



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:22 PM UTC

PDB ID : 3UKV / pdb_00003ukv
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)

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
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

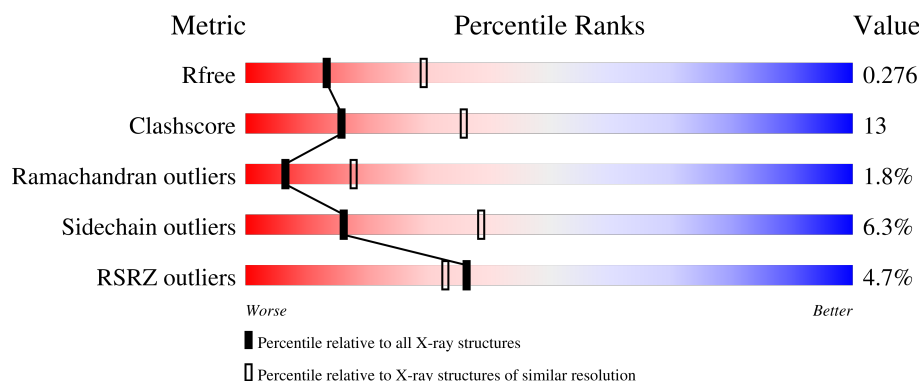
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	212	0% 66% 25% 8%
1	B	212	0% 68% 22% 8%
1	C	212	4% 64% 24% 9%
1	D	212	9% 36% 17% 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

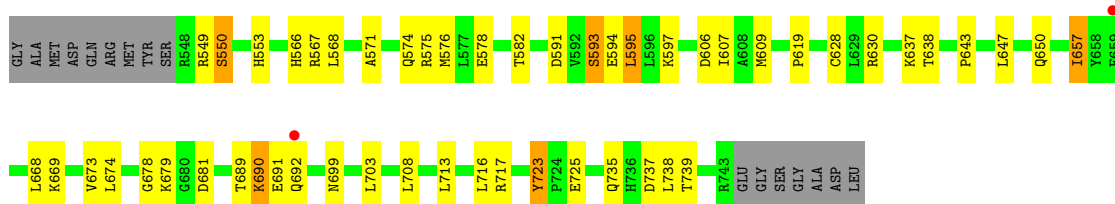
- Molecule 2 is water.

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

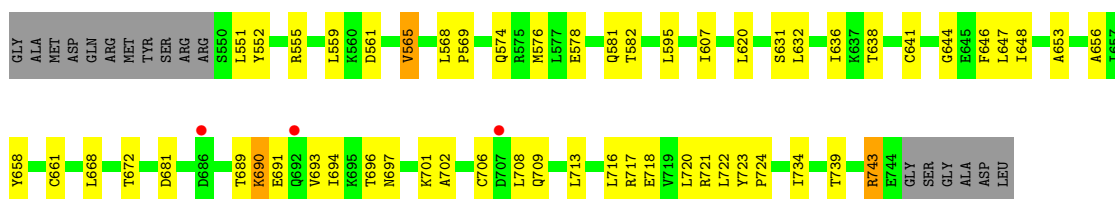
3 Residue-property plots

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.

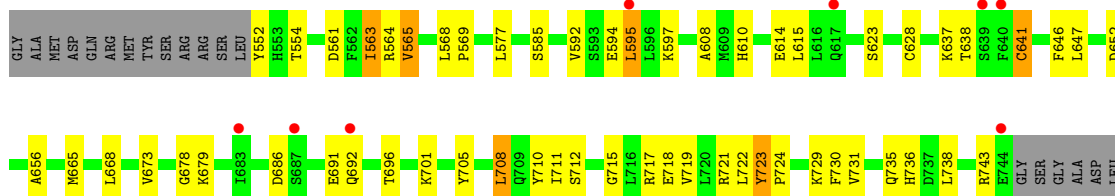
- Molecule 1: Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family



