



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:56 am GMT

PDB ID : 4AH9  
Title : Parallel screening of a low molecular weight compound library: do differences in methodology affect hit identification  
Authors : Wielens, J.; Heady, S.J.; Rhodes, D.I.; Mulder, R.J.; Dolezal, O.; Deadman, J.J.; Newman, J.; Chalmers, D.K.; Parker, M.W.; Peat, T.S.; Scanlon, M.J.  
Deposited on : 2012-02-06  
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

<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 : 1.7.2 (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

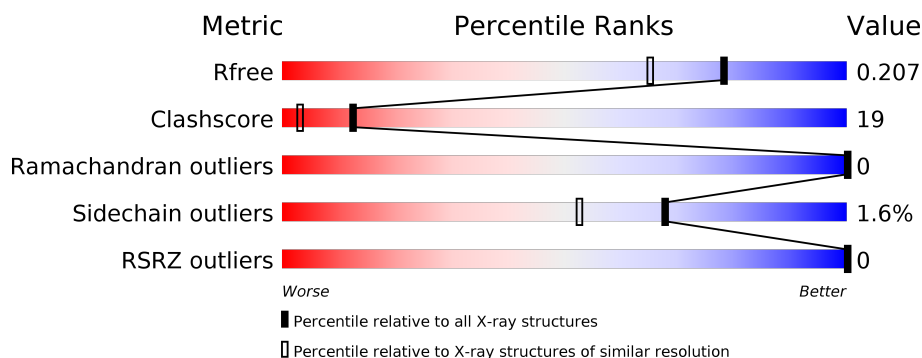
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (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. 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	183	
1	B	183	

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	SO4	A	1215	-	-	-	X
3	SO4	A	1216	-	-	X	-
3	SO4	B	1210	-	-	-	X
3	SO4	B	1211	-	-	-	X
3	SO4	B	1213	-	-	X	-
3	SO4	B	1214	-	X	-	X
4	EDO	A	1217	-	-	-	X
4	EDO	A	1218	-	-	-	X
4	EDO	B	1215	-	-	-	X
5	CL	A	1223	-	-	X	-
6	GOL	A	1226	-	-	X	-
7	TAM	A	1227	-	-	X	X
7	TAM	B	1220	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2845 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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	12	0
			1256	801	215	236	4			
1	B	150	Total	C	N	O	S	0	13	0
			1242	797	211	230	4			

There are 46 discrepancies between the modelled and reference sequences:

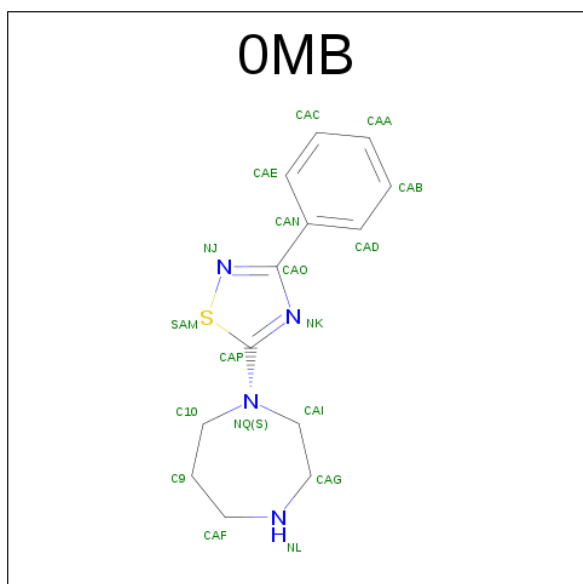
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P12497
A	31	GLY	-	EXPRESSION TAG	UNP P12497
A	32	SER	-	EXPRESSION TAG	UNP P12497
A	33	SER	-	EXPRESSION TAG	UNP P12497
A	34	HIS	-	EXPRESSION TAG	UNP P12497
A	35	HIS	-	EXPRESSION TAG	UNP P12497
A	36	HIS	-	EXPRESSION TAG	UNP P12497
A	37	HIS	-	EXPRESSION TAG	UNP P12497
A	38	HIS	-	EXPRESSION TAG	UNP P12497
A	39	HIS	-	EXPRESSION TAG	UNP P12497
A	40	SER	-	EXPRESSION TAG	UNP P12497
A	41	SER	-	EXPRESSION TAG	UNP P12497
A	42	GLY	-	EXPRESSION TAG	UNP P12497
A	43	LEU	-	EXPRESSION TAG	UNP P12497
A	44	VAL	-	EXPRESSION TAG	UNP P12497
A	45	PRO	-	EXPRESSION TAG	UNP P12497
A	46	ARG	-	EXPRESSION TAG	UNP P12497
A	47	GLY	-	EXPRESSION TAG	UNP P12497
A	48	SER	-	EXPRESSION TAG	UNP P12497
A	49	HIS	-	EXPRESSION TAG	UNP P12497
A	56	SER	CYS	ENGINEERED MUTATION	UNP P12497
A	139	ASP	PHE	ENGINEERED MUTATION	UNP P12497
A	185	HIS	PHE	ENGINEERED MUTATION	UNP P12497
B	30	MET	-	EXPRESSION TAG	UNP P12497
B	31	GLY	-	EXPRESSION TAG	UNP P12497

