



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:17 AM UTC

PDB ID : 1OTG / pdb_00001otg
Title : 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE
Authors : Subramanya, H.S.; Roper, D.I.; Dauter, Z.; Dodson, E.J.; Davies, G.J.; Wilson, K.S.; Wigley, D.B.
Deposited on : 1995-11-09
Resolution : 2.10 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

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>.

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

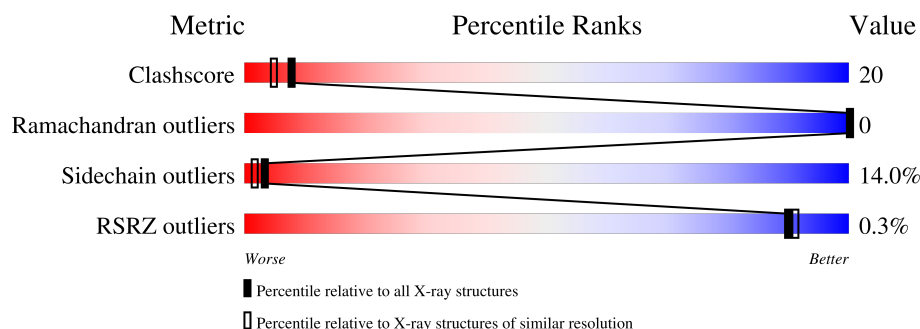
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 ≥ 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	125	
1	B	125	
1	C	125	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3227 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.

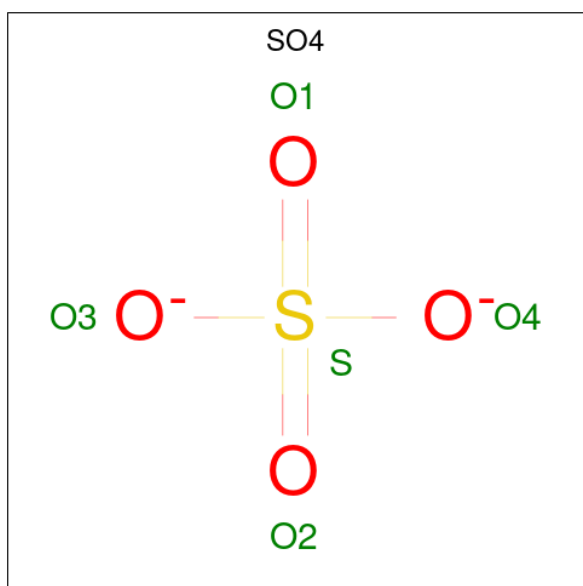
- Molecule 1 is a protein called 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			997	640	174	178	5			
1	B	125	Total	C	N	O	S	0	0	0
			997	640	174	178	5			
1	C	125	Total	C	N	O	S	0	0	0
			997	640	174	178	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	PHE	SER	conflict	UNP Q05354
B	61	PHE	SER	conflict	UNP Q05354
C	61	PHE	SER	conflict	UNP Q05354

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

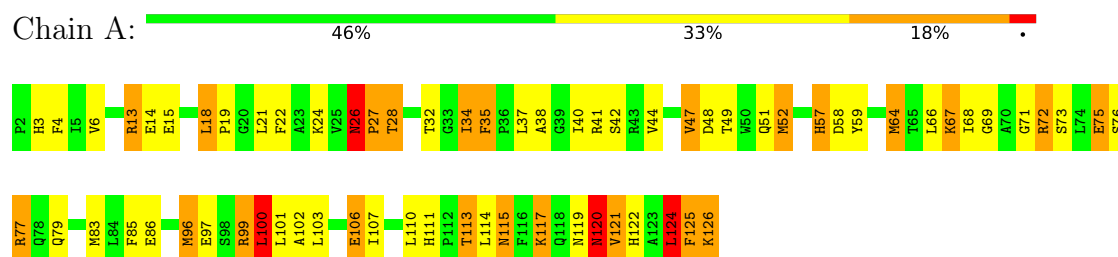
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 57 57	0	0
3	B	64	Total O 64 64	0	0
3	C	80	Total O 80 80	0	0

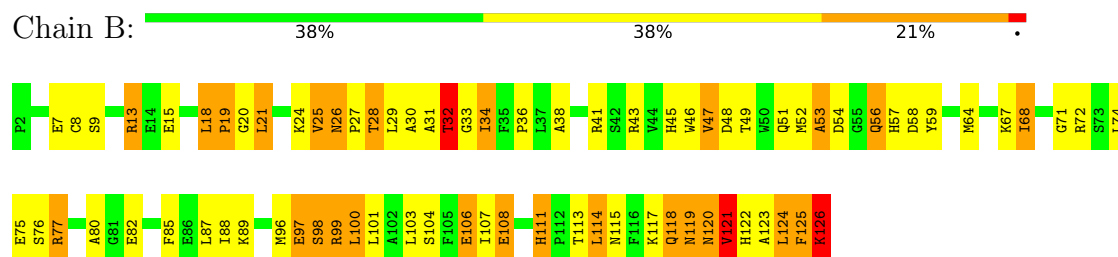
3 Residue-property plots

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.

