



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:20 PM UTC

PDB ID : 5KC1 / pdb_00005kc1
Title : Structure of the C-terminal dimerization domain of Atg38
Authors : Ohashi, Y.; Soler, N.; Garcia-Ortegon, M.; Zhang, L.; Perisic, O.; Masson, G.R.; Johnson, C.M.; Williams, R.J.
Deposited on : 2016-06-04
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

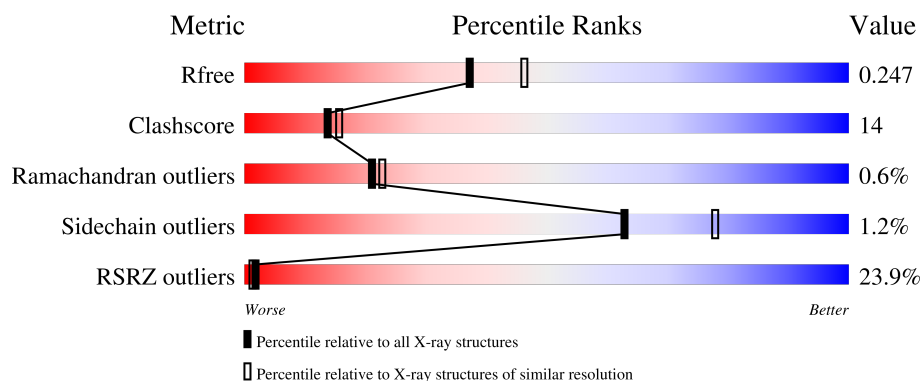
1 Overall quality at a glance

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	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	

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Mol	Chain	Length	Quality of chain
1	F	226	
1	G	226	
1	H	226	
1	I	226	
1	J	226	
1	K	226	
1	L	226	

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	EDO	I	305	-	-	X	-
6	NH4	K	307	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4567 atoms, of which 8 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 Autophagy-related protein 38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	S	0	0	0
			271	171	45	54	1			
1	D	51	Total	C	N	O	S	0	0	0
			447	287	79	79	2			
1	A	29	Total	C	N	O	S	0	1	0
			243	154	43	45	1			
1	B	57	Total	C	N	O	S	0	0	0
			493	312	88	91	2			
1	G	33	Total	C	N	O	S	0	0	0
			263	164	45	53	1			
1	H	53	Total	C	N	O	S	0	0	0
			461	296	81	82	2			
1	K	24	Total	C	N	O	S	0	0	0
			194	122	34	37	1			
1	L	60	Total	C	N	O	S	0	0	0
			515	327	90	96	2			
1	E	30	Total	C	N	O	S	0	0	0
			239	151	41	46	1			
1	F	61	Total	C	N	O	S	0	0	0
			520	330	91	97	2			
1	I	29	Total	C	N	O	S	0	0	0
			234	148	40	45	1			
1	J	58	Total	C	N	O	S	0	0	0
			500	319	88	91	2			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

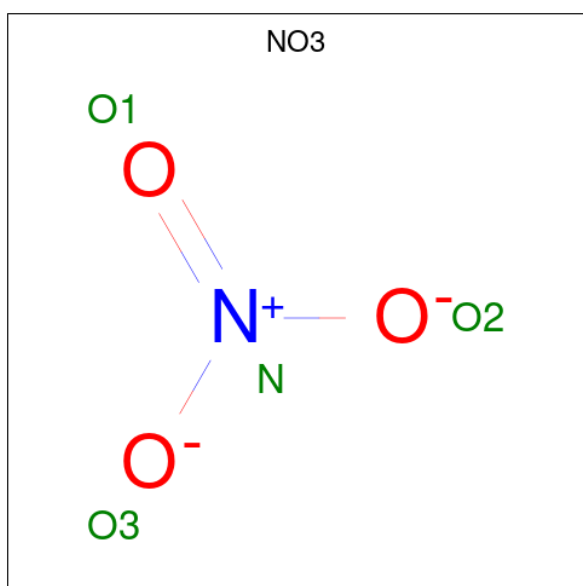
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Na	0	0
			1	1		
2	D	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Na 1	0	0
2	K	3	Total 3	Na 3	0	0
2	E	1	Total 1	Na 1	0	0
2	F	4	Total 4	Na 4	0	0
2	I	2	Total 2	Na 2	0	0

