WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 10:48 PM EST

PDB ID	:	3UKV
Title	:	Structure of the C-linker/CNBHD of zELK channels in P 1 21 1 space group, crystallized in the presence of cAMP
Authors	:	Brelidze, T.I.
Deposited on	:	2011-11-09
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

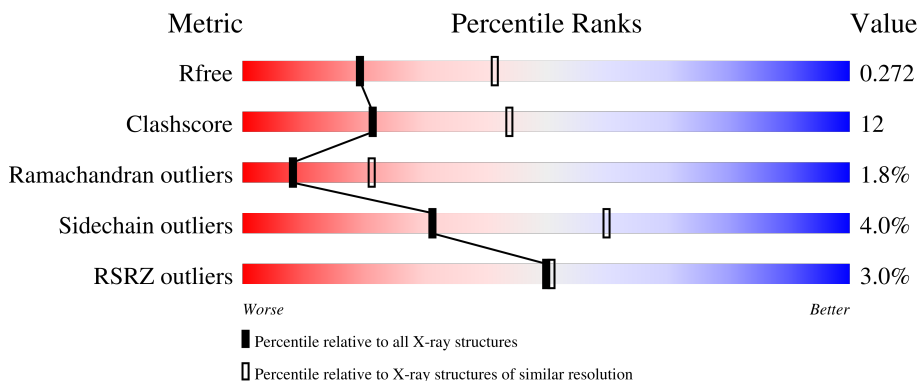|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		12
Ramachandran outliers		1.8%
Sidechain outliers		4.0%
RSRZ outliers		3.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	212	70% · 21% · 8%
1	B	212	%· 73% · 17% · 8%
1	C	212	2% · 66% · 24% · 9%
1	D	212	6% · 38% · 16% · 44%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5306 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 Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	196	Total	C	N	O	S	0	0	0
			1495	958	250	279	8			
1	A	195	Total	C	N	O	S	0	0	0
			1490	951	251	280	8			
1	C	193	Total	C	N	O	S	0	0	0
			1444	925	242	269	8			
1	D	119	Total	C	N	O	S	0	0	0
			832	532	143	151	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	539	GLY	-	expression tag	UNP A8WHX9
B	540	ALA	-	expression tag	UNP A8WHX9
B	541	MET	-	expression tag	UNP A8WHX9
B	542	ASP	-	expression tag	UNP A8WHX9
A	539	GLY	-	expression tag	UNP A8WHX9
A	540	ALA	-	expression tag	UNP A8WHX9
A	541	MET	-	expression tag	UNP A8WHX9
A	542	ASP	-	expression tag	UNP A8WHX9
C	539	GLY	-	expression tag	UNP A8WHX9
C	540	ALA	-	expression tag	UNP A8WHX9
C	541	MET	-	expression tag	UNP A8WHX9
C	542	ASP	-	expression tag	UNP A8WHX9
D	539	GLY	-	expression tag	UNP A8WHX9
D	540	ALA	-	expression tag	UNP A8WHX9
D	541	MET	-	expression tag	UNP A8WHX9
D	542	ASP	-	expression tag	UNP A8WHX9

- Molecule 2 is water.

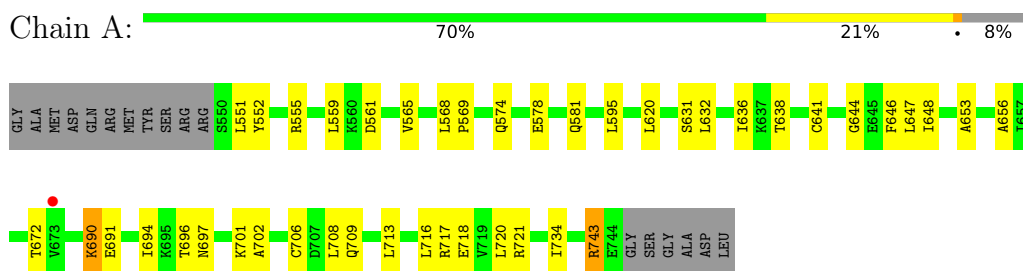| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	17	Total 17	O 17	0	0
2	A	10	Total 10	O 10	0	0
2	C	12	Total 12	O 12	0	0
2	D	6	Total 6	O 6	0	0