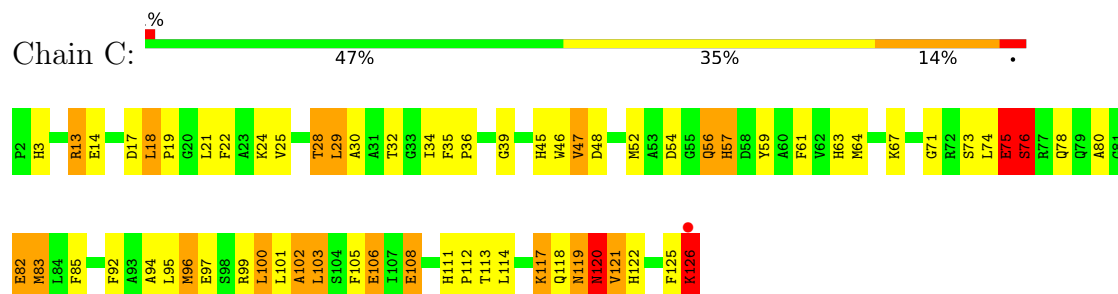
• Molecule 1: 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.30Å 90.30Å 129.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 88.8 (10.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.09Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3227	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.15	0/1022	2.48	71/1382 (5.1%)
1	B	1.25	0/1022	2.66	99/1382 (7.2%)
1	C	1.22	0/1022	2.40	57/1382 (4.1%)
All	All	1.21	0/3066	2.51	227/4146 (5.5%)

There are no bond length outliers.