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



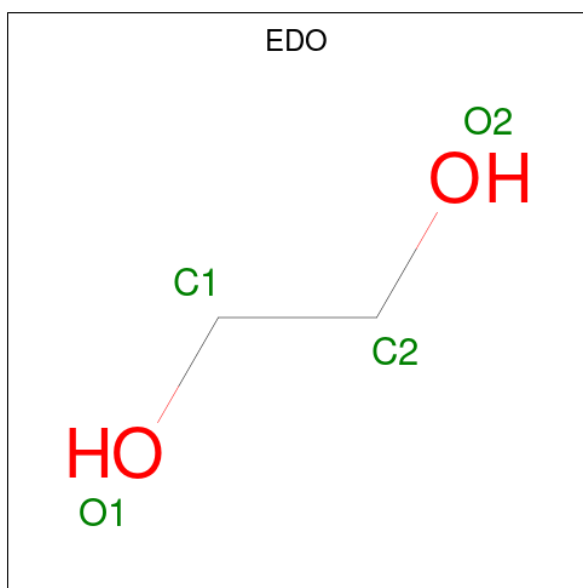
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	N 1	O 3	0	0
3	D	1	Total 4	N 1	O 3	0	0
3	D	1	Total 4	N 1	O 3	0	0
3	A	1	Total 4	N 1	O 3	0	0
3	A	1	Total 4	N 1	O 3	0	0
3	B	1	Total 4	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	N	O	0	0
			4	1	3		
3	G	1	Total	N	O	0	0
			4	1	3		
3	G	1	Total	N	O	0	0
			4	1	3		
3	G	1	Total	N	O	0	0
			4	1	3		
3	H	1	Total	N	O	0	0
			4	1	3		
3	K	1	Total	N	O	0	0
			4	1	3		
3	K	1	Total	N	O	0	0
			4	1	3		
3	K	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		
3	I	1	Total	N	O	0	0
			4	1	3		
3	I	1	Total	N	O	0	0
			4	1	3		
3	J	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

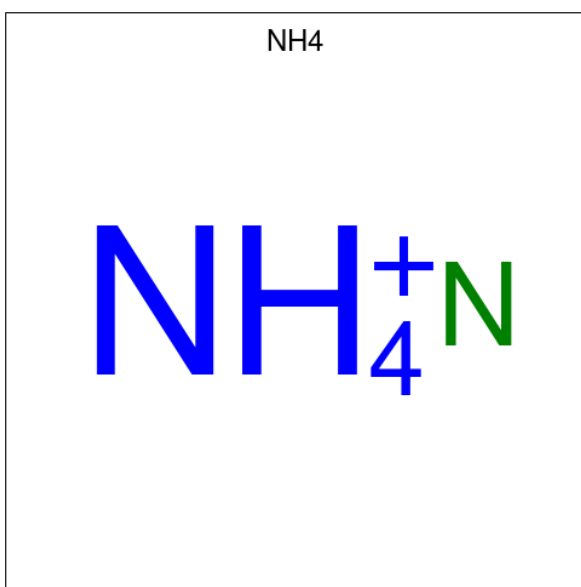


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

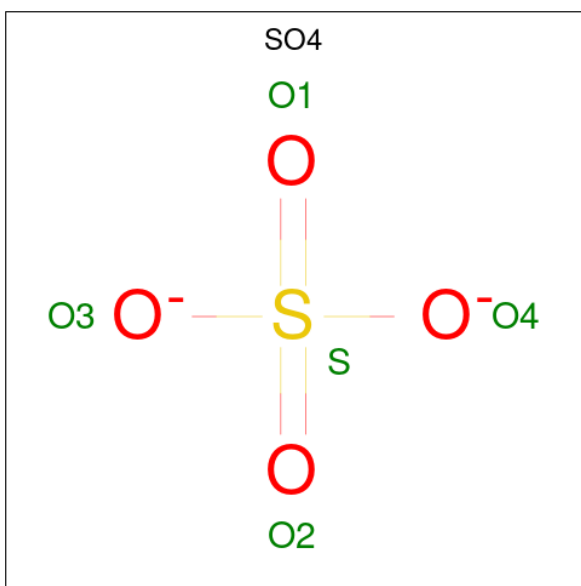
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Cl 2 2	0	0
5	E	2	Total Cl 2 2	0	0
5	F	2	Total Cl 2 2	0	0

- Molecule 6 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	H	N	0	0
			5	4	1		
6	J	1	Total	H	N	0	0
			5	4	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total I 1 1	0	0

