



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID : 4FCV
Title : Crystal structure of the C-terminal domain of ClpB
Authors : Biter, A.B.; Lee, S.; Sung, N.; Tsai, F.T.F.
Deposited on : 2012-05-25
Resolution : 3.40 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

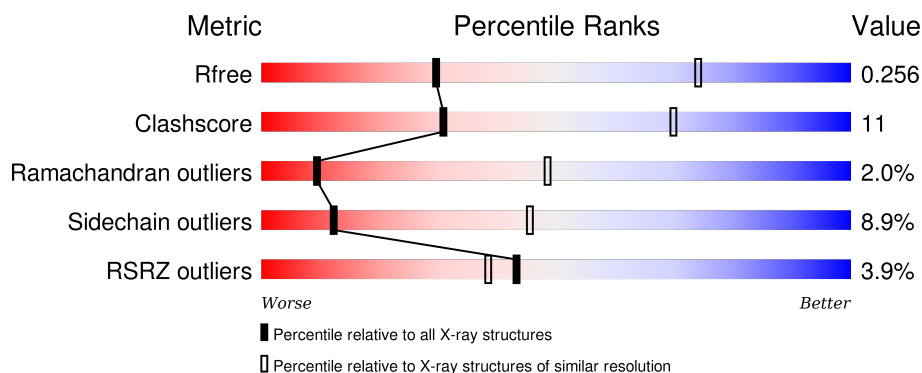
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	311	<div> <div>5%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	B	311	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>5%</div> <div>.</div> </div>
1	C	311	<div> <div>4%</div> <div>73%</div> <div>23%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7527 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 Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	Se	0	0	0
			2482	1575	449	451	7			
1	B	311	Total	C	N	O	Se	0	0	0
			2482	1575	449	451	7			
1	C	311	Total	C	N	O	Se	0	0	0
			2482	1575	449	451	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	MSE	-	EXPRESSION TAG	UNP Q9RA63
A	543	LEU	-	EXPRESSION TAG	UNP Q9RA63
A	668	ALA	GLU	ENGINEERED MUTATION	UNP Q9RA63
A	683	MSE	ILE	ENGINEERED MUTATION	UNP Q9RA63
A	706	MSE	LEU	ENGINEERED MUTATION	UNP Q9RA63
A	770	MSE	LEU	ENGINEERED MUTATION	UNP Q9RA63
B	542	MSE	-	EXPRESSION TAG	UNP Q9RA63
B	543	LEU	-	EXPRESSION TAG	UNP Q9RA63
B	668	ALA	GLU	ENGINEERED MUTATION	UNP Q9RA63
B	683	MSE	ILE	ENGINEERED MUTATION	UNP Q9RA63
B	706	MSE	LEU	ENGINEERED MUTATION	UNP Q9RA63
B	770	MSE	LEU	ENGINEERED MUTATION	UNP Q9RA63
C	542	MSE	-	EXPRESSION TAG	UNP Q9RA63
C	543	LEU	-	EXPRESSION TAG	UNP Q9RA63
C	668	ALA	GLU	ENGINEERED MUTATION	UNP Q9RA63
C	683	MSE	ILE	ENGINEERED MUTATION	UNP Q9RA63
C	706	MSE	LEU	ENGINEERED MUTATION	UNP Q9RA63
C	770	MSE	LEU	ENGINEERED MUTATION	UNP Q9RA63