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	GLU	CB-CG-CD	18.12	143.41	112.60
1	A	115	ASN	CA-CB-CG	-12.95	99.65	112.60
1	A	115	ASN	OD1-CG-ND2	12.78	135.38	122.60
1	B	20	GLY	CA-C-O	-11.11	108.46	120.90
1	A	125	PHE	O-C-N	10.48	130.35	121.65
1	B	31	ALA	CA-C-N	10.28	135.93	120.31
1	B	31	ALA	C-N-CA	10.28	135.93	120.31
1	A	99	ARG	NE-CZ-NH2	-10.16	110.06	119.20
1	A	48	ASP	CA-CB-CG	9.80	122.41	112.60
1	B	115	ASN	OD1-CG-ND2	9.61	132.21	122.60
1	B	32	THR	CA-C-O	9.49	130.89	119.97
1	B	20	GLY	O-C-N	9.44	131.25	122.19
1	B	106	GLU	CB-CG-CD	9.42	128.61	112.60
1	C	75	GLU	CA-C-N	9.31	132.55	120.44
1	C	75	GLU	C-N-CA	9.31	132.55	120.44
1	A	115	ASN	CA-C-O	-9.16	110.50	120.30
1	C	106	GLU	CG-CD-OE2	-9.12	97.43	118.40
1	B	99	ARG	NE-CZ-NH2	-8.92	111.17	119.20
1	B	56	GLN	CB-CG-CD	-8.91	97.44	112.60
1	A	79	GLN	CA-CB-CG	8.85	131.80	114.10
1	B	76	SER	CB-CA-C	-8.80	95.88	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	SER	CA-C-O	-8.77	108.43	119.31
1	B	56	GLN	OE1-CD-NE2	8.74	131.34	122.60
1	C	106	GLU	CG-CD-OE1	8.67	138.34	118.40
1	A	13	ARG	CD-NE-CZ	-8.62	112.33	124.40
1	B	115	ASN	CA-CB-CG	-8.48	104.12	112.60
1	B	80	ALA	CA-C-N	8.43	129.30	119.94
1	B	80	ALA	C-N-CA	8.43	129.30	119.94
1	C	76	SER	CB-CA-C	-8.40	97.69	110.88
1	A	99	ARG	NE-CZ-NH1	8.31	129.81	121.50
1	B	125	PHE	CA-CB-CG	-8.23	105.57	113.80
1	C	35	PHE	O-C-N	8.19	128.68	121.39
1	B	108	GLU	CB-CG-CD	8.09	126.36	112.60
1	A	85	PHE	CA-CB-CG	-8.07	105.73	113.80
1	C	80	ALA	CA-C-N	8.02	128.84	119.94
1	C	80	ALA	C-N-CA	8.02	128.84	119.94
1	A	57	HIS	CA-CB-CG	-7.98	105.82	113.80
1	A	47	VAL	N-CA-CB	-7.92	101.35	111.64
1	C	119	ASN	O-C-N	-7.82	114.12	123.27
1	A	69	GLY	CA-C-O	7.81	128.61	121.58
1	B	126	LYS	CA-C-O	-7.70	107.71	120.80
1	A	52	MET	O-C-N	-7.59	114.69	123.27
1	B	97	GLU	CB-CG-CD	7.56	125.45	112.60
1	C	45	HIS	CA-C-O	-7.55	112.47	120.40
1	A	51	GLN	N-CA-CB	7.50	122.19	110.71
1	C	106	GLU	CB-CG-CD	7.44	125.25	112.60
1	C	35	PHE	CA-CB-CG	-7.43	106.36	113.80
1	A	99	ARG	O-C-N	7.40	131.61	123.10
1	B	97	GLU	CA-C-O	7.29	128.15	120.42
1	C	82	GLU	CB-CA-C	-7.21	98.82	110.79
1	B	71	GLY	CA-C-O	-7.05	111.17	119.07
1	B	82	GLU	CB-CA-C	-7.04	99.83	110.88
1	B	32	THR	O-C-N	-7.03	113.62	122.27
1	B	114	LEU	CA-C-N	7.02	132.67	122.77
1	B	114	LEU	C-N-CA	7.02	132.67	122.77
1	B	32	THR	N-CA-CB	-7.00	99.43	110.28
1	A	72	ARG	CA-CB-CG	-6.98	100.14	114.10
1	A	125	PHE	N-CA-C	-6.97	102.06	108.75
1	B	33	GLY	CA-C-N	6.97	131.62	120.82
1	B	33	GLY	C-N-CA	6.97	131.62	120.82
1	B	119	ASN	OD1-CG-ND2	-6.92	115.67	122.60
1	B	56	GLN	N-CA-C	6.92	119.85	111.82
1	A	15	GLU	CG-CD-OE2	6.91	134.30	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	CB-CA-C	6.91	122.25	109.54
1	A	40	ILE	N-CA-CB	6.82	118.39	110.82
1	A	99	ARG	CA-C-O	-6.78	114.19	121.45
1	B	117	LYS	CA-CB-CG	-6.75	100.61	114.10
1	C	99	ARG	NE-CZ-NH1	-6.72	114.78	121.50
1	A	71	GLY	CA-C-O	-6.63	109.04	120.57
1	B	45	HIS	CA-CB-CG	-6.62	107.18	113.80
1	A	26	ASN	CA-CB-CG	-6.61	105.99	112.60
1	B	57	HIS	CA-CB-CG	-6.55	107.25	113.80
1	A	113	THR	CA-C-O	-6.54	110.89	119.06
1	C	48	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	100	LEU	N-CA-CB	-6.54	99.22	109.87