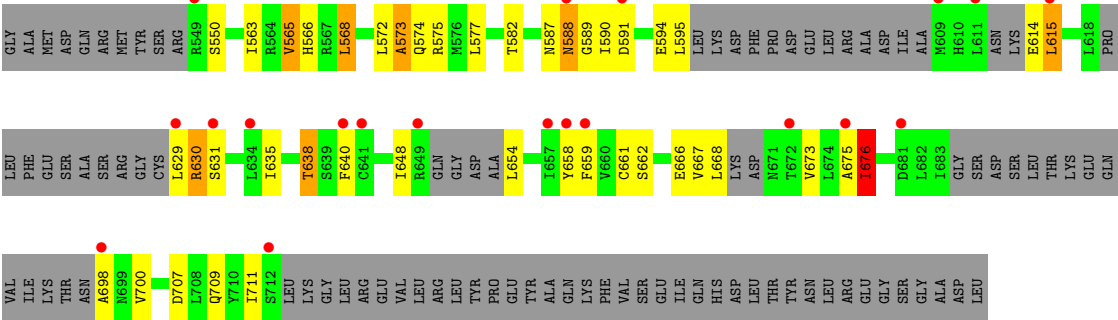
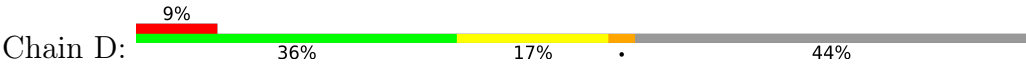
- Molecule 1: Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family



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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
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.215 , 0.277 0.216 , 0.276	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)	0.33 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

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	0.64	0/1514	0.92	2/2055 (0.1%)
1	B	0.62	0/1520	0.96	4/2064 (0.2%)
1	C	0.57	0/1468	0.95	2/1998 (0.1%)
1	D	0.51	0/841	0.89	3/1139 (0.3%)
All	All	0.60	0/5343	0.94	11/7256 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	TYR	CA-C-N	9.40	129.48	119.05
1	C	723	TYR	C-N-CA	9.40	129.48	119.05
1	A	723	TYR	CA-C-N	8.11	128.06	119.05
1	A	723	TYR	C-N-CA	8.11	128.06	119.05
1	D	568	LEU	CA-C-N	6.42	126.76	119.83
1	D	568	LEU	C-N-CA	6.42	126.76	119.83
1	B	723	TYR	CA-C-N	6.29	125.85	119.19
1	B	723	TYR	C-N-CA	6.29	125.85	119.19
1	B	692	GLN	CA-C-O	5.83	121.32	117.94
1	B	692	GLN	CB-CA-C	-5.64	108.95	117.07
1	D	588	ASN	N-CA-C	5.43	119.42	112.26

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	37	0
1	B	1495	0	1454	32	0
1	C	1444	0	1380	41	0
1	D	832	0	708	30	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	136	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 13.

All (136) 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:606:ASP:HA	1:B:609:MET:HE3	1.68	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:576:MET:HE3	1:A:607:ILE:HD13	1.82	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:D:587:ASN:C	1:D:589:GLY:HA3	2.27	0.58
1:B:566:HIS:O	1:B:567:ARG:C	2.46	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:C:722:LEU:C	1:C:724:PRO:HD3	2.29	0.57
1:D:594:GLU:O	1:D:595:LEU:C	2.48	0.56
1:B:595:LEU:HD12	1:B:595:LEU:H	1.71	0.56
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: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: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:B:681:ASP:CG	1:B:739:THR:HG21	2.35	0.52
1:C:623:SER:OG	1:C:729:LYS:HD2	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:730:PHE:CD2	1:C:730:PHE:C	2.90	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:C:678:GLY:O	1:C:679:LYS:C	2.56	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: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
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:C:647:LEU:HB2	1:C:665:MET:HE1	1.98	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: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:A:722:LEU:C	1:A:724:PRO:HD3	2.42	0.44
1:D:565:VAL:HG12	1:D:566:HIS:ND1	2.33	0.44
1:A:681:ASP:CG	1:A:739:THR:HG21	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:LEU:C	1:D:631:SER:H	2.26	0.43
1:C:614:GLU:O	1:C:615:LEU:C	2.61	0.43
1:D:572:LEU:C	1:D:574:GLN:N	2.77	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:608:ALA:C	1:C:610:HIS:H	2.27	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:607:ILE:HD13	1:A:576:MET:HE3	2.01	0.42
1:D:629:LEU:C	1:D:631:SER:N	2.76	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:D:587:ASN:C	1:D:589:GLY:CA	2.93	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: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	0.40
1:B:689:THR:O	1:B:690:LYS:C	2.63	0.40
1:B:678:GLY:O	1:B:679:LYS:C	2.64	0.40
1:A:568:LEU:HA	1:A:569:PRO:HD3	1.88	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	193/212 (91%)	181 (94%)	10 (5%)	2 (1%)	12	32
1	B	194/212 (92%)	175 (90%)	15 (8%)	4 (2%)	5	15
1	C	191/212 (90%)	173 (91%)	17 (9%)	1 (0%)	24	48
1	D	105/212 (50%)	83 (79%)	17 (16%)	5 (5%)	2	3
All	All	683/848 (80%)	612 (90%)	59 (9%)	12 (2%)	6	18

