



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:47 AM UTC

PDB ID : 5LMF / pdb_00005lmf
Title : Structure of C-terminal domain from *S. cerevisiae* Pat1 decapping activator bound to Dcp2 HLM3 peptide (region 484-500)
Authors : Charenton, C.; Gaudon-Plesse, C.; Fourati, Z.; Taverniti, V.; Back, R.; Kolesnikova, O.; Seraphin, B.; Graille, M.
Deposited on : 2016-07-30
Resolution : 2.15 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

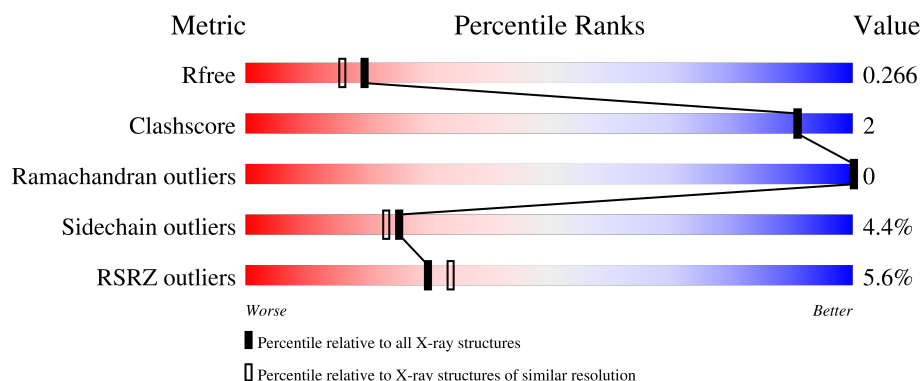
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	369	4% 77% 8% 15%
1	B	369	5% 77% 9% 14%
2	C	17	24% 88% 12%
2	D	17	6% 82% 12% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5591 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 DNA topoisomerase 2-associated protein PAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2551	1650	416	477	8			
1	B	318	Total	C	N	O	S	0	0	0
			2600	1681	424	487	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	MET	-	initiating methionine	UNP P25644
A	429	HIS	-	expression tag	UNP P25644
A	430	HIS	-	expression tag	UNP P25644
A	431	HIS	-	expression tag	UNP P25644
A	432	HIS	-	expression tag	UNP P25644
A	433	HIS	-	expression tag	UNP P25644
A	434	HIS	-	expression tag	UNP P25644
A	706	ALA	GLN	conflict	UNP P25644
A	713	ALA	LEU	conflict	UNP P25644
B	428	MET	-	initiating methionine	UNP P25644
B	429	HIS	-	expression tag	UNP P25644
B	430	HIS	-	expression tag	UNP P25644
B	431	HIS	-	expression tag	UNP P25644
B	432	HIS	-	expression tag	UNP P25644
B	433	HIS	-	expression tag	UNP P25644
B	434	HIS	-	expression tag	UNP P25644
B	706	ALA	GLN	conflict	UNP P25644
B	713	ALA	LEU	conflict	UNP P25644

- Molecule 2 is a protein called mRNA decapping protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	0	0	0
			129	80	23	26			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	0	0	0
			129	80	23	26			

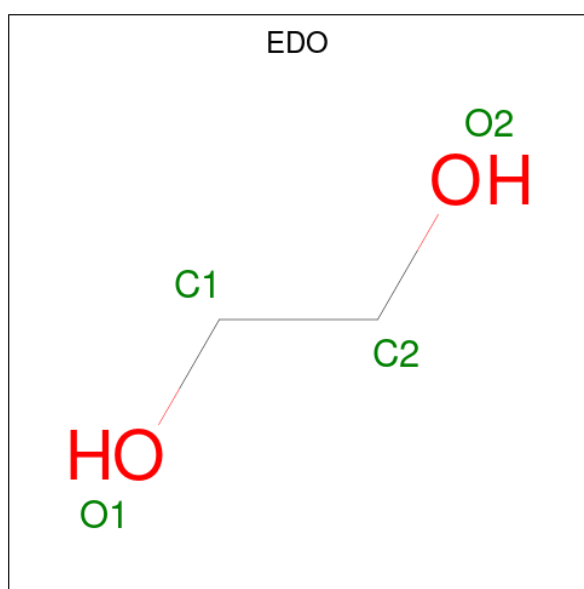
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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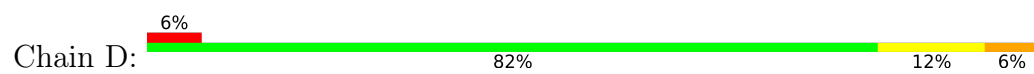
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	B	58	Total O 58 58	0	0
6	D	3	Total O 3 3	0	0