1	C	14	GLU	CG-CD-OE1	6.53	133.41	118.40
1	C	97	GLU	CB-CA-C	-6.51	99.78	110.85
1	C	63	HIS	CA-CB-CG	-6.51	107.29	113.80
1	C	56	GLN	CA-C-O	-6.50	110.79	119.11
1	B	31	ALA	O-C-N	-6.50	113.79	122.43
1	A	40	ILE	CA-CB-CG1	6.49	121.43	110.40
1	A	58	ASP	CA-C-O	-6.48	114.08	121.66
1	B	15	GLU	N-CA-CB	6.46	120.17	110.22
1	A	120	ASN	CA-CB-CG	6.44	119.04	112.60
1	C	97	GLU	CG-CD-OE1	6.44	133.22	118.40
1	B	77	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	B	98	SER	N-CA-C	6.42	120.85	112.89
1	C	47	VAL	N-CA-CB	-6.42	103.29	111.64
1	A	66	LEU	CA-C-O	-6.36	113.66	120.46
1	A	115	ASN	N-CA-CB	-6.35	100.74	110.65
1	B	30	ALA	CA-C-O	-6.34	113.83	120.55
1	B	97	GLU	CA-CB-CG	6.32	126.74	114.10
1	A	77	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	B	51	GLN	CA-C-N	-6.29	113.82	122.93
1	B	51	GLN	C-N-CA	-6.29	113.82	122.93
1	C	82	GLU	O-C-N	6.28	128.78	122.12
1	B	25	VAL	N-CA-C	6.27	116.94	110.36
1	B	115	ASN	N-CA-CB	-6.25	100.96	110.77
1	B	18	LEU	CB-CA-C	6.24	122.46	110.17
1	B	67	LYS	N-CA-CB	6.23	120.35	110.57
1	A	124	LEU	O-C-N	6.23	129.51	122.22
1	A	13	ARG	CB-CG-CD	-6.22	96.99	111.30
1	C	57	HIS	O-C-N	6.21	130.85	122.59
1	B	74	LEU	O-C-N	6.20	129.22	122.15
1	C	126	LYS	CA-CB-CG	6.18	126.46	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ASN	CB-CG-ND2	-6.12	107.22	116.40
1	B	72	ARG	CA-CB-CG	-6.12	101.86	114.10
1	C	99	ARG	NH1-CZ-NH2	6.10	127.23	119.30
1	B	124	LEU	CA-C-O	6.09	126.98	119.97
1	A	73	SER	CA-C-O	-6.07	114.82	121.87
1	B	108	GLU	CA-CB-CG	6.06	126.23	114.10
1	B	51	GLN	N-CA-CB	6.05	120.57	110.59
1	B	59	TYR	CA-CB-CG	6.03	124.76	113.90
1	B	56	GLN	CA-CB-CG	-6.00	102.09	114.10
1	C	30	ALA	CA-C-O	-5.99	114.20	120.55
1	A	35	PHE	O-C-N	5.96	128.64	121.60
1	C	74	LEU	O-C-N	-5.96	115.80	122.12
1	A	58	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	49	THR	CA-C-O	-5.93	113.93	120.33
1	C	32	THR	N-CA-C	-5.90	105.93	113.01
1	B	7	GLU	CB-CG-CD	-5.90	102.57	112.60
1	C	61	PHE	CA-CB-CG	-5.90	107.90	113.80
1	B	76	SER	O-C-N	5.88	128.85	122.15
1	C	17	ASP	CA-C-N	5.88	127.43	120.09
1	C	17	ASP	C-N-CA	5.88	127.43	120.09
1	C	13	ARG	CA-CB-CG	-5.87	102.36	114.10
1	C	97	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	64	MET	CA-CB-CG	-5.83	102.44	114.10
1	C	71	GLY	CA-C-O	-5.82	112.39	119.03
1	B	125	PHE	CB-CA-C	5.82	122.00	110.42
1	B	115	ASN	CA-C-O	-5.82	114.08	120.24
1	C	102	ALA	CA-C-O	5.80	126.62	120.36
1	B	89	LYS	CA-CB-CG	5.79	125.68	114.10
1	A	75	GLU	O-C-N	5.78	128.02	122.07
1	B	9	SER	N-CA-CB	5.76	118.44	109.97
1	C	29	LEU	CA-C-O	5.76	126.53	120.42
1	C	76	SER	CA-C-O	5.75	126.86	120.82
1	A	47	VAL	CB-CA-C	5.75	118.93	110.77
1	A	86	GLU	N-CA-CB	5.74	118.33	110.01
1	A	3	HIS	O-C-N	5.73	130.12	123.30
1	B	34	ILE	CA-CB-CG2	5.72	120.22	110.50
1	A	13	ARG	N-CA-C	5.71	118.23	111.33
1	A	76	SER	CA-CB-OG	5.70	122.50	111.10
1	B	47	VAL	N-CA-CB	-5.68	103.52	111.25
1	B	99	ARG	CD-NE-CZ	5.68	132.36	124.40
1	B	13	ARG	O-C-N	-5.67	116.19	122.09
1	C	25	VAL	O-C-N	5.67	127.67	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ASN	CA-C-O	-5.67	114.21	120.33
1	B	111	HIS	CA-CB-CG	-5.66	108.14	113.80
1	B	56	GLN	N-CA-CB	-5.64	101.54	110.28
1	A	125	PHE	CA-CB-CG	-5.63	108.17	113.80
1	B	121	VAL	CA-CB-CG1	5.60	119.92	110.40
