



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:39 PM UTC

PDB ID : 6NVT / pdb_00006nvt
Title : Crystal structure of TLA-1 extended spectrum Beta-lactamase
Authors : Rudino-Pinera, E.; Cifuentes-Castro, V.H.; Rodriguez-Almazan, C.
Deposited on : 2019-02-05
Resolution : 2.20 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

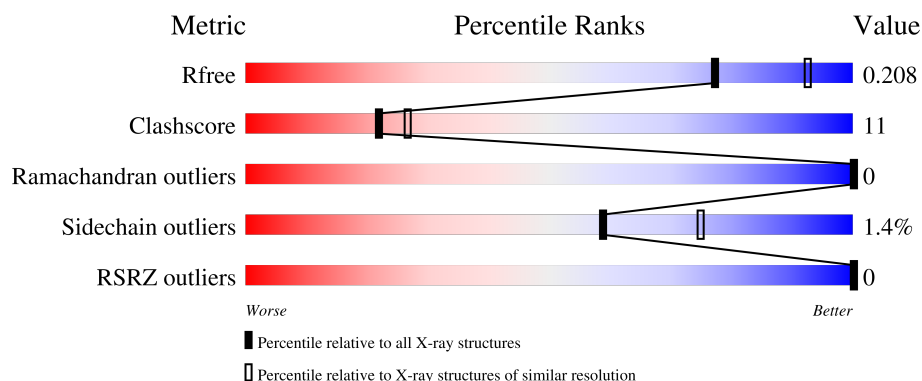
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

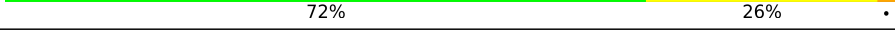
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	276	 77% 21% .
1	B	276	 76% 21% .
1	C	276	 73% 24% .
1	D	276	 72% 26% .

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
4	ACT	A	309	-	-	X	-
4	ACT	A	310	-	-	X	-
4	ACT	A	312	-	-	X	-
4	ACT	A	313	-	-	X	-
4	ACT	A	314	-	-	X	-
4	ACT	A	317	-	-	X	-
4	ACT	A	318	-	-	X	-
4	ACT	A	320	-	-	X	-
4	ACT	B	309	-	-	X	-
4	ACT	C	315	-	-	X	-
4	ACT	C	317	-	-	X	-
4	ACT	C	319	-	-	X	-
4	ACT	C	320	-	-	X	-
4	ACT	D	309	-	-	X	-
4	ACT	D	310	-	-	X	-
4	ACT	D	311	-	-	X	-
4	ACT	D	312	-	-	X	-
4	ACT	D	314	-	-	X	-
4	ACT	D	315	-	-	X	-
4	ACT	D	316	-	-	X	-
4	ACT	D	318	-	-	X	-
4	ACT	D	319	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10170 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	7	3	0
			2201	1402	371	423	5			
1	B	276	Total	C	N	O	S	9	3	0
			2201	1405	368	423	5			
1	C	276	Total	C	N	O	S	16	5	0
			2213	1412	371	425	5			
1	D	276	Total	C	N	O	S	9	4	0
			2213	1410	369	429	5			

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



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		

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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	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		

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	4	Total Cl 4 4	0	0
3	D	2	Total Cl 2 2	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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	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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	0
			254	254		
5	B	263	Total	O	0	0
			263	263		
5	C	256	Total	O	0	0
			256	256		
5	D	263	Total	O	0	0
			263	263		

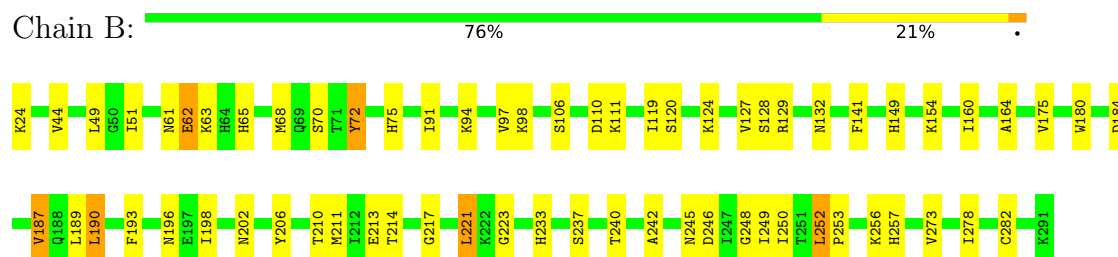
3 Residue-property plots

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.

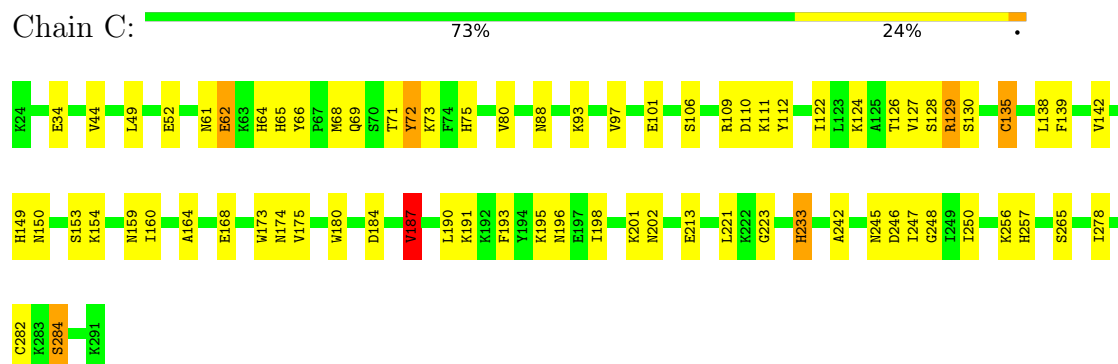
• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase

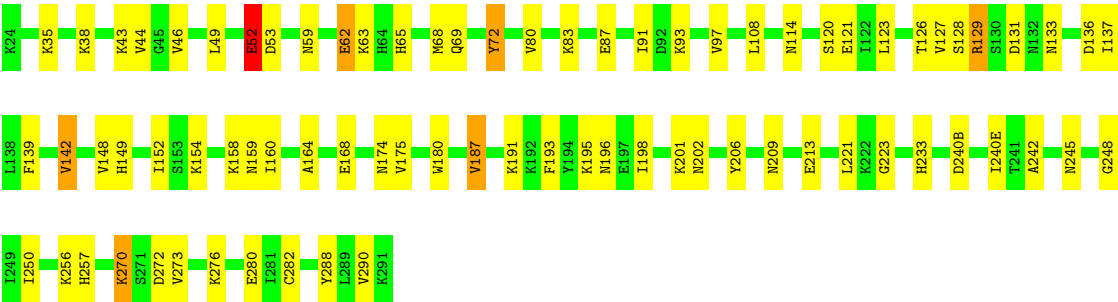


• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.06Å 99.01Å 99.70Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	35.15 – 2.20 35.15 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.15-2.20) 99.7 (35.15-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.181 , 0.208 0.183 , 0.208	Depositor DCC
R_{free} test set	4863 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for l,k,-h 0.009 for -h,-l,-k 0.007 for -h,l,k 0.469 for k,h,-l 0.469 for -k,-h,-l 0.008 for l,h,k 0.007 for k,l,h 0.007 for -l,-h,k 0.007 for -k,-l,h 0.477 for h,-k,-l 0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10170	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4, CL

