



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:27 PM UTC

PDB ID : 1N11 / pdb_00001n11
Title : D34 REGION OF HUMAN ANKYRIN-R AND LINKER
Authors : Michaely, P.; Tomchick, D.R.; Machius, M.; Anderson, R.G.W.
Deposited on : 2002-10-16
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

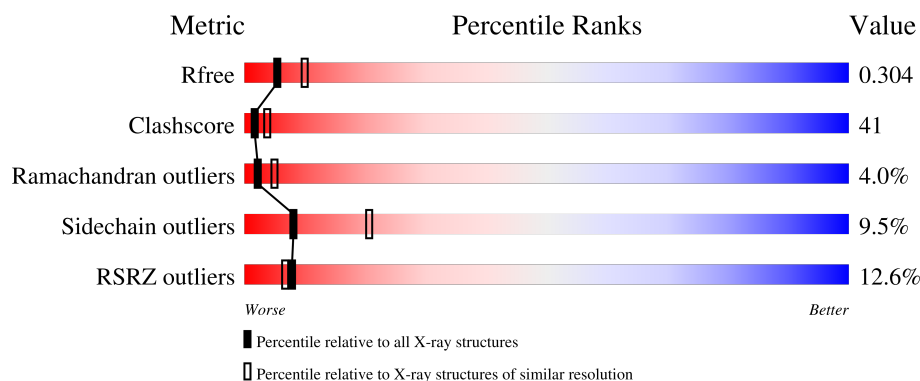
1 Overall quality at a glance

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	437	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1007	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1010	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3084 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 Ankyrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3074	1934	567	563	10	0	3	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	GLY	-	cloning artifact	UNP P16157
A	392	SER	-	cloning artifact	UNP P16157
A	393	PRO	-	cloning artifact	UNP P16157
A	394	GLY	-	cloning artifact	UNP P16157
A	395	ILE	-	cloning artifact	UNP P16157
A	396	SER	-	cloning artifact	UNP P16157
A	397	GLY	-	cloning artifact	UNP P16157
A	398	GLY	-	cloning artifact	UNP P16157
A	399	GLY	-	cloning artifact	UNP P16157
A	400	GLY	-	cloning artifact	UNP P16157
A	401	GLY	-	cloning artifact	UNP P16157

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Br	0	0
			1	1		

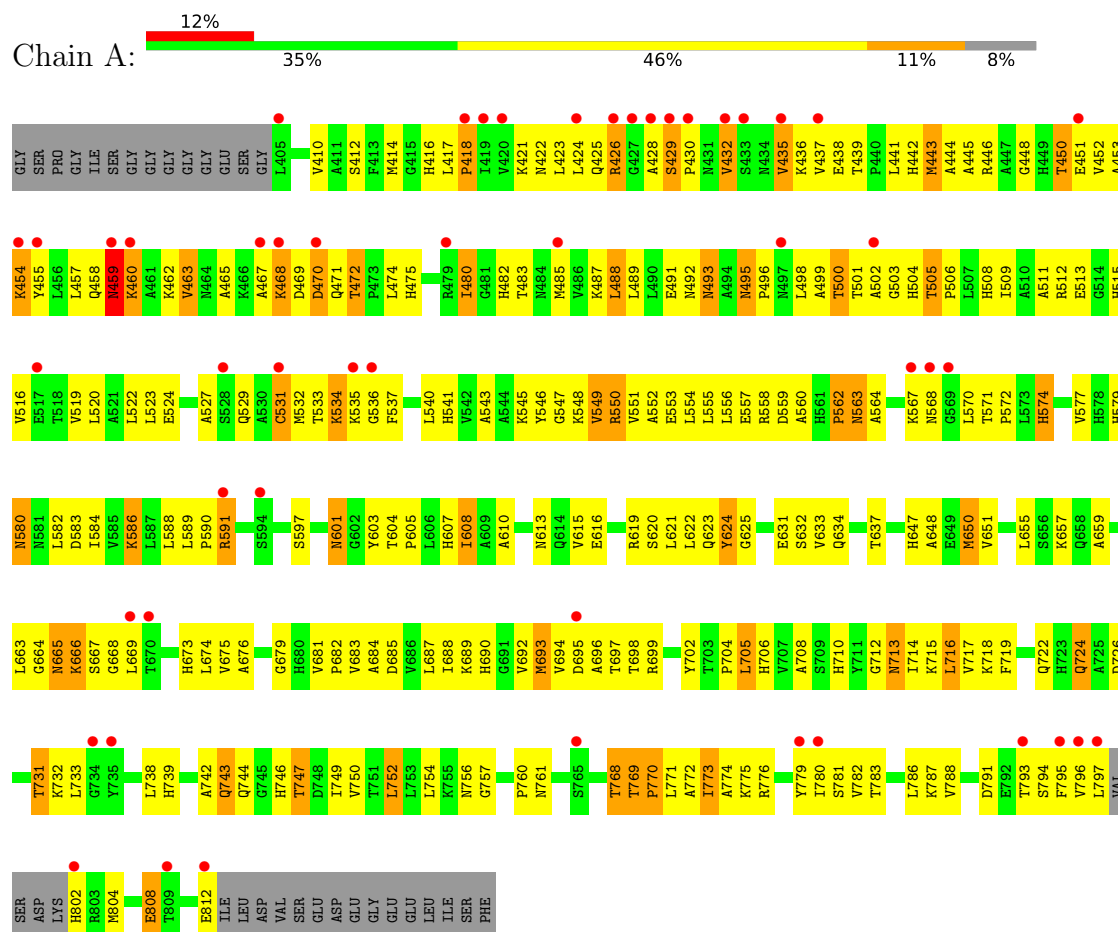
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Cl	0	0
			9	9		