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: Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family
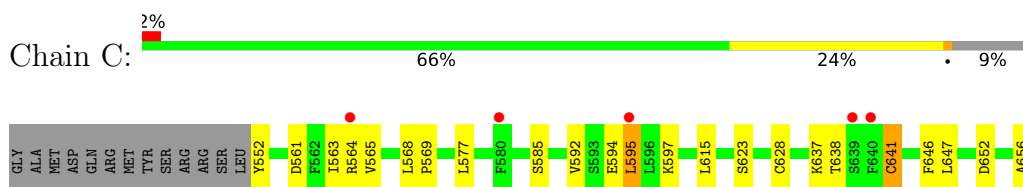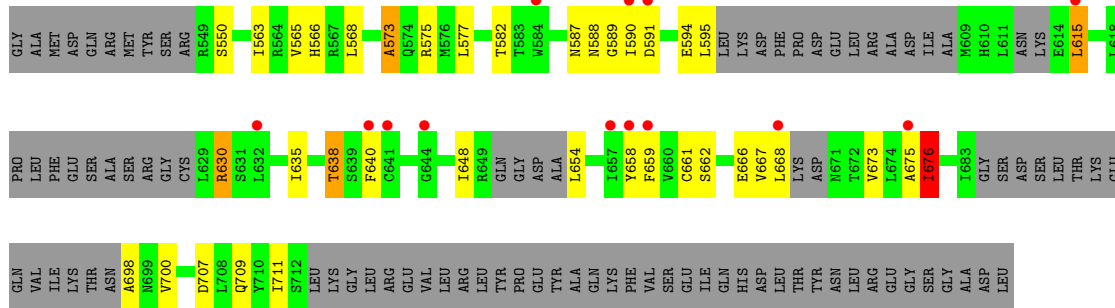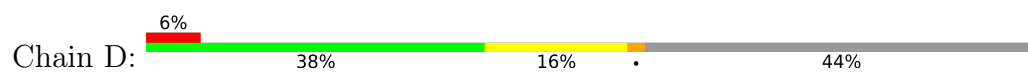

• Molecule 1: Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family

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Chain D:
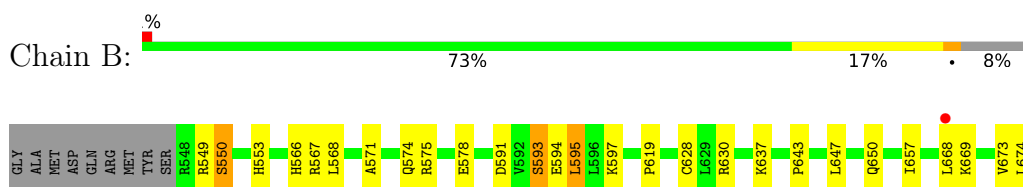
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.33Å 106.42Å 77.52Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	48.76 – 2.70 48.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.76-2.70) 95.3 (48.76-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.215 , 0.277 0.211 , 0.272	Depositor DCC
R_{free} test set	1224 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5306	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.50	0/1514	0.64	0/2055
1	B	0.48	0/1520	0.66	0/2064
1	C	0.44	0/1468	0.61	0/1998
1	D	0.37	0/841	0.56	0/1139
All	All	0.46	0/5343	0.62	0/7256

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1490	0	1456	33	0
1	B	1495	0	1454	27	0
1	C	1444	0	1380	38	0
1	D	832	0	708	27	0
2	A	10	0	0	0	0
2	B	17	0	0	1	0
2	C	12	0	0	4	0
2	D	6	0	0	4	0
All	All	5306	0	4998	123	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 12.

