



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 01:11 PM EDT

PDB ID : 9Q6W / pdb\_00009q6w  
Title : Crystal Structure of Vibrio cholerae PilU, a PilT-dependent Retraction ATPase - Crystal Form 2  
Authors : Minasov, G.; Shukla, S.; Shuvalova, L.; Brunzelle, J.S.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)  
Deposited on : 2025-08-22  
Resolution : 2.70 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.

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

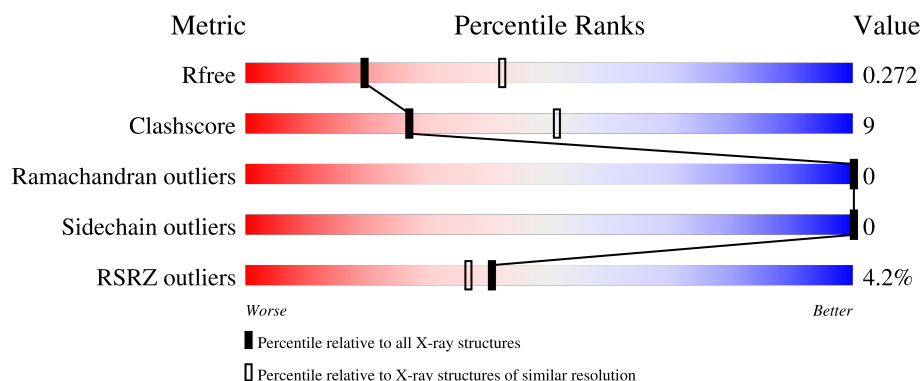
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 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	386	 3% 73% 18% 9%
1	B	386	 4% 71% 20% 9%
1	C	386	 4% 73% 18% 9%

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	414	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8648 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 Twitching motility protein PilT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2751	1714	504	519	14			
1	B	351	Total	C	N	O	S	0	0	0
			2743	1708	503	518	14			
1	C	352	Total	C	N	O	S	0	0	0
			2751	1714	504	519	14			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q9KUQ2
A	-16	ALA	-	expression tag	UNP Q9KUQ2
A	-15	GLY	-	expression tag	UNP Q9KUQ2
A	-14	GLY	-	expression tag	UNP Q9KUQ2
A	-13	SER	-	expression tag	UNP Q9KUQ2
A	-12	GLY	-	expression tag	UNP Q9KUQ2
A	-11	GLY	-	expression tag	UNP Q9KUQ2
A	-10	HIS	-	expression tag	UNP Q9KUQ2
A	-9	HIS	-	expression tag	UNP Q9KUQ2
A	-8	HIS	-	expression tag	UNP Q9KUQ2
A	-7	HIS	-	expression tag	UNP Q9KUQ2
A	-6	HIS	-	expression tag	UNP Q9KUQ2
A	-5	HIS	-	expression tag	UNP Q9KUQ2
A	-4	ALA	-	expression tag	UNP Q9KUQ2
A	-3	GLY	-	expression tag	UNP Q9KUQ2
A	-2	GLY	-	expression tag	UNP Q9KUQ2
A	-1	ALA	-	expression tag	UNP Q9KUQ2
A	0	GLY	-	expression tag	UNP Q9KUQ2
A	1	GLY	-	expression tag	UNP Q9KUQ2
B	-17	MET	-	expression tag	UNP Q9KUQ2
B	-16	ALA	-	expression tag	UNP Q9KUQ2
B	-15	GLY	-	expression tag	UNP Q9KUQ2
B	-14	GLY	-	expression tag	UNP Q9KUQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	expression tag	UNP Q9KUQ2
B	-12	GLY	-	expression tag	UNP Q9KUQ2
B	-11	GLY	-	expression tag	UNP Q9KUQ2
B	-10	HIS	-	expression tag	UNP Q9KUQ2
B	-9	HIS	-	expression tag	UNP Q9KUQ2
B	-8	HIS	-	expression tag	UNP Q9KUQ2
B	-7	HIS	-	expression tag	UNP Q9KUQ2
B	-6	HIS	-	expression tag	UNP Q9KUQ2
B	-5	HIS	-	expression tag	UNP Q9KUQ2
B	-4	ALA	-	expression tag	UNP Q9KUQ2
B	-3	GLY	-	expression tag	UNP Q9KUQ2
B	-2	GLY	-	expression tag	UNP Q9KUQ2
B	-1	ALA	-	expression tag	UNP Q9KUQ2
B	0	GLY	-	expression tag	UNP Q9KUQ2
B	1	GLY	-	expression tag	UNP Q9KUQ2
C	-17	MET	-	expression tag	UNP Q9KUQ2
C	-16	ALA	-	expression tag	UNP Q9KUQ2
C	-15	GLY	-	expression tag	UNP Q9KUQ2
C	-14	GLY	-	expression tag	UNP Q9KUQ2
C	-13	SER	-	expression tag	UNP Q9KUQ2
C	-12	GLY	-	expression tag	UNP Q9KUQ2
C	-11	GLY	-	expression tag	UNP Q9KUQ2
C	-10	HIS	-	expression tag	UNP Q9KUQ2
C	-9	HIS	-	expression tag	UNP Q9KUQ2
C	-8	HIS	-	expression tag	UNP Q9KUQ2
C	-7	HIS	-	expression tag	UNP Q9KUQ2
C	-6	HIS	-	expression tag	UNP Q9KUQ2
C	-5	HIS	-	expression tag	UNP Q9KUQ2
C	-4	ALA	-	expression tag	UNP Q9KUQ2
C	-3	GLY	-	expression tag	UNP Q9KUQ2
C	-2	GLY	-	expression tag	UNP Q9KUQ2
C	-1	ALA	-	expression tag	UNP Q9KUQ2
C	0	GLY	-	expression tag	UNP Q9KUQ2
C	1	GLY	-	expression tag	UNP Q9KUQ2