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: Ankyrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.33Å 137.33Å 197.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 97.9 (30.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.319 , 0.303 0.320 , 0.304	Depositor DCC
R_{free} test set	1155 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3084	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: BR, 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	0.63	2/3136 (0.1%)	1.18	26/4266 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	CYS	CB-SG	-11.89	1.42	1.81
1	A	693	MET	SD-CE	5.06	1.92	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	VAL	N-CA-C	12.02	122.98	110.36
1	A	551	VAL	N-CA-C	-9.94	101.19	110.53
1	A	559	ASP	N-CA-C	8.89	123.63	111.90
1	A	724	GLN	N-CA-C	8.72	123.39	111.54
1	A	429	SER	CA-C-N	7.52	126.79	118.97
1	A	429	SER	C-N-CA	7.52	126.79	118.97
1	A	450	THR	N-CA-C	7.26	119.88	111.02
1	A	769	THR	N-CA-C	-6.77	99.74	110.10
1	A	459	ASN	N-CA-C	6.58	118.15	110.97
1	A	632	SER	N-CA-C	-6.55	102.06	110.19
1	A	779	TYR	N-CA-C	-6.54	98.54	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	ALA	N-CA-C	6.47	117.99	111.07
1	A	780	ILE	N-CA-C	5.90	116.94	111.45
1	A	442	HIS	N-CA-C	-5.87	104.79	111.07
1	A	757	GLY	N-CA-C	5.83	123.64	115.43
1	A	495	ASN	CA-C-N	5.82	126.92	120.45
1	A	495	ASN	C-N-CA	5.82	126.92	120.45
1	A	454	LYS	N-CA-C	-5.70	106.17	113.01
1	A	631	GLU	N-CA-C	5.68	118.50	109.24
1	A	534	LYS	N-CA-C	-5.55	106.35	113.23
1	A	625	GLY	N-CA-C	5.38	121.92	114.92
1	A	500	THR	N-CA-C	-5.37	102.81	110.59
1	A	564	ALA	N-CA-C	-5.14	102.87	110.48
1	A	705	LEU	N-CA-C	-5.04	104.74	111.24
1	A	681	VAL	CB-CA-C	-5.02	108.93	113.70
1	A	697	THR	N-CA-C	5.01	117.92	109.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	TYR	Sidechain

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	3074	0	3134	256	0
2	A	1	0	0	0	0
3	A	9	0	0	5	0
All	All	3084	0	3134	256	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 41.