All (123) 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:595:LEU:H	1:C:595:LEU:HD23	1.36	0.89
1:D:615:LEU:HD12	1:D:659:PHE:HB3	1.55	0.88
1:A:561:ASP:O	1:A:565:VAL:HG12	1.80	0.82
1:B:735:GLN:HB2	2:B:40:HOH:O	1.82	0.79
1:A:718:GLU:HG3	1:A:721:ARG:HH21	1.47	0.79
1:D:654:LEU:N	2:D:29:HOH:O	2.16	0.78
1:B:594:GLU:HG2	1:B:597:LYS:HB2	1.69	0.74
1:A:690:LYS:CB	1:A:691:GLU:HA	2.18	0.73
1:C:721:ARG:NH1	1:C:722:LEU:HD11	2.05	0.71
1:C:595:LEU:H	1:C:595:LEU:CD2	2.02	0.71
1:B:619:PRO:HD2	1:B:737:ASP:OD1	1.91	0.71
1:C:735:GLN:HB3	2:C:24:HOH:O	1.91	0.69
1:B:550:SER:OG	1:B:553:HIS:HD2	1.76	0.69
1:B:595:LEU:HD22	1:A:559:LEU:HD13	1.75	0.69
1:D:630:ARG:HG2	1:D:630:ARG:O	1.91	0.69
1:D:662:SER:OG	1:D:707:ASP:HB2	1.93	0.67
1:C:646:PHE:CZ	1:C:701:LYS:HD2	2.30	0.66
1:C:736:HIS:CE1	2:C:24:HOH:O	2.49	0.65
1:B:647:LEU:HD13	1:B:708:LEU:CD1	2.26	0.65
1:D:675:ALA:O	1:D:676:ILE:HG12	1.95	0.65
1:C:652:ASP:O	1:C:696:THR:HG23	1.99	0.62
1:B:647:LEU:HD13	1:B:708:LEU:HD13	1.81	0.62
1:A:661:CYS:SG	1:A:709:GLN:HG3	2.40	0.62
1:A:718:GLU:CG	1:A:721:ARG:HH21	2.11	0.62
1:C:552:TYR:N	2:C:41:HOH:O	2.31	0.62
1:A:646:PHE:CZ	1:A:701:LYS:HD2	2.35	0.61
1:D:698:ALA:N	2:D:32:HOH:O	2.34	0.60
1:D:615:LEU:HD12	1:D:659:PHE:CB	2.30	0.60
1:A:552:TYR:OH	1:A:581:GLN:HB3	2.02	0.60
1:A:697:ASN:HB3	1:A:743:ARG:O	2.01	0.60
1:A:574:GLN:O	1:A:578:GLU:HG3	2.03	0.59
1:B:628:CYS:HA	1:B:723:TYR:CE2	2.39	0.58
1:C:656:ALA:HB1	1:C:711:ILE:O	2.03	0.58
1:B:574:GLN:OE1	1:B:578:GLU:HG3	2.04	0.58
1:C:647:LEU:CD1	1:C:708:LEU:HD13	2.34	0.58
1:C:718:GLU:O	1:C:722:LEU:HD13	2.05	0.57
1:D:588:ASN:N	1:D:589:GLY:CA	2.67	0.57
1:C:561:ASP:O	1:C:565:VAL:HG13	2.05	0.57
1:B:690:LYS:CB	1:B:691:GLU:HA	2.35	0.57
1:B:595:LEU:HD12	1:B:595:LEU:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:ARG:HH11	1:C:743:ARG:HG3	1.70	0.56
1:A:697:ASN:ND2	1:A:743:ARG:O	2.38	0.56
1:B:571:ALA:O	1:B:575:ARG:HG3	2.07	0.55
1:B:650:GLN:HB2	1:B:699:ASN:ND2	2.22	0.55
1:A:647:LEU:HG	1:A:648:ILE:HD12	1.89	0.54
1:D:587:ASN:C	1:D:589:GLY:HA3	2.27	0.54
1:A:653:ALA:HA	1:A:694:ILE:O	2.07	0.54
1:C:686:ASP:O	2:C:45:HOH:O	2.18	0.54
1:A:718:GLU:HG3	1:A:721:ARG:NH2	2.20	0.54
1:C:592:VAL:O	1:C:592:VAL:HG22	2.08	0.53
1:B:591:ASP:O	1:B:637:LYS:HE3	2.08	0.53
1:C:722:LEU:HD12	1:C:722:LEU:N	2.23	0.53
1:B:566:HIS:O	1:B:567:ARG:C	2.46	0.53
1:C:641:CYS:O	1:C:705:TYR:HA	2.08	0.53
1:C:721:ARG:HH11	1:C:722:LEU:HD11	1.73	0.53
1:B:647:LEU:CD1	1:B:708:LEU:HD13	2.38	0.53
1:C:722:LEU:C	1:C:724:PRO:HD3	2.29	0.52
1:C:623:SER:OG	1:C:729:LYS:HD2	2.09	0.52
1:D:594:GLU:O	1:D:595:LEU:C	2.48	0.52
1:D:661:CYS:HB2	1:D:707:ASP:O	2.10	0.52
1:D:638:THR:HG22	1:D:709:GLN:HG2	1.92	0.51
1:A:691:GLU:CB	1:A:717:ARG:NE	2.74	0.51
1:D:587:ASN:HB2	1:D:658:TYR:OH	2.11	0.51
1:B:713:LEU:O	1:B:717:ARG:HG3	2.11	0.50
1:D:590:ILE:HG23	2:D:36:HOH:O	2.11	0.50
1:C:637:LYS:HB2	1:C:710:TYR:CZ	2.47	0.50
1:C:743:ARG:HG3	1:C:743:ARG:NH1	2.24	0.50
1:A:551:LEU:O	1:A:555:ARG:HB2	2.11	0.49
1:A:713:LEU:O	1:A:717:ARG:HG3	2.12	0.49
1:A:646:PHE:CE2	1:A:701:LYS:HD2	2.48	0.48
1:D:648:ILE:HB	1:D:700:VAL:HB	1.95	0.48
1:B:566:HIS:O	1:B:568:LEU:HD23	2.13	0.48
1:C:563:ILE:HG23	1:C:568:LEU:HB2	1.96	0.47
1:B:681:ASP:CG	1:B:739:THR:HG21	2.35	0.47