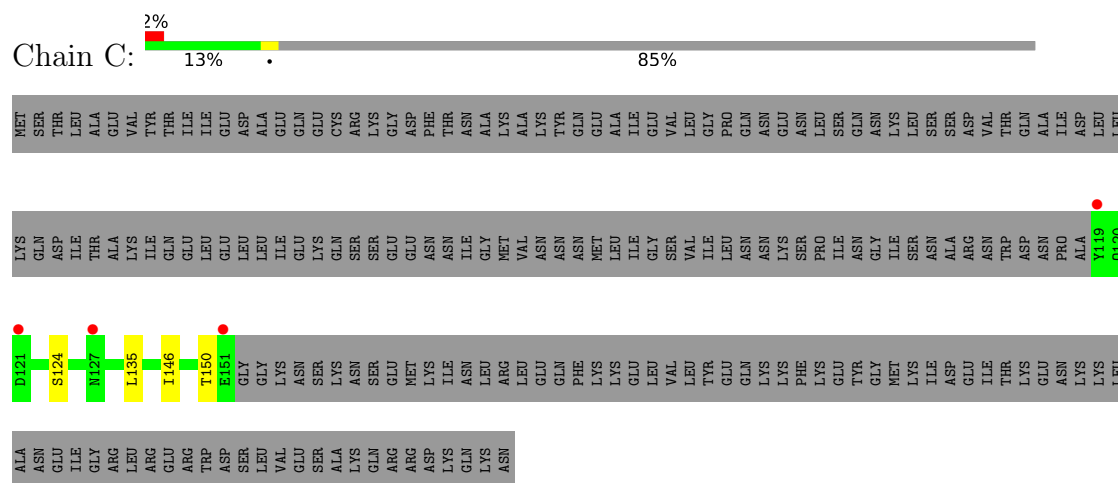
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	3	Total O 3 3	0	0
9	D	1	Total O 1 1	0	0
9	A	9	Total O 9 9	0	0
9	B	1	Total O 1 1	0	0
9	G	7	Total O 7 7	0	0
9	H	3	Total O 3 3	0	0
9	K	4	Total O 4 4	0	0
9	L	2	Total O 2 2	0	0
9	E	4	Total O 4 4	0	0
9	F	2	Total O 2 2	0	0
9	I	3	Total O 3 3	0	0
9	J	4	Total O 4 4	0	0

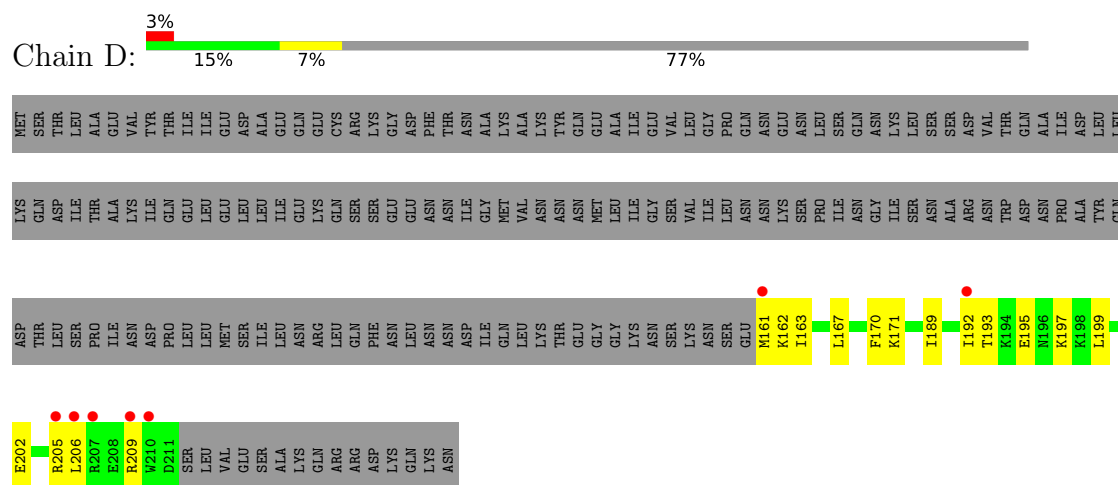
3 Residue-property plots [i](#)

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.

