



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:32 pm BST

PDB ID : 1X6M  
Title : Crystal structure of the glutathione-dependent formaldehyde-activating enzyme (Gfa)  
Authors : Neculai, A.M.; Neculai, D.; Vorholt, J.A.; Becker, S.  
Deposited on : 2004-08-11  
Resolution : 2.35 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 : 2.11  
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) : 2.11

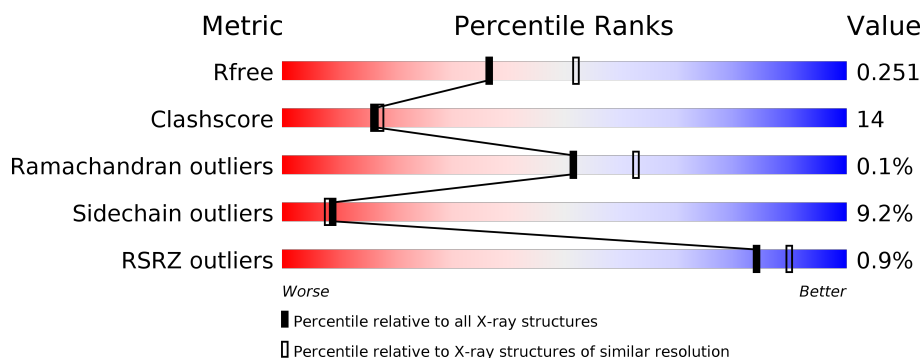
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	196	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>78%</span> <span>18%</span> <span>• •</span> </div> </div>
1	B	196	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>70%</span> <span>26%</span> <span>• •</span> </div> </div>
1	C	196	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>74%</span> <span>21%</span> <span>• •</span> </div> </div>
1	D	196	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>2%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>68%</span> <span>25%</span> <span>6%</span> <span>•</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	505	-	-	X	-
4	GOL	B	601	-	-	X	-
4	GOL	B	602	-	-	X	-
4	GOL	B	603	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6262 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 Glutathione-dependent formaldehyde-activating enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	3	0
			1496	932	277	276	11			
1	B	196	Total	C	N	O	S	0	2	0
			1494	931	276	276	11			
1	C	194	Total	C	N	O	S	0	0	0
			1469	915	269	274	11			
1	D	194	Total	C	N	O	S	0	1	0
			1475	919	271	274	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q51669
A	2	HIS	-	CLONING ARTIFACT	UNP Q51669
A	3	MET	-	CLONING ARTIFACT	UNP Q51669
B	1	GLY	-	CLONING ARTIFACT	UNP Q51669
B	2	HIS	-	CLONING ARTIFACT	UNP Q51669
B	3	MET	-	CLONING ARTIFACT	UNP Q51669
C	1	GLY	-	CLONING ARTIFACT	UNP Q51669
C	2	HIS	-	CLONING ARTIFACT	UNP Q51669
C	3	MET	-	CLONING ARTIFACT	UNP Q51669
D	1	GLY	-	CLONING ARTIFACT	UNP Q51669
D	2	HIS	-	CLONING ARTIFACT	UNP Q51669
D	3	MET	-	CLONING ARTIFACT	UNP Q51669

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

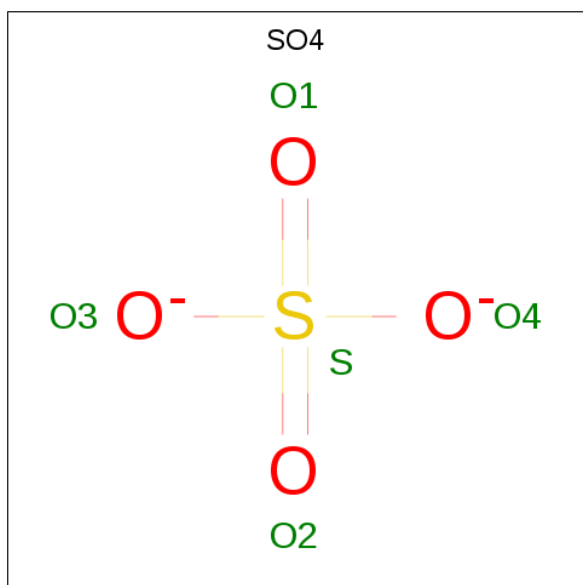
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