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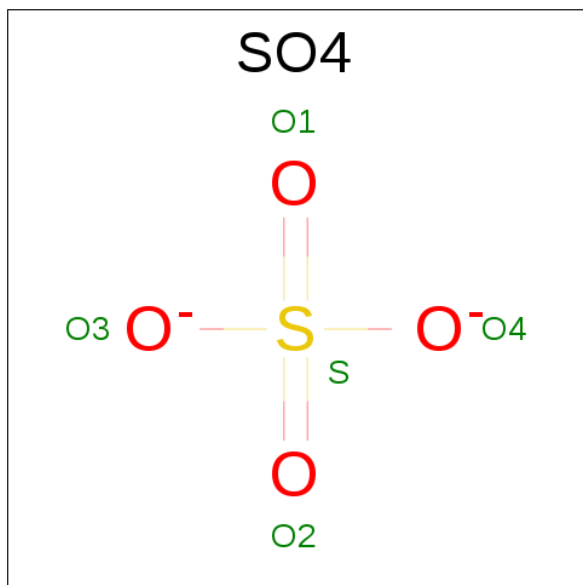
Chain	Residue	Modelled	Actual	Comment	Reference
B	32	SER	-	EXPRESSION TAG	UNP P12497
B	33	SER	-	EXPRESSION TAG	UNP P12497
B	34	HIS	-	EXPRESSION TAG	UNP P12497
B	35	HIS	-	EXPRESSION TAG	UNP P12497
B	36	HIS	-	EXPRESSION TAG	UNP P12497
B	37	HIS	-	EXPRESSION TAG	UNP P12497
B	38	HIS	-	EXPRESSION TAG	UNP P12497
B	39	HIS	-	EXPRESSION TAG	UNP P12497
B	40	SER	-	EXPRESSION TAG	UNP P12497
B	41	SER	-	EXPRESSION TAG	UNP P12497
B	42	GLY	-	EXPRESSION TAG	UNP P12497
B	43	LEU	-	EXPRESSION TAG	UNP P12497
B	44	VAL	-	EXPRESSION TAG	UNP P12497
B	45	PRO	-	EXPRESSION TAG	UNP P12497
B	46	ARG	-	EXPRESSION TAG	UNP P12497
B	47	GLY	-	EXPRESSION TAG	UNP P12497
B	48	SER	-	EXPRESSION TAG	UNP P12497
B	49	HIS	-	EXPRESSION TAG	UNP P12497
B	56	SER	CYS	ENGINEERED MUTATION	UNP P12497
B	139	ASP	PHE	ENGINEERED MUTATION	UNP P12497
B	185	HIS	PHE	ENGINEERED MUTATION	UNP P12497

- Molecule 2 is 1-(3-PHENYL-1,2,4-THIADIAZOL-5-YL)-1,4-DIAZEPANE (three-letter code: OMB) (formula: C<sub>13</sub>H<sub>16</sub>N<sub>4</sub>S).



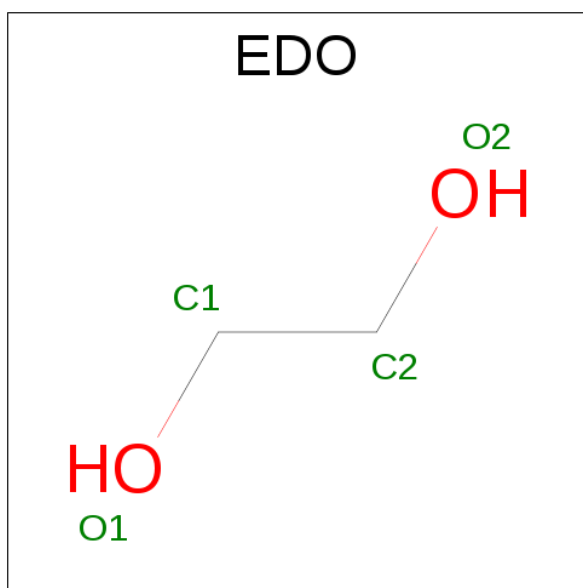
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			18	13	4	1		
2	B	1	Total	C	N	S	0	0
			18	13	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