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

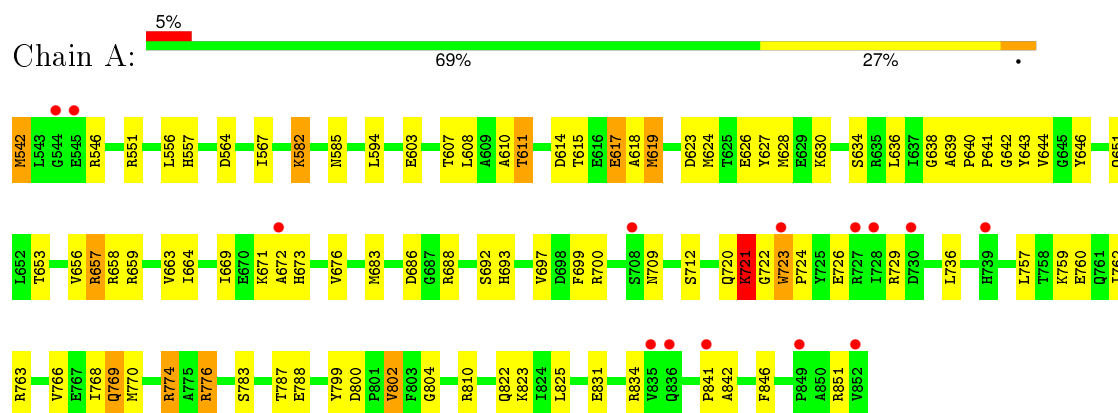


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

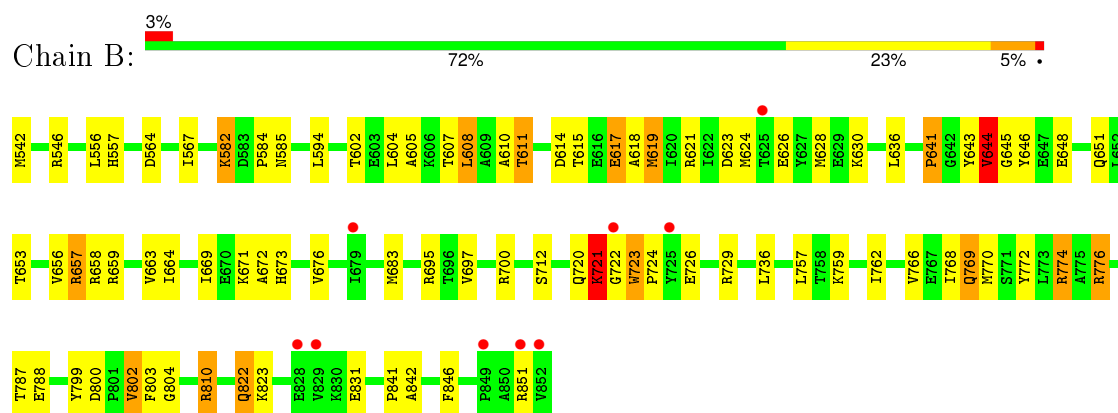
3 Residue-property plots

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.

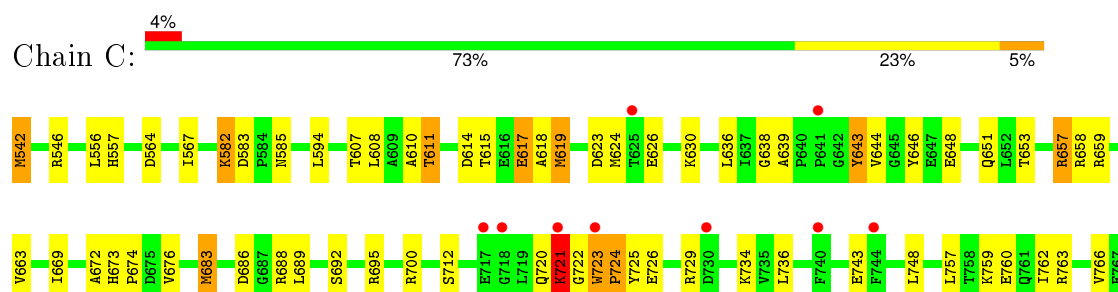
• Molecule 1: Chaperone protein ClpB

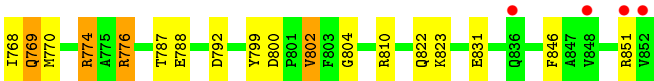


• Molecule 1: Chaperone protein ClpB



• Molecule 1: Chaperone protein ClpB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.15Å 116.81Å 68.94Å 90.00° 119.52° 90.00°	Depositor
Resolution (Å)	41.85 – 3.40 41.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.85-3.40) 99.1 (41.85-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.233 , 0.261 0.236 , 0.256	Depositor DCC
R_{free} test set	647 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.7	EDS
Estimated twinning fraction	0.049 for -h-l,k,h 0.049 for l,k,-h-l 0.040 for h,-k,-h-l 0.044 for -h-l,-k,l 0.041 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 12853 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7527	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ADP

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	0.45	1/2518 (0.0%)	0.61	1/3388 (0.0%)
1	B	0.47	1/2518 (0.0%)	0.60	0/3388
1	C	0.48	0/2518	0.60	1/3388 (0.0%)
All	All	0.47	2/7554 (0.0%)	0.60	2/10164 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	641	PRO	C-O	5.54	1.34	1.23
1	B	643	TYR	C-N	5.43	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	GLY	O-C-N	5.74	131.88	122.70
1	C	643	TYR	CG-CD2-CE2	-5.32	117.05	121.30

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	2482	0	2549	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2482	0	2549	57	0
1	C	2482	0	2549	55	0
2	A	27	0	12	3	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
All	All	7527	0	7683	166	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 11.

