



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:56 am BST

PDB ID : 4OJJ  
Title : Structure of C-terminal domain from *S. cerevisiae* Pat1 decapping activator  
(Space group : P212121)  
Authors : Fourati-Kammoun, Z.; Kolesnikova, O.; Back, R.; Keller, J.; Lazar, N.;  
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Deposited on : 2014-01-21  
Resolution : 2.32 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](mailto: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.

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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 : 2.11  
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) : 2.11

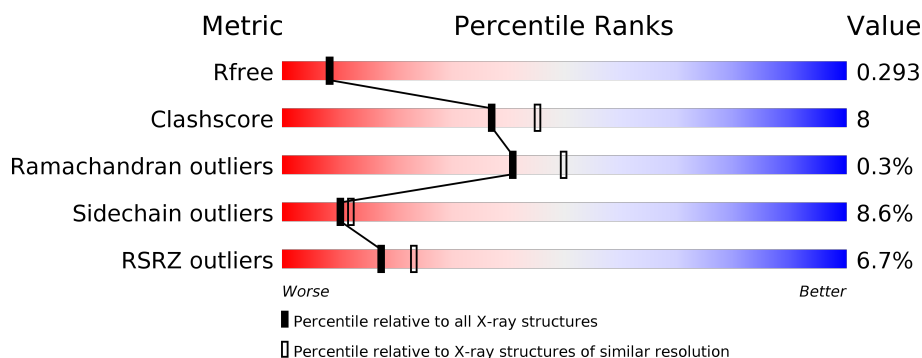
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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  $\geq 3$ , 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	330	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• 5%</div> </div> </div>
1	B	330	<div> <div>12%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>• 16%</div> </div> </div>
1	C	330	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7750 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	C	323	Total	C	N	O	S	0	0	0
			2652	1711	435	498	8			
1	A	314	Total	C	N	O	S	0	1	0
			2578	1669	419	482	8			
1	B	278	Total	C	N	O	S	0	0	0
			2283	1481	371	425	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	797	HIS	-	EXPRESSION TAG	UNP P25644
C	798	HIS	-	EXPRESSION TAG	UNP P25644
C	799	HIS	-	EXPRESSION TAG	UNP P25644
C	800	HIS	-	EXPRESSION TAG	UNP P25644
C	801	HIS	-	EXPRESSION TAG	UNP P25644
C	802	HIS	-	EXPRESSION TAG	UNP P25644
A	797	HIS	-	EXPRESSION TAG	UNP P25644
A	798	HIS	-	EXPRESSION TAG	UNP P25644
A	799	HIS	-	EXPRESSION TAG	UNP P25644
A	800	HIS	-	EXPRESSION TAG	UNP P25644
A	801	HIS	-	EXPRESSION TAG	UNP P25644
A	802	HIS	-	EXPRESSION TAG	UNP P25644
B	797	HIS	-	EXPRESSION TAG	UNP P25644
B	798	HIS	-	EXPRESSION TAG	UNP P25644
B	799	HIS	-	EXPRESSION TAG	UNP P25644
B	800	HIS	-	EXPRESSION TAG	UNP P25644
B	801	HIS	-	EXPRESSION TAG	UNP P25644
B	802	HIS	-	EXPRESSION TAG	UNP P25644

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

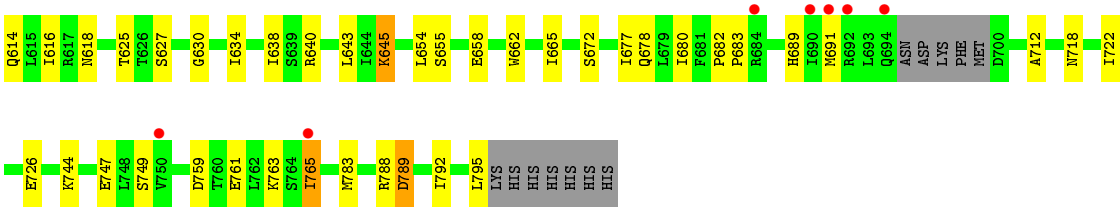
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	147	Total O 147 147	0	0
5	A	60	Total O 60 60	0	0
5	B	24	Total O 24 24	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.43 Å 173.54 Å 175.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 2.32 43.86 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.86-2.32) 99.1 (43.86-2.32)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.32 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.230 , 0.293 0.230 , 0.293	Depositor DCC
$R_{free}$ test set	2459 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.42	0/2623	0.59	0/3540
1	B	0.34	0/2316	0.52	0/3120
1	C	0.50	1/2696 (0.0%)	0.62	1/3638 (0.0%)
All	All	0.43	1/7635 (0.0%)	0.58	1/10298 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	737	GLU	CG-CD	5.32	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	778	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2578	0	2673	43	0
1	B	2283	0	2386	46	0
1	C	2652	0	2732	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	C	4	0	6	0	0
4	C	1	0	0	0	0
5	A	60	0	0	5	0
5	B	24	0	0	2	0
5	C	147	0	0	4	1
All	All	7750	0	7797	120	1