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	1.90	29/2244 (1.3%)	1.24	25/3030 (0.8%)
1	B	1.90	31/2248 (1.4%)	1.21	22/3035 (0.7%)
1	C	1.88	28/2263 (1.2%)	1.23	27/3056 (0.9%)
1	D	1.89	30/2257 (1.3%)	1.18	23/3048 (0.8%)
All	All	1.89	118/9012 (1.3%)	1.21	97/12169 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	2
All	All	0	5

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	THR	C-N	9.53	1.55	1.34
1	B	240	THR	C-N	8.06	1.52	1.34
1	C	128	SER	C-O	-7.04	1.15	1.24
1	A	240	THR	C-O	-6.65	1.16	1.24
1	B	240	THR	CA-C	6.58	1.60	1.52
1	C	247	ILE	C-O	-6.58	1.17	1.24
1	C	126	THR	C-O	-6.42	1.16	1.24
1	B	97	VAL	C-O	-6.36	1.17	1.24
1	A	97	VAL	C-O	-6.27	1.17	1.24
1	B	127	VAL	C-O	-6.22	1.18	1.24
1	D	128	SER	C-O	-6.15	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	160	ILE	C-O	-6.08	1.17	1.24
1	C	97	VAL	C-O	-5.97	1.17	1.24
1	B	128	SER	C-O	-5.89	1.17	1.24
1	C	122	ILE	C-O	-5.86	1.17	1.24
1	B	75	HIS	C-O	-5.83	1.17	1.24
1	C	160	ILE	C-O	-5.79	1.18	1.24
1	A	69	GLN	C-O	-5.78	1.18	1.24
1	D	131	ASP	C-O	-5.78	1.17	1.24
1	C	129[A]	ARG	CA-C	5.77	1.60	1.52
1	C	129[B]	ARG	CA-C	5.77	1.60	1.52
1	D	221	LEU	C-O	-5.75	1.17	1.24
1	A	128	SER	C-O	-5.72	1.17	1.24
1	D	121	GLU	C-O	-5.68	1.17	1.24
1	A	176	GLN	C-O	-5.67	1.17	1.24
1	B	149	HIS	C-O	-5.67	1.17	1.24
1	A	190	LEU	C-O	-5.66	1.17	1.24
1	A	126	THR	C-O	-5.63	1.17	1.24
1	D	250	ILE	C-O	-5.62	1.18	1.24
1	A	237	SER	C-O	-5.61	1.16	1.23
1	A	109	ARG	C-O	-5.58	1.17	1.24
1	A	160	ILE	C-O	-5.58	1.18	1.24
1	A	193	PHE	C-O	-5.58	1.17	1.24
1	A	142	VAL	C-O	-5.58	1.18	1.24
1	C	175	VAL	C-O	-5.57	1.17	1.24
1	D	46	VAL	C-O	-5.57	1.18	1.24
1	D	97	VAL	C-O	-5.56	1.18	1.24
1	B	237	SER	C-O	-5.56	1.17	1.23
1	B	44	VAL	C-O	-5.53	1.18	1.24
1	A	115	VAL	C-O	-5.52	1.18	1.23
1	B	106	SER	C-O	-5.48	1.18	1.24
1	D	127	VAL	C-O	-5.48	1.18	1.24
1	A	221	LEU	C-O	-5.48	1.17	1.24
1	B	214	THR	C-O	-5.47	1.17	1.23
1	C	142	VAL	C-O	-5.47	1.18	1.24
1	C	168	GLU	C-O	-5.46	1.17	1.24
1	C	193	PHE	C-O	-5.44	1.17	1.24
1	A	129[A]	ARG	CA-C	5.44	1.60	1.52
1	A	129[B]	ARG	CA-C	5.44	1.60	1.52
1	D	137	ILE	C-O	-5.44	1.17	1.24
1	A	122	ILE	C-O	-5.42	1.17	1.24
1	C	278	ILE	C-O	-5.42	1.18	1.24
1	D	273	VAL	C-O	-5.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	VAL	C-O	-5.40	1.17	1.24
1	B	190	LEU	C-O	-5.40	1.17	1.24
1	A	189	LEU	C-O	-5.38	1.17	1.24
1	C	106	SER	C-O	-5.38	1.19	1.24
1	C	71	THR	C-O	-5.37	1.17	1.24
1	C	190	LEU	C-O	-5.37	1.17	1.24
1	B	221	LEU	C-O	-5.36	1.17	1.24
1	A	71	THR	C-O	-5.35	1.17	1.24
1	A	157	VAL	C-O	-5.33	1.18	1.24
1	D	123	LEU	C-O	-5.33	1.17	1.24
1	B	273	VAL	C-O	-5.32	1.17	1.24
1	C	69	GLN	C-O	-5.32	1.19	1.24
1	B	278	ILE	C-O	-5.31	1.18	1.24
1	B	233	HIS	C-O	-5.29	1.17	1.23
1	D	133	ASN	C-O	-5.29	1.17	1.24
1	D	193	PHE	C-O	-5.29	1.18	1.24
1	D	136	ASP	C-O	-5.28	1.18	1.24
1	D	126	THR	C-O	-5.28	1.18	1.24
1	D	142	VAL	C-O	-5.28	1.18	1.24
1	A	131	ASP	C-O	-5.26	1.17	1.24
1	B	250	ILE	C-O	-5.26	1.18	1.24
1	C	138	LEU	C-O	-5.23	1.18	1.24
1	B	141	PHE	C-O	-5.22	1.18	1.24
1	C	282	CYS	C-O	-5.22	1.18	1.24
1	C	187	VAL	C-O	-5.22	1.18	1.24
1	C	109	ARG	C-O	-5.21	1.18	1.24
1	A	175	VAL	C-O	-5.21	1.18	1.24
1	C	250	ILE	C-O	-5.19	1.18	1.24
1	C	135	CYS	C-O	-5.18	1.18	1.24
1	C	173	TRP	C-O	-5.18	1.18	1.24
1	D	272	ASP	C-O	-5.18	1.18	1.24
1	B	72[A]	TYR	CA-C	5.18	1.60	1.52
1	B	72[B]	TYR	CA-C	5.18	1.60	1.52
1	B	282	CYS	C-O	-5.18	1.18	1.24
1	C	110	ASP	C-O	-5.17	1.18	1.24
1	D	44	VAL	C-O	-5.16	1.18	1.24
1	A	36	TYR	C-O	-5.16	1.17	1.24
1	B	106	SER	N-CA	-5.15	1.42	1.46
1	A	278	ILE	C-O	-5.13	1.18	1.24
1	B	193	PHE	C-O	-5.13	1.18	1.24
1	D	108	LEU	C-O	-5.13	1.18	1.24
1	C	75	HIS	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	PHE	C-O	-5.12	1.18	1.24
1	B	160	ILE	C-O	-5.11	1.18	1.24
1	C	127	VAL	C-O	-5.11	1.18	1.24
1	A	139	PHE	C-O	-5.10	1.18	1.24
1	D	240(E)	ILE	C-O	-5.08	1.18	1.24
1	A	247	ILE	C-O	-5.08	1.19	1.24
1	A	99	LYS	C-O	-5.07	1.18	1.24
1	B	119	ILE	C-O	-5.07	1.18	1.24
1	B	132	ASN	C-O	-5.06	1.18	1.24
1	D	191	LYS	C-O	-5.06	1.18	1.24
1	D	72[A]	TYR	CA-C	5.04	1.59	1.52
1	D	72[B]	TYR	CA-C	5.04	1.59	1.52
1	D	139	PHE	C-O	-5.03	1.18	1.24
1	B	211	MET	C-O	-5.03	1.18	1.24
1	D	69	GLN	C-O	-5.03	1.19	1.24
1	B	189	LEU	C-O	-5.02	1.18	1.24
1	D	282	CYS	C-O	-5.02	1.18	1.24
1	D	168	GLU	C-O	-5.01	1.18	1.24
1	D	280	GLU	C-O	-5.01	1.18	1.24
1	A	127	VAL	C-O	-5.00	1.18	1.24
1	B	110	ASP	C-O	-5.00	1.18	1.24
1	B	180	TRP	C-O	-5.00	1.17	1.23
1	B	217	GLY	C-O	-5.00	1.17	1.24