- Molecule 1: DNA topoisomerase 2-associated protein PAT1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.36Å 122.92Å 126.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.48 – 2.15 31.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.9 (31.48-2.15) 97.9 (31.48-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.16Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.212 , 0.246 0.227 , 0.266	Depositor DCC
R_{free} test set	2064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: MG, EDO, 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	0.87	0/2591	1.42	7/3492 (0.2%)
1	B	0.86	0/2640	1.41	9/3557 (0.3%)
2	C	0.87	0/130	1.35	0/174
2	D	0.77	0/130	1.40	0/174
All	All	0.86	0/5491	1.41	16/7397 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	614	GLN	CA-C-N	5.56	127.67	120.44
1	B	614	GLN	C-N-CA	5.56	127.67	120.44
1	B	583	LYS	CA-C-N	5.48	127.58	120.56
1	B	583	LYS	C-N-CA	5.48	127.58	120.56
1	B	548	LYS	CA-C-N	5.41	127.53	120.28
1	B	548	LYS	C-N-CA	5.41	127.53	120.28
1	A	544	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	604	ASN	CA-C-N	5.25	127.62	120.54
1	A	604	ASN	C-N-CA	5.25	127.62	120.54
1	B	512	HIS	CA-C-N	5.23	127.62	120.46
1	B	512	HIS	C-N-CA	5.23	127.62	120.46
1	A	795	LEU	CA-C-N	5.19	131.04	121.70
1	A	795	LEU	C-N-CA	5.19	131.04	121.70
1	B	604	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	709	ALA	CA-C-N	5.13	127.42	120.44
1	A	709	ALA	C-N-CA	5.13	127.42	120.44

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	2551	0	2638	10	0
1	B	2600	0	2688	10	0
2	C	129	0	135	0	0
2	D	129	0	135	3	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	18	1	0
5	B	24	0	36	3	0
6	A	82	0	0	0	0
6	B	58	0	0	0	0
6	D	3	0	0	0	0
All	All	5591	0	5650	19	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 2.

All (19) 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:625:THR:HB	1:B:680:ILE:HG22	1.67	0.77
1:A:736:ASN:HA	5:A:1005:EDO:H11	1.73	0.69
1:A:625:THR:HB	1:A:680:ILE:HG22	1.75	0.67
1:A:724:ILE:HD12	2:D:492:LEU:HD22	1.82	0.62
1:B:577:THR:HA	5:B:807:EDO:H11	1.87	0.57
1:B:533:ILE:HD12	1:B:536:MET:HG3	1.91	0.52
1:A:695:ASN:HB2	1:B:695:ASN:HB2	1.93	0.50
1:A:533:ILE:HD12	1:A:591:ILE:HD11	1.98	0.46
1:A:792:ILE:HD13	2:D:496:LEU:HD21	1.98	0.45
1:A:481:LEU:HD13	1:A:526:MET:HE2	1.99	0.43
1:A:553:GLN:O	1:A:557:ASN:HB2	2.17	0.43
1:A:698:PHE:HE1	1:A:741:LEU:HD21	1.82	0.43
1:B:689:HIS:CE1	5:B:807:EDO:H12	2.54	0.43
1:B:689:HIS:HE1	5:B:807:EDO:H12	1.84	0.43
1:B:754:ARG:HB2	1:B:758:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:LEU:HD22	2:D:493:LEU:HG	2.01	0.42
1:B:632:ASN:O	1:B:636:ILE:HG12	2.19	0.42
1:B:621:VAL:HG12	1:B:673:LEU:HD21	2.02	0.41
1:B:599:LEU:HD22	1:B:608:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/369 (84%)	305 (99%)	3 (1%)	0	100	100
1	B	312/369 (85%)	306 (98%)	6 (2%)	0	100	100
2	C	15/17 (88%)	15 (100%)	0	0	100	100
2	D	15/17 (88%)	15 (100%)	0	0	100	100
All	All	650/772 (84%)	641 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/338 (86%)	281 (97%)	10 (3%)	32	33
1	B	297/338 (88%)	283 (95%)	14 (5%)	23	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	15/15 (100%)	13 (87%)	2 (13%)	4	1
2	D	15/15 (100%)	14 (93%)	1 (7%)	15	10
All	All	618/706 (88%)	591 (96%)	27 (4%)	25	23

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	552	LEU
1	A	559	LEU
1	A	563	GLN
1	A	589	MET
1	A	615	LEU
1	A	644	ILE
1	A	664	GLU
1	A	746	LYS
1	A	782	VAL
1	A	789	ASP
1	B	481	LEU
1	B	501	GLN
1	B	565	ILE
1	B	591	ILE
1	B	640	ARG
1	B	643	LEU
1	B	653	ILE
1	B	656	SER
1	B	692	ARG
1	B	696	ASP
1	B	724	ILE
1	B	746	LYS
1	B	751	LEU
1	B	782	VAL
2	C	496	LEU
2	C	497	LYS
2	D	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	ASN
1	A	553	GLN