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%)	148 (96%)	7 (4%)	24	52
1	B	154/186 (83%)	146 (95%)	8 (5%)	21	47
1	C	143/186 (77%)	132 (92%)	11 (8%)	12	30
1	D	68/186 (37%)	61 (90%)	7 (10%)	7	18
All	All	520/744 (70%)	487 (94%)	33 (6%)	16	39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	550	SER
1	B	582	THR
1	B	593	SER
1	B	595	LEU
1	B	630	ARG
1	B	638	THR
1	B	657	ILE
1	B	725	GLU
1	A	565	VAL
1	A	582	THR
1	A	595	LEU
1	A	631	SER
1	A	638	THR
1	A	689	THR
1	A	693	VAL
1	C	554	THR
1	C	563	ILE
1	C	564	ARG
1	C	565	VAL
1	C	595	LEU
1	C	638	THR
1	C	641	CYS
1	C	708	LEU
1	C	712	SER
1	C	731	VAL
1	C	738	LEU
1	D	565	VAL
1	D	591	ASP
1	D	614	GLU
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	553	HIS
1	B	699	ASN
1	A	574	GLN
1	A	610	HIS
1	C	650	GLN
1	D	709	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](#)

There are no ligands in this entry.

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	195/212 (91%)	-0.05	3 (1%) 72 70	35, 56, 86, 138	0
1	B	196/212 (92%)	-0.13	2 (1%) 79 78	33, 55, 84, 143	0
1	C	193/212 (91%)	0.06	8 (4%) 41 37	34, 61, 115, 163	0
1	D	119/212 (56%)	0.95	20 (16%) 4 3	52, 84, 129, 168	0
All	All	703/848 (82%)	0.13	33 (4%) 36 33	33, 60, 113, 168	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	549	ARG	4.7
1	D	640	PHE	4.4
1	A	692	GLN	3.4
1	D	657	ILE	3.3
1	C	595	LEU	3.2
1	D	611	LEU	3.1
1	D	698	ALA	3.1
1	C	687	SER	3.0
1	D	659	PHE	3.0
1	D	629	LEU	2.9
1	D	591	ASP	2.8
1	D	675	ALA	2.7
1	D	712	SER	2.6
1	D	658	TYR	2.6
1	C	744	GLU	2.5
1	D	672	THR	2.5
1	D	631	SER	2.4
1	D	641	CYS	2.4
1	C	640	PHE	2.4
1	D	609	MET	2.3
1	A	686	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	659	PHE	2.3
1	C	692	GLN	2.2
1	D	649	ARG	2.2
1	D	615	LEU	2.2
1	D	681	ASP	2.2
1	D	634	LEU	2.1
1	A	707	ASP	2.1
1	C	639	SER	2.1
1	C	617	GLN	2.1
1	C	683	ILE	2.1
1	B	692	GLN	2.1
1	D	588	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.