



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:58 AM UTC

PDB ID : 4OJJ / pdb_00004ojj
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.;
Gaudon-Plesse, C.; Seraphin, B.; Graille, M.
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

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

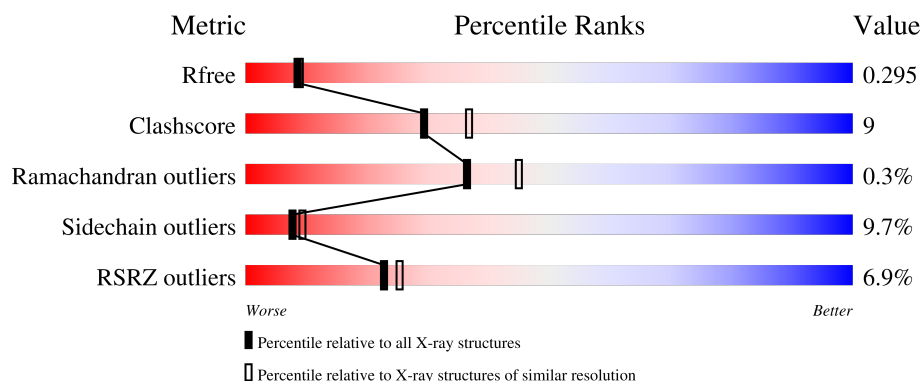
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 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	330	5% 68% 22% 5% 5%
1	B	330	11% 60% 22% • 16%
1	C	330	2% 77% 18% • •

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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

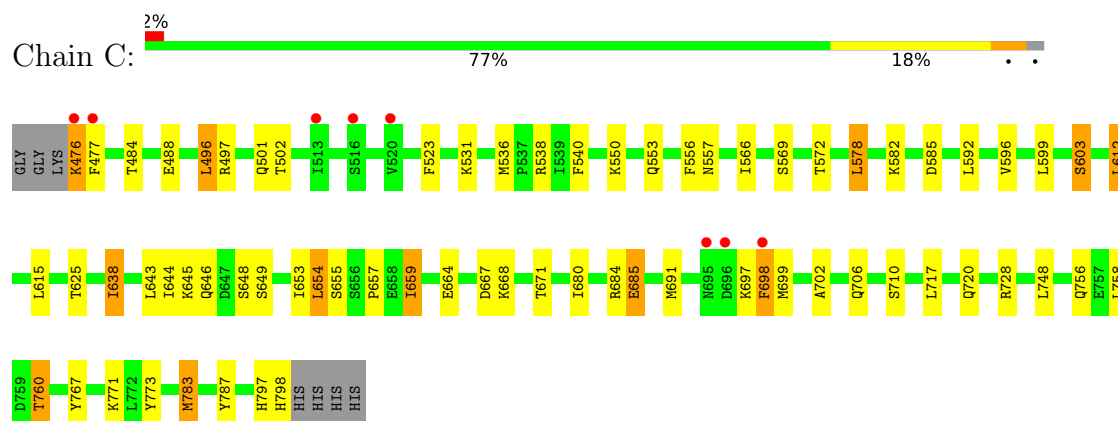
- Molecule 5 is water.

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

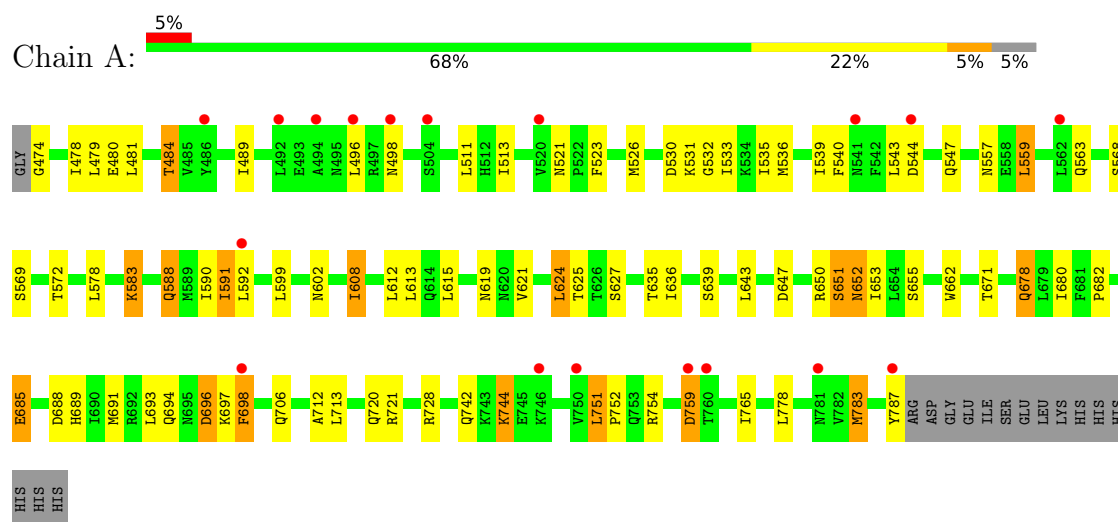
3 Residue-property plots

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.