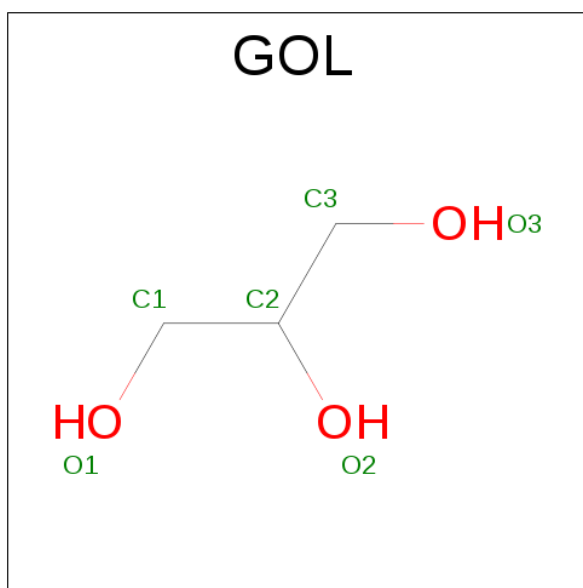


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

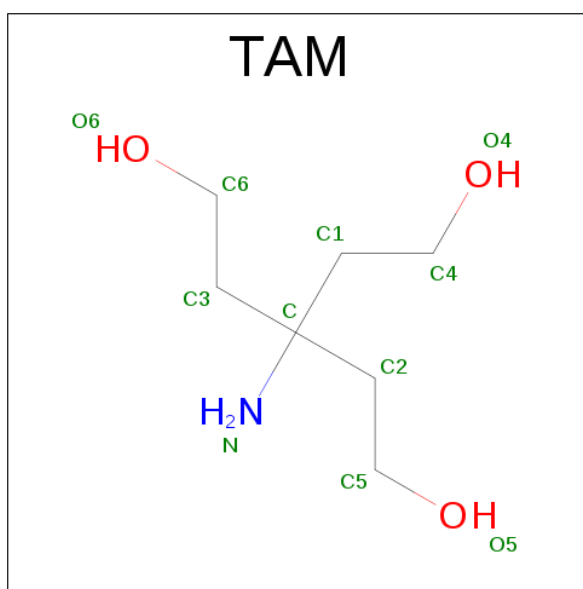
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	3	Total Cl 3 3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	7	1	3		
7	B	1	Total	C	N	O	0	0
			11	7	1	3		

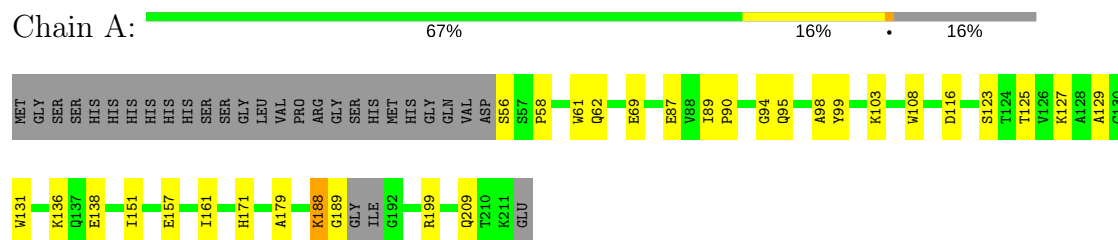
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	103	Total	O	0	0
			103	103		
8	B	84	Total	O	0	0
			84	84		

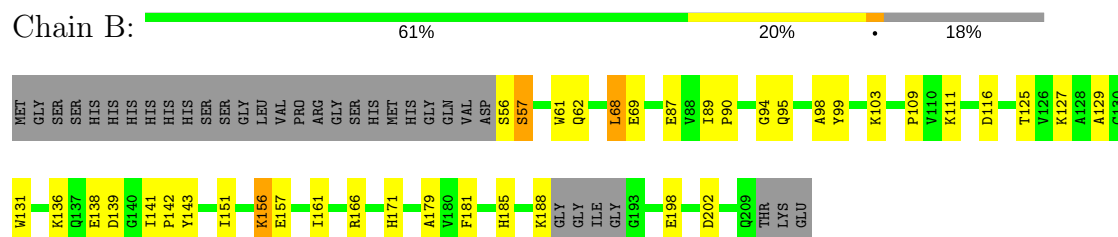
### 3 Residue-property plots [i](#)

