



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 06:03 AM EDT

PDB ID : 3N1X  
Title : X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase T201C Mutant  
Authors : Sazinsky, M.H.; McCormick, M.S.; Lippard, S.J.  
Deposited on : 2010-05-17  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

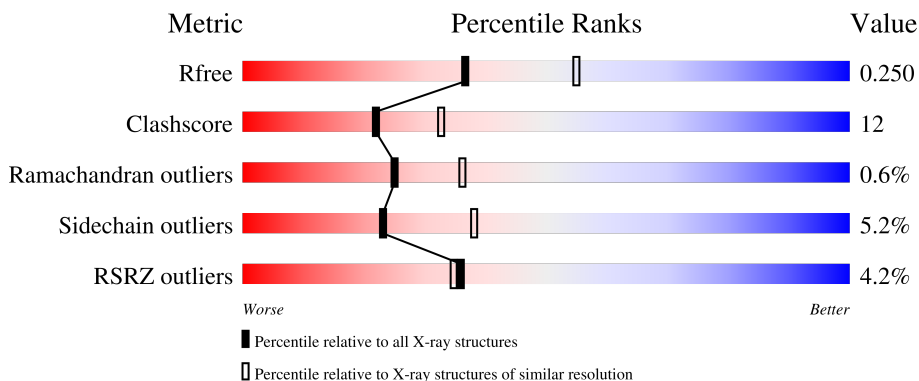
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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	498	 4% (red), 68% (green), 26% (yellow), 5% (orange)
2	B	330	 5% (red), 68% (green), 26% (yellow), ... (orange)
3	C	86	 % (red), 62% (green), 33% (yellow), 5% (orange)

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7520 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 Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	4021	2567	673	754	27	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	THR	engineered mutation	UNP Q6IV66

- Molecule 2 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	324	2658	1685	469	494	10	0	0	0

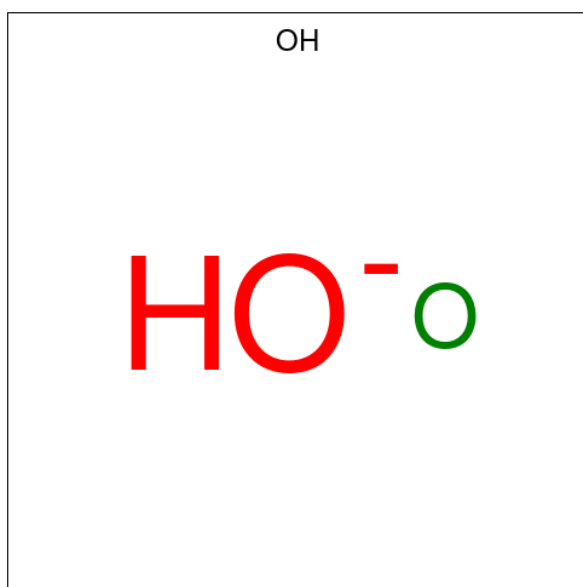
- Molecule 3 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	85	689	432	123	129	5	0	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0

- Molecule 6 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
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