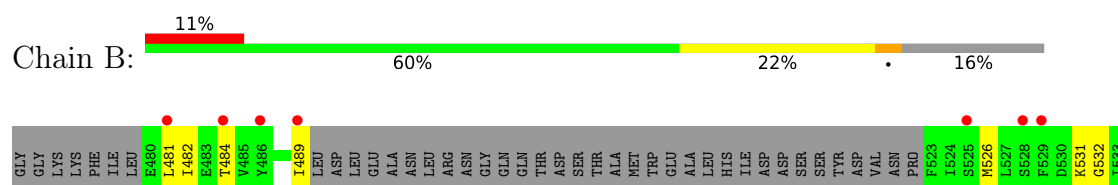
• Molecule 1: DNA topoisomerase 2-associated protein PAT1

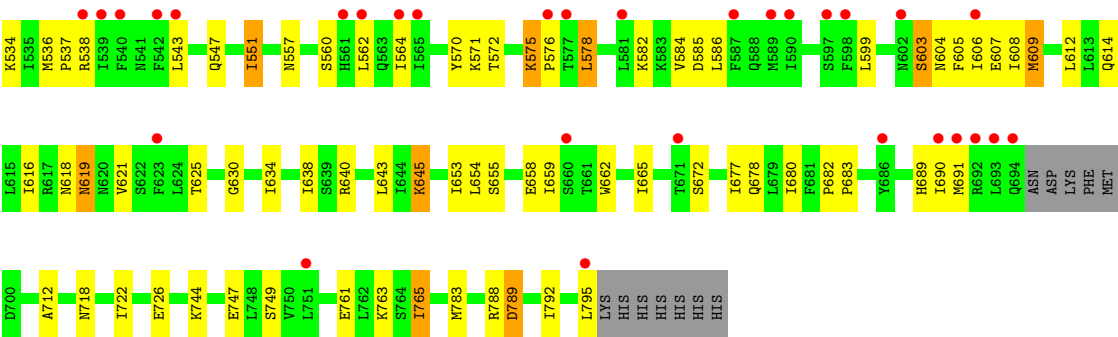


• Molecule 1: DNA topoisomerase 2-associated protein PAT1



• Molecule 1: DNA topoisomerase 2-associated protein PAT1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	36.43Å 173.54Å 175.44Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.230 , 0.293 0.232 , 0.295	Depositor DCC
R_{free} test set	2459 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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: EDO, MG, 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	0.53	0/2623	0.94	11/3540 (0.3%)
1	B	0.44	0/2316	0.83	1/3120 (0.0%)
1	C	0.66	0/2696	0.92	1/3638 (0.0%)
All	All	0.55	0/7635	0.90	13/10298 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	SER	N-CA-C	8.80	124.08	113.16
1	A	751	LEU	CA-C-N	7.54	127.08	119.24
1	A	751	LEU	C-N-CA	7.54	127.08	119.24
1	A	682	PRO	O-C-N	6.97	124.42	121.15
1	A	521	ASN	CA-C-N	6.62	128.11	119.84
1	A	521	ASN	C-N-CA	6.62	128.11	119.84
1	A	682	PRO	CA-C-N	5.74	127.02	119.84
1	A	682	PRO	C-N-CA	5.74	127.02	119.84
1	B	619	ASN	N-CA-C	5.50	116.89	108.42
1	A	536	MET	CA-C-N	-5.35	113.39	119.28
1	A	536	MET	C-N-CA	-5.35	113.39	119.28
1	A	559	LEU	N-CA-C	5.17	117.31	111.11
1	C	699	MET	N-CA-C	-5.02	102.48	109.96

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	2578	0	2673	44	0
1	B	2283	0	2386	48	0
1	C	2652	0	2732	41	0
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	4	0
5	B	24	0	0	2	0
5	C	147	0	0	4	1
All	All	7750	0	7797	131	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 9.