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	THR	O-C-N	10.54	139.56	122.70
1	A	62	GLU	N-CA-C	10.25	123.50	111.71
1	B	240	THR	O-C-N	10.00	138.69	122.70
1	A	68	MET	N-CA-C	9.59	121.82	111.36
1	A	62	GLU	CA-C-O	9.55	130.89	120.10
1	D	68	MET	N-CA-C	9.51	121.73	111.36
1	A	240	THR	CA-C-N	-9.44	96.43	117.20
1	A	129[A]	ARG	CA-C-O	9.42	130.70	119.59
1	A	129[B]	ARG	CA-C-O	9.42	130.70	119.59
1	B	68	MET	N-CA-C	9.17	121.35	111.36
1	C	284[A]	SER	N-CA-C	9.13	123.68	112.54
1	C	284[B]	SER	N-CA-C	9.13	123.68	112.54
1	C	72[A]	TYR	CA-C-O	9.11	130.58	119.10
1	C	72[B]	TYR	CA-C-O	9.11	130.58	119.10
1	A	248	GLY	N-CA-C	9.09	123.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129[A]	ARG	CA-C-O	8.81	129.99	119.59
1	C	129[B]	ARG	CA-C-O	8.81	129.99	119.59
1	C	68	MET	N-CA-C	8.74	120.89	111.36
1	C	248	GLY	N-CA-C	8.36	122.59	110.80
1	B	72[A]	TYR	CA-C-O	8.29	129.54	119.10
1	B	72[B]	TYR	CA-C-O	8.29	129.54	119.10
1	C	198	ILE	N-CA-C	8.25	118.58	111.90
1	A	198	ILE	N-CA-C	8.03	118.40	111.90
1	D	198	ILE	N-CA-C	7.97	118.67	111.81
1	D	72[A]	TYR	CA-C-O	7.90	129.05	119.10
1	D	72[B]	TYR	CA-C-O	7.90	129.05	119.10
1	D	248	GLY	N-CA-C	7.74	120.99	110.69
1	C	62	GLU	N-CA-C	7.58	119.54	111.28
1	B	248	GLY	N-CA-C	7.57	121.48	110.80
1	C	129[A]	ARG	N-CA-C	7.53	122.59	112.88
1	C	129[B]	ARG	N-CA-C	7.53	122.59	112.88
1	B	198	ILE	N-CA-C	7.45	117.93	111.90
1	B	62	GLU	N-CA-C	7.38	119.32	111.28
1	D	175	VAL	N-CA-C	7.38	118.14	110.62
1	B	240	THR	CA-C-N	-7.36	101.00	117.20
1	A	129[A]	ARG	N-CA-C	7.13	122.08	112.88
1	A	129[B]	ARG	N-CA-C	7.13	122.08	112.88
1	D	62	GLU	N-CA-C	7.05	119.04	111.36
1	A	51	ILE	N-CA-C	6.82	116.94	110.53
1	C	198	ILE	CB-CA-C	-6.78	104.79	111.30
1	A	159	ASN	N-CA-C	6.72	120.81	111.74
1	B	175	VAL	N-CA-C	6.71	117.46	110.62
1	A	223	GLY	N-CA-C	6.65	120.71	112.73
1	C	257	HIS	N-CA-C	6.56	119.69	109.52
1	C	175	VAL	N-CA-C	6.52	117.28	110.62
1	B	257	HIS	N-CA-C	6.33	119.33	109.52
1	B	127	VAL	N-CA-C	6.25	116.43	110.74
1	A	198	ILE	CB-CA-C	-6.22	105.33	111.30
1	B	164	ALA	N-CA-C	6.21	119.61	109.24
1	C	164	ALA	N-CA-C	6.20	119.59	109.24
1	B	51	ILE	N-CA-C	6.18	116.34	110.53
1	C	223	GLY	N-CA-C	6.18	120.14	112.73
1	A	245	ASN	N-CA-C	6.17	119.08	109.52
1	B	198	ILE	CB-CA-C	-6.07	105.48	111.30
1	B	223	GLY	N-CA-C	6.02	119.96	112.73
1	B	245	ASN	N-CA-C	6.00	118.81	109.52
1	C	127	VAL	N-CA-C	5.99	116.63	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	VAL	CA-C-N	5.94	132.40	121.70
1	D	290	VAL	C-N-CA	5.94	132.40	121.70
1	D	128	SER	N-CA-C	5.90	117.79	111.36
1	A	257	HIS	N-CA-C	5.89	118.66	109.52
1	D	233	HIS	N-CA-C	5.88	117.72	108.96
1	D	53	ASP	N-CA-C	5.87	116.03	108.34
1	C	159	ASN	N-CA-C	5.79	119.55	111.74
1	C	72[A]	TYR	N-CA-C	5.76	119.79	112.87
1	C	72[B]	TYR	N-CA-C	5.76	119.79	112.87
1	C	233	HIS	N-CA-C	5.72	116.95	108.60
1	D	257	HIS	N-CA-C	5.69	118.33	109.52
1	A	164	ALA	N-CA-C	5.68	118.73	109.24
1	D	242	ALA	N-CA-C	5.63	117.10	111.07
1	D	164	ALA	N-CA-C	5.59	118.56	109.06
1	B	233	HIS	N-CA-C	5.55	116.71	108.60
1	D	223	GLY	N-CA-C	5.53	119.36	112.73
1	A	267	SER	N-CA-C	5.52	118.24	109.24
1	C	245	ASN	N-CA-C	5.51	118.56	109.85
1	B	242	ALA	N-CA-C	5.48	116.94	111.07
1	B	24	LYS	O-C-N	-5.43	114.32	123.00
1	D	127	VAL	N-CA-C	5.42	115.63	110.53
1	A	174[A]	ASN	N-CA-C	5.37	119.09	112.54
1	A	174[B]	ASN	N-CA-C	5.37	119.09	112.54
1	A	242	ALA	N-CA-C	5.34	117.10	111.28
1	C	126	THR	N-CA-C	5.33	116.89	111.14
1	A	180	TRP	N-CA-C	5.31	117.76	109.52
1	D	245	ASN	N-CA-C	5.31	117.75	109.52
1	A	46	VAL	N-CA-C	5.22	116.24	108.46
1	B	252	LEU	CA-C-N	5.18	124.98	119.28
1	B	252	LEU	C-N-CA	5.18	124.98	119.28
1	D	206	TYR	N-CA-C	5.17	116.61	111.07
1	C	180	TRP	N-CA-C	5.12	117.45	109.52
1	C	242	ALA	N-CA-C	5.12	116.55	111.07
1	B	111	LYS	N-CA-C	5.09	116.91	111.36
1	C	44	VAL	N-CA-C	5.09	115.29	108.17
1	D	129	ARG	N-CA-C	5.06	119.41	112.88
1	D	180	TRP	N-CA-C	5.02	117.30	109.52
1	D	72[A]	TYR	N-CA-C	5.02	118.89	112.87
1	D	72[B]	TYR	N-CA-C	5.02	118.89	112.87
1	A	55	PHE	N-CA-C	5.01	117.56	110.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	GLU	Mainchain
1	C	284[A]	SER	Mainchain
1	C	284[B]	SER	Mainchain
1	D	52[A]	GLU	Mainchain
1	D	52[B]	GLU	Mainchain