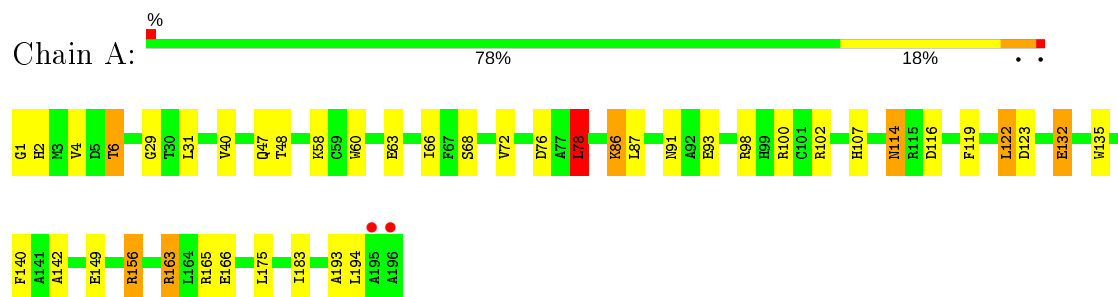
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		
5	B	85	Total	O	0	0
			85	85		
5	C	40	Total	O	0	0
			40	40		
5	D	48	Total	O	0	0
			48	48		

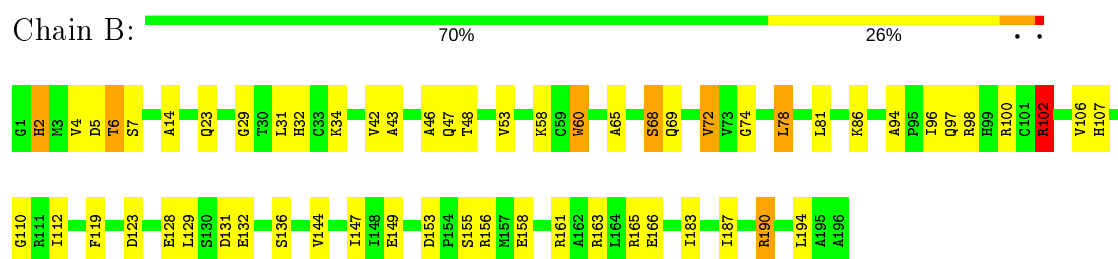
### 3 Residue-property plots [i](#)

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.

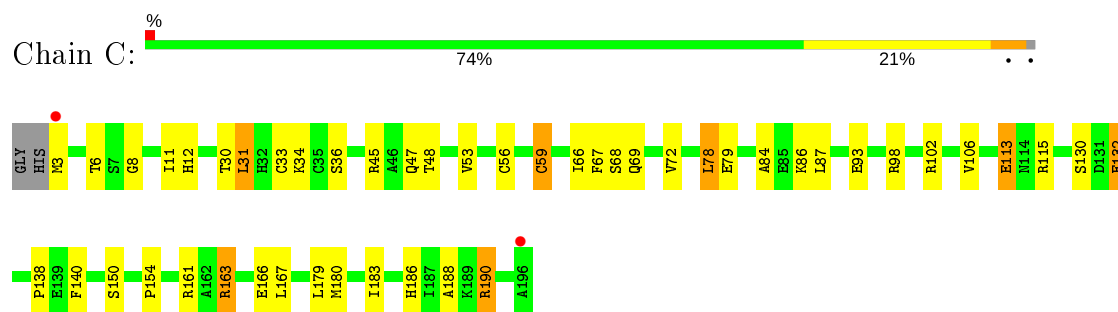
- Molecule 1: Glutathione-dependent formaldehyde-activating enzyme