All (166) 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:774:ARG:HG3	1:B:774:ARG:HH11	1.43	0.83
1:A:582:LYS:HE3	1:A:582:LYS:HA	1.61	0.83
1:A:774:ARG:HH11	1:A:774:ARG:HG3	1.43	0.81
1:C:774:ARG:HH11	1:C:774:ARG:HG3	1.47	0.80
1:C:582:LYS:HE3	1:C:582:LYS:HA	1.64	0.80
1:A:653:THR:O	1:A:657:ARG:HB2	1.83	0.79
1:B:582:LYS:HA	1:B:582:LYS:HE3	1.62	0.78
1:C:653:THR:O	1:C:657:ARG:HB2	1.83	0.78
1:B:653:THR:O	1:B:657:ARG:HB2	1.85	0.76
1:B:585:ASN:HA	1:B:700:ARG:HD2	1.69	0.73
1:B:607:THR:O	1:B:611:THR:CG2	2.36	0.73
1:C:607:THR:O	1:C:611:THR:CG2	2.37	0.72
1:A:603:GLU:CG	2:A:901:ADP:H2'	2.22	0.70
1:A:825:LEU:O	1:B:546:ARG:HD3	1.92	0.70
1:C:638:GLY:O	1:C:692:SER:HB2	1.92	0.70
1:C:769:GLN:HA	1:C:769:GLN:HE21	1.58	0.69
1:C:618:ALA:HA	1:C:659:ARG:HD3	1.74	0.67
1:C:607:THR:O	1:C:611:THR:HG22	1.96	0.65
1:B:594:LEU:HD11	1:B:736:LEU:HD11	1.78	0.65
1:B:607:THR:O	1:B:611:THR:HG22	1.96	0.65
1:C:726:GLU:HG2	1:C:729:ARG:HH12	1.62	0.65
1:A:638:GLY:O	1:A:692:SER:HB2	1.97	0.65
1:B:726:GLU:HG2	1:B:729:ARG:HH12	1.60	0.64
1:A:624:MSE:HE1	1:A:676:VAL:HG11	1.79	0.64
1:A:585:ASN:HA	1:A:700:ARG:HD2	1.79	0.64
1:B:823:LYS:HE2	1:B:846:PHE:HB2	1.80	0.64
1:A:603:GLU:HG2	2:A:901:ADP:H2'	1.80	0.64
1:A:594:LEU:HD11	1:A:736:LEU:HD11	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:THR:O	1:A:611:THR:CG2	2.46	0.62
1:B:607:THR:O	1:B:611:THR:HG23	1.98	0.62
1:A:823:LYS:HE2	1:A:846:PHE:HB2	1.82	0.62
1:A:726:GLU:HG2	1:A:729:ARG:HH12	1.64	0.61
1:C:823:LYS:HE2	1:C:846:PHE:HB2	1.82	0.60
1:B:723:TRP:CD1	1:B:723:TRP:N	2.70	0.60
1:C:723:TRP:CD1	1:C:723:TRP:N	2.69	0.60
1:C:607:THR:O	1:C:611:THR:HG23	2.00	0.60
1:A:723:TRP:CD1	1:A:723:TRP:N	2.70	0.60
1:B:774:ARG:HG3	1:B:774:ARG:NH1	2.16	0.59
1:A:721:LYS:O	1:A:723:TRP:N	2.36	0.59
1:A:636:LEU:HA	1:A:651:GLN:HE22	1.69	0.58
1:A:774:ARG:NH1	1:A:774:ARG:HG3	2.17	0.58
1:C:624:MSE:CE	1:C:672:ALA:HB2	2.33	0.58
1:B:803:PHE:HZ	1:C:734:LYS:HG2	1.69	0.58
1:B:721:LYS:O	1:B:723:TRP:N	2.37	0.58
1:C:594:LEU:HD11	1:C:736:LEU:HD11	1.86	0.57
1:A:776:ARG:HH21	1:B:584:PRO:HD3	1.69	0.57
1:A:556:LEU:HD23	1:A:611:THR:HG21	1.87	0.57
1:A:769:GLN:HA	1:A:769:GLN:HE21	1.70	0.56
1:C:762:ILE:O	1:C:766:VAL:HG23	2.06	0.56
1:C:721:LYS:O	1:C:723:TRP:N	2.39	0.56
1:A:542:MSE:SE	1:A:546:ARG:HG2	2.56	0.56
1:A:825:LEU:O	1:B:546:ARG:CD	2.53	0.56
1:B:624:MSE:CE	1:B:672:ALA:HB2	2.36	0.56
1:B:757:LEU:HD12	1:B:799:TYR:HE1	1.70	0.56
1:B:621:ARG:HD2	1:C:743:GLU:OE2	2.06	0.56
1:C:624:MSE:HE1	1:C:676:VAL:HG11	1.88	0.55