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 8.

All (120) 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:C:655:SER:HB2	1:C:657:PRO:HD2	1.64	0.78
1:B:564:ILE:HD11	1:B:584:VAL:HA	1.70	0.72
1:B:678:GLN:HE21	1:B:726:GLU:HB3	1.55	0.72
1:A:744:LYS:HB3	1:A:765:ILE:HD13	1.72	0.71
1:B:562:LEU:HG	1:B:564:ILE:HG22	1.74	0.69
1:A:647:ASP:OD1	1:A:650:ARG:NH2	2.28	0.66
1:B:575:LYS:HG2	1:B:689:HIS:CE1	2.32	0.64
1:B:606:ILE:HD11	1:B:658:GLU:HG2	1.81	0.63
1:B:482:ILE:HG12	1:B:526:MET:HG3	1.81	0.63
1:A:474:GLY:N	5:A:938:HOH:O	2.34	0.61
1:A:651:SER:N	1:A:652:ASN:HA	2.15	0.61
1:A:569:SER:HB3	1:A:572:THR:HG22	1.82	0.61
1:C:476:LYS:HD3	1:C:477:PHE:H	1.67	0.60
1:C:569:SER:HB3	1:C:572:THR:HG22	1.84	0.59
1:C:625:THR:HB	1:C:680:ILE:HG22	1.84	0.59
1:B:543:LEU:HD22	1:B:547:GLN:HB3	1.85	0.58
1:A:678:GLN:H	1:A:678:GLN:CD	2.07	0.57
1:C:702:ALA:O	1:C:706:GLN:HG3	2.04	0.57
1:B:625:THR:HB	1:B:680:ILE:HG22	1.87	0.56
1:B:557:ASN:OD1	1:B:614:GLN:NE2	2.38	0.56
1:B:578:LEU:O	1:B:582:LYS:NZ	2.25	0.56
1:A:652:ASN:O	1:A:652:ASN:ND2	2.29	0.55
1:A:480:GLU:O	1:A:484:THR:HG22	2.07	0.55
1:A:532:GLY:O	1:A:535[A]:ILE:HG12	2.08	0.54
1:B:570:TYR:CD1	1:B:683:PRO:HD3	2.42	0.54
1:C:553:GLN:NE2	5:C:1101:HOH:O	2.39	0.54
1:A:615:LEU:O	1:A:619:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:ARG:HD2	5:A:902:HOH:O	2.07	0.54
1:A:628:LYS:NZ	5:A:945:HOH:O	2.41	0.53
1:B:599:LEU:HD22	1:B:608:ILE:HD13	1.92	0.52
1:C:599:LEU:O	1:C:603:SER:HB2	2.10	0.52
1:A:588:GLN:O	1:A:592:LEU:HB2	2.10	0.52
1:B:609:MET:HE1	1:B:665:ILE:HD12	1.92	0.52
1:C:496:LEU:HD23	1:C:497:ARG:N	2.25	0.52
1:B:712:ALA:HB1	1:B:783:MET:HE1	1.91	0.51
1:C:648:SER:HB3	1:C:653:ILE:HB	1.92	0.51
1:C:538:ARG:HG3	5:C:1020:HOH:O	2.10	0.51
1:A:712:ALA:HB1	1:A:783:MET:HE1	1.92	0.51
1:A:489:ILE:HD11	1:A:539:ILE:HG13	1.92	0.51
1:A:530:ASP:OD1	1:A:583:LYS:NZ	2.33	0.51
1:B:678:GLN:H	1:B:678:GLN:CD	2.12	0.51
1:A:511:LEU:O	1:A:523:PHE:HB2	2.11	0.50
1:C:578:LEU:HD13	1:C:582:LYS:HE3	1.93	0.50
1:A:533:ILE:HD12	1:A:591:ILE:HD11	1.93	0.50
1:B:557:ASN:OD1	1:B:618:ASN:ND2	2.45	0.50
1:B:640:ARG:NH2	5:B:919:HOH:O	2.45	0.49
1:B:761:GLU:O	1:B:765:ILE:HD12	2.13	0.49
1:A:689:HIS:O	1:A:693:LEU:HG	2.13	0.48
1:C:476:LYS:HD3	1:C:477:PHE:N	2.27	0.48
1:A:619:ASN:HB3	1:A:624:LEU:HD11	1.95	0.48
1:B:718:ASN:O	1:B:722:ILE:HG13	2.14	0.48
1:A:480:GLU:OE2	5:A:931:HOH:O	2.18	0.48
1:A:540:PHE:HA	1:A:543:LEU:HD12	1.96	0.48
1:B:534:LYS:HE3	1:B:586:LEU:HD21	1.95	0.48
1:A:539:ILE:HG22	1:A:543:LEU:HD11	1.95	0.48
1:A:678:GLN:H	1:A:678:GLN:NE2	2.12	0.48
1:B:606:ILE:HA	1:B:609:MET:HG3	1.95	0.48
1:C:667:ASP:O	1:C:671:THR:HG23	2.13	0.48
1:B:489:ILE:HG21	1:B:538:ARG:HH11	1.78	0.47