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: INTEGRASE



#### • Molecule 1: INTEGRASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.59Å 70.59Å 66.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.08 – 1.70 35.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (61.08-1.70) 98.8 (35.30-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.166 , 0.209 0.165 , 0.207	Depositor DCC
$R_{free}$ test set	2021 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.488 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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, CL, EDO, SO4, OMB, TAM

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	1.24	3/1307 (0.2%)	1.17	3/1771 (0.2%)
1	B	1.22	3/1293 (0.2%)	1.12	4/1755 (0.2%)
All	All	1.23	6/2600 (0.2%)	1.15	7/3526 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	TRP	CD2-CE2	8.24	1.51	1.41
1	A	131	TRP	CD2-CE2	6.39	1.49	1.41
1	A	108	TRP	CD2-CE2	6.00	1.48	1.41
1	B	157	GLU	CD-OE1	5.41	1.31	1.25
1	B	61	TRP	CD2-CE2	5.25	1.47	1.41
1	B	131	TRP	CD2-CE2	5.24	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	157	GLU	OE1-CD-OE2	-6.54	115.46	123.30
1	A	116	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	116	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	166	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	B	68	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	A	116	ASP	CB-CG-OD2	-5.34	113.49	118.30

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	1256	0	1276	32	0
1	B	1242	0	1268	56	0
2	A	18	0	16	1	0
2	B	18	0	16	2	0
3	A	25	0	0	3	0
3	B	25	0	0	2	0
4	A	24	0	36	2	0
4	B	12	0	18	3	0
5	A	3	0	0	3	0
5	B	1	0	0	0	0
6	A	6	0	8	4	0
6	B	6	0	7	2	0
7	A	11	0	17	11	0
7	B	11	0	17	6	0
8	A	103	0	0	17	0
8	B	84	0	0	12	0
All	All	2845	0	2679	100	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 19.