- Molecule 2 is SULFATE ION (CCD ID: 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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	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		
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		

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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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

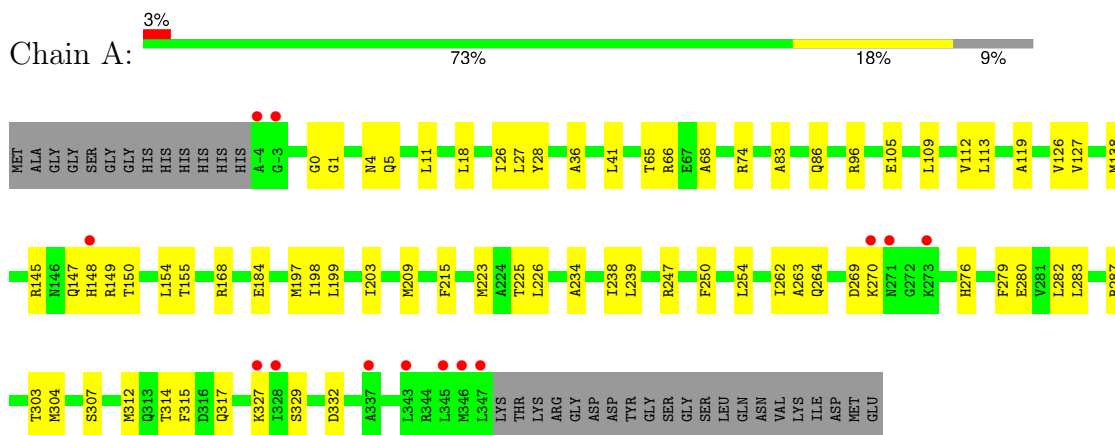


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	38	Total 38	O 38	0	0
3	C	41	Total 41	O 41	0	0