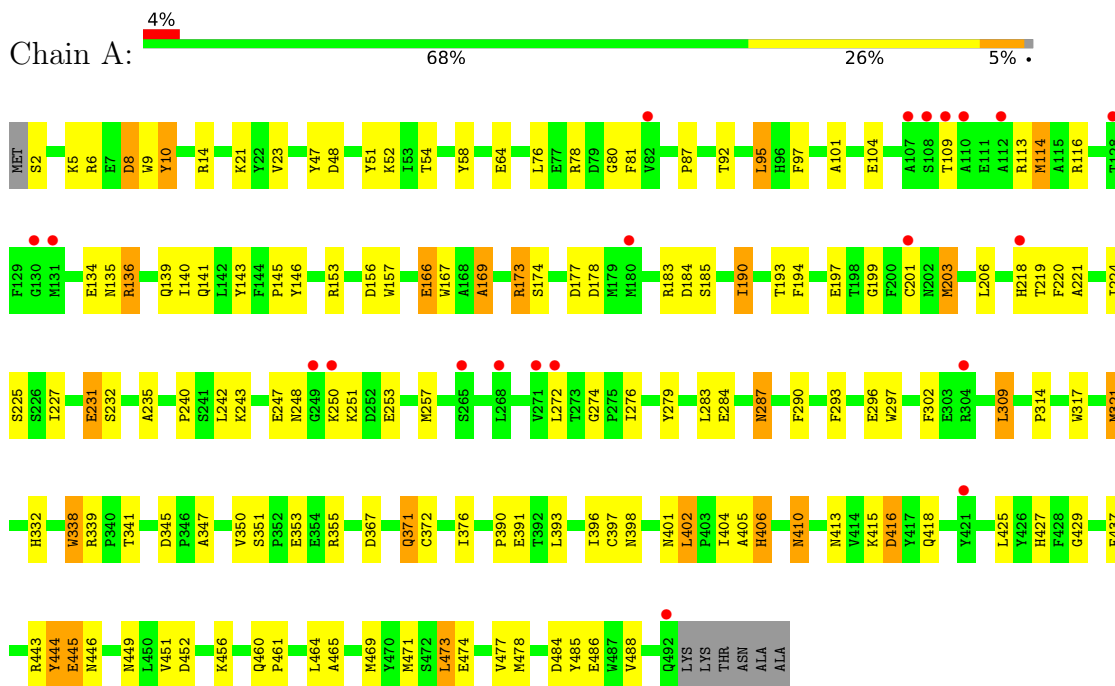
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	62	Total	O	0	0
			62	62		
8	C	5	Total	O	0	0
			5	5		

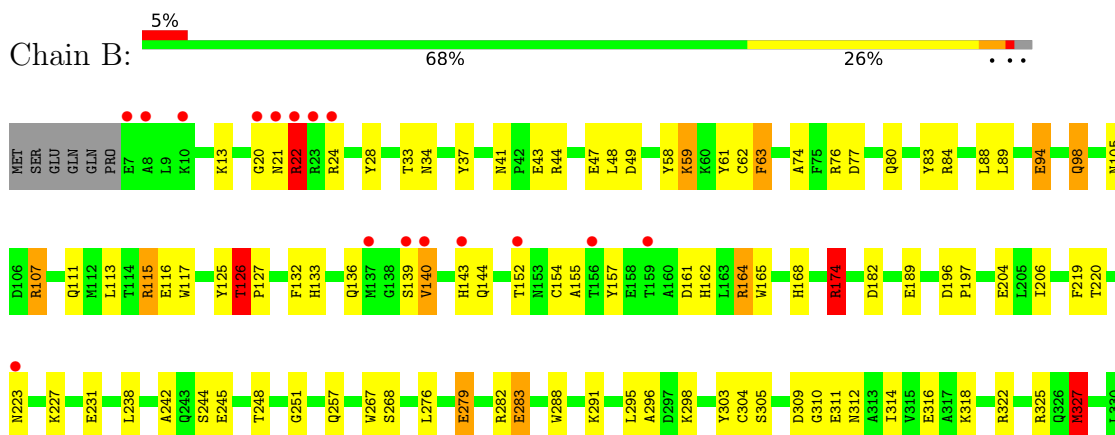
### 3 Residue-property plots [i](#)

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: Toluene o-xylene monooxygenase component