1:A:694:GLN:HG3	1:A:696:ASP:HB3	1.97	0.47
1:C:649:SER:HB2	1:A:728:ARG:CZ	2.44	0.47
1:B:605:PHE:O	1:B:609:MET:HG2	2.14	0.47
1:B:604:ASN:ND2	1:B:607:GLU:OE2	2.49	0.46
1:C:566:ILE:HA	1:C:572:THR:HG21	1.97	0.46
1:C:645:LYS:O	1:C:649:SER:HB3	2.16	0.46
1:C:685:GLU:H	1:C:685:GLU:HG3	1.14	0.46
1:C:556:PHE:CD1	1:C:615:LEU:HD12	2.50	0.46
1:C:771:LYS:NZ	5:C:1070:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ILE:O	1:B:680:ILE:HG23	2.15	0.46
1:B:551:ILE:HD13	1:B:551:ILE:HA	1.70	0.45
1:B:599:LEU:HA	1:B:603:SER:HB2	1.99	0.45
1:B:640:ARG:HA	1:B:643:LEU:HD12	1.99	0.45
1:B:788:ARG:HD3	1:B:789:ASP:H	1.82	0.45
1:B:680:ILE:O	1:B:682:PRO:HD3	2.17	0.45
1:A:612:LEU:HD13	1:A:662:TRP:HZ3	1.82	0.45
1:C:773:TYR:CE1	1:C:787:TYR:HE2	2.34	0.44
1:B:526:MET:HG2	1:B:532:GLY:HA3	1.98	0.44
1:B:481:LEU:HA	1:B:484:THR:HG22	2.00	0.44
1:B:744:LYS:O	1:B:747:GLU:HG2	2.18	0.44
1:A:535[B]:ILE:HG23	1:A:539:ILE:HG13	1.99	0.44
1:A:599:LEU:HD12	1:A:636:ILE:HG22	2.00	0.44
1:C:728:ARG:HD2	5:C:1126:HOH:O	2.17	0.44
1:B:638:ILE:HD12	1:B:662:TRP:HH2	1.82	0.44
1:B:744:LYS:HD2	1:B:747:GLU:OE1	2.18	0.44
1:C:653:ILE:O	1:C:654:LEU:HB2	2.17	0.43
1:C:645:LYS:HE2	1:C:659:ILE:HD13	1.98	0.43
1:A:751:LEU:HA	1:A:752:PRO:HD3	1.74	0.43
1:C:578:LEU:HA	1:C:578:LEU:HD23	1.83	0.43
1:C:612:LEU:HD21	1:C:638:ILE:HD11	2.01	0.43
1:C:638:ILE:HG22	1:C:710:SER:HB3	2.00	0.43
1:A:685:GLU:HG3	1:A:685:GLU:H	1.56	0.42
1:B:718:ASN:ND2	5:B:910:HOH:O	2.36	0.42
1:A:625:THR:HB	1:A:680:ILE:HG22	2.02	0.42
1:A:564:ILE:O	1:A:568:SER:OG	2.28	0.42
1:B:763:LYS:HD3	1:B:763:LYS:HA	1.76	0.42
1:A:608:ILE:H	1:A:608:ILE:HG12	1.57	0.42
1:C:712:ALA:HB1	1:C:783:MET:HE1	2.02	0.42
1:A:754:ARG:NH1	1:A:759:ASP:OD1	2.53	0.42
1:B:576:PRO:HD2	1:B:689:HIS:CD2	2.55	0.42
1:A:697:LYS:O	1:A:698:PHE:HB2	2.20	0.42
1:B:609:MET:CE	1:B:665:ILE:HD12	2.49	0.42
1:B:612:LEU:O	1:B:616:ILE:HG13	2.20	0.42
1:B:605:PHE:HD1	1:B:658:GLU:HB3	1.86	0.41
1:B:645:LYS:HG3	1:B:662:TRP:HD1	1.85	0.41
1:C:592:LEU:O	1:C:596:VAL:HG23	2.20	0.41
1:C:698:PHE:HZ	1:C:767:TYR:HE2	1.69	0.41
1:C:773:TYR:CE1	1:C:787:TYR:CE2	3.08	0.41
1:A:544:ASP:OD1	1:A:547:GLN:HG3	2.21	0.41
1:B:722:ILE:O	1:B:726:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:LEU:HD23	1:A:671:THR:HG23	2.03	0.41
1:A:568:SER:HB2	1:A:627:SER:HB2	2.02	0.41
1:A:635:THR:O	1:A:639:SER:OG	2.32	0.41
1:B:630:GLY:O	1:B:634:ILE:HG13	2.21	0.41
1:C:756:GLN:O	1:C:760:THR:HG23	2.21	0.41
1:B:712:ALA:HB1	1:B:783:MET:CE	2.51	0.40
1:C:664:GLU:O	1:C:668:LYS:HG3	2.21	0.40
1:A:498:ASN:HA	5:A:914:HOH:O	2.20	0.40
1:A:531:LYS:O	1:A:535[A]:ILE:HG23	2.21	0.40
1:B:536:MET:N	1:B:537:PRO:HD2	2.36	0.40
1:A:590:ILE:HG22	1:A:591:ILE:HD13	2.03	0.40