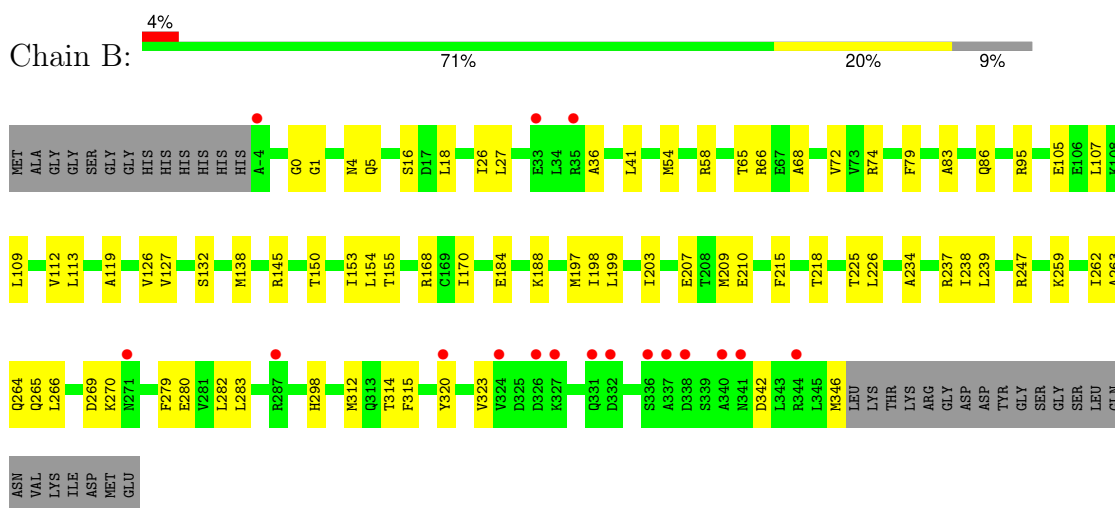
### 3 Residue-property plots [i](#)

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.

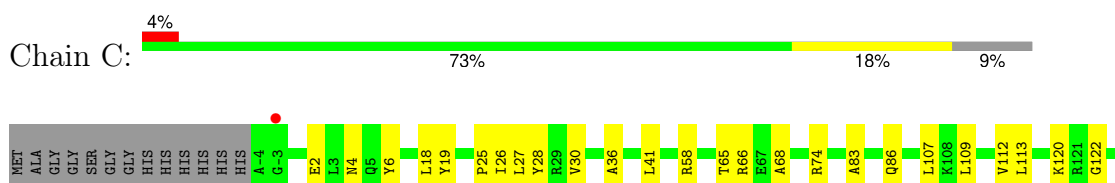
#### • Molecule 1: Twitching motility protein PilT

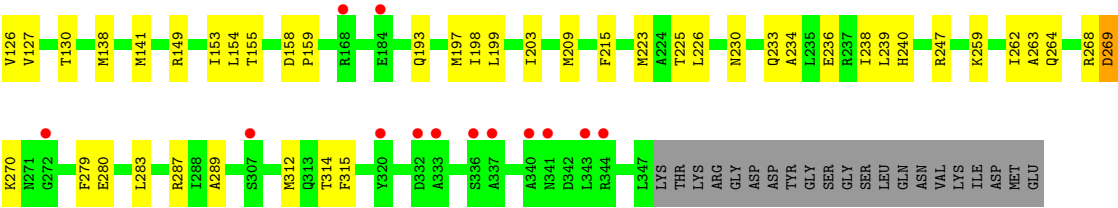


#### • Molecule 1: Twitching motility protein PilT



#### • Molecule 1: Twitching motility protein PilT





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.83Å 120.83Å 175.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.70 29.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.1 (29.58-2.70) 92.1 (29.58-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, $R_{free}$	0.223 , 0.270 0.222 , 0.272	Depositor DCC
$R_{free}$ test set	1386 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: 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	0.46	0/2788	1.01	3/3759 (0.1%)
1	B	0.46	0/2780	1.04	6/3748 (0.2%)
1	C	0.46	0/2788	1.01	5/3759 (0.1%)
All	All	0.46	0/8356	1.02	14/11266 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	PHE	N-CA-CB	6.58	119.80	110.12
1	B	210	GLU	CB-CA-C	6.51	121.93	110.85
1	B	188	LYS	CB-CA-C	-6.21	101.12	110.88
1	B	315	PHE	N-CA-CB	6.18	119.21	110.12
1	C	86	GLN	CB-CA-C	5.78	118.68	110.24
1	B	264	GLN	N-CA-CB	-5.74	101.69	111.69
1	B	86	GLN	CB-CA-C	5.74	118.62	110.24
1	C	264	GLN	N-CA-CB	-5.74	101.70	111.69
1	C	269	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	264	GLN	N-CA-CB	-5.65	101.85	111.69
1	A	86	GLN	CB-CA-C	5.60	118.42	110.24
1	A	315	PHE	CA-CB-CG	5.43	119.23	113.80
1	B	237	ARG	CA-CB-CG	5.33	124.77	114.10
1	C	287	ARG	N-CA-CB	5.09	117.39	110.01

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	2751	0	2780	52	0
1	B	2743	0	2769	55	0
1	C	2751	0	2780	50	0
2	A	95	0	0	2	0
2	B	95	0	0	1	0
2	C	85	0	0	1	0
3	A	49	0	0	1	0
3	B	38	0	0	2	0
3	C	41	0	0	1	0
All	All	8648	0	8329	155	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 9.