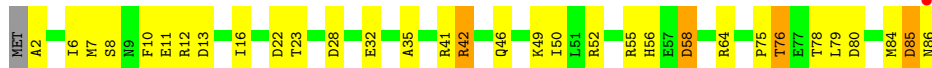


- Molecule 2: Toluene o-xylene monooxygenase component



- Molecule 3: Toluene o-xylene monooxygenase component

Chain C:  %



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.29Å 183.29Å 68.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.02 – 2.40 38.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.02-2.40) 99.2 (38.02-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.90 (at 2.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.184 , 0.242 0.193 , 0.250	Depositor DCC
$R_{free}$ test set	2592 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: OH, FE, SO4, 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	1.46	28/4148 (0.7%)	1.26	33/5637 (0.6%)
2	B	1.54	32/2730 (1.2%)	1.20	14/3711 (0.4%)
3	C	1.29	1/703 (0.1%)	1.28	6/952 (0.6%)
All	All	1.48	61/7581 (0.8%)	1.24	53/10300 (0.5%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	PHE	CE2-CZ	8.88	1.54	1.37
2	B	283	GLU	CB-CG	8.02	1.67	1.52
2	B	182	ASP	CB-CG	7.98	1.68	1.51
2	B	311	GLU	CG-CD	7.68	1.63	1.51
1	A	101	ALA	CA-CB	7.18	1.67	1.52
2	B	116	GLU	CG-CD	7.15	1.62	1.51
2	B	155	ALA	CA-CB	7.07	1.67	1.52
2	B	74	ALA	CA-CB	6.68	1.66	1.52
1	A	231	GLU	CB-CG	6.54	1.64	1.52
2	B	165	TRP	CZ3-CH2	6.54	1.50	1.40
2	B	311	GLU	CD-OE2	6.40	1.32	1.25
1	A	253	GLU	CG-CD	6.39	1.61	1.51
3	C	32	GLU	CG-CD	6.38	1.61	1.51
1	A	201	CYS	CB-SG	-6.36	1.71	1.82
2	B	140	VAL	CB-CG1	6.30	1.66	1.52
1	A	64	GLU	CG-CD	6.26	1.61	1.51
1	A	402	LEU	CG-CD2	6.19	1.74	1.51
2	B	157	TYR	CE2-CZ	6.12	1.46	1.38
2	B	44	ARG	CB-CG	6.12	1.69	1.52
1	A	64	GLU	CB-CG	6.09	1.63	1.52
2	B	283	GLU	CG-CD	6.03	1.60	1.51
2	B	37	TYR	CD1-CE1	5.98	1.48	1.39
2	B	251	GLY	N-CA	5.89	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	TYR	CG-CD1	5.70	1.46	1.39
1	A	353	GLU	CG-CD	5.67	1.60	1.51
2	B	98	GLN	CG-CD	5.66	1.64	1.51
1	A	444	TYR	CE2-CZ	5.61	1.45	1.38
2	B	63	PHE	CE1-CZ	5.60	1.48	1.37
1	A	157	TRP	CB-CG	5.51	1.60	1.50
2	B	61	TYR	CE1-CZ	5.50	1.45	1.38
1	A	143	TYR	CD2-CE2	5.49	1.47	1.39
1	A	465	ALA	CA-CB	5.49	1.64	1.52
1	A	284	GLU	CG-CD	5.49	1.60	1.51
2	B	47	GLU	CG-CD	5.44	1.60	1.51
1	A	51	TYR	CD2-CE2	5.44	1.47	1.39
1	A	58	TYR	CD1-CE1	-5.42	1.31	1.39
2	B	94	GLU	CG-CD	5.39	1.60	1.51
2	B	174	ARG	CB-CG	-5.39	1.38	1.52
2	B	43	GLU	CG-CD	5.38	1.60	1.51
2	B	62	CYS	CB-SG	5.37	1.91	1.82
1	A	437	PHE	CG-CD1	5.36	1.46	1.38
1	A	146	TYR	CD2-CE2	5.35	1.47	1.39
1	A	437	PHE	CD1-CE1	5.33	1.50	1.39
2	B	303	TYR	CD2-CE2	5.31	1.47	1.39
2	B	296	ALA	CA-CB	5.30	1.63	1.52
1	A	231	GLU	CG-CD	5.29	1.59	1.51
2	B	132	PHE	CE2-CZ	5.29	1.47	1.37
1	A	169	ALA	CA-CB	5.28	1.63	1.52
1	A	23	VAL	CB-CG1	5.26	1.63	1.52
1	A	167	TRP	CB-CG	5.25	1.59	1.50
2	B	28	TYR	CE1-CZ	5.25	1.45	1.38
1	A	350	VAL	CB-CG2	5.12	1.63	1.52
2	B	231	GLU	CB-CG	5.12	1.61	1.52
2	B	279	GLU	CG-CD	5.12	1.59	1.51
1	A	166	GLU	CG-CD	5.11	1.59	1.51
1	A	279	TYR	CD1-CE1	5.11	1.47	1.39
1	A	10	TYR	CE2-CZ	5.05	1.45	1.38
2	B	116	GLU	CD-OE1	5.05	1.31	1.25
1	A	338	TRP	CE3-CZ3	5.05	1.47	1.38
2	B	58	TYR	CG-CD1	5.03	1.45	1.39
2	B	291	LYS	CD-CE	5.00	1.63	1.51