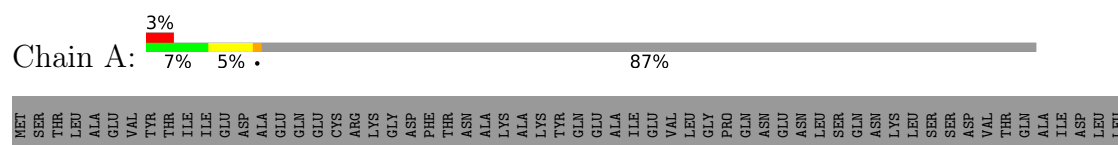
• Molecule 1: Autophagy-related protein 38

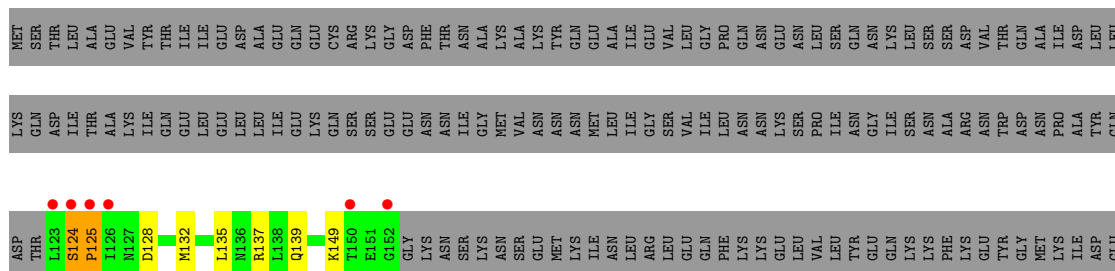


• Molecule 1: Autophagy-related protein 38



• Molecule 1: Autophagy-related protein 38





ILE	THR	LYS	GLY	ASN	LYS	LYS	LEU	ALA	ASN	GLU	ILE	GLY	ARG	LEU	ARG	GLU	ARG	TRP	ASP	SER	VAL	GLU	SER	ALA	LYS	GLN	ARG	ASP	LYS	GLN	LYS	ASN
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● Molecule 1: Autophagy-related protein 38



MET	SER	THR	LEU	ALA	GLU	VAL	TYR	THR	ILE	ILE	GLU	ASP	ALA	LEU	ILE	GLN	GLU	CYS	ARG	LYS	GLY	ASP	PHE	GLU	ASN	THR	ASN	ILE	ALA	LYS	GLN	ALA	LYS	TYR	GLN	GLU	ALA	ILE	GLY	VAL	SER	LEU	GLY	PRO	ASN	ASN	GLN	LYS	ASN	ASN	PRO	ILE	SER	LEU	SER	ASP	VAL	ASN	TRP	THR	GLN	ASP	ALA	ILE	ASP	ALA	TYR	LEU	GLN
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LYS	GLN	ASP	THR	ILE	THR	ALA	LYS	ILE	GLN	GLU	ILE	GLU	LEU	LEU	LEU	ILE	GLN	GLU	GLN	SER	SER	GLU	ASN	GLU	ASP	ASN	THR	ASN	ILE	GLY	MET	VAL	VAL	LYS	ASN	LYS	LYS	ASN	TYR	ASN	GLN	MET	GLU	LEU	ALA	ILE	LYS	GLY	ASN	SER	VAL	ILE	PRO	ASN	SER	ASN	PRO	ILE	ASN	GLY	ASN	GLN	ILE	LYS	ILE	SER	ASN	ALA	SER	ASP	VAL	ASN	TRP	THR	GLN	ASP	ALA	ILE	ASP	ALA	TYR	LEU	GLN
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ASP	THR	LEU	SER	PRO	ILE	ASN	ASP	PRO	GLN	LEU	LEU	MET	SER	ILE	LEU	GLN	ARG	GLN	PHE	ASN	ASN	ASP	ILE	GLN	VAL	LYS	ASN	LYS	THR	THR	GLU	GLY	GLY	LYS	ASN	SER	K157	K158	S159	E160	M161	L174	K180	K188	I192	T193	K194	E195	M196	K197	K198	L199	A200	E201	E202	I203
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K204	R205	L206	R207	E208	R209	V210	D211	S212	L213	V214	E215	S216	D217	LYS	GLN	ARG	ARG	ASP	LYS	GLN	ASN
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● Molecule 1: Autophagy-related protein 38