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	2201	0	2248	29	1
1	B	2201	0	2249	30	0
1	C	2213	0	2262	44	0
1	D	2213	0	2246	60	1
2	A	35	0	0	2	0
2	B	35	0	0	1	0
2	C	50	0	0	3	0
2	D	30	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	4	0	0	3	0
3	D	2	0	0	1	0
4	A	48	0	36	24	1
4	B	24	0	18	8	0
4	C	28	0	21	7	0
4	D	48	0	36	29	0
5	A	254	0	0	21	0
5	B	263	0	0	11	0
5	C	256	0	0	16	0
5	D	263	0	0	20	1
All	All	10170	0	9116	194	2

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 11.

All (194) 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:D:62:GLU:OE2	4:D:314:ACT:H1	1.36	1.24
1:D:174[A]:ASN:ND2	5:D:401:HOH:O	1.60	1.23
1:D:52[B]:GLU:CG	1:D:256:LYS:HD2	1.71	1.19
1:D:52[A]:GLU:HG3	1:D:256:LYS:HD2	1.16	1.16
1:D:52[B]:GLU:HG3	1:D:256:LYS:HD2	1.16	1.16
4:D:312:ACT:H2	5:D:575:HOH:O	1.48	1.12
1:D:52[B]:GLU:HG3	1:D:256:LYS:CD	1.80	1.10
1:D:52[A]:GLU:HG3	1:D:256:LYS:CD	1.80	1.10
4:A:312:ACT:O	5:A:401:HOH:O	1.67	1.09
1:B:62:GLU:HG2	1:B:184:ASP:OD1	1.51	1.08
4:B:309:ACT:CH3	5:B:411:HOH:O	2.01	1.08
1:D:201:LYS:HE3	5:D:528:HOH:O	1.52	1.08
2:C:310:SO4:O1	5:C:402:HOH:O	1.70	1.06
4:D:309:ACT:O	5:D:402:HOH:O	1.71	1.06
4:A:318:ACT:OXT	5:A:402:HOH:O	1.76	1.03
4:B:309:ACT:H2	5:B:411:HOH:O	1.57	1.03
4:C:319:ACT:OXT	4:C:320:ACT:H2	1.60	1.01
1:B:256[B]:LYS:NZ	1:C:202:ASN:OD1	1.95	0.99
1:B:62:GLU:CG	1:B:184:ASP:OD1	2.11	0.97
1:D:149:HIS:ND1	5:D:404:HOH:O	1.97	0.96
1:A:129[A]:ARG:NH1	5:A:403:HOH:O	1.78	0.95
4:A:320:ACT:O	5:A:404:HOH:O	1.83	0.95
1:A:217:GLY:H	4:A:314:ACT:H2	1.28	0.94
1:D:288:TYR:OH	4:D:318:ACT:H1	1.67	0.94
1:D:35:LYS:HA	1:D:38:LYS:HD2	1.48	0.94
1:D:52[A]:GLU:CG	1:D:256:LYS:HD2	1.71	0.94
1:D:114:ASN:ND2	4:D:320:ACT:OXT	1.99	0.93
1:C:52:GLU:CG	1:C:256:LYS:HD2	2.00	0.91
1:C:154:LYS:HD2	1:C:154:LYS:N	1.86	0.89
1:D:62:GLU:OE2	4:D:314:ACT:CH3	2.20	0.88
4:D:309:ACT:OXT	5:D:403:HOH:O	1.93	0.87
1:C:52:GLU:HG3	1:C:256:LYS:HD2	1.54	0.86
1:A:150:ASN:O	1:A:154:LYS:HE2	1.75	0.85
1:B:65:HIS:HE1	5:B:580:HOH:O	1.58	0.85
4:D:319:ACT:H1	5:D:598:HOH:O	1.77	0.84
4:D:312:ACT:CH3	5:D:575:HOH:O	2.12	0.84
1:A:52:GLU:HG3	1:A:256:LYS:HD2	1.57	0.83
1:A:52:GLU:CG	1:A:256:LYS:HD2	2.07	0.82
4:A:310:ACT:H2	5:A:463:HOH:O	1.79	0.82
4:C:315:ACT:OXT	5:C:403:HOH:O	1.98	0.82
1:D:59:ASN:HB3	1:D:62:GLU:OE1	1.80	0.81
1:A:256:LYS:HE2	5:A:603:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LYS:CE	4:D:319:ACT:H3	2.11	0.81
1:A:49:LEU:HD22	1:A:187:VAL:HG13	1.63	0.80
1:D:62:GLU:CD	4:D:314:ACT:H1	2.06	0.80
1:D:62:GLU:CD	4:D:314:ACT:CH3	2.55	0.79
4:B:311:ACT:O	5:B:401:HOH:O	2.02	0.78
1:A:256:LYS:CE	5:A:603:HOH:O	2.30	0.77
1:D:52[B]:GLU:HG2	1:D:256:LYS:HD2	1.67	0.77
1:B:94:LYS:H	4:B:312:ACT:H2	1.52	0.75
4:C:319:ACT:OXT	4:C:320:ACT:CH3	2.34	0.75
1:D:195:LYS:HE2	4:D:319:ACT:H3	1.67	0.74
1:C:52:GLU:HG3	1:C:256:LYS:CD	2.17	0.74
1:D:52[B]:GLU:CG	1:D:256:LYS:CD	2.54	0.74
1:A:49:LEU:HD22	1:A:187:VAL:CG1	2.19	0.73
1:D:93:LYS:NZ	4:D:310:ACT:H2	2.02	0.73
1:C:49:LEU:HD22	1:C:187:VAL:HG13	1.70	0.72