All (53) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	A	173	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	A	443	ARG	NE-CZ-NH1	11.50	126.05	120.30
3	C	42	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	A	136	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	A	443	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	136	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	A	173	ARG	NE-CZ-NH1	9.52	125.06	120.30
2	B	115	ARG	NE-CZ-NH1	8.42	124.51	120.30
2	B	164	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	156	ASP	CB-CG-OD2	7.82	125.34	118.30
1	A	339	ARG	NE-CZ-NH1	-7.67	116.47	120.30
2	B	44	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	416	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	257	MET	CG-SD-CE	-7.17	88.72	100.20
3	C	58	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	116	ARG	NE-CZ-NH1	-7.10	116.75	120.30
2	B	325	ARG	NE-CZ-NH2	-7.08	116.76	120.30
3	C	58	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	339	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	B	174	ARG	NE-CZ-NH2	6.63	123.61	120.30
3	C	42	ARG	CG-CD-NE	-6.49	98.17	111.80
1	A	48	ASP	CB-CG-OD1	6.49	124.14	118.30
3	C	41	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	177	ASP	CB-CG-OD1	6.44	124.09	118.30
2	B	115	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	201	CYS	CA-CB-SG	-6.31	102.64	114.00
1	A	153	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	14	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	248	ASN	C-N-CA	-6.19	109.30	122.30
1	A	141	GLN	CA-CB-CG	-6.16	99.85	113.40
1	A	287	ASN	CB-CA-C	6.13	122.65	110.40
1	A	478	MET	CG-SD-CE	-6.09	90.45	100.20
1	A	345	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	184	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	114	MET	CG-SD-CE	-5.92	90.73	100.20
2	B	182	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	473	LEU	CB-CG-CD2	-5.88	101.00	111.00
2	B	84	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	48	ASP	CB-CG-OD2	-5.67	113.19	118.30
2	B	44	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	8	ASP	CB-CG-OD2	-5.38	113.46	118.30
2	B	59	LYS	CD-CE-NZ	5.34	123.98	111.70
1	A	183	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	321	MET	CG-SD-CE	-5.28	91.76	100.20
2	B	174	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	190	ILE	CB-CA-C	-5.19	101.21	111.60
1	A	184	ASP	CB-CG-OD1	5.15	122.94	118.30
3	C	41	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	153	ARG	CG-CD-NE	-5.12	101.05	111.80
2	B	283	GLU	CA-CB-CG	5.10	124.63	113.40
2	B	327	MET	CG-SD-CE	5.07	108.30	100.20

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	4021	0	3770	92	0
2	B	2658	0	2554	67	0
3	C	689	0	678	29	0
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	A	4	0	6	0	0
7	B	5	0	0	0	0
8	A	73	0	0	0	0
8	B	62	0	0	0	0
8	C	5	0	0	0	0
All	All	7520	0	7008	169	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 12.

