



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 PM GMT

PDB ID : 4OJJ
Title : X-ray structure of the C-terminal domain of Pat1 (decapping activator)
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

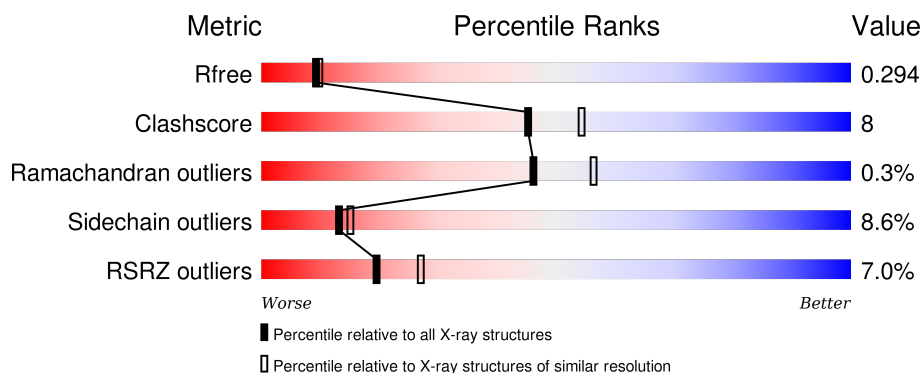
1 Overall quality at a glance

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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>13%</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: C₂H₆O₂).



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

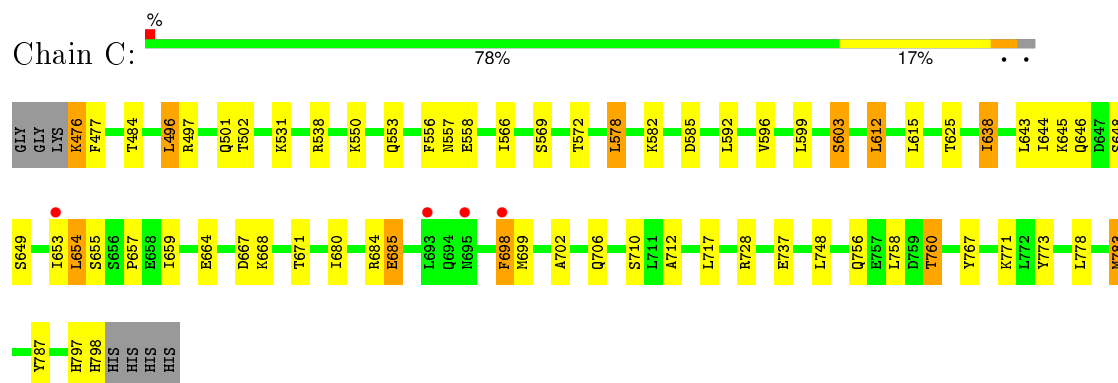
- Molecule 5 is water.

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

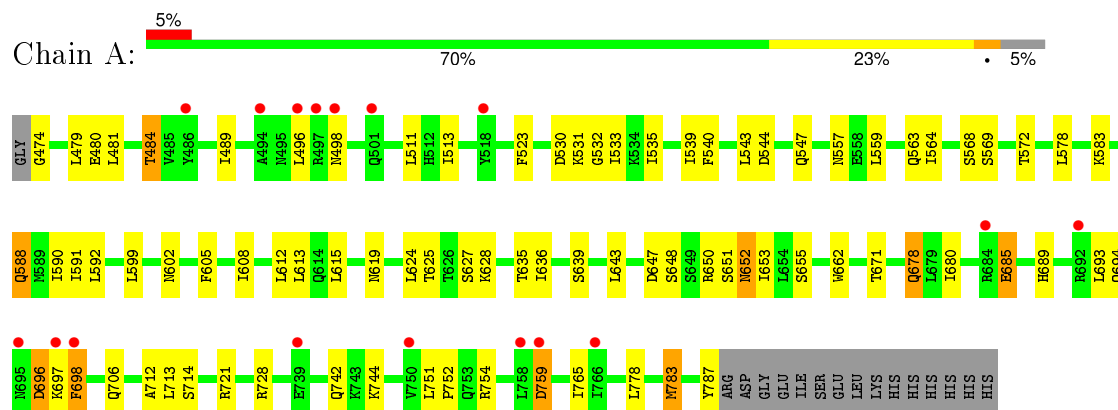
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

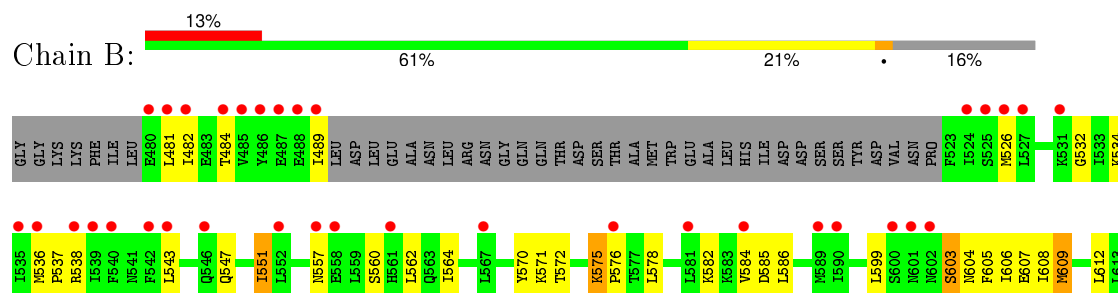
- Molecule 1: DNA topoisomerase 2-associated protein PAT1