All (155) 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:C:263:ALA:HB3	1:C:280:GLU:HB3	1.69	0.74
1:B:263:ALA:HB3	1:B:280:GLU:HB3	1.69	0.73
1:A:263:ALA:HB3	1:A:280:GLU:HB3	1.70	0.72
1:B:132:SER:O	1:B:266:LEU:CD1	2.39	0.69
1:C:153:ILE:HG23	1:C:197:MET:HE3	1.74	0.68
1:A:145:ARG:HG2	1:A:197:MET:HE3	1.75	0.67
1:B:132:SER:O	1:B:266:LEU:HD11	1.93	0.67
1:B:155:THR:HG22	1:B:199:LEU:HB3	1.76	0.67
1:A:126:VAL:HB	1:A:138:MET:HE2	1.77	0.67
1:B:126:VAL:HB	1:B:138:MET:HE2	1.77	0.66
1:C:155:THR:HG22	1:C:199:LEU:HB3	1.77	0.66
1:A:155:THR:HG22	1:A:199:LEU:HB3	1.77	0.66
1:B:153:ILE:HG23	1:B:197:MET:HE3	1.76	0.66
1:C:126:VAL:HB	1:C:138:MET:HE2	1.79	0.65
1:B:282:LEU:C	1:B:282:LEU:HD23	2.23	0.64
1:A:168:ARG:NH1	2:A:414:SO4:O3	2.30	0.64
1:C:2:GLU:HG2	1:C:6:TYR:CE2	2.34	0.63
1:C:58:ARG:NH1	2:C:402:SO4:O2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD12	1:A:312:MET:HE3	1.83	0.60
1:A:304:MET:HA	1:A:312:MET:HE2	1.83	0.59
1:A:109:LEU:HD23	1:A:279:PHE:CZ	2.37	0.59
1:A:250:PHE:CE2	1:A:254:LEU:HD11	2.38	0.58
1:C:153:ILE:HG23	1:C:197:MET:CE	2.33	0.58
1:B:27:LEU:HD23	1:B:36:ALA:HA	1.86	0.58
1:C:283:LEU:HB2	1:C:312:MET:HE2	1.85	0.58
1:A:27:LEU:HD23	1:A:36:ALA:HA	1.85	0.58
1:C:27:LEU:HD23	1:C:36:ALA:HA	1.86	0.58
1:B:283:LEU:HB2	1:B:312:MET:HE2	1.87	0.57
1:C:4:ASN:ND2	1:C:74:ARG:HH22	2.02	0.57
1:A:270:LYS:NZ	3:A:501:HOH:O	2.39	0.56
1:B:153:ILE:HG23	1:B:197:MET:CE	2.35	0.56
1:C:230:ASN:HD21	1:C:233:GLN:HE21	1.54	0.56
1:B:113:LEU:HD22	1:B:262:ILE:CD1	2.36	0.55
1:C:113:LEU:HD22	1:C:262:ILE:CD1	2.36	0.55
1:B:18:LEU:HD11	1:B:26:ILE:HG23	1.88	0.55
1:C:109:LEU:HD23	1:C:279:PHE:CZ	2.41	0.55
1:A:18:LEU:HD13	1:A:28:TYR:CE1	2.42	0.55
1:C:113:LEU:HD22	1:C:262:ILE:HD11	1.89	0.55
1:A:65:THR:O	1:A:66:ARG:HB2	2.06	0.55
1:C:18:LEU:HD11	1:C:26:ILE:HG23	1.89	0.55
1:B:0:GLY:O	1:B:4:ASN:ND2	2.40	0.55
1:C:4:ASN:ND2	1:C:74:ARG:NH2	2.55	0.55
1:A:113:LEU:HD22	1:A:262:ILE:CD1	2.37	0.55
1:C:65:THR:O	1:C:66:ARG:HB2	2.06	0.54
1:B:109:LEU:HD23	1:B:279:PHE:CZ	2.42	0.54
1:C:18:LEU:HD13	1:C:28:TYR:CE1	2.43	0.54
1:A:0:GLY:O	1:A:4:ASN:ND2	2.41	0.54
1:A:113:LEU:HD22	1:A:262:ILE:HD11	1.89	0.53
1:B:113:LEU:HD22	1:B:262:ILE:HD11	1.90	0.53
1:A:269:ASP:OD1	1:A:276:HIS:ND1	2.41	0.53
1:B:283:LEU:O	1:B:312:MET:HE2	2.09	0.53
1:B:320:TYR:O	1:B:323:VAL:HG22	2.09	0.53
1:A:127:VAL:HG12	1:A:226:LEU:HB2	1.91	0.53
1:B:154:LEU:C	1:B:154:LEU:HD23	2.34	0.53
1:B:65:THR:O	1:B:66:ARG:HB2	2.07	0.52