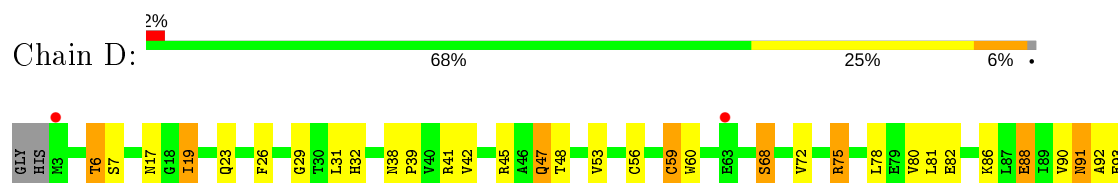
- Molecule 1: Glutathione-dependent formaldehyde-activating enzyme

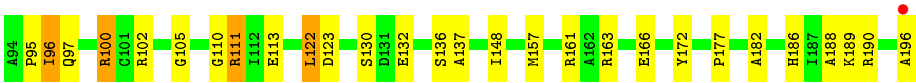


- Molecule 1: Glutathione-dependent formaldehyde-activating enzyme



- Molecule 1: Glutathione-dependent formaldehyde-activating enzyme







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.36 Å 118.86 Å 95.99 Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	74.29 – 2.35 74.29 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.29-2.35) 99.8 (74.29-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.250 0.189 , 0.251	Depositor DCC
$R_{free}$ test set	3455 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% 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: GOL, ZN, SO4

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	0.95	1/1546 (0.1%)	0.96	4/2096 (0.2%)
1	B	0.98	1/1537 (0.1%)	1.00	5/2084 (0.2%)
1	C	0.80	1/1502 (0.1%)	0.92	5/2038 (0.2%)
1	D	0.84	1/1513 (0.1%)	0.87	3/2053 (0.1%)
All	All	0.90	4/6098 (0.1%)	0.94	17/8271 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	TRP	CB-CG	-6.29	1.39	1.50
1	D	82	GLU	CG-CD	5.24	1.59	1.51
1	C	140	PHE	CE2-CZ	5.06	1.47	1.37
1	A	132	GLU	CG-CD	5.06	1.59	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	C	78	LEU	CA-CB-CG	7.41	132.34	115.30
1	C	59	CYS	CA-CB-SG	7.32	127.18	114.00
1	A	78	LEU	CA-CB-CG	7.19	131.85	115.30
1	B	163	ARG	NE-CZ-NH1	6.72	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	102	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	D	122	LEU	CA-CB-CG	6.06	129.24	115.30
1	C	161	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	156	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	B	78	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	78	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	100	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	D	59	CYS	CA-CB-SG	5.19	123.35	114.00
1	A	194	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	163	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	190	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLY	Peptide

## 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	1496	0	1460	28	0
1	B	1494	0	1455	49	0
1	C	1469	0	1430	34	0
1	D	1475	0	1433	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	15	0	0	3	0
4	B	18	0	24	17	0
4	C	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	8	1	0
5	A	82	0	0	2	0
5	B	85	0	0	7	0
5	C	40	0	0	4	0
5	D	48	0	0	1	0
All	All	6262	0	5818	171	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 14.