1:D:63:LYS:HG2	5:D:513:HOH:O	1.88	0.72
1:B:49:LEU:HD22	1:B:187:VAL:HG13	1.72	0.71
1:B:98:LYS:NZ	5:B:405:HOH:O	2.24	0.71
4:A:314:ACT:H1	5:A:559:HOH:O	1.91	0.70
1:A:271:SER:H	4:A:312:ACT:H2	1.55	0.70
1:A:62:GLU:OE2	4:A:317:ACT:H1	1.93	0.69
5:C:505:HOH:O	4:D:312:ACT:H3	1.91	0.69
2:A:307:SO4:O4	5:A:405:HOH:O	2.08	0.69
1:D:158:LYS:HG2	4:D:311:ACT:O	1.94	0.68
1:A:120:SER:HB3	4:A:313:ACT:H1	1.76	0.67
1:C:93:LYS:HZ1	4:D:315:ACT:H3	1.60	0.67
1:D:80:VAL:HG12	1:D:142:VAL:HG13	1.77	0.67
4:A:310:ACT:H1	5:A:521:HOH:O	1.94	0.66
1:D:65:HIS:HD2	5:D:603:HOH:O	1.78	0.66
1:C:49:LEU:HD22	1:C:187:VAL:CG1	2.25	0.66
1:D:62:GLU:OE1	4:D:314:ACT:CH3	2.43	0.66
1:A:49:LEU:HB2	1:A:187:VAL:HG13	1.79	0.64
1:D:49:LEU:HD12	1:D:187:VAL:HG13	1.79	0.64
1:C:49:LEU:HB2	1:C:187:VAL:HG13	1.78	0.64
1:C:184:ASP:OD1	5:C:404:HOH:O	2.16	0.63
4:A:309:ACT:H2	4:A:317:ACT:OXT	1.97	0.63
1:B:62:GLU:C	1:B:62:GLU:CD	2.67	0.62
1:D:62:GLU:OE1	4:D:314:ACT:H3	1.99	0.62
1:C:201:LYS:HE3	5:C:557:HOH:O	1.98	0.62
1:C:52:GLU:HG2	1:C:256:LYS:HD2	1.80	0.61
1:C:129[A]:ARG:HG2	5:C:498:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:HIS:ND1	5:C:410:HOH:O	2.31	0.61
4:A:318:ACT:H2	5:A:591:HOH:O	2.00	0.60
1:A:271:SER:N	4:A:312:ACT:H2	2.15	0.60
1:D:195:LYS:NZ	4:D:319:ACT:H3	2.15	0.60
1:A:62:GLU:H	1:A:62:GLU:CD	2.09	0.59
1:D:52[A]:GLU:CG	1:D:256:LYS:CD	2.54	0.59
1:D:93:LYS:HZ3	4:D:310:ACT:H2	1.66	0.59
1:C:174[A]:ASN:OD1	5:C:405:HOH:O	2.17	0.59
1:B:49:LEU:HD22	1:B:187:VAL:CG1	2.33	0.58
1:B:61:ASN:H	4:B:310:ACT:H3	1.68	0.58
1:D:43:LYS:CD	5:D:420:HOH:O	2.51	0.58
1:C:52:GLU:CG	1:C:256:LYS:CD	2.78	0.58
1:A:65:HIS:HD2	5:A:601:HOH:O	1.87	0.57
1:A:49:LEU:CD2	1:A:187:VAL:HG13	2.34	0.56
1:B:98:LYS:NZ	4:B:309:ACT:H1	2.20	0.56
1:D:129:ARG:NH1	5:D:405:HOH:O	2.19	0.56
1:D:196:ASN:HA	3:D:308:CL:CL	2.44	0.55
1:B:91:ILE:HG12	1:B:120:SER:HB2	1.87	0.55
1:B:154:LYS:N	1:B:154:LYS:HE2	2.22	0.55
1:A:180:TRP:HE1	4:A:320:ACT:H3	1.72	0.55
1:D:91:ILE:HG12	1:D:120:SER:HB2	1.88	0.54
1:B:49:LEU:HB2	1:B:187:VAL:HG13	1.88	0.54
1:C:201:LYS:HG2	5:C:557:HOH:O	2.06	0.54
4:B:313:ACT:H2	5:B:646:HOH:O	2.07	0.54
1:D:35:LYS:HA	1:D:38:LYS:CD	2.30	0.53
1:C:153:SER:C	1:C:154:LYS:HD2	2.33	0.53
1:A:256:LYS:HE3	5:A:603:HOH:O	1.98	0.53
1:B:124:LYS:NZ	1:B:213:GLU:OE1	2.41	0.53
1:D:43:LYS:HD3	5:D:420:HOH:O	2.09	0.53
1:D:83:LYS:O	1:D:87:GLU:HG3	2.09	0.53
2:A:304:SO4:O1	5:A:406:HOH:O	2.17	0.52
1:C:201:LYS:CG	5:C:557:HOH:O	2.58	0.52
1:B:202:ASN:OD1	1:C:256:LYS:NZ	2.42	0.52
1:B:221:LEU:HG	1:B:246:ASP:HB3	1.92	0.52
1:A:271:SER:H	4:A:312:ACT:CH3	2.21	0.51
1:C:65:HIS:HE1	5:C:420:HOH:O	1.93	0.51
4:A:318:ACT:CH3	5:A:591:HOH:O	2.55	0.51
1:C:233:HIS:NE2	3:C:311:CL:CL	2.58	0.51
1:D:93:LYS:HZ2	4:D:310:ACT:H2	1.75	0.51
1:C:150:ASN:O	1:C:154:LYS:HG2	2.10	0.51
2:C:308:SO4:O3	5:C:406:HOH:O	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:310:ACT:CH3	5:A:521:HOH:O	2.57	0.49
1:C:111:LYS:HD3	1:C:112:TYR:CE2	2.47	0.49
1:B:190:LEU:HB3	1:B:249:ILE:HD11	1.94	0.49