1	B	57	HIS	O-C-N	5.60	130.47	122.74
1	A	27	PRO	O-C-N	-5.57	115.83	122.24
1	A	122	HIS	CA-C-N	5.57	127.75	120.28
1	A	122	HIS	C-N-CA	5.57	127.75	120.28
1	B	123	ALA	O-C-N	-5.56	116.23	122.12
1	B	125	PHE	N-CA-C	-5.55	98.97	110.80
1	B	68	ILE	CA-C-O	-5.53	115.87	121.67
1	B	121	VAL	CA-C-O	-5.53	113.23	119.42
1	C	36	PRO	CA-C-O	-5.52	115.32	121.23
1	B	34	ILE	CB-CG1-CD1	-5.52	102.21	113.80
1	A	14	GLU	CG-CD-OE1	5.50	131.06	118.40
1	B	47	VAL	CB-CA-C	5.50	119.02	110.83
1	C	29	LEU	N-CA-CB	-5.49	102.03	110.16
1	B	41	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	B	107	ILE	N-CA-CB	5.47	118.69	111.25
1	C	39	GLY	CA-C-N	5.47	129.46	121.80
1	C	39	GLY	C-N-CA	5.47	129.46	121.80
1	A	4	PHE	CA-C-O	-5.45	114.49	120.70
1	A	22	PHE	O-C-N	5.43	127.88	122.12
1	C	96	MET	CA-C-N	5.43	128.00	120.29
1	C	96	MET	C-N-CA	5.43	128.00	120.29
1	B	75	GLU	CG-CD-OE1	5.40	130.81	118.40
1	B	122	HIS	N-CA-CB	5.39	118.52	110.22
1	C	39	GLY	CA-C-O	-5.38	111.21	120.57
1	B	52	MET	CA-CB-CG	-5.38	103.34	114.10
1	C	94	ALA	CA-C-O	-5.38	113.78	119.97
1	A	117	LYS	CA-C-N	5.38	128.85	121.33
1	A	117	LYS	C-N-CA	5.38	128.85	121.33
1	B	13	ARG	CA-CB-CG	-5.37	103.36	114.10
1	C	96	MET	CA-C-O	5.37	126.17	120.10
1	B	36	PRO	CA-C-O	-5.37	115.22	121.34
1	A	106	GLU	CG-CD-OE2	-5.36	106.06	118.40
1	B	15	GLU	CB-CA-C	-5.36	100.71	110.63
1	B	119	ASN	CB-CG-ND2	5.36	124.44	116.40
1	C	117	LYS	N-CA-C	5.33	116.94	108.79
1	B	118	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	B	26	ASN	CB-CG-ND2	5.31	124.37	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	SER	N-CA-CB	5.30	118.01	110.16
1	B	41	ARG	CD-NE-CZ	5.29	131.81	124.40
1	C	85	PHE	CA-CB-CG	-5.29	108.50	113.80
1	A	85	PHE	CA-C-O	5.29	126.16	120.55
1	B	41	ARG	CA-C-N	5.29	130.30	123.00
1	B	41	ARG	C-N-CA	5.29	130.30	123.00
1	A	41	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	73	SER	O-C-N	5.27	128.80	122.79
1	B	85	PHE	CA-CB-CG	-5.26	108.54	113.80
1	B	19	PRO	CA-C-O	5.23	127.49	119.55
1	B	71	GLY	CA-C-N	5.22	128.88	121.42
1	B	71	GLY	C-N-CA	5.22	128.88	121.42
1	A	67	LYS	N-CA-CB	5.21	118.92	110.42
1	C	92	PHE	N-CA-C	5.21	119.62	113.16
1	C	14	GLU	CG-CD-OE2	-5.21	106.42	118.40
1	B	36	PRO	N-CD-CG	-5.20	95.39	103.20
1	C	108	GLU	CB-CA-C	-5.20	99.44	109.37
1	C	14	GLU	CA-CB-CG	-5.19	103.72	114.10
1	C	22	PHE	O-C-N	5.18	127.61	122.12
1	B	53	ALA	CA-C-O	5.18	127.91	120.51
1	A	97	GLU	CA-C-O	-5.17	113.22	119.27
1	C	3	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	77	ARG	CA-C-N	5.15	127.50	120.54
1	A	77	ARG	C-N-CA	5.15	127.50	120.54
1	C	120	ASN	CA-C-O	-5.14	113.06	119.28
1	B	75	GLU	CG-CD-OE2	-5.12	106.62	118.40
1	A	86	GLU	CB-CA-C	-5.12	102.85	110.88
1	A	28	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	126	LYS	CB-CA-C	5.08	119.76	110.10
1	A	15	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	A	96	MET	CB-CA-C	5.05	119.97	110.63
1	B	8	CYS	CA-C-O	-5.05	114.72	120.32
1	A	24	LYS	CB-CA-C	-5.04	100.58	110.11
1	A	100	LEU	CA-C-O	-5.04	114.64	120.49
1	A	76	SER	N-CA-CB	-5.04	102.71	110.12
1	B	119	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	42	SER	CA-C-O	-5.03	114.95	120.43
1	B	18	LEU	CD1-CG-CD2	-5.02	99.76	110.80