All (171) 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:B:74:GLY:H	4:B:603:GOL:H12	1.17	1.07
1:C:45:ARG:NH2	1:C:79:GLU:OE1	1.90	1.05
1:B:14:ALA:CB	4:B:602:GOL:H12	1.96	0.96
1:C:186:HIS:CD2	1:C:190:ARG:HH11	1.83	0.96
1:A:114:ASN:HD22	1:A:116:ASP:H	1.13	0.92
1:B:14:ALA:HB2	4:B:602:GOL:H12	1.53	0.90
1:A:6:THR:HG21	1:A:166:GLU:OE1	1.72	0.89
1:A:114:ASN:ND2	1:A:116:ASP:H	1.72	0.86
1:C:186:HIS:HD2	1:C:190:ARG:HH11	1.20	0.86
1:B:98:ARG:HD2	4:B:601:GOL:H32	1.56	0.86
1:C:47:GLN:HE21	1:C:48:THR:H	1.20	0.86
1:D:111:ARG:HH11	1:D:111:ARG:HG3	1.41	0.85
1:D:102:ARG:HH11	1:D:102:ARG:HG3	1.42	0.84
1:D:182:ALA:HB1	4:D:605:GOL:H31	1.61	0.81
1:B:6:THR:HG21	1:B:166:GLU:OE1	1.80	0.81
1:C:179:LEU:HD23	4:C:604:GOL:H12	1.62	0.80
1:B:74:GLY:N	4:B:603:GOL:H12	1.97	0.79
1:D:47:GLN:HE21	1:D:48:THR:H	1.29	0.78
1:D:88:GLU:OE2	1:D:100:ARG:NH2	2.19	0.75
1:D:111:ARG:HH11	1:D:111:ARG:CG	1.99	0.74
1:D:111:ARG:HD3	1:D:113:GLU:OE2	1.87	0.74
1:B:14:ALA:HB1	4:B:602:GOL:H12	1.70	0.74
1:B:47:GLN:HE21	1:B:48:THR:H	1.34	0.73
1:D:75:ARG:NH1	1:D:75:ARG:HG3	2.03	0.73
1:A:60:TRP:O	1:A:68:SER:HB2	1.90	0.71
1:B:2:HIS:NE2	1:B:166:GLU:OE2	2.24	0.71
1:D:111:ARG:NH1	1:D:123:ASP:OD1	2.24	0.70
1:D:75:ARG:HH11	1:D:75:ARG:HG3	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ARG:HH11	1:D:75:ARG:CG	2.03	0.70
1:D:29:GLY:HA3	1:D:132:GLU:OE1	1.91	0.69
1:C:8:GLY:HA2	5:C:634:HOH:O	1.92	0.69
1:C:186:HIS:HD2	1:C:190:ARG:NH1	1.91	0.69
1:B:86:LYS:O	1:B:102:ARG:HG2	1.94	0.67
1:B:98:ARG:CD	4:B:601:GOL:H32	2.26	0.66
1:D:111:ARG:NH1	1:D:111:ARG:HG3	2.05	0.66
1:C:180:MET:CE	1:C:183:ILE:HD12	2.25	0.65
1:B:144:VAL:O	1:B:147:ILE:HG12	1.95	0.65
1:D:163:ARG:NH2	1:D:166:GLU:OE1	2.24	0.65
1:C:163:ARG:HD3	5:C:611:HOH:O	1.97	0.64
1:B:43:ALA:HB2	1:B:81:LEU:HD11	1.78	0.64
1:C:69:GLN:HE21	1:C:138:PRO:HG3	1.63	0.64
1:B:190:ARG:HH11	1:B:190:ARG:HB2	1.61	0.63
1:A:114:ASN:HD22	1:A:116:ASP:N	1.93	0.62