1:A:607:THR:O	1:A:611:THR:HG22	2.06	0.55
1:A:757:LEU:HD12	1:A:799:TYR:HE1	1.72	0.55
1:A:607:THR:O	1:A:611:THR:HG23	2.06	0.55
1:B:624:MSE:HE1	1:B:676:VAL:HG11	1.89	0.55
1:A:766:VAL:O	1:A:770:MSE:HG2	2.06	0.55
1:A:800:ASP:OD2	1:A:802:VAL:HG22	2.07	0.55
1:C:624:MSE:HE2	1:C:672:ALA:CB	2.37	0.54
1:B:766:VAL:O	1:B:770:MSE:HG2	2.07	0.54
1:A:762:ILE:O	1:A:766:VAL:HG23	2.07	0.54
1:B:762:ILE:O	1:B:766:VAL:HG23	2.08	0.54
1:B:556:LEU:HD23	1:B:611:THR:HG21	1.88	0.54
1:C:800:ASP:OD2	1:C:802:VAL:HG22	2.09	0.53
1:C:624:MSE:HE2	1:C:672:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:GLN:HE21	1:B:769:GLN:HA	1.74	0.53
1:C:624:MSE:CE	1:C:672:ALA:CB	2.87	0.52
1:C:766:VAL:O	1:C:770:MSE:HG2	2.10	0.52
1:C:585:ASN:HA	1:C:700:ARG:HD2	1.92	0.52
1:B:624:MSE:HE2	1:B:672:ALA:HB2	1.92	0.52
1:C:639:ALA:O	1:C:646:TYR:HD2	1.93	0.52
1:C:774:ARG:NH1	1:C:774:ARG:HG3	2.19	0.52
1:B:624:MSE:HE2	1:B:672:ALA:CB	2.40	0.52
1:A:841:PRO:HD2	1:A:842:ALA:H	1.76	0.51
1:C:618:ALA:HA	1:C:659:ARG:HH11	1.76	0.51
1:B:636:LEU:HA	1:B:651:GLN:HE22	1.74	0.51
1:C:556:LEU:HD23	1:C:611:THR:HG21	1.93	0.50
1:A:634:SER:HB2	1:A:639:ALA:HA	1.93	0.50
1:A:646:TYR:CZ	1:A:693:HIS:CE1	3.00	0.50
1:B:624:MSE:CE	1:B:672:ALA:CB	2.90	0.50
1:B:800:ASP:OD2	1:B:802:VAL:HG22	2.10	0.50
1:B:803:PHE:CZ	1:C:734:LYS:HG2	2.47	0.49
1:B:557:HIS:CE1	1:B:567:ILE:HD12	2.47	0.49
1:C:757:LEU:HD12	1:C:799:TYR:HE1	1.78	0.48
1:A:628:MSE:HG2	1:A:671:LYS:O	2.13	0.48
1:A:618:ALA:HA	1:A:659:ARG:HD3	1.95	0.47
1:B:623:ASP:O	1:B:626:GLU:HG2	2.15	0.47
1:B:602:THR:O	1:B:605:ALA:HB3	2.15	0.47
1:B:618:ALA:HA	1:B:659:ARG:HD3	1.97	0.47
1:A:618:ALA:HA	1:A:659:ARG:HH11	1.80	0.47
1:A:603:GLU:HG3	2:A:901:ADP:H2'	1.96	0.47
1:A:630:LYS:HE2	1:A:673:HIS:HE2	1.79	0.46
1:A:624:MSE:CE	1:A:672:ALA:HB2	2.45	0.46
1:A:557:HIS:CE1	1:A:567:ILE:HD12	2.51	0.46
1:A:623:ASP:O	1:A:626:GLU:HG2	2.15	0.46
1:B:628:MSE:HG2	1:B:671:LYS:O	2.15	0.46
1:B:636:LEU:HD22	1:B:676:VAL:HG13	1.98	0.46
1:C:760:GLU:HA	1:C:763:ARG:HH11	1.81	0.45
1:C:619:MSE:HA	1:C:663:VAL:O	2.17	0.45
1:B:619:MSE:HA	1:B:663:VAL:O	2.17	0.45
1:C:623:ASP:O	1:C:626:GLU:HG2	2.17	0.45
1:A:776:ARG:HA	1:A:776:ARG:HD2	1.57	0.45
1:A:841:PRO:CD	1:A:842:ALA:H	2.29	0.45
1:C:557:HIS:CE1	1:C:567:ILE:HD12	2.51	0.45
1:B:787:THR:HG22	1:B:788:GLU:N	2.32	0.44
1:B:656:VAL:HG22	1:B:664:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:MSE:HG3	1:C:669:ILE:HA	1.99	0.44
1:C:776:ARG:HD2	1:C:776:ARG:HA	1.60	0.43
1:A:624:MSE:HG3	1:A:669:ILE:HA	2.00	0.43
1:B:610:ALA:O	1:B:614:ASP:HA	2.18	0.43