All (169) 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:402:LEU:CD2	1:A:402:LEU:CG	1.74	1.59
2:B:219:PHE:O	2:B:223:ASN:HB2	1.53	1.06
1:A:445:GLU:HG2	1:A:446:ASN:H	1.16	1.06
1:A:445:GLU:HG2	1:A:446:ASN:N	1.70	1.05
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.22	1.04
1:A:445:GLU:CG	1:A:446:ASN:N	2.27	0.96
2:B:305:SER:HB3	2:B:314:ILE:HD11	1.52	0.90
2:B:126:THR:HB	2:B:189:GLU:CG	2.01	0.90
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.20	0.89
2:B:126:THR:OG1	2:B:127:PRO:HD3	1.72	0.88
1:A:139:GLN:HE22	2:B:83:TYR:H	1.19	0.88
1:A:372:CYS:O	1:A:376:ILE:HD13	1.75	0.85
1:A:474:GLU:O	1:A:477:VAL:HG22	1.76	0.84
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.12	0.83
2:B:126:THR:HB	2:B:189:GLU:HG3	1.62	0.80
2:B:327:MET:HA	2:B:327:MET:CE	2.11	0.80
1:A:8:ASP:O	2:B:174:ARG:HD2	1.85	0.77
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.67	0.77
1:A:76:LEU:CD1	1:A:218:HIS:HB2	2.14	0.76
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.05	0.75
1:A:445:GLU:HG2	2:B:49:ASP:OD1	1.85	0.75
3:C:2:ALA:HA	3:C:23:THR:OG1	1.86	0.73
1:A:2:SER:N	2:B:105:ASN:HD22	1.85	0.73
1:A:9:TRP:HB3	2:B:174:ARG:HG3	1.71	0.72
2:B:219:PHE:O	2:B:223:ASN:CB	2.37	0.70
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.91	0.69
2:B:126:THR:HG21	2:B:189:GLU:OE1	1.93	0.68
3:C:52:ARG:HH11	3:C:52:ARG:HG3	1.59	0.67
3:C:55:ARG:HD2	3:C:58:ASP:OD1	1.94	0.67
1:A:9:TRP:CB	2:B:174:ARG:HG3	2.24	0.67
2:B:162:HIS:HE1	2:B:227:LYS:HZ3	1.42	0.67
1:A:203:MET:HG3	1:A:297:TRP:HB3	1.78	0.66
3:C:56:HIS:HD2	3:C:80:ASP:OD1	1.79	0.65
1:A:367:ASP:HB3	1:A:410:ASN:ND2	2.12	0.65
3:C:75:PRO:O	3:C:76:THR:CB	2.45	0.65
3:C:75:PRO:O	3:C:76:THR:HB	1.97	0.64
1:A:402:LEU:CD2	1:A:402:LEU:CD1	2.70	0.64
1:A:398:ASN:HD22	1:A:427:HIS:H	1.45	0.64
2:B:21:ASN:O	2:B:22:ARG:HB2	1.98	0.63
2:B:59:LYS:HA	2:B:63:PHE:HD2	1.64	0.62
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.34	0.62
1:A:92:THR:HG23	1:A:276:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLU:H	1:A:477:VAL:CG2	2.13	0.62
2:B:327:MET:HA	2:B:327:MET:HE2	1.81	0.62
1:A:402:LEU:CD2	1:A:402:LEU:CB	2.75	0.61
2:B:204:GLU:OE1	2:B:298:LYS:NZ	2.33	0.61
2:B:126:THR:HB	2:B:189:GLU:HG2	1.79	0.61
2:B:21:ASN:O	2:B:22:ARG:CB	2.50	0.59
2:B:126:THR:CB	2:B:127:PRO:HD3	2.33	0.59
2:B:143:HIS:CG	2:B:152:THR:HG23	2.37	0.59
3:C:75:PRO:O	3:C:76:THR:HG22	2.02	0.58
1:A:405:ALA:O	1:A:406:HIS:HB2	2.01	0.58
1:A:243:LYS:O	1:A:247:GLU:HG3	2.05	0.57
1:A:317:TRP:O	1:A:321:MET:HG2	2.05	0.57
2:B:219:PHE:HE1	2:B:223:ASN:HD22	1.50	0.56
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.87	0.56