1:D:6:THR:HG21	1:D:166:GLU:OE1	1.98	0.62
1:D:100:ARG:HD3	1:D:105:GLY:HA2	1.81	0.62
1:A:2:HIS:CE1	1:A:4:VAL:O	2.52	0.61
1:D:91:ASN:HD21	1:D:93:GLU:HG2	1.66	0.61
1:A:40:VAL:HG11	1:A:87:LEU:HD21	1.82	0.60
1:D:47:GLN:HE21	1:D:48:THR:N	1.99	0.60
1:D:161:ARG:HD2	3:D:507:SO4:O1	2.02	0.60
1:D:32[B]:HIS:ND1	1:D:41:ARG:HG2	2.17	0.60
1:C:59:CYS:HB3	1:C:98:ARG:NH2	2.17	0.59
1:D:96:ILE:HD11	1:D:110:GLY:HA3	1.85	0.59
4:B:601:GOL:O2	5:B:631:HOH:O	2.16	0.58
1:D:91:ASN:ND2	1:D:93:GLU:H	2.01	0.58
1:B:156:ARG:NH2	5:B:681:HOH:O	2.35	0.58
1:B:29:GLY:HA3	1:B:132:GLU:OE1	2.03	0.58
1:D:38:ASN:O	1:D:86:LYS:HE2	2.03	0.58
1:D:92:ALA:HA	1:D:97:GLN:HE21	1.69	0.57
1:C:180:MET:HE2	1:C:183:ILE:HD12	1.87	0.56
1:C:47:GLN:HE21	1:C:48:THR:N	1.97	0.56
1:A:2:HIS:NE2	1:A:166:GLU:OE2	2.26	0.56
1:D:111:ARG:HH12	1:D:123:ASP:CG	2.09	0.56
1:C:66:ILE:HG13	1:C:67:PHE:HD1	1.70	0.56
1:B:60:TRP:HB2	1:B:107:HIS:CD2	2.42	0.55
1:A:47:GLN:HE21	1:A:48:THR:H	1.54	0.55
1:B:2:HIS:CE1	1:B:166:GLU:OE2	2.60	0.55
1:B:194:LEU:HD11	1:C:154:PRO:HD3	1.89	0.55
1:A:165:ARG:NH1	5:A:572:HOH:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:CYS:HB2	5:C:619:HOH:O	2.07	0.55
1:D:75:ARG:HH12	1:D:111:ARG:CZ	2.20	0.55
1:D:31:LEU:HB2	1:D:42:VAL:HG23	1.89	0.55
1:C:66:ILE:HG13	1:C:67:PHE:CD1	2.41	0.54
1:D:96:ILE:CD1	1:D:110:GLY:HA3	2.37	0.54
1:B:183:ILE:O	1:B:187:ILE:HG12	2.07	0.54
1:C:186:HIS:CD2	1:C:190:ARG:NH1	2.65	0.54
1:B:34:LYS:HG3	1:B:106:VAL:HG21	1.90	0.54
1:A:175:LEU:HD12	1:A:183:ILE:HD11	1.90	0.53
1:D:102:ARG:NH1	1:D:102:ARG:HG3	2.17	0.53
1:D:19:ILE:CD1	1:D:137:ALA:HB1	2.37	0.53
1:A:114:ASN:HD22	1:A:114:ASN:C	2.12	0.53
1:C:53:VAL:HA	1:C:68:SER:O	2.08	0.53
1:B:47:GLN:HE21	1:B:48:THR:N	2.03	0.52
1:B:153:ASP:OD2	1:B:155:SER:OG	2.19	0.52
1:C:115:ARG:HB2	5:C:639:HOH:O	2.09	0.52
1:D:95:PRO:HG2	3:D:505:SO4:O1	2.10	0.51
1:A:66:ILE:CD1	1:A:156:ARG:HH12	2.24	0.51
1:C:6:THR:HG23	1:C:163:ARG:HB2	1.93	0.50