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	997	0	982	43	0
1	B	997	0	982	46	0
1	C	997	0	982	47	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	57	0	0	0	0
3	B	64	0	0	1	0
3	C	80	0	0	2	0
All	All	3227	0	2946	119	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 20.

All (119) 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:54:ASP:OD1	1:B:56:GLN:HB2	1.51	1.09
1:C:126:LYS:HE2	1:C:126:LYS:C	1.93	0.93
1:A:28:THR:HG22	1:A:83:MET:HE3	1.52	0.92
1:A:111:HIS:CD2	1:A:114:LEU:H	1.89	0.91
1:A:120:ASN:HD21	1:B:100:LEU:HA	1.40	0.85
1:C:24:LYS:O	1:C:28:THR:HG23	1.79	0.82
1:A:126:LYS:HE2	1:A:126:LYS:C	2.06	0.81
1:B:54:ASP:CG	1:B:56:GLN:HB2	2.05	0.81
1:B:118:GLN:NE2	1:C:96:MET:HE3	1.95	0.81
1:B:106:GLU:OE1	3:B:139:HOH:O	1.97	0.81
1:B:125:PHE:O	1:B:126:LYS:HE3	1.81	0.80
1:A:111:HIS:HD2	1:A:114:LEU:H	1.27	0.80
1:A:6:VAL:HG22	1:A:64:MET:HG2	1.66	0.78
1:B:118:GLN:HE21	1:C:96:MET:HE3	1.49	0.78
1:C:119:ASN:HD21	1:C:121:VAL:HG13	1.49	0.77
1:C:111:HIS:CD2	1:C:114:LEU:H	2.03	0.77
1:C:126:LYS:C	1:C:126:LYS:CE	2.58	0.76
1:B:120:ASN:HD21	1:C:100:LEU:HA	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:HIS:CD2	1:A:113:THR:H	2.04	0.76
1:A:28:THR:CG2	1:A:83:MET:HE3	2.16	0.75
1:B:24:LYS:O	1:B:28:THR:HG23	1.86	0.74
1:B:32:THR:HG22	1:B:34:ILE:H	1.55	0.72
1:A:106:GLU:HG2	1:A:107:ILE:N	2.04	0.71
1:A:111:HIS:HD2	1:A:113:THR:H	1.38	0.71
1:A:28:THR:HG22	1:A:83:MET:CE	2.20	0.70
1:A:68:ILE:HD11	1:A:77:ARG:HD3	1.72	0.70
1:C:111:HIS:HD2	1:C:113:THR:H	1.39	0.70
1:C:119:ASN:ND2	1:C:121:VAL:HG13	2.07	0.69
1:C:96:MET:CE	1:C:103:LEU:HD22	2.24	0.68
1:B:32:THR:CG2	1:B:34:ILE:HB	2.24	0.68
1:C:96:MET:HE3	1:C:103:LEU:HD22	1.77	0.67
1:C:111:HIS:CD2	1:C:113:THR:H	2.13	0.67
1:C:78:GLN:O	1:C:82:GLU:HG3	1.94	0.66
1:A:52:MET:HE1	1:A:102:ALA:HB2	1.77	0.66
1:A:26:ASN:HB2	1:A:27:PRO:HD3	1.77	0.66
1:B:38:ALA:HB2	1:B:125:PHE:CD2	2.32	0.65
1:C:57:HIS:HD2	1:C:59:TYR:OH	1.78	0.65
1:C:111:HIS:HD2	1:C:114:LEU:H	1.44	0.64
1:A:38:ALA:HB2	1:A:125:PHE:CD1	2.35	0.61
1:A:100:LEU:HA	1:C:120:ASN:HD21	1.64	0.61
1:B:120:ASN:C	1:B:120:ASN:HD22	2.09	0.60
1:B:18:LEU:N	1:B:19:PRO:CD	2.64	0.60
1:A:37:LEU:HD21	1:B:54:ASP:HB3	1.84	0.60
1:B:32:THR:CG2	1:B:34:ILE:H	2.16	0.58
1:A:125:PHE:O	1:A:126:LYS:HD3	2.03	0.58
1:B:111:HIS:HD2	1:B:113:THR:H	1.51	0.58
1:B:24:LYS:O	1:B:28:THR:CG2	2.52	0.57
1:A:32:THR:OG1	1:A:34:ILE:HG13	2.05	0.56
1:B:111:HIS:HD2	1:B:114:LEU:H	1.53	0.56
1:C:13:ARG:HG3	1:C:46:TRP:CH2	2.40	0.56
1:A:67:LYS:NZ	1:B:108:GLU:OE2	2.38	0.56
1:B:111:HIS:CD2	1:B:114:LEU:H	2.24	0.55
1:A:68:ILE:C	1:A:110:LEU:HD12	2.30	0.55
1:A:26:ASN:HD22	1:A:26:ASN:N	2.05	0.55
1:B:21:LEU:HD22	1:B:25:VAL:HG23	1.87	0.54
1:A:121:VAL:HG23	1:A:125:PHE:HE1	1.71	0.54
1:A:101:LEU:H	1:C:120:ASN:HD21	1.56	0.54
1:C:24:LYS:O	1:C:28:THR:CG2	2.52	0.53
1:C:120:ASN:C	1:C:120:ASN:HD22	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:HIS:CD2	1:B:113:THR:H	2.27	0.53
1:C:18:LEU:N	1:C:19:PRO:CD	2.71	0.53
1:C:122:HIS:O	1:C:126:LYS:HB3	2.09	0.52
1:C:96:MET:HE2	1:C:101:LEU:HD23	1.92	0.51
1:A:96:MET:HE3	1:C:118:GLN:NE2	2.26	0.51
1:A:26:ASN:CB	1:A:27:PRO:HD3	2.40	0.50