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.88	0.56
1:A:139:GLN:NE2	2:B:83:TYR:H	1.97	0.56
2:B:33:THR:HB	2:B:34:ASN:HD22	1.71	0.56
1:A:97:PHE:CD2	1:A:145:PRO:HB3	2.40	0.55
1:A:95:LEU:HD12	1:A:95:LEU:C	2.27	0.55
1:A:231:GLU:OE1	5:A:501:OH:O	2.25	0.55
2:B:94:GLU:O	2:B:98:GLN:HG2	2.07	0.55
1:A:427:HIS:HE1	3:C:76:THR:CG2	2.08	0.55
1:A:95:LEU:HD11	1:A:272:LEU:HD22	1.87	0.55
1:A:413:ASN:OD1	1:A:415:LYS:HE2	2.08	0.54
2:B:126:THR:CG2	2:B:189:GLU:OE1	2.55	0.54
2:B:219:PHE:CE1	2:B:223:ASN:ND2	2.76	0.54
2:B:327:MET:HA	2:B:327:MET:HE3	1.88	0.54
1:A:218:HIS:O	1:A:219:THR:C	2.46	0.53
1:A:190:ILE:HD12	1:A:242:LEU:CD2	2.38	0.53
3:C:52:ARG:HG3	3:C:52:ARG:NH1	2.23	0.52
1:A:485:TYR:O	1:A:488:VAL:HB	2.09	0.52
1:A:416:ASP:H	3:C:56:HIS:CE1	2.28	0.52
2:B:161:ASP:O	2:B:164:ARG:HB3	2.11	0.51
2:B:305:SER:CB	2:B:314:ILE:HD11	2.32	0.51
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.58	0.51
1:A:220:PHE:CE2	1:A:224:ILE:HG13	2.46	0.51
1:A:193:THR:HA	1:A:197:GLU:OE1	2.11	0.50
3:C:85:ASP:O	3:C:86:ASN:CB	2.59	0.50
1:A:449:ASN:O	1:A:452:ASP:HB2	2.11	0.50
2:B:127:PRO:HA	2:B:189:GLU:HB3	1.93	0.50
2:B:107:ARG:O	2:B:107:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:ALA:O	3:C:23:THR:N	2.42	0.50
3:C:2:ALA:O	3:C:22:ASP:HA	2.12	0.49
1:A:445:GLU:CG	2:B:49:ASP:OD1	2.60	0.49
3:C:75:PRO:O	3:C:76:THR:CG2	2.60	0.49
2:B:77:ASP:HB2	2:B:154:CYS:SG	2.53	0.49
2:B:125:TYR:O	2:B:126:THR:C	2.50	0.49
1:A:460:GLN:HA	1:A:461:PRO:C	2.33	0.49
3:C:50:ILE:N	3:C:84:MET:O	2.26	0.48
3:C:28:ASP:OD1	3:C:64:ARG:HB3	2.13	0.48
3:C:13:ASP:OD1	3:C:42:ARG:HD2	2.13	0.48
1:A:218:HIS:O	1:A:221:ALA:N	2.47	0.48
1:A:391:GLU:HA	1:A:464:LEU:HD11	1.94	0.48
2:B:223:ASN:ND2	2:B:268:SER:OG	2.47	0.48
1:A:135:ASN:O	1:A:139:GLN:HG3	2.13	0.47
1:A:444:TYR:O	1:A:445:GLU:C	2.53	0.47
1:A:351:SER:O	1:A:355:ARG:HG3	2.14	0.47
1:A:341:THR:HA	1:A:473:LEU:HD13	1.95	0.47
1:A:76:LEU:CD1	1:A:218:HIS:CB	2.90	0.47
2:B:304:CYS:HB2	2:B:314:ILE:HG12	1.97	0.47
3:C:6:ILE:HD13	3:C:79:LEU:HD12	1.96	0.47
1:A:396:ILE:CG2	1:A:401:ASN:HA	2.45	0.46
1:A:166:GLU:HA	1:A:471:MET:HB3	1.98	0.46
1:A:169:ALA:O	1:A:173:ARG:HG3	2.15	0.46
1:A:332:HIS:HE1	1:A:347:ALA:O	1.99	0.46
2:B:133:HIS:O	2:B:136:GLN:HB3	2.15	0.46
2:B:312:ASN:O	2:B:316:GLU:HG3	2.16	0.46
1:A:76:LEU:HD11	1:A:218:HIS:HB2	1.95	0.46
1:A:76:LEU:HD11	1:A:218:HIS:CB	2.46	0.45
2:B:117:TRP:CZ2	2:B:242:ALA:HA	2.52	0.45
2:B:117:TRP:CE3	2:B:245:GLU:HG3	2.52	0.45
2:B:305:SER:HB3	2:B:314:ILE:CD1	2.35	0.45
2:B:126:THR:HG1	2:B:127:PRO:HD3	1.79	0.45
1:A:6:ARG:HD2	1:A:54:THR:HG23	1.99	0.44
1:A:445:GLU:HG3	1:A:446:ASN:N	2.24	0.44
3:C:7:MET:HG2	3:C:76:THR:O	2.16	0.44