1:C:61:ASN:H	4:C:317:ACT:H2	1.78	0.48
1:D:80:VAL:HG12	1:D:142:VAL:CG1	2.43	0.48
1:D:149:HIS:CE1	5:D:404:HOH:O	2.58	0.48
1:B:70:SER:HB2	5:B:403:HOH:O	2.14	0.48
1:C:62:GLU:OE1	4:C:317:ACT:O	2.32	0.48
1:C:124:LYS:NZ	1:C:213:GLU:OE2	2.46	0.47
1:D:270:LYS:HA	4:D:315:ACT:H1	1.96	0.47
1:D:49:LEU:CD1	1:D:187:VAL:HG13	2.44	0.47
1:A:61:ASN:HA	4:A:309:ACT:H2	1.95	0.47
1:A:201:LYS:NZ	5:A:418:HOH:O	2.43	0.47
1:C:101:GLU:OE2	1:D:240(B):ASP:OD2	2.32	0.47
1:C:196:ASN:HA	3:C:313:CL:CL	2.52	0.47
1:D:52[B]:GLU:HG3	1:D:256:LYS:CE	2.42	0.46
1:D:52[A]:GLU:HG3	1:D:256:LYS:CE	2.42	0.46
1:B:62:GLU:OE1	1:B:63:LYS:N	2.48	0.46
1:C:265:SER:HB3	3:C:312:CL:CL	2.52	0.46
1:B:129:ARG:NH1	5:B:402:HOH:O	2.20	0.46
4:A:314:ACT:H3	5:A:609:HOH:O	2.16	0.46
1:B:49:LEU:CD2	1:B:187:VAL:HG13	2.45	0.46
1:B:252:LEU:HB3	1:B:253:PRO:HD2	1.98	0.46
1:C:129[A]:ARG:NH1	5:C:408:HOH:O	2.28	0.46
1:A:30:LYS:HZ1	4:A:317:ACT:H3	1.81	0.46
2:B:306:SO4:O1	5:B:403:HOH:O	2.21	0.46
1:D:288:TYR:OH	4:D:318:ACT:CH3	2.51	0.46
1:A:120:SER:CB	4:A:313:ACT:H1	2.45	0.45
1:B:65:HIS:HD2	5:B:605:HOH:O	2.00	0.45
1:C:88:ASN:HD22	4:D:316:ACT:H3	1.82	0.45
1:D:148:VAL:O	1:D:152:ILE:HG12	2.16	0.45
1:D:65:HIS:CD2	5:D:603:HOH:O	2.61	0.45
4:D:316:ACT:CH3	5:D:462:HOH:O	2.64	0.45
4:B:309:ACT:H3	5:B:411:HOH:O	1.90	0.45
1:C:49:LEU:CD2	1:C:187:VAL:HG13	2.43	0.45
1:A:54:ASN:ND2	5:A:424:HOH:O	2.50	0.45
1:B:206:TYR:O	1:B:210:THR:HG23	2.17	0.44
4:C:315:ACT:H3	5:C:511:HOH:O	2.18	0.43
4:A:320:ACT:H2	5:A:617:HOH:O	2.17	0.43
1:B:62:GLU:C	1:B:62:GLU:OE1	2.61	0.43
1:C:93:LYS:HZ1	4:D:315:ACT:CH3	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASN:H	4:D:311:ACT:H2	1.84	0.43
1:A:61:ASN:HA	4:A:309:ACT:CH3	2.49	0.43
4:A:314:ACT:CH3	5:A:609:HOH:O	2.66	0.42
1:B:196:ASN:HA	3:B:308:CL:CL	2.57	0.42
1:C:34:GLU:OE2	4:C:317:ACT:H3	2.19	0.42
1:D:52[A]:GLU:HG2	1:D:256:LYS:HD2	1.67	0.42
1:D:276:LYS:NZ	5:D:416:HOH:O	2.41	0.42
1:A:48:VAL:HG22	1:A:260:ILE:HG13	2.02	0.42
1:C:221:LEU:HG	1:C:246:ASP:HB3	2.02	0.42
1:D:43:LYS:NZ	5:D:420:HOH:O	2.46	0.42
1:A:154:LYS:HA	1:A:154:LYS:HD3	1.74	0.42
1:B:62:GLU:CD	1:B:62:GLU:O	2.63	0.42
1:B:62:GLU:HG3	1:B:184:ASP:OD1	2.11	0.42
1:C:49:LEU:HD12	1:C:49:LEU:HA	1.87	0.41
1:C:195:LYS:HE2	5:C:574:HOH:O	2.20	0.41
1:D:270:LYS:HD2	5:D:547:HOH:O	2.21	0.41
2:C:301:SO4:O4	5:C:407:HOH:O	2.20	0.41
1:C:191:LYS:O	1:C:195:LYS:HG3	2.20	0.41
1:D:154:LYS:N	1:D:154:LYS:HD2	2.36	0.41
1:C:256:LYS:HD3	1:C:256:LYS:HA	1.92	0.41
1:C:73:LYS:HE2	1:C:135:CYS:HB2	2.03	0.41
1:B:202:ASN:OD1	1:C:256:LYS:CE	2.68	0.41
1:C:93:LYS:NZ	4:D:315:ACT:H3	2.32	0.41
1:D:49:LEU:HG	1:D:187:VAL:CG1	2.51	0.41
1:D:209:ASN:O	1:D:213[B]:GLU:HG2	2.21	0.41
1:D:49:LEU:CG	1:D:187:VAL:HG13	2.51	0.40
1:D:35:LYS:NZ	5:D:431:HOH:O	2.55	0.40
1:A:111:LYS:HD3	1:A:112:TYR:CE2	2.57	0.40
1:C:64:HIS:HB3	1:C:66:TYR:CE1	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:312:ACT:CH3	5:D:522:HOH:O[1_545]	1.63	0.57
1:A:256:LYS:NZ	1:D:202:ASN:OD1[2_5411]	1.69	0.51