1:C:610:ALA:O	1:C:614:ASP:HA	2.17	0.43
1:C:615:THR:OG1	1:C:617:GLU:HG2	2.18	0.43
1:A:760:GLU:HA	1:A:763:ARG:HH11	1.84	0.43
1:B:776:ARG:HD2	1:B:776:ARG:HA	1.60	0.43
1:A:624:MSE:HE2	1:A:672:ALA:CB	2.47	0.43
1:B:822:GLN:HB2	1:B:822:GLN:HE21	1.61	0.43
1:C:787:THR:HG22	1:C:788:GLU:N	2.34	0.43
1:C:800:ASP:O	1:C:804:GLY:N	2.52	0.43
1:A:640:PRO:O	1:A:643:TYR:HB2	2.18	0.43
1:B:641:PRO:HA	1:B:646:TYR:CZ	2.54	0.43
1:B:800:ASP:O	1:B:804:GLY:N	2.52	0.43
1:A:624:MSE:CE	1:A:672:ALA:CB	2.96	0.42
1:B:841:PRO:HD2	1:B:842:ALA:H	1.84	0.42
1:C:724:PRO:HB2	1:C:725:TYR:H	1.65	0.42
1:A:551:ARG:HE	1:A:551:ARG:HB3	1.65	0.42
1:B:615:THR:OG1	1:B:617:GLU:HG2	2.19	0.42
1:C:542:MSE:SE	1:C:546:ARG:HG2	2.69	0.42
1:B:615:THR:HG23	1:B:618:ALA:HB2	2.01	0.42
1:A:774:ARG:HH11	1:A:774:ARG:CG	2.23	0.42
1:B:624:MSE:HG3	1:B:669:ILE:HA	2.00	0.42
1:C:689:LEU:HA	1:C:689:LEU:HD12	1.87	0.42
1:B:644:VAL:HG23	1:B:645:GLY:H	1.84	0.42
1:B:810:ARG:NH2	1:C:748:LEU:O	2.53	0.42
1:C:636:LEU:HD22	1:C:676:VAL:HG13	2.01	0.42
1:B:657:ARG:NH2	1:B:695:ARG:HD2	2.35	0.41
1:A:686:ASP:C	1:A:688:ARG:N	2.74	0.41
1:A:615:THR:OG1	1:A:617:GLU:HG2	2.20	0.41
1:A:653:THR:HB	1:A:697:VAL:HG21	2.02	0.41
1:A:783:SER:HB2	1:A:834:ARG:HA	2.02	0.41
1:C:763:ARG:HD2	1:C:792:ASP:OD2	2.20	0.41
1:B:653:THR:HB	1:B:697:VAL:HG21	2.03	0.41
1:C:636:LEU:HA	1:C:651:GLN:HE22	1.86	0.41
1:A:639:ALA:O	1:A:646:TYR:HD2	2.04	0.41
1:A:656:VAL:HG22	1:A:664:ILE:HD11	2.03	0.41
1:A:619:MSE:HA	1:A:663:VAL:O	2.21	0.41
1:C:630:LYS:HE2	1:C:673:HIS:HE2	1.85	0.41
1:A:610:ALA:O	1:A:614:ASP:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:ARG:NH2	1:C:695:ARG:HD2	2.35	0.41
1:A:787:THR:HG22	1:A:788:GLU:N	2.36	0.41
1:B:630:LYS:HE2	1:B:673:HIS:HE2	1.84	0.41
1:B:772:TYR:OH	1:C:583:ASP:HA	2.21	0.41
1:A:800:ASP:O	1:A:804:GLY:N	2.54	0.41
1:C:695:ARG:HE	1:C:695:ARG:HB2	1.74	0.40
1:A:624:MSE:HE2	1:A:672:ALA:HB2	2.02	0.40
1:B:618:ALA:HA	1:B:659:ARG:HH11	1.85	0.40
1:C:686:ASP:C	1:C:688:ARG:N	2.74	0.40
1:C:683:MSE:HB2	1:C:689:LEU:HD13	2.02	0.40
1:A:626:GLU:HG3	1:A:627:TYR:CE1	2.57	0.40
1:C:673:HIS:HA	1:C:674:PRO:HD3	1.93	0.40
1:B:604:LEU:O	1:B:608:LEU:HB2	2.22	0.40
1:A:709:ASN:OD1	1:A:709:ASN:N	2.52	0.40
1:A:656:VAL:HG21	1:A:699:PHE:CE2	2.56	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	309/311 (99%)	281 (91%)	22 (7%)	6 (2%)	10	49
1	B	309/311 (99%)	280 (91%)	22 (7%)	7 (2%)	8	45
1	C	309/311 (99%)	281 (91%)	22 (7%)	6 (2%)	10	49
All	All	927/933 (99%)	842 (91%)	66 (7%)	19 (2%)	9	48