MET	SER	THR	LEU	ALA	GLU	VAL	TYR	THR	ILE	ILE	GLU	ASP	ALA	LEU	ILE	GLN	GLU	CYS	ARG	LYS	GLY	ASP	PHE	THR	ASN	ILE	ALA	LYS	VAL	LYS	ASN	GLN	GLU	ALA	ILE	GLY	VAL	LEU	PRO	GLN	ASN	ASN	GLN	LYS	ASN	ASN	PRO	ILE	SER	GLN	ASN	LYS	SER	LEU	SER	ASP	VAL	ASN	TRP	THR	GLN	ALA	ILE	ASP	TYR	LEU	GLN
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LYS	GLN	ASP	THR	ILE	THR	ALA	LYS	ILE	GLN	GLU	LEU	GLU	LEU	LEU	ILE	GLN	GLU	LYS	SER	SER	GLU	ASN	GLU	ASP	PHE	ASN	ASN	ILE	GLY	MET	VAL	VAL	LYS	ASN	LYS	ASN	TYR	ASN	MET	GLU	LEU	ALA	ILE	GLY	ASN	SER	VAL	ILE	PRO	ASN	PRO	ILE	ASN	GLY	ASN	GLY	TYR	GLU	GLN	LYS	ALA	SER	ASP	VAL	ASN	TRP	THR	GLN	ASP	ALA	ILE	ASP	TYR	LEU	GLN
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D121	T122	S123	P125	I126	M132	R137	L138	N141	M144	D145	I146	Q147	L148	K149	THR	GLY	GLY	LYS	ASN	SER	LYS	ASN	GLY	VAL	GLU	SER	ALA	LYS	VAL	ALA	LYS	ASN	LYS	ASN	GLN	MET	LYS	ILE	ASN	GLY	LEU	ARG	LEU	GLU	GLN	PHE	ASN	ASN	LYS	LYS	PRO	ASN	PRO	ILE	ASN	GLY	ASN	GLY	TYR	GLU	GLN	LYS	LYS	PHE	ASN	TRP	THR	GLN	ASP	ALA	ILE	ASP	TYR	LEU	GLN
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ASP	GLU	ILE	THR	GLY	ASN	LYS	LYS	LEU	ALA	ASN	GLU	ILE	GLY	ARG	TRP	ASP	SER	SER	VAL	GLU	SER	ALA	LYS	VAL	GLU	ASN	ILE	ALA	LYS	VAL	ALA	LYS	ASN	GLN	ARG	ASP	LYS	GLN	ASN	ASN	ASN
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● Molecule 1: Autophagy-related protein 38



MET	SER	THR	LEU	ALA	GLU	VAL	TYR	THR	ILE	ILE	GLU	ASP	ALA	LEU	ILE	GLN	GLU	CYS	ARG	LYS	GLY	ASP	PHE	THR	ASN	ILE	ALA	LYS	VAL	LYS	ASN	GLN	ALA	ILE	GLY	VAL	LEU	GLY	PRO	GLN	ASN	ASN	GLN	LYS	ASN	ASN	PRO	ILE	SER	GLN	ASN	SER	ASP	VAL	ASN	TRP	THR	GLN	ASP	ALA	ILE	ASP	ALA	TYR	LEU	GLN
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LYS	GLN	ASP	THR	ILE	THR	ALA	LYS	ILE	GLN	GLU	LEU	GLU	LEU	LEU	ILE	GLN	GLU	LYS	SER	SER	GLU	ASN	GLU	ASP	PHE	ASN	ASN	ILE	GLY	MET	VAL	VAL	LYS	ASN	LYS	ASN	TYR	ASN	MET	GLU	LEU	ALA	ILE	GLY	ASN	SER	VAL	ILE	PRO	ASN	PRO	ILE	ASN	GLY	ASN	GLY	TYR	GLU	GLN	LYS	ALA	SER	ASP	VAL	ASN	TRP	THR	GLN	ASP	ALA	ILE	ASP	ALA	TYR	LEU	GLN
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ASP	THR	SER	PRO	ILE	ASN	ASP	PRO	GLN	LEU	LEU	MET	SER	ILE	ASN	ASN	ARG	LEU	GLN	PHE	ASN	ASN	ASP	ILE	ASN	ILE	GLY	LYS	VAL	LYS	ASN	GLN	ALA	LYS	ASN	SER	K157	K158	S159	E160	M161	K162	I163	R166	Q169	F170	K171	K172	E173	L174	K180	K181	F182	K183	E184	K188
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I188	D190	I191	T192	T193	K194	E195	K196	L199	E202	T203	G204	R205	E207	E208	R209	V210	S212	L213	V214	GLU	SER	ALA	LYS	GLN	ARG	ASP	LYS	GLN	LYS	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.38Å 249.38Å 50.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 2.20 58.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.00-2.20) 99.7 (58.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX dev_1810	Depositor
R, R_{free}	0.205 , 0.241 0.210 , 0.247	Depositor DCC
R_{free} test set	2862 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4567	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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: NH4, IOD, EDO, NA, SO4, NO3, 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	0.43	0/248	0.68	0/335
1	B	0.33	0/498	0.67	0/657
1	C	0.44	0/274	0.83	2/372 (0.5%)
1	D	0.31	0/452	0.62	0/596
1	E	0.48	0/241	0.70	0/326
1	F	0.33	0/525	0.68	0/694
1	G	0.46	0/265	0.70	0/359
1	H	0.34	0/466	0.64	0/615
1	I	0.43	0/236	0.88	2/320 (0.6%)
1	J	0.35	0/505	0.66	0/667
1	K	0.45	0/196	0.70	0/266
1	L	0.32	0/520	0.63	0/687
All	All	0.37	0/4426	0.69	4/5894 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	SER	CA-C-N	5.45	125.53	119.32
1	C	124	SER	C-N-CA	5.45	125.53	119.32
1	I	124	SER	CA-C-N	5.22	125.53	119.47
1	I	124	SER	C-N-CA	5.22	125.53	119.47