All (1) 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)
5:C:1103:HOH:O	5:C:1105:HOH:O[1_455]	2.09	0.11

## 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	313/330 (95%)	303 (97%)	9 (3%)	1 (0%)	41	50
1	B	272/330 (82%)	264 (97%)	7 (3%)	1 (0%)	34	41
1	C	321/330 (97%)	316 (98%)	4 (1%)	1 (0%)	41	50
All	All	906/990 (92%)	883 (98%)	20 (2%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	654	LEU

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Mol	Chain	Res	Type
1	A	698	PHE
1	B	560	SER

### 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	298/311 (96%)	269 (90%)	29 (10%)	8	9
1	B	265/311 (85%)	246 (93%)	19 (7%)	14	18
1	C	306/311 (98%)	279 (91%)	27 (9%)	10	11
All	All	869/933 (93%)	794 (91%)	75 (9%)	10	12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	476	LYS
1	C	484	THR
1	C	496	LEU
1	C	501	GLN
1	C	502	THR
1	C	531	LYS
1	C	550	LYS
1	C	557	ASN
1	C	558	GLU
1	C	578	LEU
1	C	585	ASP
1	C	603	SER
1	C	612	LEU
1	C	638	ILE
1	C	643	LEU
1	C	644	ILE
1	C	646	GLN
1	C	684	ARG
1	C	685	GLU
1	C	698	PHE