All (131) 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:609:MET:HE2	1:B:665:ILE:HD12	1.60	0.81
1:C:655:SER:HB2	1:C:657:PRO:HD2	1.64	0.78
1:C:691:MET:HE3	1:C:697:LYS:HA	1.67	0.75
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:C:536:MET:HE3	1:C:540:PHE:HE2	1.60	0.67
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:C:523:PHE:CZ	1:C:536:MET:HE1	2.34	0.62
1:A:678:GLN:H	1:A:678:GLN:CD	2.07	0.62
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:A:530:ASP:OD1	1:A:583:LYS:NZ	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:609:MET:HE1	1:B:662:TRP:HA	1.83	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: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:678:GLN:H	1:B:678:GLN:CD	2.12	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
1:A:720:GLN:HB3	1:A:783:MET:HE1	1.88	0.54
1:A:721:ARG:HD2	5:A:902:HOH:O	2.07	0.54
1:C:523:PHE:HZ	1:C:536:MET:HE1	1.74	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:C:496:LEU:HD23	1:C:497:ARG:N	2.25	0.52
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:489:ILE:HD11	1:A:539:ILE:HG13	1.92	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:712:ALA:HB1	1:B:783:MET:HE1	1.94	0.49
1:B:761:GLU:O	1:B:765:ILE:HD12	2.13	0.49
1:C:476:LYS:HD3	1:C:477:PHE:N	2.27	0.48
1:A:689:HIS:O	1:A:693:LEU:HG	2.13	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:C:667:ASP:O	1:C:671:THR:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:566:ILE:HA	1:C:572:THR:HG21	1.97	0.46
1:B:604:ASN:ND2	1:B:607:GLU:OE2	2.49	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
1:C:523:PHE:CE1	1:C:536:MET:HE1	2.50	0.46
1:B:677:ILE:O	1:B:680:ILE:HG23	2.15	0.46
1:B:609:MET:HE1	1:B:662:TRP:CA	2.45	0.45
1:B:551:ILE:HD13	1:B:551:ILE:HA	1.70	0.45
1:A:526:MET:HE3	1:A:526:MET:HB2	1.87	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:720:GLN:HB3	1:C:783:MET:HE1	1.98	0.44
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:C:728:ARG:HD2	5:C:1126:HOH:O	2.17	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: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:645:LYS:HE2	1:C:659:ILE:HD13	1.98	0.43
1:C:653:ILE:O	1:C:654:LEU:HB2	2.17	0.43
1:A:751:LEU:HA	1:A:752:PRO:HD3	1.74	0.43
1:C:578:LEU:HD23	1:C:578:LEU:HA	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:H	1:A:685:GLU:HG3	1.56	0.42
1:B:718:ASN:ND2	5:B:910:HOH:O	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:GLN:CG	1:C:783:MET:HE1	2.50	0.42
1:A:625:THR:HB	1:A:680:ILE:HG22	2.02	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:A:754:ARG:NH1	1:A:759:ASP:OD1	2.53	0.42
1:B:609:MET:HE2	1:B:609:MET:HB3	1.86	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:612:LEU:O	1:B:616:ILE:HG13	2.20	0.42
1:C:783:MET:HE2	1:C:783:MET:HA	2.01	0.41
1:A:712:ALA:HB1	1:A:783:MET:HE3	2.02	0.41
1:B:605:PHE:HD1	1:B:658:GLU:HB3	1.86	0.41
1:C:592:LEU:O	1:C:596:VAL:HG23	2.20	0.41
1:B:645:LYS:HG3	1:B:662:TRP:HD1	1.85	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:C:717:LEU:HD23	1:A:671:THR:HG23	2.03	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
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:A:688:ASP:HA	1:A:691:MET:HE3	2.03	0.41
1:C:664:GLU:O	1:C:668:LYS:HG3	2.21	0.40
1:B:712:ALA:HB1	1:B:783:MET:CE	2.51	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:C:536:MET:HE3	1:C:540:PHE:CE2	2.48	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%)	36	45
1	B	272/330 (82%)	264 (97%)	7 (3%)	1 (0%)	30	37
1	C	321/330 (97%)	316 (98%)	4 (1%)	1 (0%)	36	45
All	All	906/990 (92%)	883 (98%)	20 (2%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	654	LEU
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%)	265 (89%)	33 (11%)	6	6
1	B	265/311 (85%)	241 (91%)	24 (9%)	9	11
1	C	306/311 (98%)	279 (91%)	27 (9%)	9	12
All	All	869/933 (93%)	785 (90%)	84 (10%)	8	9

