



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:04 AM BST

PDB ID : 5LMF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

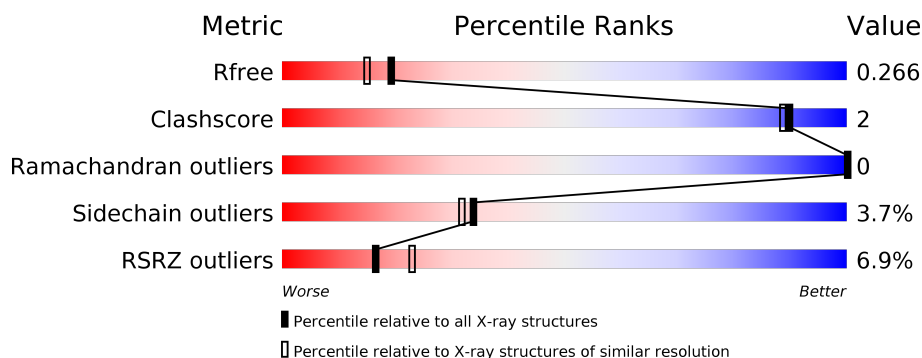
1 Overall quality at a glance

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>15%</div> </div> </div>
1	B	369	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>14%</div> </div> </div>
2	C	17	<div> <div>12%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
2	D	17	<div> <div> <div></div> <div>71%</div> <div>24%</div> <div>6%</div> </div> </div>

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			

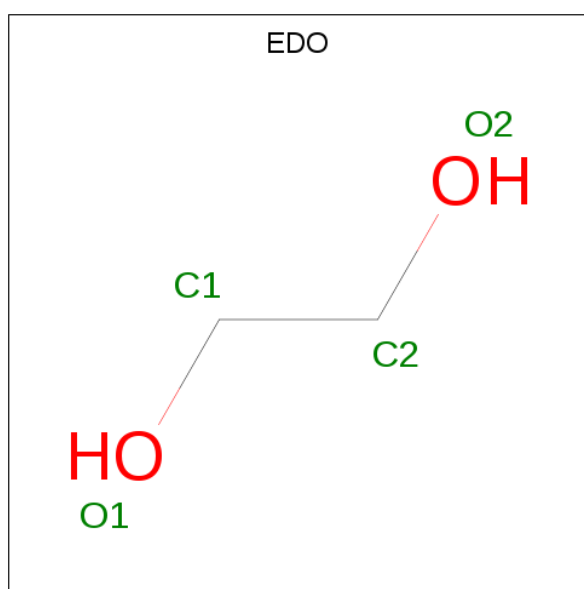
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: 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 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

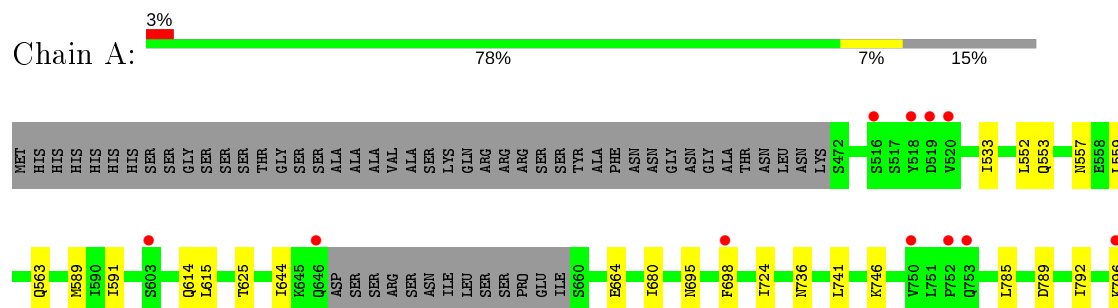
- Molecule 6 is water.