1:A:656:ALA:HB3	1:A:658:TYR:CZ	2.50	0.47
1:D:666:GLU:OE1	1:D:668:LEU:HD21	2.15	0.47
1:C:691:GLU:HA	1:C:717:ARG:CZ	2.44	0.47
1:B:595:LEU:HD12	1:B:595:LEU:N	2.30	0.46
1:C:722:LEU:N	1:C:722:LEU:CD1	2.78	0.46
1:D:711:ILE:O	2:D:30:HOH:O	2.21	0.46
1:B:669:LYS:CB	1:B:674:LEU:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ILE:HG21	1:A:696:THR:HG21	1.96	0.46
1:A:641:CYS:HB2	1:A:706:CYS:HB2	1.98	0.46
1:D:565:VAL:HG12	1:D:566:HIS:CE1	2.50	0.46
1:C:637:LYS:HB2	1:C:710:TYR:CE1	2.51	0.45
1:A:644:GLY:N	1:A:702:ALA:O	2.45	0.45
1:A:718:GLU:CG	1:A:721:ARG:NH2	2.79	0.45
1:D:573:ALA:O	1:D:577:LEU:HG	2.17	0.45
1:B:668:LEU:HD23	1:B:673:VAL:HA	1.98	0.45
1:A:647:LEU:HG	1:A:648:ILE:CD1	2.46	0.45
1:A:647:LEU:HD13	1:A:708:LEU:CD1	2.46	0.45
1:C:730:PHE:CD2	1:C:730:PHE:C	2.90	0.45
1:A:620:LEU:HD13	1:A:734:ILE:HA	1.98	0.44
1:B:657:ILE:HD13	1:B:716:LEU:HD22	1.99	0.44
1:A:668:LEU:HA	1:A:672:THR:O	2.17	0.44
1:B:628:CYS:HB2	1:B:723:TYR:CG	2.52	0.44
1:D:550:SER:HB3	1:D:640:PHE:CZ	2.53	0.44
1:A:644:GLY:O	1:A:701:LYS:HE2	2.17	0.44
1:C:678:GLY:O	1:C:679:LYS:C	2.56	0.44
1:D:565:VAL:HG12	1:D:566:HIS:ND1	2.33	0.44
1:D:588:ASN:N	1:D:589:GLY:HA2	2.33	0.44
1:C:577:LEU:HD23	1:C:577:LEU:HA	1.89	0.43
1:C:594:GLU:O	1:C:597:LYS:HB2	2.18	0.43
1:A:647:LEU:CG	1:A:648:ILE:HD12	2.48	0.43
1:D:563:ILE:HG23	1:D:568:LEU:HB2	2.01	0.43
1:C:628:CYS:HA	1:C:723:TYR:CE2	2.54	0.42
1:C:568:LEU:HA	1:C:569:PRO:HD2	1.81	0.42
1:B:703:LEU:HD23	1:B:703:LEU:HA	1.91	0.42
1:C:563:ILE:HA	1:C:568:LEU:HG	2.01	0.42
1:C:585:SER:HA	1:C:646:PHE:O	2.19	0.41
1:C:615:LEU:HD23	1:C:615:LEU:O	2.19	0.41
1:C:668:LEU:HD21	1:C:673:VAL:HG22	2.03	0.41
1:C:715:GLY:O	1:C:719:VAL:HG23	2.19	0.41
1:C:723:TYR:N	1:C:724:PRO:HD3	2.35	0.41
1:B:643:PRO:HB3	1:B:703:LEU:O	2.21	0.41
1:A:716:LEU:O	1:A:720:LEU:HG	2.20	0.41
1:D:588:ASN:N	1:D:589:GLY:HA3	2.36	0.41
1:D:661:CYS:HB2	1:D:707:ASP:HB3	2.03	0.41
1:D:575:ARG:H	1:D:575:ARG:HG3	1.75	0.41
1:B:595:LEU:HD22	1:A:559:LEU:CD1	2.48	0.41
1:A:632:LEU:O	1:A:636:ILE:HG13	2.21	0.41
1:D:667:VAL:HG12	1:D:667:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:HA	1:A:569:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	193/212 (91%)	181 (94%)	10 (5%)	2 (1%)	15	37
1	B	194/212 (92%)	175 (90%)	15 (8%)	4 (2%)	7	18
1	C	191/212 (90%)	173 (91%)	17 (9%)	1 (0%)	29	54
1	D	105/212 (50%)	83 (79%)	17 (16%)	5 (5%)	2	4
All	All	683/848 (80%)	612 (90%)	59 (9%)	12 (2%)	8	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	549	ARG
1	B	690	LYS
1	A	743	ARG
1	B	593	SER
1	A	690	LYS
1	C	692	GLN
1	D	573	ALA
1	D	630	ARG
1	D	582	THR
1	B	738	LEU
1	D	676	ILE
1	D	673	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	155/186 (83%)	152 (98%)	3 (2%)	57	82
1	B	154/186 (83%)	150 (97%)	4 (3%)	46	75
1	C	143/186 (77%)	134 (94%)	9 (6%)	18	40
1	D	68/186 (37%)	63 (93%)	5 (7%)	13	32
All	All	520/744 (70%)	499 (96%)	21 (4%)	31	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	550	SER
1	B	593	SER
1	B	595	LEU
1	B	630	ARG
1	A	595	LEU
1	A	631	SER
1	A	638	THR
1	C	564	ARG
1	C	595	LEU
1	C	638	THR
1	C	641	CYS
1	C	685	SER
1	C	708	LEU
1	C	712	SER
1	C	731	VAL
1	C	738	LEU
1	D	591	ASP
1	D	615	LEU
1	D	635	ILE
1	D	638	THR
1	D	676	ILE