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	476	LYS
1	C	484	THR
1	C	488	GLU
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	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	659	ILE
1	C	684	ARG
1	C	685	GLU
1	C	698	PHE
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	478	ILE
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	583	LYS
1	A	588	GLN
1	A	591	ILE
1	A	602	ASN
1	A	608	ILE
1	A	613	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	621	VAL
1	A	624	LEU
1	A	643	LEU
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	742	GLN
1	A	744	LYS
1	A	759	ASP
1	A	778	LEU
1	A	783	MET
1	A	787	TYR
1	B	531	LYS
1	B	551	ILE
1	B	571	LYS
1	B	572	THR
1	B	575	LYS
1	B	578	LEU
1	B	585	ASP
1	B	603	SER
1	B	609	MET
1	B	619	ASN
1	B	621	VAL
1	B	645	LYS
1	B	653	ILE
1	B	654	LEU
1	B	655	SER
1	B	659	ILE
1	B	672	SER
1	B	690	ILE
1	B	691	MET
1	B	749	SER
1	B	765	ILE
1	B	789	ASP
1	B	792	ILE
1	B	795	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	500	GLN
1	A	521	ASN
1	A	553	GLN
1	A	557	ASN
1	A	614	GLN
1	A	618	ASN
1	B	547	GLN
1	B	618	ASN
1	B	678	GLN
1	B	689	HIS
1	B	718	ASN
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 oligosaccharides 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	0.51	0	2,2,2	0.28	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, 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	314/330 (95%)	0.61	18 (5%) 29 32	31, 57, 85, 98	1 (0%)
1	B	278/330 (84%)	1.03	37 (13%) 7 8	47, 70, 106, 114	0
1	C	323/330 (97%)	0.14	8 (2%) 58 61	28, 45, 67, 81	0
All	All	915/990 (92%)	0.57	63 (6%) 23 25	28, 56, 99, 114	1 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	ILE	4.9
1	B	562	LEU	4.7
1	B	542	PHE	4.4
1	A	496	LEU	4.2
1	B	481	LEU	4.1
1	A	781	ASN	3.8
1	B	539	ILE	3.6
1	B	694	GLN	3.5
1	B	590	ILE	3.3
1	B	543	LEU	3.2
1	B	486	TYR	3.2
1	A	541	ASN	3.1
1	B	693	LEU	3.0
1	B	577	THR	2.9
1	B	528	SER	2.9
1	A	492	LEU	2.9
1	B	691	MET	2.8
1	C	476	LYS	2.8
1	C	516	SER	2.7
1	B	623	PHE	2.7
1	B	484	THR	2.7
1	B	576	PRO	2.7
1	B	538	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	698	PHE	2.6
1	A	787	TYR	2.6
1	A	520	VAL	2.6
1	A	562	LEU	2.6
1	C	520	VAL	2.5
1	B	597	SER	2.5
1	A	698	PHE	2.5
1	B	660	SER	2.5
1	C	513	ILE	2.4
1	B	540	PHE	2.4
1	A	746	LYS	2.4
1	A	760	THR	2.4
1	A	544	ASP	2.3
1	B	525	SER	2.3
1	B	589	MET	2.3
1	A	486	TYR	2.3
1	A	759	ASP	2.3
1	C	695	ASN	2.3
1	A	498	ASN	2.3
1	A	750	VAL	2.3
1	B	795	LEU	2.2
1	B	686	TYR	2.2
1	A	494	ALA	2.2
1	B	598	PHE	2.2
1	B	564	ILE	2.1
1	C	696	ASP	2.1
1	A	504	SER	2.1
1	B	565	ILE	2.1
1	B	751	LEU	2.1
1	C	477	PHE	2.1
1	B	587	PHE	2.1
1	B	606	ILE	2.1
1	A	592	LEU	2.0
1	B	581	LEU	2.0
1	B	602	ASN	2.0
1	B	692	ARG	2.0
1	B	529	PHE	2.0
1	B	671	THR	2.0
1	B	561	HIS	2.0
1	B	690	ILE	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
3	EDO	C	902	4/4	0.84	0.10	57,59,60,61	0
2	MG	C	901	1/1	0.95	0.16	34,34,34,34	0
4	CL	C	903	1/1	0.97	0.05	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.