All (256) 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:A:731:THR:HG22	1:A:733:LEU:H	1.12	1.09
1:A:550:ARG:H	1:A:550:ARG:HD3	1.12	1.09
1:A:468:LYS:H	1:A:468:LYS:HE2	1.23	1.03
1:A:601:ASN:HD22	1:A:601:ASN:H	1.12	0.91
1:A:567:LYS:H	1:A:567:LYS:HD2	1.40	0.86
1:A:545:LYS:HG3	1:A:579:HIS:CE1	2.09	0.86
1:A:550:ARG:HD3	1:A:550:ARG:N	1.90	0.86
1:A:533:THR:CG2	1:A:535:LYS:HG2	2.08	0.83
1:A:533:THR:HG21	1:A:535:LYS:HG2	1.60	0.82
1:A:457:LEU:HD21	1:A:463:VAL:HG13	1.61	0.82
1:A:567:LYS:HD2	1:A:567:LYS:N	1.95	0.80
1:A:468:LYS:H	1:A:468:LYS:CE	1.95	0.80
1:A:582:LEU:HD13	1:A:616:GLU:HG3	1.63	0.79
1:A:714:ILE:HG13	1:A:749:ILE:HG12	1.65	0.79
1:A:568:ASN:HB2	1:A:570:LEU:HD12	1.63	0.78
1:A:613:ASN:HB2	1:A:647:HIS:CG	2.20	0.77
1:A:468:LYS:HE2	1:A:468:LYS:N	2.01	0.74
1:A:713:ASN:OD1	1:A:715:LYS:HB2	1.88	0.74
1:A:548:LYS:HB3	1:A:550:ARG:NH2	2.04	0.72
1:A:459:ASN:HD22	1:A:459:ASN:N	1.87	0.72
1:A:550:ARG:H	1:A:550:ARG:CD	1.99	0.71
1:A:613:ASN:HB2	1:A:647:HIS:CD2	2.25	0.71
1:A:793:THR:C	1:A:795:PHE:H	1.98	0.71
1:A:459:ASN:O	1:A:460:LYS:HB3	1.88	0.71
1:A:783:THR:O	1:A:787:LYS:HB2	1.91	0.71
1:A:619:ARG:HH11	1:A:619:ARG:HG2	1.55	0.71
1:A:421:LYS:HG2	1:A:455:TYR:CE2	2.26	0.71
1:A:532:MET:HE2	1:A:536:GLY:C	2.17	0.69
1:A:582:LEU:HD21	1:A:586:LYS:HD2	1.72	0.69
1:A:610:ALA:HA	1:A:650:MET:SD	2.32	0.69
1:A:487:LYS:O	1:A:491:GLU:HB2	1.91	0.69
1:A:417:LEU:HG	1:A:421:LYS:HE3	1.74	0.69
1:A:601:ASN:H	1:A:601:ASN:ND2	1.90	0.69
1:A:435:VAL:HG12	1:A:436:LYS:HD2	1.75	0.68
1:A:713:ASN:CB	3:A:1010:CL:CL	2.78	0.68
1:A:731:THR:HG22	1:A:733:LEU:N	1.97	0.68
1:A:457:LEU:HD21	1:A:463:VAL:CG1	2.23	0.68
1:A:467:ALA:HB1	1:A:468:LYS:HE3	1.76	0.68
1:A:545:LYS:HE3	1:A:579:HIS:HE1	1.58	0.68
1:A:747:THR:HG21	1:A:781:SER:HB2	1.76	0.68
1:A:580:ASN:HD22	1:A:580:ASN:C	2.02	0.68
1:A:698:THR:HG21	1:A:808:GLU:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:HG2	1:A:469:ASP:H	1.60	0.66
1:A:508:HIS:O	1:A:511:ALA:HB3	1.95	0.66
1:A:601:ASN:HD22	1:A:601:ASN:N	1.84	0.66
1:A:679:GLY:HA2	1:A:716:LEU:HD13	1.78	0.65
1:A:655:LEU:HD11	1:A:687:LEU:HD23	1.79	0.65
1:A:516:VAL:HG21	1:A:550:ARG:HG2	1.77	0.64
1:A:545:LYS:HG3	1:A:579:HIS:HE1	1.62	0.64