1:A:104:GLU:O	1:A:134:GLU:HB3	2.18	0.44
3:C:10:PHE:CE1	3:C:35:ALA:HA	2.52	0.44
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.52	0.44
1:A:371:GLN:H	1:A:371:GLN:HG2	1.64	0.44
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.52	0.44
1:A:10:TYR:CZ	1:A:52:LYS:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:O	1:A:81:PHE:C	2.56	0.44
1:A:190:ILE:O	1:A:194:PHE:HB3	2.17	0.43
2:B:318:LYS:O	2:B:322:ARG:HG3	2.18	0.43
2:B:126:THR:CB	2:B:127:PRO:CD	2.97	0.43
2:B:276:LEU:HD22	2:B:282:ARG:HB2	2.01	0.43
1:A:367:ASP:HB3	1:A:410:ASN:HD21	1.82	0.43
1:A:178:ASP:HA	2:B:48:LEU:HD11	2.01	0.43
2:B:295:LEU:HD23	2:B:295:LEU:HA	1.80	0.43
1:A:404:ILE:HG12	1:A:429:GLY:HA2	2.01	0.42
1:A:416:ASP:H	3:C:56:HIS:HE1	1.67	0.42
1:A:474:GLU:H	1:A:477:VAL:HG22	1.83	0.42
1:A:398:ASN:ND2	1:A:427:HIS:H	2.15	0.42
2:B:304:CYS:O	2:B:310:GLY:HA2	2.19	0.42
1:A:293:PHE:CD2	1:A:293:PHE:C	2.93	0.42
1:A:109:THR:HG23	2:B:144:GLN:HB2	2.01	0.42
1:A:232:SER:HA	1:A:235:ALA:HB3	2.02	0.42
2:B:196:ASP:O	2:B:197:PRO:C	2.58	0.42
1:A:78:ARG:HD3	1:A:78:ARG:HA	1.94	0.42
1:A:199:GLY:HA3	1:A:302:PHE:CZ	2.55	0.42
1:A:309:LEU:HD13	1:A:309:LEU:HA	1.85	0.42
1:A:396:ILE:HG12	1:A:451:VAL:HG23	2.02	0.42
1:A:418:GLN:HE22	3:C:78:THR:H	1.68	0.42
1:A:393:LEU:N	1:A:393:LEU:HD23	2.34	0.41
2:B:312:ASN:ND2	2:B:316:GLU:OE1	2.52	0.41
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.55	0.41
2:B:111:GLN:OE1	2:B:111:GLN:N	2.46	0.41
2:B:117:TRP:CH2	2:B:242:ALA:HA	2.55	0.41
3:C:13:ASP:OD2	3:C:42:ARG:NH1	2.52	0.41
1:A:274:GLY:HA2	1:A:290:PHE:CG	2.56	0.41
3:C:46:GLN:O	3:C:49:LYS:HB2	2.21	0.41
1:A:114:MET:HA	1:A:185:SER:OG	2.20	0.41
1:A:224:ILE:HD13	1:A:224:ILE:HA	1.86	0.41
1:A:140:ILE:CG2	1:A:227:ILE:HD11	2.51	0.41
2:B:220:THR:HG21	2:B:288:TRP:HB3	2.02	0.41
3:C:8:SER:O	3:C:16:ILE:HA	2.21	0.41
2:B:88:LEU:HD23	2:B:88:LEU:HA	1.98	0.41
2:B:125:TYR:HB2	2:B:238:LEU:HD21	2.03	0.41
1:A:396:ILE:HG22	1:A:401:ASN:HA	2.03	0.40
2:B:298:LYS:HE2	2:B:298:LYS:HB3	1.90	0.40
1:A:474:GLU:H	1:A:477:VAL:HG21	1.86	0.40
1:A:484:ASP:O	1:A:485:TYR:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLU:C	1:A:488:VAL:H	2.24	0.40
1:A:136:ARG:HB2	2:B:83:TYR:CD1	2.56	0.40
2:B:139:SER:OG	2:B:162:HIS:HD2	2.05	0.40
1:A:76:LEU:HD13	1:A:218:HIS:HB2	2.01	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/498 (98%)	451 (92%)	37 (8%)	2 (0%)	34	48
2	B	322/330 (98%)	310 (96%)	9 (3%)	3 (1%)	17	25
3	C	83/86 (96%)	74 (89%)	9 (11%)	0	100	100
All	All	895/914 (98%)	835 (93%)	55 (6%)	5 (1%)	25	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	GLU
1	A	406	HIS
2	B	22	ARG
2	B	126	THR
2	B	20	GLY