All (100) 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:141[B]:ILE:CD1	1:B:142:PRO:HD2	1.20	1.61
1:B:141[B]:ILE:HD12	1:B:142:PRO:CD	1.13	1.56
1:B:69:GLU:OE2	6:B:1219:GOL:O1	1.54	1.21
1:B:62[B]:GLN:NE2	1:B:151[B]:ILE:HD11	1.53	1.21
6:A:1226:GOL:H12	8:A:2012:HOH:O	1.43	1.16
1:A:69:GLU:OE2	6:A:1226:GOL:O1	1.64	1.14
1:B:141[B]:ILE:HD11	1:B:142:PRO:HD2	1.23	1.09
1:B:141[B]:ILE:CD1	1:B:142:PRO:CD	1.97	1.05
1:B:141[B]:ILE:HD12	1:B:142:PRO:N	1.70	1.05
6:A:1226:GOL:C1	8:A:2012:HOH:O	2.04	0.97
5:A:1223:CL:CL	7:A:1227:TAM:H42	2.02	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:N	8:A:2002:HOH:O	1.96	0.96
1:B:141[B]:ILE:HD12	1:B:142:PRO:HD3	1.49	0.92
1:B:62[B]:GLN:NE2	1:B:151[B]:ILE:CD1	2.36	0.88
1:A:94:GLY:HA3	7:A:1227:TAM:H11	1.57	0.87
1:B:95[B]:GLN:CD	8:B:2023:HOH:O	2.12	0.87
1:B:141[B]:ILE:HG23	1:B:143:TYR:CE2	2.12	0.84
1:B:62[B]:GLN:HE22	1:B:151[B]:ILE:HD11	1.38	0.84
1:A:127:LYS:HE3	8:A:2059:HOH:O	1.79	0.83
1:B:171:HIS:HD2	3:B:1213:SO4:O2	1.63	0.82
1:B:94:GLY:HA3	7:B:1220:TAM:H11	1.62	0.81
1:B:156:LYS:HB2	1:B:156:LYS:NZ	1.99	0.77
1:B:95[B]:GLN:NE2	8:B:2023:HOH:O	2.17	0.77
6:A:1226:GOL:O1	8:A:2012:HOH:O	2.02	0.75
4:A:1219:EDO:H21	8:A:2101:HOH:O	1.86	0.74
1:B:62[B]:GLN:HE21	1:B:151[B]:ILE:HD11	1.48	0.74
7:B:1220:TAM:H42	8:B:2022:HOH:O	1.87	0.72
1:B:68:LEU:O	1:B:69:GLU:HB2	1.91	0.70
1:B:57:SER:OG	8:B:2002:HOH:O	1.89	0.69
1:A:58:PRO:HB2	4:A:1217:EDO:H22	1.76	0.68
1:A:123:SER:OG	7:A:1227:TAM:H12	1.94	0.68
5:A:1224:CL:CL	7:A:1227:TAM:H62	2.32	0.66
1:B:127:LYS:HE3	8:B:2045:HOH:O	1.96	0.66
1:B:62[B]:GLN:HE21	1:B:151[B]:ILE:CD1	2.04	0.65
1:B:139:ASP:OD1	1:B:141[B]:ILE:HG22	1.95	0.65
1:A:171:HIS:HD2	3:A:1216:SO4:O1	1.81	0.63
1:B:156:LYS:HB2	1:B:156:LYS:HZ2	1.63	0.63
1:A:69:GLU:HG3	8:A:2009:HOH:O	1.98	0.63
8:A:2099:HOH:O	1:B:95[B]:GLN:OE1	2.16	0.62
1:B:156:LYS:CB	1:B:156:LYS:NZ	2.62	0.62
1:B:141[B]:ILE:CG2	1:B:143:TYR:CE2	2.82	0.60
1:B:69:GLU:OE2	6:B:1219:GOL:C1	2.49	0.60
1:A:87[B]:GLU:OE2	1:A:89:ILE:CG2	2.50	0.59
3:A:1215:SO4:O1	8:A:2023:HOH:O	2.17	0.59
1:B:111:LYS:HD2	4:B:1216:EDO:H21	1.86	0.57
1:B:171:HIS:CD2	3:B:1213:SO4:O2	2.53	0.57
1:A:209:GLN:NE2	1:B:202[B]:ASP:OD1	2.37	0.56
1:A:69:GLU:CG	8:A:2009:HOH:O	2.54	0.56
1:A:125[B]:THR:H	7:A:1227:TAM:HN1	1.54	0.56
1:A:69:GLU:CA	8:A:2009:HOH:O	2.54	0.55
1:B:125:THR:OG1	7:B:1220:TAM:N	2.40	0.55
1:A:125[A]:THR:H	7:A:1227:TAM:HN1	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:218:0MB:HAI2	1:B:198:GLU:OE2	2.06	0.54
1:A:171:HIS:CD2	3:A:1216:SO4:O1	2.60	0.53
1:B:56:SER:CB	8:B:2003:HOH:O	2.57	0.52
1:B:69:GLU:HA	8:B:2008:HOH:O	2.08	0.52
1:A:123:SER:OG	7:A:1227:TAM:C1	2.58	0.52
1:B:89:ILE:HB	1:B:90:PRO:HD2	1.92	0.51
1:B:141[B]:ILE:CG2	1:B:143:TYR:CZ	2.93	0.51
1:B:87[B]:GLU:OE2	1:B:89:ILE:CG2	2.59	0.51
1:B:127:LYS:CE	8:B:2045:HOH:O	2.55	0.50
1:B:141[B]:ILE:HG23	1:B:143:TYR:CZ	2.47	0.50
1:B:69:GLU:CA	8:B:2008:HOH:O	2.60	0.49
1:A:136[A]:LYS:HE2	1:A:138:GLU:OE2	2.12	0.49
1:A:199:ARG:NH2	8:A:2016:HOH:O	2.46	0.49
1:B:69:GLU:N	8:B:2008:HOH:O	2.46	0.49
1:A:188:LYS:HA	1:A:189:GLY:HA2	1.65	0.48
1:A:95[A]:GLN:HG3	7:A:1227:TAM:C5	2.44	0.48
1:B:156:LYS:HB2	1:B:156:LYS:HZ3	1.79	0.48
1:B:141[B]:ILE:CD1	1:B:142:PRO:HD3	2.22	0.48
1:A:209:GLN:HE22	1:B:202[B]:ASP:CG	2.18	0.47
1:B:181:PHE:O	1:B:185:HIS:HD2	1.96	0.47
1:B:94:GLY:H	7:B:1220:TAM:H42	1.80	0.47
7:B:1220:TAM:C4	8:B:2022:HOH:O	2.56	0.46
1:B:129:ALA:HA	4:B:1217:EDO:H21	1.97	0.46
1:A:87[B]:GLU:OE2	1:A:89:ILE:HG21	2.15	0.45
5:A:1223:CL:CL	7:A:1227:TAM:C4	2.90	0.45
1:B:87[B]:GLU:OE2	1:B:89:ILE:HG21	2.17	0.45
1:A:69:GLU:N	8:A:2009:HOH:O	2.51	0.44
8:A:2083:HOH:O	4:B:1217:EDO:H11	2.18	0.44
1:B:109:PRO:HD3	2:B:218:0MB:CAD	2.48	0.44
1:B:89:ILE:HB	1:B:90:PRO:CD	2.48	0.43
2:B:218:0MB:HAF1	2:B:218:0MB:HAI1	1.64	0.43
1:B:68:LEU:O	1:B:69:GLU:CB	2.60	0.43
1:A:125[A]:THR:OG1	7:A:1227:TAM:N	2.52	0.43
1:A:127:LYS:CE	8:A:2059:HOH:O	2.52	0.43
7:B:1220:TAM:HN1	7:B:1220:TAM:H61	1.34	0.42
1:B:161:ILE:HG21	1:B:179:ALA:HA	2.01	0.42
7:A:1227:TAM:H41	7:A:1227:TAM:H32	1.76	0.42
1:B:156:LYS:HG3	8:B:2063:HOH:O	2.18	0.42
1:A:98:ALA:HB1	1:A:129:ALA:HB2	2.01	0.42
1:A:99:TYR:CE2	1:A:103[B]:LYS:HD2	2.55	0.42
1:A:95[B]:GLN:NE2	8:A:2034:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:HE2	1:B:138:GLU:OE2	2.21	0.41
1:A:62[B]:GLN:NE2	1:A:151:ILE:HG13	2.37	0.41
1:B:98:ALA:HB1	1:B:129:ALA:HB2	2.03	0.41
1:A:89:ILE:HB	1:A:90:PRO:HD2	2.03	0.40
1:B:99:TYR:CE2	1:B:103[B]:LYS:HD2	2.56	0.40
1:A:69:GLU:HA	8:A:2009:HOH:O	2.18	0.40
1:A:161:ILE:HG21	1:A:179:ALA:HA	2.03	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	162/183 (88%)	158 (98%)	4 (2%)	0	100	100
1	B	159/183 (87%)	158 (99%)	1 (1%)	0	100	100
All	All	321/366 (88%)	316 (98%)	5 (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	137/150 (91%)	136 (99%)	1 (1%)	87	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	136/150 (91%)	133 (98%)	3 (2%)	57 38
All	All	273/300 (91%)	269 (98%)	4 (2%)	68 55