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Mol	Chain	Res	Type
1	C	699	MET
1	C	748	LEU
1	C	758	LEU
1	C	760	THR
1	C	783	MET
1	C	797	HIS
1	C	798	HIS
1	A	479	LEU
1	A	481	LEU
1	A	484	THR
1	A	496	LEU
1	A	513	ILE
1	A	557	ASN
1	A	559	LEU
1	A	563	GLN
1	A	578	LEU
1	A	588	GLN
1	A	602	ASN
1	A	605	PHE
1	A	613	LEU
1	A	643	LEU
1	A	648	SER
1	A	652	ASN
1	A	653	ILE
1	A	655	SER
1	A	678	GLN
1	A	685	GLU
1	A	696	ASP
1	A	706	GLN
1	A	713	LEU
1	A	714	SER
1	A	742	GLN
1	A	759	ASP
1	A	778	LEU
1	A	783	MET
1	A	787	TYR
1	B	551	ILE
1	B	571	LYS
1	B	572	THR
1	B	575	LYS
1	B	585	ASP
1	B	603	SER

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Mol	Chain	Res	Type
1	B	609	MET
1	B	627	SER
1	B	645	LYS
1	B	654	LEU
1	B	655	SER
1	B	672	SER
1	B	691	MET
1	B	749	SER
1	B	759	ASP
1	B	765	ILE
1	B	789	ASP
1	B	792	ILE
1	B	795	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	557	ASN
1	A	614	GLN
1	B	618	ASN
1	B	678	GLN
1	B	774	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	EDO	C	902	-	3,3,3	0.55	0	2,2,2	0.23	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
3	EDO	C	902	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	314/330 (95%)	0.33	16 (5%) 28 35	31, 57, 85, 98	0
1	B	278/330 (84%)	0.88	41 (14%) 2 3	47, 70, 106, 114	0
1	C	323/330 (97%)	0.14	4 (1%) 79 83	28, 45, 67, 81	0
All	All	915/990 (92%)	0.43	61 (6%) 17 23	28, 56, 99, 114	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	PHE	9.0
1	B	487	GLU	7.5
1	B	539	ILE	5.7
1	B	540	PHE	5.7
1	B	481	LEU	5.5
1	B	538	ARG	4.8
1	B	561	HIS	4.7
1	B	543	LEU	4.6
1	B	527	LEU	4.4
1	A	496	LEU	4.0
1	B	485	VAL	4.0
1	B	484	THR	3.9
1	A	498	ASN	3.9
1	B	531	LYS	3.6
1	B	536	MET	3.4
1	B	546	GLN	3.4
1	B	602	ASN	3.4
1	B	765	ILE	3.3
1	B	750	VAL	3.3
1	B	525	SER	3.2
1	A	750	VAL	3.2
1	B	482	ILE	3.2
1	B	590	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	557	ASN	3.2
1	A	758	LEU	3.1
1	A	698	PHE	3.1
1	B	567	LEU	3.1
1	A	494	ALA	3.0
1	B	488	GLU	3.0
1	B	486	TYR	3.0
1	B	694	GLN	2.9
1	B	601	ASN	2.8
1	C	698	PHE	2.7
1	B	690	ILE	2.7
1	B	558	GLU	2.7
1	B	576	PRO	2.6
1	C	653	ILE	2.6
1	B	684	ARG	2.5
1	A	695	ASN	2.5
1	B	489	ILE	2.5
1	B	535	ILE	2.5
1	A	497	ARG	2.4
1	A	766	ILE	2.4
1	B	692	ARG	2.4
1	A	739	GLU	2.4
1	A	518	TYR	2.4
1	B	581	LEU	2.3
1	B	589	MET	2.3
1	B	600	SER	2.3
1	A	684	ARG	2.3
1	B	524	ILE	2.3
1	B	480	GLU	2.2
1	B	552	LEU	2.2
1	B	691	MET	2.2
1	A	486	TYR	2.1
1	C	693	LEU	2.1
1	A	692	ARG	2.1
1	A	759	ASP	2.1
1	C	695	ASN	2.1
1	B	584	VAL	2.0
1	A	697	LYS	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 [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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
3	EDO	C	902	4/4	0.86	0.20	57,59,60,61	0
4	CL	C	903	1/1	0.94	0.07	72,72,72,72	0
2	MG	C	901	1/1	0.98	0.29	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.