1:D:96:ILE:HG23	3:D:505:SO4:O1	2.10	0.50
1:D:19:ILE:HD13	1:D:137:ALA:HB1	1.93	0.50
1:D:23:GLN:HE21	1:D:26:PHE:HD2	1.60	0.50
1:C:180:MET:HE1	1:C:183:ILE:HD12	1.92	0.50
1:D:42:VAL:HG12	1:D:80:VAL:HG22	1.94	0.49
1:D:6:THR:HG23	1:D:163:ARG:HD3	1.94	0.49
1:D:88:GLU:OE2	1:D:100:ARG:HD2	2.12	0.49
1:B:112:ILE:HD13	1:B:119:PHE:HB2	1.93	0.49
1:C:12:HIS:HD2	1:C:67:PHE:O	1.95	0.49
1:D:59:CYS:HB2	5:D:613:HOH:O	2.12	0.49
1:C:113:GLU:OE2	1:C:113:GLU:HA	2.13	0.49
1:A:86:LYS:O	1:A:102:ARG:HG2	2.13	0.48
1:B:5:ASP:OD2	1:B:7:SER:HB2	2.13	0.48
1:B:6:THR:HG21	1:B:166:GLU:CD	2.33	0.48
1:D:31:LEU:HB2	1:D:42:VAL:CG2	2.43	0.48
1:A:78:LEU:HG	1:A:123:ASP:OD2	2.13	0.48
4:B:601:GOL:H11	5:B:610:HOH:O	2.12	0.48
1:D:172:TYR:CZ	1:D:177:PRO:HD3	2.49	0.48
1:D:92:ALA:HA	1:D:97:GLN:NE2	2.28	0.48
1:A:66:ILE:HD11	1:A:156:ARG:HH12	1.79	0.47
1:A:114:ASN:HD21	1:A:116:ASP:HB2	1.78	0.47
1:B:47:GLN:HA	1:B:47:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HG3	1:C:106:VAL:HG21	1.97	0.47
1:B:53:VAL:HA	1:B:68:SER:O	2.14	0.47
1:B:128:GLU:CB	4:B:602:GOL:H11	2.45	0.47
1:B:128:GLU:HB3	4:B:602:GOL:H11	1.97	0.47
1:D:148:ILE:HD11	1:D:157:MET:HG3	1.97	0.46
1:A:58:LYS:HD3	1:A:58:LYS:HA	1.77	0.46
1:A:100:ARG:HA	1:A:107:HIS:HA	1.98	0.46
1:D:186:HIS:CD2	1:D:190:ARG:HE	2.34	0.46
1:D:90:VAL:HG22	1:D:100:ARG:CZ	2.45	0.46
1:D:91:ASN:HD22	1:D:92:ALA:N	2.13	0.46
1:A:47:GLN:HE22	1:A:135:TRP:HA	1.81	0.45
1:B:32[A]:HIS:NE2	1:B:131:ASP:OD2	2.45	0.45
1:C:130:SER:OG	1:C:132:GLU:HG2	2.17	0.45
1:A:149:GLU:HA	1:D:188:ALA:HB2	1.98	0.45
1:C:11:ILE:HG23	1:C:67:PHE:CD1	2.51	0.45
1:A:98:ARG:HD2	5:A:583:HOH:O	2.16	0.45
1:D:60:TRP:O	1:D:68:SER:HB2	2.16	0.45
1:A:47:GLN:HE21	1:A:48:THR:N	2.14	0.45
1:C:179:LEU:CD2	4:C:604:GOL:H12	2.41	0.44
1:D:91:ASN:C	1:D:91:ASN:HD22	2.21	0.44
1:B:2:HIS:HE1	1:B:6:THR:HB	1.83	0.44
1:D:102:ARG:HH11	1:D:102:ARG:CG	2.21	0.44
1:B:46:ALA:HB1	5:B:655:HOH:O	2.16	0.43