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	277/276 (100%)	274 (99%)	3 (1%)	0	100	100
1	B	277/276 (100%)	273 (99%)	4 (1%)	0	100	100
1	C	279/276 (101%)	275 (99%)	4 (1%)	0	100	100
1	D	278/276 (101%)	275 (99%)	3 (1%)	0	100	100
All	All	1111/1104 (101%)	1097 (99%)	14 (1%)	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	250/247 (101%)	245 (98%)	5 (2%)	48	64
1	B	250/247 (101%)	247 (99%)	3 (1%)	63	78
1	C	252/247 (102%)	246 (98%)	6 (2%)	43	58
1	D	251/247 (102%)	245 (98%)	6 (2%)	43	58
All	All	1003/988 (102%)	983 (98%)	20 (2%)	59	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80[A]	VAL
1	A	80[B]	VAL

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Mol	Chain	Res	Type
1	A	158	LYS
1	A	187	VAL
1	A	270	LYS
1	B	72[A]	TYR
1	B	72[B]	TYR
1	B	187	VAL
1	C	72[A]	TYR
1	C	72[B]	TYR
1	C	80[A]	VAL
1	C	80[B]	VAL
1	C	130	SER
1	C	187	VAL
1	D	52[A]	GLU
1	D	52[B]	GLU
1	D	72[A]	TYR
1	D	72[B]	TYR
1	D	187	VAL
1	D	270	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	C	59	ASN
1	C	88	ASN
1	C	245	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 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
2	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	B	307	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	D	303	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	C	307	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.15	0
4	ACT	C	319	-	3,3,3	1.01	0	3,3,3	0.94	0
2	SO4	D	305	-	4,4,4	0.22	0	6,6,6	0.21	0
4	ACT	D	309	-	3,3,3	0.82	0	3,3,3	0.85	0
4	ACT	A	315	-	3,3,3	1.02	0	3,3,3	1.45	0
4	ACT	B	311	-	3,3,3	1.30	1 (33%)	3,3,3	0.36	0
4	ACT	D	312	-	3,3,3	0.99	0	3,3,3	1.27	0
4	ACT	D	313	-	3,3,3	1.04	0	3,3,3	0.95	0
2	SO4	B	304	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	C	310	-	4,4,4	0.41	0	6,6,6	0.71	0
4	ACT	A	309	-	3,3,3	0.64	0	3,3,3	1.09	0
4	ACT	C	321	-	3,3,3	0.89	0	3,3,3	1.68	1 (33%)
4	ACT	D	316	-	3,3,3	0.92	0	3,3,3	2.03	2 (66%)
4	ACT	C	317	-	3,3,3	0.96	0	3,3,3	1.78	2 (66%)
2	SO4	C	308	-	4,4,4	0.56	0	6,6,6	0.58	0
4	ACT	D	318	-	3,3,3	1.12	0	3,3,3	1.13	0
2	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	B	303	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	C	303	-	4,4,4	0.32	0	6,6,6	0.24	0
2	SO4	A	302	-	4,4,4	0.28	0	6,6,6	0.15	0
4	ACT	A	312	-	3,3,3	1.28	1 (33%)	3,3,3	1.79	1 (33%)
4	ACT	D	315	-	3,3,3	1.13	0	3,3,3	1.87	2 (66%)
4	ACT	B	313	-	3,3,3	1.13	0	3,3,3	0.89	0
4	ACT	A	310	-	3,3,3	1.36	1 (33%)	3,3,3	1.41	1 (33%)
4	ACT	A	319	-	3,3,3	1.01	0	3,3,3	1.95	2 (66%)
4	ACT	D	317	-	3,3,3	1.08	0	3,3,3	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	305	-	4,4,4	0.37	0	6,6,6	0.20	0
4	ACT	A	320	-	3,3,3	0.98	0	3,3,3	1.31	1 (33%)
2	SO4	A	307	-	4,4,4	0.37	0	6,6,6	0.50	0
4	ACT	B	309	-	3,3,3	0.94	0	3,3,3	1.47	1 (33%)
4	ACT	A	311	-	3,3,3	1.01	0	3,3,3	0.72	0
4	ACT	C	318	-	3,3,3	0.80	0	3,3,3	1.84	1 (33%)
4	ACT	D	310	-	3,3,3	1.06	0	3,3,3	1.68	1 (33%)
2	SO4	A	301	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	B	306	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	C	309	-	4,4,4	0.31	0	6,6,6	0.68	0
4	ACT	A	316	-	3,3,3	0.80	0	3,3,3	1.43	0
4	ACT	B	312	-	3,3,3	1.13	0	3,3,3	1.06	0
2	SO4	A	306	-	4,4,4	0.36	0	6,6,6	0.40	0
2	SO4	C	306	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	A	304	-	4,4,4	0.25	0	6,6,6	0.29	0
4	ACT	C	315	-	3,3,3	1.25	1 (33%)	3,3,3	0.98	0
2	SO4	D	306	-	4,4,4	0.33	0	6,6,6	0.30	0
4	ACT	C	316	-	3,3,3	1.07	0	3,3,3	1.80	1 (33%)
4	ACT	D	320	-	3,3,3	1.17	0	3,3,3	1.41	1 (33%)
4	ACT	A	317	-	3,3,3	1.00	0	3,3,3	1.13	0
2	SO4	A	303	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	D	302	-	4,4,4	0.23	0	6,6,6	0.20	0
4	ACT	D	314	-	3,3,3	1.06	0	3,3,3	1.48	1 (33%)
4	ACT	A	313	-	3,3,3	0.78	0	3,3,3	1.06	0
4	ACT	D	319	-	3,3,3	1.07	0	3,3,3	1.04	0
2	SO4	C	301	-	4,4,4	0.24	0	6,6,6	0.20	0
4	ACT	B	310	-	3,3,3	1.12	0	3,3,3	1.52	1 (33%)
4	ACT	A	318	-	3,3,3	0.73	0	3,3,3	1.44	0
4	ACT	D	311	-	3,3,3	1.14	0	3,3,3	0.83	0
2	SO4	B	305	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	C	304	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	D	301	-	4,4,4	0.31	0	6,6,6	0.14	0
4	ACT	A	314	-	3,3,3	0.81	0	3,3,3	1.70	1 (33%)
2	SO4	C	305	-	4,4,4	0.29	0	6,6,6	0.15	0
4	ACT	C	320	-	3,3,3	0.93	0	3,3,3	0.76	0
4	ACT	B	314	-	3,3,3	0.88	0	3,3,3	1.78	1 (33%)
2	SO4	D	304	-	4,4,4	0.26	0	6,6,6	0.17	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	310	ACT	OXT-C	-2.24	1.20	1.30
4	B	311	ACT	OXT-C	-2.22	1.20	1.30
4	C	315	ACT	OXT-C	-2.16	1.20	1.30
4	A	312	ACT	OXT-C	-2.04	1.21	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	319	ACT	OXT-C-O	-2.54	112.59	122.03
4	A	312	ACT	OXT-C-O	-2.50	112.75	122.03
4	B	314	ACT	OXT-C-CH3	2.47	125.39	115.05
4	C	318	ACT	OXT-C-CH3	2.46	125.37	115.05
4	D	316	ACT	OXT-C-CH3	2.44	125.28	115.05
4	D	314	ACT	OXT-C-O	-2.43	113.00	122.03
4	D	316	ACT	OXT-C-O	-2.38	113.21	122.03
4	B	310	ACT	OXT-C-O	-2.34	113.34	122.03
4	D	310	ACT	OXT-C-CH3	2.33	124.82	115.05
4	C	316	ACT	OXT-C-CH3	2.33	124.80	115.05
4	D	315	ACT	OXT-C-O	-2.32	113.40	122.03
4	C	317	ACT	OXT-C-O	-2.19	113.90	122.03
4	D	315	ACT	OXT-C-CH3	2.16	124.10	115.05
4	D	320	ACT	OXT-C-O	-2.15	114.04	122.03
4	A	320	ACT	OXT-C-O	-2.14	114.08	122.03
4	C	317	ACT	OXT-C-CH3	2.10	123.88	115.05
4	B	309	ACT	OXT-C-CH3	2.06	123.70	115.05
4	A	310	ACT	OXT-C-O	-2.04	114.45	122.03
4	C	321	ACT	OXT-C-CH3	2.04	123.61	115.05
4	A	314	ACT	OXT-C-O	-2.03	114.51	122.03
4	A	319	ACT	OXT-C-CH3	2.01	123.47	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	319	ACT	2	0
4	D	309	ACT	2	0
4	B	311	ACT	1	0
4	D	312	ACT	3	0
2	C	310	SO4	1	0
4	A	309	ACT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	316	ACT	2	0
4	C	317	ACT	3	0
2	C	308	SO4	1	0
4	D	318	ACT	2	0
4	A	312	ACT	4	1
4	D	315	ACT	4	0
4	B	313	ACT	1	0
4	A	310	ACT	3	0
4	A	320	ACT	3	0
2	A	307	SO4	1	0
4	B	309	ACT	4	0
4	D	310	ACT	3	0
2	B	306	SO4	1	0
4	B	312	ACT	1	0
2	A	304	SO4	1	0
4	C	315	ACT	2	0
4	D	320	ACT	1	0
4	A	317	ACT	3	0
4	D	314	ACT	6	0
4	A	313	ACT	2	0
4	D	319	ACT	4	0
2	C	301	SO4	1	0
4	B	310	ACT	1	0
4	A	318	ACT	3	0
4	D	311	ACT	2	0
4	A	314	ACT	4	0
4	C	320	ACT	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, 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	276/276 (100%)	-1.47	0 100 100	16, 35, 52, 81	3 (1%)
1	B	276/276 (100%)	-1.46	0 100 100	16, 36, 53, 84	3 (1%)
1	C	276/276 (100%)	-1.47	0 100 100	16, 36, 53, 86	5 (1%)
1	D	276/276 (100%)	-1.47	0 100 100	17, 36, 53, 85	4 (1%)
All	All	1104/1104 (100%)	-1.47	0 100 100	16, 36, 53, 86	15 (1%)