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	243	0	257	22	0
1	B	493	0	513	16	0
1	C	271	0	272	6	0
1	D	447	0	472	16	0
1	E	239	0	247	17	0
1	F	520	0	543	21	0
1	G	263	0	266	7	0
1	H	461	0	488	24	0
1	I	234	0	242	12	0
1	J	500	0	527	17	0
1	K	194	0	196	9	0
1	L	515	0	538	14	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	4	0	0	0	0
2	I	2	0	0	0	0
2	K	3	0	0	0	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	8	0	0	0	0
3	F	4	0	0	1	0
3	G	16	0	0	0	0
3	H	4	0	0	0	0
3	I	8	0	0	0	0
3	J	4	0	0	0	0
3	K	12	0	0	2	0
4	A	8	0	12	3	0
4	C	8	0	12	3	0
4	I	4	0	6	7	0
4	J	8	0	12	0	0
4	K	4	0	6	1	0
4	L	4	0	6	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2	0	0	0	0
6	J	1	4	0	0	0
6	K	1	4	0	0	0
7	K	5	0	0	1	0
8	E	1	0	0	1	0
9	A	9	0	0	1	0
9	B	1	0	0	0	0
9	C	3	0	0	0	0
9	D	1	0	0	0	0
9	E	4	0	0	0	0
9	F	2	0	0	0	0
9	G	7	0	0	1	0
9	H	3	0	0	0	0
9	I	3	0	0	1	0
9	J	4	0	0	0	0
9	K	4	0	0	0	0
9	L	2	0	0	0	0
All	All	4559	8	4615	132	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 14.

The worst 5 of 132 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD13	1:A:126:ILE:HA	1.33	1.09
1:L:203:ILE:HD12	1:J:199:LEU:HD13	1.61	0.82
1:G:135:LEU:HD21	1:F:174:LEU:CD2	2.14	0.78
1:E:124:SER:H	1:E:125:PRO:CD	1.98	0.76
4:I:305:EDO:H12	1:J:170:PHE:HB2	1.67	0.76

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	28/226 (12%)	25 (89%)	2 (7%)	1 (4%)	2	1
1	B	55/226 (24%)	55 (100%)	0	0	100	100
1	C	31/226 (14%)	31 (100%)	0	0	100	100
1	D	49/226 (22%)	49 (100%)	0	0	100	100
1	E	28/226 (12%)	26 (93%)	0	2 (7%)	1	0
1	F	59/226 (26%)	59 (100%)	0	0	100	100
1	G	31/226 (14%)	31 (100%)	0	0	100	100
1	H	51/226 (23%)	51 (100%)	0	0	100	100
1	I	27/226 (12%)	27 (100%)	0	0	100	100
1	J	56/226 (25%)	56 (100%)	0	0	100	100
1	K	22/226 (10%)	18 (82%)	4 (18%)	0	100	100
1	L	58/226 (26%)	58 (100%)	0	0	100	100
All	All	495/2712 (18%)	486 (98%)	6 (1%)	3 (1%)	21	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	124	SER
1	E	125	PRO
1	A	126	ILE