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	B	57	SER
1	B	156	LYS
1	B	188	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	209	GLN
1	B	155	ASN
1	B	171	HIS
1	B	185	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 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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	A	1212	-	4,4,4	0.21	0	6,6,6	1.30	2 (33%)
3	SO4	A	1213	-	4,4,4	0.45	0	6,6,6	1.15	0
3	SO4	A	1214	-	4,4,4	0.36	0	6,6,6	1.07	0
3	SO4	A	1215	-	4,4,4	0.84	0	6,6,6	2.25	3 (50%)
3	SO4	A	1216	-	4,4,4	0.37	0	6,6,6	0.43	0
4	EDO	A	1217	-	3,3,3	0.43	0	2,2,2	0.83	0
4	EDO	A	1218	-	3,3,3	0.36	0	2,2,2	0.69	0
4	EDO	A	1219	-	3,3,3	0.62	0	2,2,2	1.15	0
4	EDO	A	1220	-	3,3,3	0.87	0	2,2,2	0.53	0
4	EDO	A	1221	-	3,3,3	0.48	0	2,2,2	1.03	0
4	EDO	A	1222	-	3,3,3	0.58	0	2,2,2	0.32	0
6	GOL	A	1226	-	5,5,5	0.34	0	5,5,5	1.13	0
7	TAM	A	1227	-	7,10,10	1.30	1 (14%)	9,12,12	4.24	8 (88%)
2	OMB	A	218	-	15,20,20	1.47	2 (13%)	14,26,26	2.29	6 (42%)
3	SO4	B	1210	-	4,4,4	0.27	0	6,6,6	1.26	1 (16%)
3	SO4	B	1211	-	4,4,4	0.71	0	6,6,6	1.32	1 (16%)
3	SO4	B	1212	-	4,4,4	0.36	0	6,6,6	1.30	2 (33%)
3	SO4	B	1213	-	4,4,4	0.29	0	6,6,6	0.67	0
3	SO4	B	1214	-	4,4,4	1.03	0	6,6,6	2.38	4 (66%)
4	EDO	B	1215	-	3,3,3	0.46	0	2,2,2	0.67	0
4	EDO	B	1216	-	3,3,3	0.26	0	2,2,2	0.88	0
4	EDO	B	1217	-	3,3,3	0.32	0	2,2,2	0.94	0
6	GOL	B	1219	-	5,5,5	0.47	0	5,5,5	0.70	0
7	TAM	B	1220	-	7,10,10	1.24	1 (14%)	9,12,12	3.32	6 (66%)
2	OMB	B	218	-	15,20,20	1.46	2 (13%)	14,26,26	2.37	7 (50%)