### 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	417/422 (99%)	398 (95%)	19 (5%)	27	43
2	B	276/282 (98%)	257 (93%)	19 (7%)	15	25
3	C	78/79 (99%)	76 (97%)	2 (3%)	46	66
All	All	771/783 (98%)	731 (95%)	40 (5%)	23	38

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	21	LYS
1	A	87	PRO
1	A	95	LEU
1	A	174	SER
1	A	203	MET
1	A	206	LEU
1	A	225	SER
1	A	250	LYS
1	A	251	LYS
1	A	283	LEU
1	A	287	ASN
1	A	296	GLU
1	A	309	LEU
1	A	371	GLN
1	A	397	CYS
1	A	410	ASN
1	A	456	LYS
1	A	469	MET
2	B	13	LYS
2	B	22	ARG
2	B	24	ARG
2	B	41	ASN
2	B	80	GLN
2	B	89	LEU
2	B	107	ARG
2	B	113	LEU
2	B	115	ARG
2	B	126	THR
2	B	140	VAL
2	B	174	ARG
2	B	206	ILE

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Mol	Chain	Res	Type
2	B	244	SER
2	B	248	THR
2	B	279	GLU
2	B	283	GLU
2	B	309	ASP
2	B	327	MET
3	C	76	THR
3	C	85	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	237	GLN
1	A	248	ASN
1	A	322	GLN
1	A	379	ASN
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	34	ASN
2	B	98	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	223	ASN
3	C	56	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 2 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
7	SO4	B	331	-	4,4,4	0.07	0	6,6,6	0.83	0
6	EDO	A	502	4	3,3,3	0.99	0	2,2,2	0.54	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
6	EDO	A	502	4	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	491/498 (98%)	-0.02	21 (4%) 35 33	42, 54, 69, 85	0
2	B	324/330 (98%)	-0.12	16 (4%) 29 28	40, 51, 71, 95	1 (0%)
3	C	85/86 (98%)	-0.32	1 (1%) 79 77	52, 61, 72, 84	0
All	All	900/914 (98%)	-0.09	38 (4%) 36 35	40, 54, 71, 95	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	HIS	6.5
2	B	22	ARG	4.1
2	B	7	GLU	3.7
3	C	86	ASN	3.6
1	A	272	LEU	3.5
2	B	140	VAL	3.5
2	B	223	ASN	3.3
2	B	23	ARG	3.2
1	A	112	ALA	3.2
1	A	268	LEU	3.0
1	A	110	ALA	3.0
2	B	21	ASN	3.0
1	A	107	ALA	2.9
1	A	109	THR	2.9
2	B	159	THR	2.8
2	B	8	ALA	2.7
2	B	137	MET	2.7
1	A	108	SER	2.7
2	B	10	LYS	2.7
2	B	24	ARG	2.6
2	B	156	THR	2.6
1	A	492	GLN	2.6
1	A	130	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	139	SER	2.6
1	A	131	MET	2.5
1	A	304	ARG	2.5
1	A	421	TYR	2.5
1	A	271	VAL	2.4
1	A	249	GLY	2.4
2	B	152	THR	2.4
2	B	143	HIS	2.3
2	B	20	GLY	2.2
1	A	82	VAL	2.1
1	A	265	SER	2.1
1	A	128	THR	2.1
1	A	180	MET	2.0
1	A	250	LYS	2.0
1	A	201	CYS	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 monosaccharides 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
6	EDO	A	502	4/4	0.93	0.63	57,60,64,66	0
7	SO4	B	331	5/5	0.93	0.18	93,96,97,98	0
4	FE	A	500	1/1	0.99	0.19	52,52,52,52	0
4	FE	A	499	1/1	1.00	0.18	48,48,48,48	0
5	OH	A	501	1/1	1.00	0.24	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.