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

Mol	Chain	Res	Type
1	B	553	HIS
1	A	553	HIS
1	C	650	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	195/212 (91%)	-0.07	1 (0%)	91	92	35, 56, 86, 138	0
1	B	196/212 (92%)	-0.08	2 (1%)	82	83	33, 55, 84, 143	0
1	C	193/212 (91%)	-0.02	5 (2%)	56	57	34, 61, 115, 163	0
1	D	119/212 (56%)	0.56	13 (10%)	5	4	52, 84, 129, 168	0
All	All	703/848 (82%)	0.05	21 (2%)	50	51	33, 60, 113, 168	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	640	PHE	4.4
1	D	657	ILE	4.0
1	D	658	TYR	3.8
1	D	668	LEU	3.3
1	B	668	LEU	3.2
1	D	675	ALA	3.0
1	D	659	PHE	2.9
1	D	641	CYS	2.9
1	D	590	ILE	2.8
1	C	640	PHE	2.7
1	D	615	LEU	2.5
1	D	632	LEU	2.4
1	A	673	VAL	2.4
1	C	564	ARG	2.3
1	B	688	LEU	2.2
1	D	584	TRP	2.2
1	C	580	PHE	2.2
1	D	644	GLY	2.1
1	C	639	SER	2.1
1	C	595	LEU	2.1
1	D	591	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.