3	0.42	0	2,2,2	0.33	0
5	LMR	B	520	-	2,8,8	0.09	0	3,10,10	0.67	0
2	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.10	0
3	EDO	B	512	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	B	513	-	3,3,3	0.50	0	2,2,2	0.38	0
2	SO4	A	509	-	4,4,4	0.11	0	6,6,6	0.23	0
3	EDO	B	518	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	B	517	-	3,3,3	0.52	0	2,2,2	0.16	0
2	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.08	0
4	MLT	A	515	-	2,8,8	0.36	0	3,10,10	0.96	0
3	EDO	A	512	-	3,3,3	0.50	0	2,2,2	0.15	0
3	EDO	B	516[A]	-	3,3,3	0.49	0	2,2,2	0.26	0
2	SO4	B	510	-	4,4,4	0.20	0	6,6,6	0.32	0
2	SO4	A	503	-	4,4,4	0.16	0	6,6,6	0.13	0
3	EDO	B	516[B]	-	3,3,3	0.48	0	2,2,2	0.17	0
2	SO4	B	511	-	4,4,4	0.25	0	6,6,6	0.42	0
2	SO4	A	507	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.23	0
3	EDO	A	513	-	3,3,3	0.44	0	2,2,2	0.33	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	511	-	4,4,4	0.12	0	6,6,6	0.27	0
2	SO4	A	502	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	B	508	-	4,4,4	0.15	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	516[B]	-	-	1/1/1/1	-
5	LMR	B	519	-	-	0/2/8/8	-
3	EDO	B	515	-	-	0/1/1/1	-
4	MLT	A	514	-	-	2/2/8/8	-
3	EDO	B	513	-	-	0/1/1/1	-
3	EDO	B	518	-	-	1/1/1/1	-
3	EDO	B	517	-	-	1/1/1/1	-
3	EDO	B	512	-	-	1/1/1/1	-
4	MLT	A	515	-	-	2/2/8/8	-
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
3	EDO	B	514	-	-	0/1/1/1	-
3	EDO	B	516[A]	-	-	1/1/1/1	-
5	LMR	B	520	-	-	2/2/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	514	MLT	C3-C2-C1	-2.45	107.98	111.10

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	514	MLT	O3-C2-C3-C4
5	B	520	LMR	O2-C2-C3-C4
4	A	515	MLT	C1-C2-C3-C4
4	A	515	MLT	O3-C2-C3-C4
3	B	516[B]	EDO	O1-C1-C2-O2
3	B	512	EDO	O1-C1-C2-O2
3	B	518	EDO	O1-C1-C2-O2
3	B	517	EDO	O1-C1-C2-O2
3	B	516[A]	EDO	O1-C1-C2-O2
4	A	514	MLT	C1-C2-C3-C4
5	B	520	LMR	C1-C2-C3-C4
3	A	513	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	514	MLT	4	0
2	B	509	SO4	1	0
3	B	515	EDO	1	0
5	B	520	LMR	2	0
3	B	512	EDO	1	0
3	B	513	EDO	1	0
2	A	509	SO4	2	0
3	B	518	EDO	2	0
3	B	517	EDO	3	0
4	A	515	MLT	5	0
3	A	512	EDO	1	0
3	A	513	EDO	3	0
2	B	508	SO4	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	478/495 (96%)	0.46	41 (8%) 10 12	23, 37, 67, 82	0
1	B	484/495 (97%)	-0.02	13 (2%) 54 58	21, 30, 51, 74	0
All	All	962/990 (97%)	0.22	54 (5%) 24 27	21, 33, 61, 82	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	5.4
1	A	45[A]	TYR	5.2
1	A	300	TYR	4.7