1:C:127:VAL:HG12	1:C:226:LEU:HB2	1.91	0.52
1:C:283:LEU:O	1:C:312:MET:HE2	2.08	0.52
1:A:18:LEU:HD11	1:A:26:ILE:HG23	1.90	0.52
1:A:112:VAL:HG21	1:A:283:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG12	1:B:226:LEU:HB2	1.92	0.52
1:B:58:ARG:NH2	3:B:502:HOH:O	2.41	0.51
1:C:239:LEU:HD11	1:C:247:ARG:HB3	1.93	0.51
1:A:239:LEU:HD11	1:A:247:ARG:HB3	1.93	0.51
1:B:54:MET:HG2	1:B:58:ARG:HD2	1.93	0.51
1:A:154:LEU:C	1:A:154:LEU:HD23	2.36	0.50
1:A:209:MET:HE2	1:A:238:ILE:HD12	1.93	0.50
1:B:265:GLN:C	1:B:266:LEU:HD12	2.37	0.50
1:A:147:GLN:O	1:A:168:ARG:HD3	2.12	0.50
1:B:239:LEU:HD11	1:B:247:ARG:HB3	1.93	0.50
1:A:105:GLU:OE2	1:A:105:GLU:N	2.43	0.49
1:B:218:THR:OG1	1:C:130:THR:HG22	2.13	0.49
1:C:112:VAL:HG21	1:C:283:LEU:HD11	1.94	0.49
1:A:280:GLU:HG3	1:A:314:THR:HA	1.94	0.49
1:B:105:GLU:OE2	1:B:105:GLU:N	2.44	0.49
1:B:112:VAL:HG21	1:B:283:LEU:HD11	1.95	0.49
1:A:119:ALA:O	1:A:145:ARG:NH1	2.45	0.49
1:C:209:MET:HE2	1:C:238:ILE:HD12	1.93	0.49
1:A:304:MET:HG2	1:A:312:MET:HE2	1.94	0.49
1:B:16:SER:O	1:B:95:ARG:HD3	2.13	0.49
1:C:230:ASN:ND2	1:C:233:GLN:HE21	2.11	0.48
1:B:119:ALA:O	1:B:145:ARG:NH1	2.45	0.48
1:B:209:MET:HE2	1:B:238:ILE:HD12	1.96	0.48
1:C:138:MET:SD	1:C:223:MET:HG2	2.54	0.48
1:A:198:ILE:HD12	1:A:215:PHE:CG	2.49	0.47
1:B:266:LEU:HD12	1:B:266:LEU:N	2.28	0.47
1:B:269:ASP:OD1	1:B:270:LYS:N	2.47	0.47
1:C:280:GLU:HG3	1:C:314:THR:HA	1.96	0.47
1:C:198:ILE:HD12	1:C:215:PHE:CG	2.50	0.47
1:C:269:ASP:OD1	1:C:270:LYS:N	2.48	0.47
1:C:268:ARG:HG2	1:C:269:ASP:N	2.29	0.46
1:B:198:ILE:HD12	1:B:215:PHE:CG	2.49	0.46
1:A:138:MET:SD	1:A:223:MET:HG2	2.55	0.46
1:B:4:ASN:CG	1:B:74:ARG:NH2	2.74	0.46
1:C:138:MET:HE3	1:C:225:THR:HG23	1.96	0.46
1:A:4:ASN:CG	1:A:74:ARG:NH2	2.74	0.46
1:A:287:ARG:HD3	1:A:303:THR:HG23	1.97	0.46
1:C:120:LYS:HG2	1:C:149:ARG:HH22	1.80	0.45
1:C:4:ASN:CG	1:C:74:ARG:NH2	2.74	0.45
1:B:184:GLU:OE1	1:B:184:GLU:N	2.41	0.45
1:A:26:ILE:CD1	1:A:41:LEU:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG11	1:B:234:ALA:CB	2.46	0.45
1:A:26:ILE:HD13	1:A:41:LEU:HD11	1.99	0.45
1:C:26:ILE:CD1	1:C:41:LEU:HD11	2.46	0.45
1:B:68:ALA:HB3	1:B:83:ALA:HB3	1.98	0.45
1:B:342:ASP:O	1:B:346:MET:HG2	2.17	0.45
1:C:30:VAL:O	1:C:30:VAL:HG23	2.17	0.45
1:C:141:MET:HE3	1:C:223:MET:SD	2.57	0.45
1:A:11:LEU:HD13	1:A:96:ARG:CZ	2.47	0.44
1:A:304:MET:HG2	1:A:312:MET:CE	2.47	0.44
1:B:298:HIS:ND1	2:B:416:SO4:O1	2.50	0.44
1:B:280:GLU:HG3	1:B:314:THR:HA	2.00	0.44