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

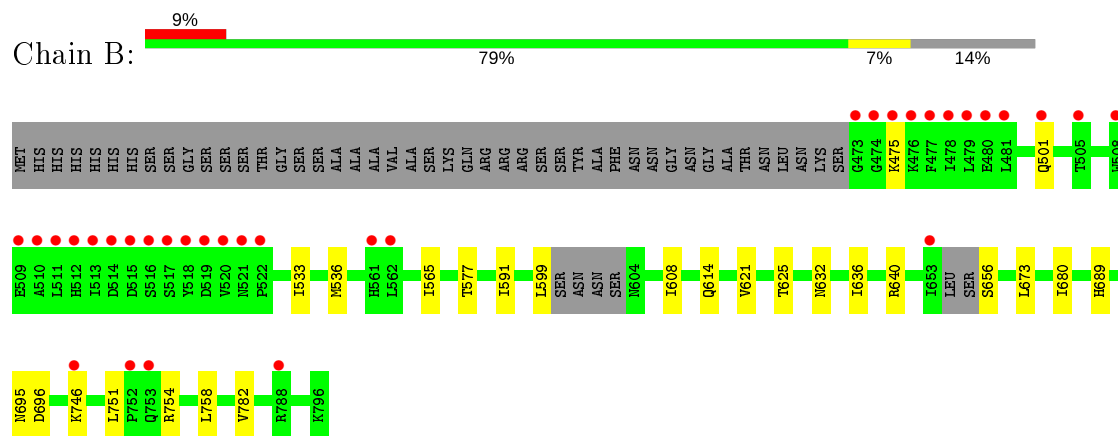
3 Residue-property plots [i](#)

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.

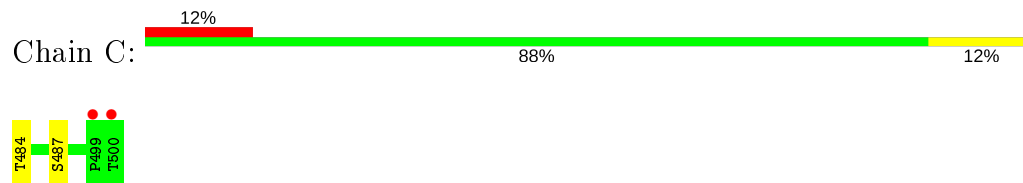
- Molecule 1: DNA topoisomerase 2-associated protein PAT1



- Molecule 1: DNA topoisomerase 2-associated protein PAT1



- Molecule 2: mRNA decapping protein 2



- Molecule 2: mRNA decapping protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.36 Å 122.92 Å 126.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.48 – 2.15 48.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.9 (31.48-2.15) 97.9 (48.93-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.16 Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.212 , 0.246 0.226 , 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 , 52.3	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	0.49	0/2591	0.63	0/3492
1	B	0.48	0/2640	0.63	0/3557
2	C	0.52	0/130	0.60	0/174
2	D	0.47	0/130	0.58	0/174
All	All	0.49	0/5491	0.62	0/7397

There are no bond length outliers.

There are no bond angle outliers.

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	9	0
1	B	2600	0	2688	10	0
2	C	129	0	135	1	0
2	D	129	0	135	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	20	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 (20) 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
2:D:484:THR:N	2:D:487:SER:HG	2.05	0.55
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
2:C:484:THR:N	2:C:487:SER:HG	2.15	0.45
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
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 ⓘ

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	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 ⓘ

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%)	280 (96%)	11 (4%)	33	31
1	B	297/338 (88%)	286 (96%)	11 (4%)	34	32
2	C	15/15 (100%)	15 (100%)	0	100	100
2	D	15/15 (100%)	14 (93%)	1 (7%)	16	11
All	All	618/706 (88%)	595 (96%)	23 (4%)	34	32

All (23) 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	614	GLN
1	A	615	LEU
1	A	644	ILE
1	A	664	GLU
1	A	746	LYS
1	A	789	ASP

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Mol	Chain	Res	Type
1	A	796	LYS
1	B	475	LYS
1	B	501	GLN
1	B	565	ILE
1	B	591	ILE
1	B	614	GLN
1	B	640	ARG
1	B	656	SER
1	B	696	ASP
1	B	746	LYS
1	B	751	LEU
1	B	782	VAL
2	D	493	LEU