1:B:31:LEU:HG	1:B:129:LEU:HB2	2.00	0.43
1:C:6:THR:HG21	1:C:166:GLU:OE1	2.19	0.43
1:D:53:VAL:HA	1:D:68:SER:O	2.18	0.43
1:B:97:GLN:O	1:B:110:GLY:HA2	2.18	0.43
1:D:91:ASN:HD22	1:D:93:GLU:H	1.66	0.43
1:D:32[B]:HIS:CE1	1:D:41:ARG:HG2	2.53	0.43
1:B:94:ALA:CB	4:B:601:GOL:H12	2.48	0.43
1:B:72:VAL:HA	1:B:123:ASP:O	2.20	0.42
1:B:23:GLN:OE1	1:B:23:GLN:HA	2.20	0.42
1:D:96:ILE:HD12	1:D:96:ILE:C	2.39	0.42
1:B:149:GLU:HA	1:C:188:ALA:HB2	2.01	0.42
1:D:31:LEU:HD12	1:D:130:SER:HB2	2.01	0.42
1:A:29:GLY:HA3	1:A:132:GLU:OE1	2.19	0.42
1:B:78:LEU:HG	1:B:123:ASP:OD2	2.20	0.42
1:B:14:ALA:HB2	4:B:602:GOL:C1	2.36	0.42
1:B:161:ARG:O	1:B:165:ARG:HG3	2.20	0.42
1:B:65:ALA:HA	5:B:617:HOH:O	2.19	0.42
1:C:31:LEU:HD12	1:C:130:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLU:H	1:C:132:GLU:HG2	1.74	0.42
1:D:91:ASN:ND2	1:D:93:GLU:HG2	2.33	0.42
1:B:32[B]:HIS:CD2	5:B:620:HOH:O	2.72	0.41
1:B:74:GLY:N	4:B:603:GOL:H31	2.35	0.41
1:C:84:ALA:HA	1:C:87:LEU:HD12	2.02	0.41
1:D:47:GLN:HA	1:D:47:GLN:HE21	1.84	0.41
1:A:119:PHE:O	1:A:122:LEU:HB2	2.21	0.41
1:D:38:ASN:N	1:D:39:PRO:CD	2.84	0.41
1:D:47:GLN:HA	1:D:47:GLN:NE2	2.36	0.41
1:C:179:LEU:HA	1:C:179:LEU:HD23	1.75	0.41
1:A:100:ARG:HB2	1:A:107:HIS:CD2	2.56	0.41
1:A:114:ASN:ND2	1:A:116:ASP:N	2.54	0.41
1:A:140:PHE:HE1	1:A:142:ALA:HB2	1.86	0.41
1:D:75:ARG:HB2	1:D:123:ASP:OD2	2.21	0.41
1:D:96:ILE:HD12	1:D:97:GLN:N	2.37	0.40
1:B:98:ARG:NE	4:B:601:GOL:O1	2.34	0.40
1:B:74:GLY:H	4:B:603:GOL:H31	1.87	0.40
1:B:96:ILE:O	4:B:601:GOL:H11	2.21	0.40
1:B:69:GLN:NE2	5:B:627:HOH:O	2.39	0.40
1:D:189:LYS:HZ2	1:D:196:ALA:HB3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/196 (100%)	187 (95%)	9 (5%)	1 (0%)	29	32
1	B	196/196 (100%)	190 (97%)	6 (3%)	0	100	100
1	C	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
1	D	193/196 (98%)	187 (97%)	6 (3%)	0	100	100
All	All	778/784 (99%)	751 (96%)	26 (3%)	1 (0%)	51	63