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 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
4	ACT	D	317	4/4	0.95	0.14	65,66,72,81	0
4	ACT	B	313	4/4	0.96	0.07	52,52,56,62	0
4	ACT	C	321	4/4	0.96	0.09	52,62,69,70	0
4	ACT	D	313	4/4	0.96	0.07	53,54,57,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	315	4/4	0.96	0.08	62,71,75,76	0
4	ACT	D	318	4/4	0.96	0.08	58,76,77,81	0
2	SO4	B	307	5/5	0.97	0.05	78,81,87,89	0
4	ACT	B	314	4/4	0.97	0.11	47,68,69,75	0
4	ACT	C	318	4/4	0.97	0.07	42,61,65,69	0
4	ACT	A	314	4/4	0.97	0.07	36,54,57,70	0
2	SO4	A	306	5/5	0.97	0.06	68,75,95,96	0
4	ACT	A	318	4/4	0.97	0.08	44,47,48,58	0
4	ACT	B	312	4/4	0.97	0.08	31,63,65,65	0
4	ACT	D	319	4/4	0.97	0.06	57,67,74,81	0
4	ACT	A	313	4/4	0.98	0.06	39,54,64,69	0
2	SO4	B	304	5/5	0.98	0.05	71,77,96,102	0
2	SO4	C	310	5/5	0.98	0.05	58,63,79,83	0
4	ACT	C	316	4/4	0.98	0.07	45,49,60,65	0
4	ACT	A	316	4/4	0.98	0.06	49,62,63,71	0
4	ACT	C	319	4/4	0.98	0.07	53,61,78,78	0
4	ACT	C	320	4/4	0.98	0.05	63,74,78,84	0
2	SO4	D	305	5/5	0.98	0.06	65,67,89,111	0
4	ACT	D	309	4/4	0.98	0.07	56,57,64,73	0
4	ACT	D	310	4/4	0.98	0.09	54,66,78,79	0
4	ACT	D	311	4/4	0.98	0.07	54,62,68,69	0
4	ACT	A	319	4/4	0.98	0.06	53,53,57,76	0
4	ACT	A	320	4/4	0.98	0.06	52,63,69,83	0
4	ACT	B	309	4/4	0.98	0.05	54,74,74,84	0
4	ACT	B	311	4/4	0.98	0.06	50,50,60,62	0
4	ACT	A	309	4/4	0.99	0.06	53,59,62,73	0
4	ACT	A	310	4/4	0.99	0.03	33,38,40,45	0
4	ACT	A	311	4/4	0.99	0.04	48,49,52,52	0
4	ACT	A	312	4/4	0.99	0.04	44,45,52,65	0
2	SO4	B	301	5/5	0.99	0.03	63,71,72,77	0
2	SO4	B	302	5/5	0.99	0.04	58,65,80,91	0
2	SO4	B	303	5/5	0.99	0.04	64,64,87,105	0
2	SO4	A	304	5/5	0.99	0.03	54,60,75,77	0
4	ACT	A	317	4/4	0.99	0.04	47,55,55,65	0
2	SO4	B	306	5/5	0.99	0.05	41,44,49,57	0
2	SO4	A	305	5/5	0.99	0.07	43,53,58,69	0
2	SO4	C	302	5/5	0.99	0.05	46,46,52,56	0
2	SO4	C	303	5/5	0.99	0.04	39,56,59,76	0
4	ACT	B	310	4/4	0.99	0.04	39,48,62,64	0
2	SO4	C	304	5/5	0.99	0.04	62,69,74,76	0
2	SO4	C	305	5/5	0.99	0.03	60,62,81,94	0
2	SO4	C	306	5/5	0.99	0.04	61,66,85,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	307	5/5	0.99	0.03	70,74,87,100	0
4	ACT	C	315	4/4	0.99	0.07	49,56,57,66	0
2	SO4	C	308	5/5	0.99	0.05	43,53,62,71	0
4	ACT	C	317	4/4	0.99	0.04	40,49,57,64	0
2	SO4	C	309	5/5	0.99	0.04	69,70,74,82	0
2	SO4	A	303	5/5	0.99	0.09	60,65,71,72	0
2	SO4	D	303	5/5	0.99	0.04	61,70,71,73	0
2	SO4	D	304	5/5	0.99	0.04	61,65,77,88	0
2	SO4	A	307	5/5	0.99	0.04	60,67,72,84	0
2	SO4	D	306	5/5	0.99	0.04	78,79,83,89	0
3	CL	B	308	1/1	0.99	0.06	38,38,38,38	0
4	ACT	D	312	4/4	0.99	0.04	50,59,59,68	0
3	CL	C	311	1/1	0.99	0.09	66,66,66,66	0
4	ACT	D	314	4/4	0.99	0.04	50,50,57,62	0
4	ACT	D	315	4/4	0.99	0.04	48,48,50,61	0
4	ACT	D	316	4/4	0.99	0.06	45,52,54,65	0
3	CL	C	313	1/1	0.99	0.06	41,41,41,41	0
3	CL	C	314	1/1	0.99	0.06	56,56,56,56	0
3	CL	D	307	1/1	0.99	0.03	57,57,57,57	0
4	ACT	D	320	4/4	0.99	0.06	48,53,54,64	0
3	CL	A	308	1/1	1.00	0.06	39,39,39,39	0
2	SO4	D	301	5/5	1.00	0.04	42,45,50,56	0
2	SO4	D	302	5/5	1.00	0.04	49,50,54,55	0
3	CL	C	312	1/1	1.00	0.09	53,53,53,53	0
2	SO4	A	302	5/5	1.00	0.02	49,51,54,57	0
2	SO4	A	301	5/5	1.00	0.05	45,46,49,50	0
2	SO4	C	301	5/5	1.00	0.05	41,41,48,52	0
3	CL	D	308	1/1	1.00	0.04	39,39,39,39	0
2	SO4	B	305	5/5	1.00	0.04	47,50,52,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.