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	721	LYS
1	B	644	VAL

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Mol	Chain	Res	Type
1	B	721	LYS
1	C	644	VAL
1	C	721	LYS
1	A	720	GLN
1	A	722	GLY
1	B	641	PRO
1	B	720	GLN
1	B	722	GLY
1	C	720	GLN
1	C	722	GLY
1	A	724	PRO
1	B	724	PRO
1	C	724	PRO
1	A	712	SER
1	B	712	SER
1	C	712	SER
1	A	644	VAL

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	262/255 (103%)	240 (92%)	22 (8%)	14	49
1	B	262/255 (103%)	238 (91%)	24 (9%)	11	43
1	C	262/255 (103%)	238 (91%)	24 (9%)	11	43
All	All	786/765 (103%)	716 (91%)	70 (9%)	12	45

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	MSE
1	A	564	ASP
1	A	582	LYS
1	A	608	LEU
1	A	611	THR

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Mol	Chain	Res	Type
1	A	617	GLU
1	A	619	MSE
1	A	657	ARG
1	A	658	ARG
1	A	683	MSE
1	A	721	LYS
1	A	723	TRP
1	A	759	LYS
1	A	768	ILE
1	A	769	GLN
1	A	774	ARG
1	A	776	ARG
1	A	802	VAL
1	A	810	ARG
1	A	822	GLN
1	A	831	GLU
1	A	851	ARG
1	B	542	MSE
1	B	564	ASP
1	B	582	LYS
1	B	608	LEU
1	B	611	THR
1	B	617	GLU
1	B	619	MSE
1	B	644	VAL
1	B	648	GLU
1	B	657	ARG
1	B	658	ARG
1	B	683	MSE
1	B	721	LYS
1	B	723	TRP
1	B	759	LYS
1	B	768	ILE
1	B	769	GLN
1	B	774	ARG
1	B	776	ARG
1	B	802	VAL
1	B	810	ARG
1	B	822	GLN
1	B	831	GLU
1	B	851	ARG
1	C	542	MSE