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	SO4	A	1212	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1213	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1214	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1215	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1216	-	-	0/0/0/0	0/0/0/0
4	EDO	A	1217	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1218	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1219	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1220	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1221	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1222	-	-	0/1/1/1	0/0/0/0
6	GOL	A	1226	-	-	0/4/4/4	0/0/0/0
7	TAM	A	1227	-	-	0/12/12/12	0/0/0/0
2	0MB	A	218	-	-	0/4/17/17	1/2/3/3
3	SO4	B	1210	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1211	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1212	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1213	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1214	-	-	0/0/0/0	0/0/0/0
4	EDO	B	1215	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1216	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1217	-	-	0/1/1/1	0/0/0/0
6	GOL	B	1219	-	-	0/4/4/4	0/0/0/0
7	TAM	B	1220	-	-	0/12/12/12	0/0/0/0
2	0MB	B	218	-	-	0/4/17/17	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1227	TAM	C1-C4	2.31	1.56	1.52
7	B	1220	TAM	C1-C4	2.47	1.57	1.52
2	B	218	0MB	CAO-NK	2.73	1.39	1.35
2	A	218	0MB	CAO-NK	3.07	1.39	1.35
2	A	218	0MB	CAP-NQ	3.67	1.37	1.32
2	B	218	0MB	CAP-NQ	4.11	1.38	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1227	TAM	C3-C-N	-7.90	90.54	107.94
7	B	1220	TAM	C3-C-N	-7.27	91.93	107.94
2	B	218	0MB	CAB-CAD-CAN	-4.87	114.39	120.57
2	A	218	0MB	CAI-CAG-NL	-4.79	106.13	112.87
3	B	1214	SO4	O3-S-O2	-3.79	88.36	109.26
3	A	1215	SO4	O4-S-O1	-3.69	88.89	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	0MB	CAC-CAE-CAN	-3.69	115.90	120.57
2	B	218	0MB	CAI-CAG-NL	-3.61	107.79	112.87
7	A	1227	TAM	C3-C-C2	-3.13	104.99	110.50
7	B	1220	TAM	C3-C-C1	-3.08	105.06	110.50
2	B	218	0MB	CAA-CAC-CAE	-2.56	116.69	120.21
2	A	218	0MB	CAA-CAB-CAD	-2.48	116.80	120.21
2	A	218	0MB	NK-CAO-NJ	-2.39	117.34	122.17
3	B	1210	SO4	O3-S-O2	-2.33	96.40	109.26
3	A	1212	SO4	O3-S-O1	-2.32	96.49	109.26
3	B	1214	SO4	O4-S-O1	-2.26	96.83	109.26
3	B	1212	SO4	O4-S-O3	-2.23	98.89	108.96
7	A	1227	TAM	C3-C-C1	-2.14	106.74	110.50
3	A	1215	SO4	O3-S-O2	-2.12	97.55	109.26
2	B	218	0MB	C10-C9-CAF	-2.07	109.01	113.82
2	B	218	0MB	NK-CAO-NJ	-2.06	118.01	122.17
3	A	1212	SO4	O4-S-O3	2.02	118.08	108.96
3	B	1212	SO4	O3-S-O1	2.18	121.27	109.26
7	A	1227	TAM	C1-C-N	2.35	113.12	107.94
2	A	218	0MB	CAB-CAD-CAN	2.38	123.58	120.57
3	B	1214	SO4	O4-S-O2	2.45	122.77	109.26
7	A	1227	TAM	C2-C-C1	2.45	114.83	110.50
3	B	1211	SO4	O4-S-O3	2.46	120.03	108.96
7	B	1220	TAM	C2-C-N	2.50	113.44	107.94
2	B	218	0MB	CAE-CAN-CAD	2.58	122.72	117.59
3	A	1215	SO4	O4-S-O3	2.61	120.70	108.96
3	B	1214	SO4	O4-S-O3	2.69	121.07	108.96
7	B	1220	TAM	O4-C4-C1	2.79	119.23	111.33
2	A	218	0MB	CAA-CAC-CAE	3.07	124.42	120.21
2	B	218	0MB	CAA-CAB-CAD	3.12	124.50	120.21
7	B	1220	TAM	C1-C-N	3.24	115.08	107.94
7	B	1220	TAM	C2-C-C1	3.39	116.48	110.50
7	A	1227	TAM	O4-C4-C1	3.72	121.87	111.33
7	A	1227	TAM	O5-C5-C2	4.40	123.78	111.33
7	A	1227	TAM	C2-C-N	6.32	121.87	107.94