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Mol	Chain	Res	Type
1	A	557	ASN
1	A	781	ASN
1	B	500	GLN
1	B	512	HIS
1	B	646	GLN
1	B	742	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
5	EDO	B	805	-	3,3,3	0.50	0	2,2,2	0.41	0
5	EDO	A	1004	-	3,3,3	0.62	0	2,2,2	0.23	0
5	EDO	B	803	-	3,3,3	0.59	0	2,2,2	0.17	0
5	EDO	A	1003	-	3,3,3	0.46	0	2,2,2	0.44	0
5	EDO	A	1005	-	3,3,3	0.48	0	2,2,2	0.40	0
5	EDO	B	806	-	3,3,3	0.42	0	2,2,2	0.19	0
5	EDO	B	802	-	3,3,3	0.58	0	2,2,2	0.27	0
5	EDO	B	804	-	3,3,3	0.54	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	807	-	3,3,3	0.45	0	2,2,2	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	805	-	-	0/1/1/1	-
5	EDO	A	1004	-	-	1/1/1/1	-
5	EDO	B	803	-	-	0/1/1/1	-
5	EDO	A	1003	-	-	1/1/1/1	-
5	EDO	A	1005	-	-	0/1/1/1	-
5	EDO	B	806	-	-	0/1/1/1	-
5	EDO	B	802	-	-	0/1/1/1	-
5	EDO	B	804	-	-	0/1/1/1	-
5	EDO	B	807	-	-	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
5	A	1004	EDO	O1-C1-C2-O2
5	A	1003	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	EDO	1	0
5	B	807	EDO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	312/369 (84%)	0.41	15 (4%) 35 40	40, 53, 87, 126	0
1	B	318/369 (86%)	0.54	17 (5%) 32 36	38, 60, 102, 119	0
2	C	17/17 (100%)	1.18	4 (23%) 2 2	51, 63, 96, 108	0
2	D	17/17 (100%)	0.46	1 (5%) 28 32	47, 56, 66, 70	0
All	All	664/772 (86%)	0.50	37 (5%) 30 34	38, 56, 93, 126	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	653	ILE	5.3
2	C	500	THR	4.3
1	A	698	PHE	4.2
1	B	520	VAL	4.2
1	B	652	ASN	3.7
1	B	796	LYS	3.1
1	A	520	VAL	2.9
1	B	513	ILE	2.9
1	B	657	PRO	2.9
1	B	659	ILE	2.8
2	C	496	LEU	2.8
1	B	473	GLY	2.7
1	B	477	PHE	2.7
1	B	562	LEU	2.6
1	B	656	SER	2.6
1	B	474	GLY	2.6
1	B	773	TYR	2.6
1	B	475	LYS	2.5
1	A	697	LYS	2.5
1	A	695	ASN	2.5
1	B	599	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	498	LYS	2.4
2	C	499	PRO	2.4
1	B	521	ASN	2.4
1	A	603	SER	2.3
1	A	606	ILE	2.3
1	A	788	ARG	2.3
1	A	644	ILE	2.2
1	A	474	GLY	2.1
2	D	500	THR	2.1
1	A	513	ILE	2.1
1	A	605	PHE	2.1
1	A	643	LEU	2.1
1	B	795	LEU	2.1
1	A	516	SER	2.1
1	A	472	SER	2.0
1	A	473	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
5	EDO	B	802	4/4	0.68	0.19	51,54,56,57	0
5	EDO	B	805	4/4	0.77	0.16	68,69,71,72	0
5	EDO	A	1005	4/4	0.81	0.19	71,73,73,73	0
5	EDO	A	1004	4/4	0.83	0.20	73,76,77,78	0
5	EDO	B	803	4/4	0.84	0.13	68,68,68,69	0
5	EDO	B	807	4/4	0.85	0.18	57,57,57,58	0
5	EDO	B	806	4/4	0.89	0.15	41,44,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	804	4/4	0.91	0.10	50,51,51,53	0
5	EDO	A	1003	4/4	0.92	0.12	54,54,55,55	0
4	CL	A	1002	1/1	0.93	0.10	67,67,67,67	0
4	CL	B	801	1/1	0.97	0.11	61,61,61,61	0
3	MG	A	1001	1/1	0.98	0.09	59,59,59,59	1

6.5 Other polymers [i](#)

There are no such residues in this entry.