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	30/206 (15%)	29 (97%)	1 (3%)	33	45
1	B	54/206 (26%)	54 (100%)	0	100	100
1	C	33/206 (16%)	33 (100%)	0	100	100
1	D	48/206 (23%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	29/206 (14%)	29 (100%)	0	100	100
1	F	57/206 (28%)	57 (100%)	0	100	100
1	G	32/206 (16%)	32 (100%)	0	100	100
1	H	50/206 (24%)	49 (98%)	1 (2%)	48	64
1	I	29/206 (14%)	28 (97%)	1 (3%)	32	44
1	J	55/206 (27%)	53 (96%)	2 (4%)	31	42
1	K	24/206 (12%)	24 (100%)	0	100	100
1	L	57/206 (28%)	56 (98%)	1 (2%)	51	68
All	All	498/2472 (20%)	492 (99%)	6 (1%)	63	78

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	137	ARG
1	J	174	LEU
1	J	194	LYS
1	H	194	LYS
1	A	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	E	139	GLN

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 51 ligands modelled in this entry, 21 are monoatomic and 2 are modelled with single atom - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NO3	G	304	-	1,3,3	0.60	0	0,3,3	-	-
3	NO3	I	304	-	1,3,3	0.67	0	0,3,3	-	-
3	NO3	G	301	-	1,3,3	0.54	0	0,3,3	-	-
4	EDO	I	305	-	3,3,3	0.40	0	2,2,2	0.46	0
3	NO3	B	302	-	1,3,3	0.63	0	0,3,3	-	-
3	NO3	A	301	-	1,3,3	0.57	0	0,3,3	-	-
4	EDO	J	304	-	3,3,3	0.58	0	2,2,2	0.21	0
4	EDO	L	301	-	3,3,3	0.48	0	2,2,2	0.35	0
4	EDO	A	304	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	J	303	-	3,3,3	0.45	0	2,2,2	0.35	0
3	NO3	H	301	-	1,3,3	0.70	0	0,3,3	-	-
3	NO3	D	304	-	1,3,3	0.60	0	0,3,3	-	-
4	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.35	0
3	NO3	D	303	-	1,3,3	0.78	0	0,3,3	-	-
7	SO4	K	309	2	4,4,4	0.26	0	6,6,6	0.30	0
3	NO3	I	303	-	1,3,3	0.55	0	0,3,3	-	-
3	NO3	G	303	-	1,3,3	0.67	0	0,3,3	-	-
3	NO3	A	302	-	1,3,3	0.64	0	0,3,3	-	-
3	NO3	K	304	-	1,3,3	0.63	0	0,3,3	-	-
3	NO3	C	302	-	1,3,3	0.55	0	0,3,3	-	-
4	EDO	C	304	-	3,3,3	0.49	0	2,2,2	0.30	0
3	NO3	G	302	-	1,3,3	0.62	0	0,3,3	-	-
4	EDO	K	308	-	3,3,3	0.46	0	2,2,2	0.36	0
3	NO3	J	301	-	1,3,3	0.59	0	0,3,3	-	-
3	NO3	K	305	2	1,3,3	0.62	0	0,3,3	-	-
3	NO3	K	306	-	1,3,3	0.69	0	0,3,3	-	-
3	NO3	F	305	-	1,3,3	0.79	0	0,3,3	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	L	301	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	K	308	-	-	1/1/1/1	-
4	EDO	J	303	-	-	0/1/1/1	-
4	EDO	C	303	-	-	1/1/1/1	-
4	EDO	I	305	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	J	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	EDO	O1-C1-C2-O2
4	K	308	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	305	EDO	7	0
4	A	303	EDO	3	0
7	K	309	SO4	1	0
3	K	304	NO3	1	0
4	C	304	EDO	3	0
4	K	308	EDO	1	0
3	K	306	NO3	1	0
3	F	305	NO3	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	29/226 (12%)	1.06	6 (20%) 2 2	21, 45, 116, 120	1 (3%)
1	B	57/226 (25%)	1.70	16 (28%) 1 1	42, 86, 160, 174	0
1	C	33/226 (14%)	0.89	4 (12%) 8 6	39, 55, 117, 152	0
1	D	51/226 (22%)	1.25	7 (13%) 6 5	43, 80, 162, 173	0
1	E	30/226 (13%)	1.33	6 (20%) 3 2	34, 48, 124, 139	0
1	F	61/226 (26%)	1.70	22 (36%) 1 0	38, 94, 161, 169	0
1	G	33/226 (14%)	0.62	2 (6%) 27 24	38, 47, 91, 135	0
1	H	53/226 (23%)	1.47	12 (22%) 2 1	42, 83, 152, 163	0
1	I	29/226 (12%)	1.23	8 (27%) 1 1	36, 55, 105, 127	0
1	J	58/226 (25%)	1.57	21 (36%) 1 0	41, 88, 163, 168	0
1	K	24/226 (10%)	0.83	4 (16%) 4 3	35, 46, 87, 122	0
1	L	60/226 (26%)	1.67	16 (26%) 1 1	38, 98, 152, 163	0
All	All	518/2712 (19%)	1.37	124 (23%) 2 1	21, 72, 157, 174	1 (0%)