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	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	158/155 (102%)	146 (92%)	12 (8%)	13	13
1	B	157/155 (101%)	146 (93%)	11 (7%)	15	15
1	C	154/155 (99%)	138 (90%)	16 (10%)	7	6
1	D	155/155 (100%)	137 (88%)	18 (12%)	5	5
All	All	624/620 (101%)	567 (91%)	57 (9%)	9	8

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	31	LEU
1	A	63	GLU
1	A	72	VAL
1	A	76	ASP
1	A	78	LEU
1	A	86	LYS
1	A	91	ASN
1	A	93	GLU
1	A	114	ASN
1	A	122	LEU
1	A	163	ARG
1	B	2	HIS
1	B	4	VAL
1	B	6	THR
1	B	42	VAL
1	B	58	LYS
1	B	68	SER
1	B	72	VAL

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	136	SER
1	B	158	GLU
1	B	190	ARG
1	C	3	MET
1	C	30	THR
1	C	31	LEU
1	C	33	CYS
1	C	36	SER
1	C	56	CYS
1	C	72	VAL
1	C	78	LEU
1	C	86	LYS
1	C	93	GLU
1	C	102	ARG
1	C	113	GLU
1	C	132	GLU
1	C	150	SER
1	C	163	ARG
1	C	167	LEU
1	D	6	THR
1	D	7	SER
1	D	17	ASN
1	D	19	ILE
1	D	45	ARG
1	D	47	GLN
1	D	56	CYS
1	D	68	SER
1	D	72	VAL
1	D	75	ARG
1	D	81	LEU
1	D	88	GLU
1	D	91	ASN
1	D	96	ILE
1	D	100	ARG
1	D	111	ARG
1	D	122	LEU
1	D	136	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	47	GLN
1	A	91	ASN
1	A	114	ASN
1	B	47	GLN
1	B	97	GLN
1	C	47	GLN
1	C	69	GLN
1	C	97	GLN
1	C	186	HIS
1	D	23	GLN
1	D	47	GLN
1	D	91	ASN
1	D	97	GLN
1	D	99	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	504	-	4,4,4	0.20	0	6,6,6	0.39	0
3	SO4	D	506	-	4,4,4	0.20	0	6,6,6	0.41	0
3	SO4	B	502	-	4,4,4	0.20	0	6,6,6	0.61	0
4	GOL	D	605	-	5,5,5	0.37	0	5,5,5	0.40	0
4	GOL	B	602	-	5,5,5	0.63	0	5,5,5	0.62	0
4	GOL	B	601	-	5,5,5	1.10	1 (20%)	5,5,5	1.89	2 (40%)
3	SO4	C	503	-	4,4,4	0.17	0	6,6,6	0.31	0
3	SO4	D	507	-	4,4,4	0.29	0	6,6,6	0.48	0
4	GOL	B	603	-	5,5,5	0.54	0	5,5,5	0.54	0
3	SO4	D	505	-	4,4,4	0.12	0	6,6,6	0.46	0
4	GOL	C	604	-	5,5,5	0.65	0	5,5,5	1.09	0
3	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.51	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
4	GOL	B	601	-	-	2/4/4/4	-
4	GOL	B	602	-	-	2/4/4/4	-
4	GOL	C	604	-	-	0/4/4/4	-
4	GOL	B	603	-	-	4/4/4/4	-
4	GOL	D	605	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	GOL	O2-C2	-2.02	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	GOL	O2-C2-C1	-2.47	98.23	109.12
4	B	601	GOL	O1-C1-C2	2.44	121.89	110.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	605	GOL	C1-C2-C3-O3
4	B	601	GOL	O1-C1-C2-C3
4	B	602	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-C3
4	D	605	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-O2
4	B	601	GOL	O1-C1-C2-O2
4	B	602	GOL	O2-C2-C3-O3
4	D	605	GOL	O1-C1-C2-O2
4	D	605	GOL	O2-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3
4	B	603	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	605	GOL	1	0
4	B	602	GOL	6	0
4	B	601	GOL	7	0
3	D	507	SO4	1	0
4	B	603	GOL	4	0
3	D	505	SO4	2	0
4	C	604	GOL	2	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	196/196 (100%)	0.43	2 (1%) 82 88	21, 31, 48, 74	0
1	B	196/196 (100%)	0.43	0 100 100	21, 31, 52, 61	0
1	C	194/196 (98%)	0.46	2 (1%) 82 88	23, 42, 59, 76	0
1	D	194/196 (98%)	0.56	3 (1%) 73 81	23, 43, 58, 76	0
All	All	780/784 (99%)	0.47	7 (0%) 84 90	21, 36, 57, 76	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	6.1
1	A	196	ALA	6.0
1	C	3	MET	3.9
1	D	3	MET	2.9
1	D	63	GLU	2.6
1	C	196	ALA	2.3
1	A	195	ALA	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	604	6/6	0.70	0.30	30,40,42,42	6
3	SO4	D	505	5/5	0.82	0.23	49,51,53,54	5
4	GOL	B	603	6/6	0.82	0.23	30,33,37,37	6
4	GOL	D	605	6/6	0.83	0.30	36,38,40,45	6
3	SO4	D	507	5/5	0.86	0.31	35,37,40,41	5
4	GOL	B	601	6/6	0.92	0.32	23,25,29,29	6
4	GOL	B	602	6/6	0.94	0.20	8,12,16,17	6
2	ZN	B	201	1/1	0.97	0.13	32,32,32,32	1
2	ZN	C	201	1/1	0.97	0.14	38,38,38,38	1
3	SO4	C	503	5/5	0.97	0.15	56,56,56,57	5
2	ZN	A	201	1/1	0.98	0.14	32,32,32,32	1
3	SO4	D	506	5/5	0.98	0.15	48,48,49,49	0
2	ZN	D	200	1/1	0.98	0.14	50,50,50,50	0
2	ZN	D	201	1/1	0.99	0.13	43,43,43,43	1
3	SO4	B	502	5/5	0.99	0.20	35,37,39,39	5
3	SO4	C	504	5/5	0.99	0.11	44,44,46,48	0
2	ZN	C	200	1/1	0.99	0.13	52,52,52,52	0
3	SO4	A	501	5/5	0.99	0.15	40,41,42,44	5
2	ZN	B	200	1/1	1.00	0.18	34,34,34,34	0
2	ZN	A	200	1/1	1.00	0.17	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.