1:A:34:ILE:HD12	1:A:35:PHE:CZ	2.47	0.50
1:A:120:ASN:HD21	1:B:101:LEU:H	1.58	0.49
1:B:29:LEU:O	1:B:32:THR:HB	2.11	0.49
1:C:54:ASP:OD1	1:C:56:GLN:HB2	2.12	0.49
1:A:120:ASN:ND2	1:B:101:LEU:H	2.10	0.49
1:C:126:LYS:C	1:C:126:LYS:NZ	2.71	0.49
1:C:75:GLU:HB2	3:C:198:HOH:O	2.12	0.48
1:B:96:MET:HG2	1:B:101:LEU:HD23	1.95	0.48
1:B:119:ASN:HD22	1:B:121:VAL:H	1.62	0.48
1:C:119:ASN:ND2	1:C:121:VAL:H	2.12	0.48
1:B:18:LEU:HD12	1:B:46:TRP:CH2	2.48	0.48
1:A:13:ARG:HH11	1:A:13:ARG:HD2	1.44	0.47
1:A:101:LEU:H	1:C:120:ASN:ND2	2.13	0.47
1:A:18:LEU:N	1:A:19:PRO:CD	2.76	0.47
1:B:119:ASN:ND2	1:B:121:VAL:H	2.12	0.47
1:C:34:ILE:HD11	3:C:144:HOH:O	2.15	0.47
1:C:73:SER:O	1:C:76:SER:HB2	2.14	0.47
1:C:125:PHE:O	1:C:126:LYS:C	2.57	0.47
1:A:120:ASN:HD22	1:A:120:ASN:C	2.23	0.46
1:B:34:ILE:HG21	1:B:34:ILE:HD13	1.50	0.46
1:A:119:ASN:C	1:A:119:ASN:HD22	2.22	0.46
1:B:126:LYS:HE3	1:B:126:LYS:C	2.40	0.46
1:C:67:LYS:HA	1:C:108:GLU:O	2.16	0.46
1:B:38:ALA:HB2	1:B:125:PHE:HD2	1.81	0.46
1:B:64:MET:HE1	1:B:88:ILE:HG21	1.98	0.46
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.85	0.44
1:C:13:ARG:HH11	1:C:13:ARG:HD3	1.65	0.44
1:A:52:MET:HE1	1:A:102:ALA:CB	2.45	0.44
1:A:111:HIS:HD2	1:A:113:THR:N	2.09	0.43
1:C:13:ARG:O	1:C:13:ARG:HG2	2.05	0.43
1:A:57:HIS:HD2	1:A:59:TYR:OH	2.01	0.43
1:B:48:ASP:OD1	1:B:48:ASP:C	2.62	0.43
1:A:34:ILE:O	1:A:72:ARG:NH1	2.52	0.43
1:A:121:VAL:HG23	1:A:125:PHE:CE1	2.52	0.43
1:B:119:ASN:ND2	1:B:121:VAL:HG13	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASN:ND2	1:C:101:LEU:H	2.17	0.42
1:B:58:ASP:O	1:B:99:ARG:NH2	2.52	0.42
1:A:34:ILE:HD12	1:A:35:PHE:CE2	2.55	0.42
1:B:43:ARG:HB2	1:C:47:VAL:HG11	2.02	0.41
1:C:13:ARG:HG3	1:C:46:TRP:CZ3	2.55	0.41
1:B:68:ILE:HD11	1:B:77:ARG:HD3	2.02	0.41
1:B:26:ASN:N	1:B:27:PRO:CD	2.84	0.41
1:C:95:LEU:HD23	1:C:95:LEU:HA	1.85	0.41
1:B:43:ARG:HB2	1:C:47:VAL:CG1	2.50	0.41
1:C:111:HIS:HA	1:C:112:PRO:HD3	1.89	0.41
1:A:44:VAL:CG1	1:B:49:THR:HB	2.51	0.41
1:C:52:MET:HE1	1:C:102:ALA:HB2	2.03	0.41
1:A:37:LEU:O	1:B:53:ALA:HA	2.21	0.41
1:B:120:ASN:C	1:B:120:ASN:ND2	2.75	0.40
1:C:64:MET:O	1:C:105:PHE:HA	2.22	0.40
1:C:111:HIS:HD2	1:C:113:THR:N	2.14	0.40
1:C:83:MET:HB2	1:C:83:MET:HE3	1.78	0.40
1:A:121:VAL:O	1:A:124:LEU:HB2	2.22	0.40
1:C:54:ASP:C	1:C:56:GLN:N	2.80	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	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	B	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	C	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
All	All	369/375 (98%)	360 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	105/105 (100%)	90 (86%)	15 (14%)	3	1
1	B	105/105 (100%)	90 (86%)	15 (14%)	3	1
1	C	105/105 (100%)	91 (87%)	14 (13%)	4	2
All	All	315/315 (100%)	271 (86%)	44 (14%)	3	2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	21	LEU
1	A	26	ASN
1	A	34	ILE
1	A	47	VAL
1	A	75	GLU
1	A	99	ARG
1	A	100	LEU
1	A	103	LEU
1	A	115	ASN
1	A	117	LYS
1	A	120	ASN
1	A	121	VAL
1	A	124	LEU
1	A	126	LYS
1	B	13	ARG
1	B	21	LEU
1	B	28	THR
1	B	32	THR
1	B	47	VAL
1	B	87	LEU
1	B	97	GLU
1	B	98	SER
1	B	100	LEU
1	B	103	LEU
1	B	104	SER