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	LEU	6.5
1	E	126	ILE	6.5
1	E	125	PRO	6.5
1	E	123	LEU	6.2
1	J	213	LEU	6.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	NH4	J	302	1/1	0.50	0.21	111,133,133,133	0
5	CL	E	303	1/1	0.62	0.14	116,116,116,116	0
6	NH4	K	307	1/1	0.67	0.77	82,99,99,99	0
3	NO3	I	304	4/4	0.68	0.17	79,87,91,106	0
3	NO3	G	303	4/4	0.68	0.22	68,69,81,98	0
3	NO3	K	305	4/4	0.69	0.22	83,89,93,104	0
2	NA	D	302	1/1	0.74	0.36	94,94,94,94	0
3	NO3	D	303	4/4	0.74	0.20	64,69,81,88	0
4	EDO	C	304	4/4	0.75	0.33	50,62,81,84	0
3	NO3	H	301	4/4	0.75	0.20	63,67,81,99	0
4	EDO	J	304	4/4	0.76	0.28	54,57,65,68	0
2	NA	F	303	1/1	0.76	0.29	90,90,90,90	0
4	EDO	A	303	4/4	0.78	0.21	75,85,89,89	0
4	EDO	A	304	4/4	0.78	0.18	103,104,109,110	0
3	NO3	K	304	4/4	0.78	0.17	68,77,80,81	0
2	NA	B	301	1/1	0.79	0.27	87,87,87,87	0
3	NO3	A	302	4/4	0.79	0.19	74,76,84,91	0
5	CL	F	306	1/1	0.81	0.11	124,124,124,124	0
2	NA	I	301	1/1	0.82	0.27	78,78,78,78	0
2	NA	I	302	1/1	0.82	0.35	86,86,86,86	0
3	NO3	K	306	4/4	0.82	0.19	50,56,60,84	0
2	NA	F	302	1/1	0.82	0.26	98,98,98,98	0
4	EDO	J	303	4/4	0.83	0.26	85,98,99,103	0
3	NO3	F	305	4/4	0.83	0.20	47,50,61,81	0
3	NO3	G	304	4/4	0.84	0.17	78,82,93,99	0
5	CL	D	306	1/1	0.85	0.26	90,90,90,90	0
8	IOD	E	304	1/1	0.85	0.52	192,192,192,192	0
4	EDO	K	308	4/4	0.86	0.17	68,69,82,95	0
4	EDO	C	303	4/4	0.86	0.22	68,80,85,99	0
2	NA	E	301	1/1	0.86	0.39	69,69,69,69	0
2	NA	K	302	1/1	0.87	0.24	76,76,76,76	0
3	NO3	D	304	4/4	0.88	0.18	56,66,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	L	301	4/4	0.88	0.22	61,68,75,83	0
5	CL	E	302	1/1	0.89	0.21	107,107,107,107	0
2	NA	K	303	1/1	0.89	0.17	73,73,73,73	0
2	NA	F	301	1/1	0.89	0.31	50,50,50,50	0
3	NO3	J	301	4/4	0.90	0.10	98,99,108,110	0
3	NO3	A	301	4/4	0.91	0.20	55,59,62,67	0
2	NA	C	301	1/1	0.91	0.45	74,74,74,74	0
4	EDO	I	305	4/4	0.91	0.52	49,53,56,59	0
2	NA	F	304	1/1	0.91	0.15	66,66,66,66	0
5	CL	F	307	1/1	0.93	0.23	100,100,100,100	0
2	NA	D	301	1/1	0.93	0.16	93,93,93,93	0
3	NO3	B	302	4/4	0.94	0.11	50,52,62,77	0
3	NO3	I	303	4/4	0.95	0.10	50,51,61,67	0
2	NA	K	301	1/1	0.95	0.12	63,63,63,63	0
3	NO3	G	301	4/4	0.95	0.14	40,40,48,50	0
3	NO3	C	302	4/4	0.95	0.10	58,59,59,69	0
3	NO3	G	302	4/4	0.96	0.11	54,55,57,60	0
7	SO4	K	309	5/5	0.96	0.20	52,54,65,77	0
5	CL	D	305	1/1	0.96	0.15	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.