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	218	0MB	C10-C9-CAF-CAG-CAI-NL-NQ

13 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1215	SO4	1	0
3	A	1216	SO4	2	0
4	A	1217	EDO	1	0
4	A	1219	EDO	1	0
6	A	1226	GOL	4	0
7	A	1227	TAM	11	0
2	A	218	0MB	1	0
3	B	1213	SO4	2	0
4	B	1216	EDO	1	0
4	B	1217	EDO	2	0
6	B	1219	GOL	2	0
7	B	1220	TAM	6	0
2	B	218	0MB	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 [i](#)

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

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	154/183 (84%)	-0.59	0 100 100	9, 16, 40, 66	14 (9%)
1	B	150/183 (81%)	-0.65	0 100 100	9, 16, 36, 52	14 (9%)
All	All	304/366 (83%)	-0.62	0 100 100	9, 16, 37, 66	28 (9%)

There are no RSRZ outliers to report.

### 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
3	SO4	B	1214	5/5	0.81	0.17	4.91	18,26,32,39	5
4	EDO	B	1215	4/4	0.95	0.18	4.53	43,48,50,62	0
4	EDO	A	1217	4/4	0.95	0.16	4.37	35,42,44,58	0
3	SO4	B	1211	5/5	0.86	0.13	3.85	29,36,44,51	5
7	TAM	A	1227	11/11	0.87	0.13	3.34	22,32,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	TAM	B	1220	11/11	0.89	0.13	2.84	25,34,42,43	0
3	SO4	A	1215	5/5	0.81	0.14	2.32	22,25,32,41	5
3	SO4	B	1210	5/5	0.98	0.10	2.27	23,23,26,28	5
4	EDO	A	1218	4/4	0.91	0.09	2.06	33,37,43,48	0
4	EDO	A	1221	4/4	0.93	0.07	1.95	34,38,38,39	0
2	OMB	B	218	18/18	0.93	0.09	1.76	16,27,45,46	0
3	SO4	A	1213	5/5	0.90	0.11	1.74	34,46,51,55	5
3	SO4	A	1212	5/5	0.98	0.11	1.62	23,23,24,29	5
6	GOL	A	1226	6/6	0.89	0.14	1.14	34,37,40,43	0
2	OMB	A	218	18/18	0.94	0.09	1.10	16,25,44,46	0
4	EDO	A	1220	4/4	0.87	0.09	1.10	34,38,44,46	0
6	GOL	B	1219	6/6	0.88	0.14	0.96	35,36,42,44	0
4	EDO	B	1217	4/4	0.95	0.07	0.60	35,41,44,44	0
4	EDO	A	1222	4/4	0.97	0.06	0.16	25,35,36,45	0
3	SO4	A	1214	5/5	0.98	0.07	-0.26	28,28,31,40	5
3	SO4	B	1212	5/5	0.97	0.07	-0.42	28,29,30,36	5
4	EDO	A	1219	4/4	0.97	0.06	-0.43	23,27,34,47	0
3	SO4	B	1213	5/5	0.96	0.09	-0.69	34,38,45,50	5
5	CL	B	1218	1/1	0.95	0.06	-1.39	66,66,66,66	0
3	SO4	A	1216	5/5	0.98	0.09	-	37,42,47,50	5
4	EDO	B	1216	4/4	0.96	0.10	-	47,52,56,61	0
5	CL	A	1223	1/1	0.89	0.07	-	61,61,61,61	0
5	CL	A	1225	1/1	0.93	0.10	-	67,67,67,67	0
5	CL	A	1224	1/1	0.96	0.03	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.