1:C:127:VAL:HG11	1:C:234:ALA:CB	2.47	0.44
1:C:68:ALA:HB3	1:C:83:ALA:HB3	1.99	0.44
1:A:197:MET:HG2	1:A:198:ILE:N	2.31	0.44
1:B:138:MET:HE3	1:B:225:THR:HG23	1.99	0.43
1:A:68:ALA:HB3	1:A:83:ALA:HB3	1.99	0.43
1:B:26:ILE:CD1	1:B:41:LEU:HD11	2.47	0.43
1:A:127:VAL:HG11	1:A:234:ALA:CB	2.47	0.43
1:A:168:ARG:NH1	2:A:414:SO4:S	2.91	0.43
1:B:26:ILE:HD13	1:B:41:LEU:HD11	2.00	0.43
1:C:122:GLY:HA3	1:C:259:LYS:HG2	1.99	0.43
1:B:282:LEU:C	1:B:282:LEU:CD2	2.90	0.43
1:C:26:ILE:HD13	1:C:41:LEU:HD11	2.00	0.43
1:B:259:LYS:NZ	3:B:506:HOH:O	2.52	0.43
1:A:148:HIS:ND1	1:A:149:ARG:HB2	2.34	0.42
1:B:1:GLY:O	1:B:5:GLN:HG3	2.19	0.42
1:C:154:LEU:HD11	1:C:193:GLN:OE1	2.18	0.42
1:C:289:ALA:HB3	3:C:510:HOH:O	2.19	0.42
1:A:184:GLU:OE1	1:A:184:GLU:N	2.41	0.42
1:A:203:ILE:HB	1:A:226:LEU:CD2	2.50	0.42
1:B:150:THR:HA	1:B:168:ARG:O	2.20	0.42
1:B:320:TYR:HA	1:B:323:VAL:HG22	2.01	0.42
1:B:72:VAL:CG2	1:B:79:PHE:HB2	2.49	0.42
1:C:120:LYS:HG2	1:C:149:ARG:NH2	2.35	0.41
1:A:1:GLY:O	1:A:5:GLN:HG3	2.21	0.41
1:A:276:HIS:ND1	1:A:327:LYS:HB3	2.36	0.41
1:C:25:PRO:O	1:C:27:LEU:HG	2.21	0.41
1:B:132:SER:O	1:B:266:LEU:HD13	2.18	0.41
1:C:107:LEU:HB2	1:C:109:LEU:HG	2.03	0.41
1:C:203:ILE:HB	1:C:226:LEU:CD2	2.50	0.41
1:A:127:VAL:HG23	1:A:263:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HE3	1:A:225:THR:HG23	2.00	0.41
1:A:149:ARG:HG2	1:A:150:THR:N	2.36	0.41
1:C:127:VAL:HG23	1:C:263:ALA:HA	2.01	0.41
1:C:236:GLU:HG2	1:C:240:HIS:NE2	2.36	0.41
1:B:203:ILE:HB	1:B:226:LEU:CD2	2.50	0.41
1:B:127:VAL:HG23	1:B:263:ALA:HA	2.02	0.41
1:B:170:ILE:HD11	1:C:19:TYR:CD2	2.56	0.41
1:B:184:GLU:HB3	1:B:207:GLU:OE2	2.21	0.40
1:A:329:SER:OG	1:A:332:ASP:OD2	2.39	0.40
1:B:107:LEU:HB2	1:B:109:LEU:HG	2.03	0.40
1:C:158:ASP:HA	1:C:159:PRO:HA	1.86	0.40
1:A:150:THR:HA	1:A:168:ARG:O	2.21	0.40
1:A:307:SER:O	1:A:312:MET:HB2	2.21	0.40
1:A:314:THR:HG1	1:A:317:GLN:HG3	1.86	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	350/386 (91%)	338 (97%)	12 (3%)	0	100	100
1	B	349/386 (90%)	338 (97%)	11 (3%)	0	100	100
1	C	350/386 (91%)	336 (96%)	14 (4%)	0	100	100
All	All	1049/1158 (91%)	1012 (96%)	37 (4%)	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	291/317 (92%)	291 (100%)	0	100	100
1	B	290/317 (92%)	290 (100%)	0	100	100
1	C	291/317 (92%)	291 (100%)	0	100	100
All	All	872/951 (92%)	872 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	HIS
1	B	232	ASN
1	C	4	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