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Mol	Chain	Res	Type
1	B	120	ASN
1	B	121	VAL
1	B	124	LEU
1	B	126	LYS
1	C	18	LEU
1	C	21	LEU
1	C	28	THR
1	C	29	LEU
1	C	75	GLU
1	C	76	SER
1	C	83	MET
1	C	100	LEU
1	C	103	LEU
1	C	106	GLU
1	C	117	LYS
1	C	120	ASN
1	C	121	VAL
1	C	126	LYS

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	26	ASN
1	A	57	HIS
1	A	111	HIS
1	A	119	ASN
1	A	120	ASN
1	B	57	HIS
1	B	111	HIS
1	B	118	GLN
1	B	119	ASN
1	B	120	ASN
1	C	57	HIS
1	C	78	GLN
1	C	111	HIS
1	C	118	GLN
1	C	119	ASN
1	C	120	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](#)

7 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	C	127	-	4,4,4	0.91	0	6,6,6	0.65	0
2	SO4	A	127	-	4,4,4	0.94	0	6,6,6	0.29	0
2	SO4	A	1	-	4,4,4	0.91	0	6,6,6	0.76	0
2	SO4	A	128	-	4,4,4	0.82	0	6,6,6	0.91	0
2	SO4	B	128	-	4,4,4	0.53	0	6,6,6	0.45	0
2	SO4	C	128	-	4,4,4	0.67	0	6,6,6	0.75	0
2	SO4	B	127	-	4,4,4	0.73	0	6,6,6	0.39	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.

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 [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, 95th 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 ²)	Q<0.9
1	A	125/125 (100%)	-0.63	0 100 100	18, 30, 55, 74	0
1	B	125/125 (100%)	-0.58	0 100 100	19, 28, 51, 68	0
1	C	125/125 (100%)	-0.82	1 (0%) 82 84	15, 26, 45, 64	0
All	All	375/375 (100%)	-0.68	1 (0%) 90 91	15, 28, 52, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	126	LYS	2.3

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, 95th 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 ²)	Q<0.9
2	SO4	A	127	5/5	0.91	0.08	99,99,99,99	0
2	SO4	A	1	5/5	0.94	0.08	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	128	5/5	0.97	0.06	62,62,63,63	0
2	SO4	B	128	5/5	0.97	0.09	50,50,50,51	0
2	SO4	C	127	5/5	0.97	0.07	48,49,49,50	0
2	SO4	B	127	5/5	0.98	0.06	45,46,47,47	0
2	SO4	C	128	5/5	0.98	0.07	41,42,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.