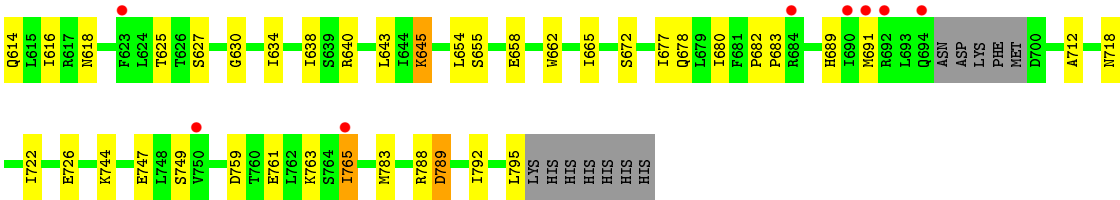


- Molecule 1: DNA topoisomerase 2-associated protein PAT1



- 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 0.229 , 0.294	Depositor DCC
R_{free} test set	2458 reflections (5.00%)	DCC
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 , 52.0	EDS
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 49175 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:578:LEU:O	1:B:582:LYS:NZ	2.25	0.56
1:B:557:ASN:OD1	1:B:614:GLN:NE2	2.38	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:B:570:TYR:CD1	1:B:683:PRO:HD3	2.42	0.54
1:A:532:GLY:O	1:A:535[A]:ILE:HG12	2.08	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: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:B:606:ILE:HA	1:B:609:MET:HG3	1.95	0.48
1:A:678:GLN:H	1:A:678:GLN:NE2	2.12	0.48
1:A:539:ILE:HG22	1:A:543:LEU:HD11	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: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

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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:B:718:ASN:ND2	5:B:910:HOH:O	2.36	0.42
1:A:685:GLU:HG3	1:A:685:GLU:H	1.56	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:C:712:ALA:HB1	1:C:783:MET:HE1	2.02	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:576:PRO:HD2	1:B:689:HIS:CD2	2.55	0.42
1:B:609:MET:CE	1:B:665:ILE:HD12	2.49	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: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:773:TYR:CE1	1:C:787:TYR:CE2	3.08	0.41
1:C:698:PHE:HZ	1:C:767:TYR:HE2	1.69	0.41
1:B:722:ILE:O	1:B:726:GLU:HG3	2.20	0.41
1:A:544:ASP:OD1	1:A:547:GLN:HG3	2.21	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 [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	313/330 (95%)	303 (97%)	9 (3%)	1 (0%)	46	56
1	B	272/330 (82%)	264 (97%)	7 (3%)	1 (0%)	39	48
1	C	321/330 (97%)	316 (98%)	4 (1%)	1 (0%)	46	56
All	All	906/990 (92%)	883 (98%)	20 (2%)	3 (0%)	46	56

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%)	10	11
1	B	265/311 (85%)	246 (93%)	19 (7%)	18	22
1	C	306/311 (98%)	279 (91%)	27 (9%)	12	14
All	All	869/933 (93%)	794 (91%)	75 (9%)	13	15

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	0.56	0	2,2,2	0.32	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	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	0.39	17 (5%) 29 38	31, 57, 85, 98	0
1	B	278/330 (84%)	0.96	43 (15%) 3 5	47, 70, 106, 114	0
1	C	323/330 (97%)	0.19	4 (1%) 81 85	28, 45, 67, 81	0
All	All	915/990 (92%)	0.49	64 (6%) 19 27	28, 56, 99, 114	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	PHE	9.3
1	B	487	GLU	7.6
1	B	539	ILE	5.9
1	B	540	PHE	5.9
1	B	481	LEU	5.8
1	B	538	ARG	4.9
1	B	543	LEU	4.9
1	B	561	HIS	4.8
1	B	527	LEU	4.6
1	A	496	LEU	4.2
1	B	485	VAL	4.1
1	B	484	THR	4.1
1	A	498	ASN	4.0
1	B	531	LYS	3.6
1	B	546	GLN	3.6
1	B	536	MET	3.6
1	B	602	ASN	3.5
1	B	765	ILE	3.5
1	B	750	VAL	3.4
1	B	482	ILE	3.3
1	B	590	ILE	3.3
1	A	750	VAL	3.3
1	A	758	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	525	SER	3.3
1	B	557	ASN	3.3
1	A	698	PHE	3.2
1	B	567	LEU	3.2
1	B	486	TYR	3.0
1	A	494	ALA	3.0
1	B	488	GLU	3.0
1	B	694	GLN	2.9
1	C	698	PHE	2.9
1	B	601	ASN	2.9
1	B	690	ILE	2.8
1	B	576	PRO	2.8
1	B	558	GLU	2.7
1	C	653	ILE	2.7
1	B	535	ILE	2.6
1	A	695	ASN	2.6
1	B	684	ARG	2.6
1	B	489	ILE	2.6
1	B	581	LEU	2.5
1	A	766	ILE	2.5
1	B	524	ILE	2.5
1	A	497	ARG	2.5
1	A	739	GLU	2.5
1	A	684	ARG	2.5
1	A	518	TYR	2.4
1	B	589	MET	2.4
1	B	692	ARG	2.4
1	B	480	GLU	2.3
1	B	600	SER	2.3
1	B	552	LEU	2.3
1	A	486	TYR	2.3
1	C	693	LEU	2.3
1	B	691	MET	2.2
1	C	695	ASN	2.2
1	A	692	ARG	2.2
1	A	759	ASP	2.1
1	B	584	VAL	2.1
1	A	697	LYS	2.1
1	A	501	GLN	2.0
1	B	526	MET	2.0
1	B	623	PHE	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	C	903	1/1	0.93	0.07	-2.24	72,72,72,72	0
3	EDO	C	902	4/4	0.86	0.19	-	57,59,60,61	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.