55 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	A	412	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	416	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	419	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	B	403	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	C	413	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	C	404	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	414	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	C	417	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	407	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	A	408	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	411	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	C	403	-	4,4,4	0.35	0	6,6,6	0.05	0
2	SO4	C	414	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	B	405	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	C	401	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	B	415	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	401	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	A	416	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	A	405	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	C	406	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	A	411	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	B	407	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	B	404	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	409	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	B	414	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	417	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	C	409	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	410	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	C	410	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	B	408	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	418	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	B	419	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	C	407	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	410	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	C	408	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	404	-	4,4,4	0.34	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	413	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	C	405	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	B	401	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	C	416	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	412	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	402	-	4,4,4	0.32	0	6,6,6	0.13	0
2	SO4	A	417	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	C	411	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	C	402	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	A	402	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	406	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	C	412	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	C	415	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	409	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	A	403	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	415	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	413	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	B	418	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	406	-	4,4,4	0.33	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	416	SO4	1	0
2	A	414	SO4	2	0
2	C	402	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	352/386 (91%)	0.23	13 (3%) 45 41	23, 42, 95, 133	0
1	B	351/386 (90%)	0.20	17 (4%) 35 32	26, 41, 98, 164	0
1	C	352/386 (91%)	0.24	14 (3%) 42 38	23, 47, 101, 132	0
All	All	1055/1158 (91%)	0.22	44 (4%) 40 37	23, 43, 99, 164	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	VAL	3.7
1	C	337	ALA	3.6
1	C	343	LEU	3.6
1	A	343	LEU	3.5
1	B	-4	ALA	3.4
1	A	346	MET	3.3
1	B	326	ASP	3.2
1	A	-3	GLY	3.1
1	B	337	ALA	3.0
1	B	332	ASP	2.9
1	C	272	GLY	2.9
1	C	340	ALA	2.9
1	B	33	GLU	2.9
1	B	340	ALA	2.9
1	A	-4	ALA	2.8
1	A	347	LEU	2.8
1	A	327	LYS	2.7
1	B	320	TYR	2.7
1	A	148	HIS	2.7
1	B	341	ASN	2.6
1	A	328	ILE	2.6
1	A	345	LEU	2.6
1	B	338	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	270	LYS	2.4
1	C	333	ALA	2.4
1	C	-3	GLY	2.3
1	C	168	ARG	2.3
1	C	184	GLU	2.2
1	B	271	ASN	2.2
1	B	287	ARG	2.2
1	B	327	LYS	2.2
1	B	35	ARG	2.2
1	B	344	ARG	2.2
1	C	344	ARG	2.2
1	A	271	ASN	2.2
1	C	332	ASP	2.2
1	B	336	SER	2.1
1	B	331	GLN	2.1
1	C	307	SER	2.1
1	C	336	SER	2.1
1	A	273	LYS	2.0
1	A	337	ALA	2.0
1	C	341	ASN	2.0
1	C	320	TYR	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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	417	5/5	0.52	0.17	108,112,116,117	0
2	SO4	A	415	5/5	0.55	0.12	106,109,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	412	5/5	0.56	0.16	98,110,112,125	0
2	SO4	B	416	5/5	0.61	0.16	87,95,99,100	0
2	SO4	B	408	5/5	0.61	0.15	103,104,107,110	0
2	SO4	A	408	5/5	0.62	0.20	104,105,106,106	0
2	SO4	C	413	5/5	0.63	0.19	94,96,102,104	0
2	SO4	B	418	5/5	0.65	0.16	108,117,121,126	0
2	SO4	B	415	5/5	0.65	0.13	123,130,131,132	0
2	SO4	A	409	5/5	0.65	0.20	93,95,104,106	0
2	SO4	C	416	5/5	0.66	0.11	94,97,101,101	0
2	SO4	A	417	5/5	0.66	0.09	122,122,126,127	0
2	SO4	B	405	5/5	0.70	0.19	96,103,109,114	0
2	SO4	A	412	5/5	0.70	0.13	83,90,95,95	0
2	SO4	A	418	5/5	0.70	0.12	115,115,117,118	0
2	SO4	C	414	5/5	0.71	0.25	110,115,118,119	0
2	SO4	C	408	5/5	0.71	0.13	89,97,101,107	0
2	SO4	B	411	5/5	0.71	0.15	79,86,90,93	0
2	SO4	A	414	5/5	0.72	0.14	88,90,97,104	0
2	SO4	B	413	5/5	0.73	0.14	109,117,118,121	0
2	SO4	A	411	5/5	0.74	0.12	81,83,86,88	0
2	SO4	B	414	5/5	0.74	0.17	90,102,106,111	0
2	SO4	A	419	5/5	0.74	0.18	94,98,100,102	0
2	SO4	C	412	5/5	0.74	0.16	98,103,107,110	0
2	SO4	A	413	5/5	0.75	0.19	96,101,102,103	0
2	SO4	C	407	5/5	0.75	0.15	95,98,102,103	0
2	SO4	C	410	5/5	0.76	0.13	71,78,78,82	0
2	SO4	B	407	5/5	0.76	0.10	106,107,109,110	0
2	SO4	A	405	5/5	0.77	0.12	91,96,101,110	0
2	SO4	C	405	5/5	0.77	0.15	87,88,92,95	0
2	SO4	A	416	5/5	0.78	0.14	111,113,116,117	0
2	SO4	B	409	5/5	0.78	0.15	76,78,82,86	0
2	SO4	C	411	5/5	0.79	0.16	97,98,104,111	0
2	SO4	C	409	5/5	0.80	0.19	93,95,96,102	0
2	SO4	B	403	5/5	0.80	0.10	86,87,90,91	0
2	SO4	B	417	5/5	0.82	0.19	84,91,92,93	0
2	SO4	C	415	5/5	0.82	0.12	117,119,120,123	0
2	SO4	A	406	5/5	0.84	0.12	80,81,85,85	0
2	SO4	B	410	5/5	0.84	0.12	79,84,89,92	0
2	SO4	A	403	5/5	0.85	0.11	82,83,84,86	0
2	SO4	B	419	5/5	0.86	0.26	107,108,112,112	0
2	SO4	A	410	5/5	0.87	0.11	74,80,87,91	0
2	SO4	C	406	5/5	0.90	0.12	67,69,72,75	0
2	SO4	A	407	5/5	0.90	0.13	58,61,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	404	5/5	0.90	0.13	63,64,66,72	0
2	SO4	B	404	5/5	0.90	0.08	66,70,71,72	0
2	SO4	C	403	5/5	0.91	0.07	60,66,67,67	0
2	SO4	B	406	5/5	0.92	0.12	63,68,71,73	0
2	SO4	C	404	5/5	0.93	0.10	64,64,70,72	0
2	SO4	C	402	5/5	0.95	0.07	33,37,40,40	0
2	SO4	B	402	5/5	0.96	0.06	40,41,44,49	0
2	SO4	A	401	5/5	0.96	0.05	33,33,36,40	0
2	SO4	A	402	5/5	0.97	0.06	44,44,46,49	0
2	SO4	C	401	5/5	0.97	0.05	37,40,41,42	0
2	SO4	B	401	5/5	0.99	0.05	35,35,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.