1	A	215	PHE	4.5
1	A	418	MET	4.2
1	A	484	ALA	4.2
1	A	169	PHE	4.1
1	B	171	ASP	4.0
1	B	173	ASP	4.0
1	A	46	ALA	3.9
1	B	484	ALA	3.9
1	A	176	VAL	3.7
1	A	213	LYS	3.6
1	A	216	ASP	3.6
1	A	219	ILE	3.5
1	A	409	ASP	3.4
1	A	249	LEU	3.4
1	A	408	LYS	3.3
1	A	417	ALA	3.3
1	A	414	HIS	3.2
1	A	258	ASP	3.2
1	B	452	LYS	3.1
1	B	369	TYR	3.1
1	A	167	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	47	PHE	3.0
1	A	412	ILE	2.9
1	A	415	MET	2.9
1	B	305	PRO	2.8
1	A	243	LYS	2.8
1	A	452	LYS	2.8
1	A	182	PHE	2.7
1	A	445	HIS	2.7
1	A	181	ALA	2.6
1	B	174	LEU	2.6
1	A	217	TYR	2.6
1	A	177	LYS	2.5
1	B	47	PHE	2.5
1	A	204	ILE	2.5
1	A	416	SER	2.4
1	B	1	SER	2.4
1	A	218	PRO	2.4
1	A	168	MET	2.3
1	A	411	ALA	2.3
1	A	200	VAL	2.3
1	B	172	LYS	2.3
1	B	170	LEU	2.3
1	A	385	TYR	2.3
1	A	413	ALA	2.3
1	B	453	ASN	2.1
1	A	137	ILE	2.1
1	A	423	LEU	2.1
1	B	306	ASN	2.1
1	A	480	THR	2.0
1	A	127	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	B	513	4/4	0.78	0.17	36,57,68,68	0
3	EDO	B	516[A]	4/4	0.78	0.34	34,43,52,52	10
3	EDO	B	516[B]	4/4	0.78	0.34	32,43,51,52	10
3	EDO	B	515	4/4	0.80	0.17	50,67,71,83	0
2	SO4	A	507	5/5	0.80	0.24	88,91,112,113	0
2	SO4	A	508	5/5	0.81	0.28	58,72,84,105	0
2	SO4	B	507	5/5	0.81	0.20	75,80,108,112	0
3	EDO	B	517	4/4	0.82	0.24	43,54,58,65	0
5	LMR	B	520	9/9	0.83	0.22	59,65,72,76	0
5	LMR	B	519	9/9	0.83	0.21	51,56,64,67	0
2	SO4	B	505	5/5	0.83	0.22	42,45,60,61	5
2	SO4	B	506	5/5	0.89	0.23	67,68,90,102	0
3	EDO	B	518	4/4	0.89	0.55	49,60,69,73	0
3	EDO	A	513	4/4	0.89	0.32	39,57,69,74	0
4	MLT	A	514	9/9	0.90	0.13	50,58,63,65	0
3	EDO	B	514	4/4	0.90	0.25	52,63,68,68	0
2	SO4	A	505	5/5	0.91	0.12	69,72,89,90	5
4	MLT	A	515	9/9	0.91	0.16	49,59,71,74	0
2	SO4	A	504	5/5	0.91	0.16	76,77,92,94	0
3	EDO	B	512	4/4	0.92	0.28	35,52,61,74	0
2	SO4	A	506	5/5	0.92	0.18	85,86,96,107	0
3	EDO	A	512	4/4	0.93	0.17	36,46,56,58	0
2	SO4	A	503	5/5	0.94	0.13	47,48,56,60	5
2	SO4	B	502	5/5	0.94	0.10	34,49,58,60	5
2	SO4	B	504	5/5	0.94	0.07	61,71,75,81	0
2	SO4	B	508	5/5	0.94	0.23	77,83,88,95	0
2	SO4	B	501	5/5	0.95	0.10	48,56,66,67	0
2	SO4	A	501	5/5	0.96	0.16	60,66,83,85	0
2	SO4	B	503	5/5	0.96	0.19	38,53,57,59	5
2	SO4	B	511	5/5	0.97	0.09	39,40,47,51	0
2	SO4	A	511	5/5	0.97	0.07	46,52,56,57	0
2	SO4	A	502	5/5	0.97	0.08	58,62,65,66	0
2	SO4	A	510	5/5	0.97	0.09	36,41,47,49	0
2	SO4	A	509	5/5	0.99	0.08	34,40,43,49	0
2	SO4	B	510	5/5	0.99	0.07	28,28,31,32	0
2	SO4	B	509	5/5	0.99	0.05	31,32,35,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.