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Mol	Chain	Res	Type
1	C	564	ASP
1	C	582	LYS
1	C	608	LEU
1	C	611	THR
1	C	617	GLU
1	C	619	MSE
1	C	643	TYR
1	C	648	GLU
1	C	657	ARG
1	C	658	ARG
1	C	683	MSE
1	C	721	LYS
1	C	723	TRP
1	C	759	LYS
1	C	768	ILE
1	C	769	GLN
1	C	774	ARG
1	C	776	ARG
1	C	802	VAL
1	C	810	ARG
1	C	822	GLN
1	C	831	GLU
1	C	851	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	746	ASN
1	A	769	GLN
1	A	822	GLN
1	B	651	GLN
1	B	746	ASN
1	B	769	GLN
1	B	822	GLN
1	C	651	GLN
1	C	769	GLN
1	C	822	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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$
2	ADP	A	901	-	22,29,29	1.09	2 (9%)	27,45,45	2.08	5 (18%)
2	ADP	B	901	-	22,29,29	1.11	2 (9%)	27,45,45	2.05	5 (18%)
2	ADP	C	901	-	22,29,29	1.04	1 (4%)	27,45,45	2.06	5 (18%)

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
2	ADP	A	901	-	-	0/12/32/32	0/3/3/3
2	ADP	B	901	-	-	0/12/32/32	0/3/3/3
2	ADP	C	901	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ADP	O4'-C1'	2.16	1.43	1.41
2	A	901	ADP	PB-O3B	2.17	1.62	1.54
2	A	901	ADP	C5-C4	2.77	1.46	1.40
2	C	901	ADP	C5-C4	2.96	1.47	1.40
2	B	901	ADP	C5-C4	3.15	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ADP	N3-C2-N1	-7.34	123.27	128.89
2	A	901	ADP	N3-C2-N1	-7.25	123.34	128.89
2	C	901	ADP	N3-C2-N1	-6.49	123.92	128.89
2	C	901	ADP	PA-O3A-PB	-4.65	117.06	132.67
2	A	901	ADP	PA-O3A-PB	-4.25	118.42	132.67
2	B	901	ADP	PA-O3A-PB	-4.14	118.77	132.67
2	A	901	ADP	C2'-C1'-N9	-3.35	109.17	114.29
2	C	901	ADP	C2'-C1'-N9	-3.01	109.69	114.29
2	A	901	ADP	C4-C5-N7	-2.94	106.78	109.48
2	B	901	ADP	C4-C5-N7	-2.39	107.28	109.48
2	C	901	ADP	C4-C5-N7	-2.05	107.59	109.48
2	B	901	ADP	C4'-O4'-C1'	2.08	112.01	109.72
2	A	901	ADP	O2B-PB-O1B	3.00	120.23	110.58
2	C	901	ADP	O2B-PB-O1B	3.12	120.62	110.58
2	B	901	ADP	O2B-PB-O1B	3.33	121.29	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ADP	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	304/311 (97%)	0.23	14 (4%) 36 32	69, 105, 172, 193	0
1	B	304/311 (97%)	0.20	9 (2%) 54 49	58, 97, 155, 177	0
1	C	304/311 (97%)	0.34	13 (4%) 39 34	62, 102, 169, 211	0
All	All	912/933 (97%)	0.26	36 (3%) 43 38	58, 102, 167, 211	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	851	ARG	4.7
1	B	852	VAL	4.7
1	C	852	VAL	4.4
1	C	717	GLU	4.0
1	A	672	ALA	3.5
1	B	829	VAL	3.5
1	A	723	TRP	3.4
1	A	852	VAL	3.3
1	B	828	GLU	3.2
1	B	679	ILE	3.1
1	B	722	GLY	2.8
1	C	740	PHE	2.8
1	A	849	PRO	2.8
1	B	849	PRO	2.7
1	B	725	TYR	2.6
1	C	721	LYS	2.5
1	C	718	GLY	2.4
1	C	730	ASP	2.3
1	A	544	GLY	2.3
1	A	728	ILE	2.3
1	C	744	PHE	2.3
1	A	730	ASP	2.3
1	A	545	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	708	SER	2.3
1	A	739	HIS	2.2
1	C	851	ARG	2.2
1	C	723	TRP	2.2
1	A	841	PRO	2.2
1	C	848	VAL	2.2
1	C	836	GLN	2.1
1	B	625	THR	2.1
1	C	625	THR	2.1
1	A	727	ARG	2.1
1	C	641	PRO	2.1
1	A	836	GLN	2.1
1	A	835	VAL	2.1

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
2	ADP	B	901	27/27	0.94	0.20	-0.38	63,66,76,76	0
2	ADP	A	901	27/27	0.94	0.17	-0.95	66,73,92,93	0
2	ADP	C	901	27/27	0.95	0.16	-1.44	69,75,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.