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

Mol	Chain	Res	Type
1	A	557	ASN
1	B	512	HIS
1	B	557	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	1005	-	3,3,3	0.53	0	2,2,2	0.37	0
5	EDO	B	805	-	3,3,3	0.57	0	2,2,2	0.37	0
5	EDO	B	804	-	3,3,3	0.60	0	2,2,2	0.24	0
5	EDO	B	803	-	3,3,3	0.66	0	2,2,2	0.13	0
5	EDO	A	1003	-	3,3,3	0.51	0	2,2,2	0.40	0
5	EDO	B	807	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	A	1004	-	3,3,3	0.69	0	2,2,2	0.18	0
5	EDO	B	802	-	3,3,3	0.64	0	2,2,2	0.22	0
5	EDO	B	806	-	3,3,3	0.46	0	2,2,2	0.15	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	A	1005	-	-	0/1/1/1	-
5	EDO	B	805	-	-	0/1/1/1	-
5	EDO	B	804	-	-	0/1/1/1	-
5	EDO	B	803	-	-	0/1/1/1	-
5	EDO	A	1003	-	-	1/1/1/1	-
5	EDO	B	807	-	-	0/1/1/1	-
5	EDO	A	1004	-	-	1/1/1/1	-
5	EDO	B	802	-	-	0/1/1/1	-
5	EDO	B	806	-	-	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.12	11 (3%) 44 52	40, 53, 87, 126	0
1	B	318/369 (86%)	0.48	33 (10%) 6 9	38, 60, 102, 119	0
2	C	17/17 (100%)	0.72	2 (11%) 4 6	51, 63, 96, 108	0
2	D	17/17 (100%)	-0.06	0 100 100	47, 56, 66, 70	0
All	All	664/772 (86%)	0.30	46 (6%) 16 23	38, 56, 93, 126	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	VAL	10.6
1	B	518	TYR	6.6
1	B	516	SER	5.5
1	B	477	PHE	5.3
2	C	500	THR	5.2
1	B	475	LYS	4.9
1	A	752	PRO	4.4
1	B	517	SER	4.2
1	B	521	ASN	4.0
1	B	515	ASP	3.8
1	A	518	TYR	3.7
1	B	508	TRP	3.5
1	A	753	GLN	3.4
1	B	481	LEU	3.4
1	B	653	ILE	3.3
1	B	505	THR	3.3
2	C	499	PRO	3.3
1	B	513	ILE	3.2
1	B	519	ASP	3.2
1	B	753	GLN	3.1
1	B	522	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	478	ILE	3.1
1	B	509	GLU	3.1
1	B	476	LYS	3.0
1	B	514	ASP	3.0
1	A	520	VAL	2.9
1	A	516	SER	2.9
1	B	473	GLY	2.8
1	A	698	PHE	2.6
1	B	746	LYS	2.6
1	B	474	GLY	2.6
1	B	479	LEU	2.6
1	A	519	ASP	2.5
1	B	511	LEU	2.4
1	A	646	GLN	2.3
1	B	480	GLU	2.3
1	A	750	VAL	2.2
1	B	561	HIS	2.2
1	A	603	SER	2.2
1	A	796	LYS	2.2
1	B	562	LEU	2.2
1	B	752	PRO	2.2
1	B	512	HIS	2.1
1	B	510	ALA	2.1
1	B	788	ARG	2.1
1	B	501	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(\AA^2)	Q<0.9
5	EDO	B	803	4/4	0.76	0.21	68,68,68,69	0
5	EDO	A	1004	4/4	0.78	0.33	73,76,77,78	0
5	EDO	A	1005	4/4	0.81	0.23	71,73,73,73	0
5	EDO	B	805	4/4	0.83	0.13	68,69,71,72	0
5	EDO	B	802	4/4	0.83	0.14	51,54,56,57	0
5	EDO	B	807	4/4	0.89	0.24	57,57,57,58	0
5	EDO	B	806	4/4	0.89	0.12	41,44,46,49	0
5	EDO	B	804	4/4	0.90	0.14	50,51,51,53	0
4	CL	B	801	1/1	0.91	0.06	61,61,61,61	0
5	EDO	A	1003	4/4	0.92	0.14	54,54,55,55	0
4	CL	A	1002	1/1	0.93	0.11	67,67,67,67	0
3	MG	A	1001	1/1	0.97	0.10	59,59,59,59	1

6.5 Other polymers [i](#)

There are no such residues in this entry.