1:A:713:ASN:HB2	3:A:1010:CL:CL	2.34	0.64
1:A:731:THR:CG2	1:A:732:LYS:N	2.62	0.63
1:A:793:THR:O	1:A:795:PHE:N	2.32	0.63
1:A:601:ASN:O	1:A:633:VAL:HG23	1.98	0.63
1:A:718:LYS:HG2	1:A:752:LEU:HD21	1.79	0.63
1:A:548:LYS:HB3	1:A:550:ARG:HH22	1.63	0.62
1:A:483:THR:N	3:A:1007:CL:CL	2.70	0.62
1:A:688:ILE:HD12	1:A:719:PHE:CE2	2.34	0.62
1:A:445:ALA:HA	1:A:485:MET:HE3	1.79	0.62
1:A:613:ASN:HB2	1:A:647:HIS:CE1	2.35	0.62
1:A:752:LEU:CD1	1:A:756:ASN:HD22	2.13	0.62
1:A:775:LYS:NZ	1:A:787:LYS:NZ	2.48	0.62
1:A:483:THR:HB	3:A:1007:CL:CL	2.37	0.61
1:A:776:ARG:HD3	1:A:802:HIS:CE1	2.36	0.61
1:A:454:LYS:O	1:A:458:GLN:HG2	2.00	0.61
1:A:698:THR:HG22	1:A:699:ARG:H	1.66	0.60
1:A:422:ASN:HD21	1:A:426:ARG:CZ	2.14	0.60
1:A:515:HIS:O	1:A:519:VAL:HG23	2.01	0.60
1:A:601:ASN:HD21	1:A:603:TYR:HB2	1.67	0.60
1:A:423:LEU:O	1:A:428:ALA:HB3	2.01	0.60
1:A:713:ASN:N	3:A:1010:CL:CL	2.72	0.59
1:A:438:GLU:OE1	1:A:443:MET:HE3	2.02	0.59
1:A:529:GLN:OE1	1:A:560:ALA:HB2	2.03	0.59
1:A:414:MET:HB3	1:A:416:HIS:CE1	2.38	0.59
1:A:417:LEU:O	1:A:421:LYS:HG3	2.03	0.59
1:A:589:LEU:HD13	1:A:624:TYR:CD1	2.38	0.59
1:A:655:LEU:HD13	1:A:690:HIS:ND1	2.18	0.59
1:A:560:ALA:O	1:A:562:PRO:HD3	2.02	0.59
1:A:768:THR:HG21	1:A:773:ILE:CD1	2.33	0.58
1:A:451[A]:GLU:OE2	1:A:452:VAL:HG23	2.03	0.58
1:A:752:LEU:O	1:A:752:LEU:HD12	2.03	0.58
1:A:666:LYS:O	1:A:699:ARG:NH2	2.33	0.57
1:A:665:ASN:C	1:A:665:ASN:HD22	2.13	0.57
1:A:545:LYS:CE	1:A:579:HIS:HE1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:GLN:HB2	1:A:746:HIS:CD2	2.40	0.57
1:A:634:GLN:O	1:A:666:LYS:HB2	2.05	0.57
1:A:615:VAL:HA	1:A:650:MET:HE1	1.87	0.56
1:A:548:LYS:HD2	1:A:550:ARG:HH22	1.69	0.56
1:A:692:VAL:HG12	1:A:693:MET:N	2.21	0.56
1:A:690:HIS:O	1:A:690:HIS:CD2	2.59	0.56
1:A:567:LYS:H	1:A:567:LYS:CD	2.16	0.55
1:A:665:ASN:C	1:A:665:ASN:ND2	2.62	0.55
1:A:705:LEU:O	1:A:706:HIS:C	2.49	0.55
1:A:552:ALA:O	1:A:556:LEU:HD12	2.06	0.55
1:A:698:THR:HG21	1:A:808:GLU:CG	2.36	0.54
1:A:505:THR:HG21	1:A:531:CYS:HB3	1.89	0.54
1:A:469:ASP:O	1:A:470:ASP:HB2	2.06	0.54
1:A:548:LYS:HA	1:A:550:ARG:HH12	1.73	0.54
1:A:435:VAL:HG12	1:A:436:LYS:H	1.73	0.54
1:A:435:VAL:HG12	1:A:436:LYS:N	2.23	0.53
1:A:422:ASN:HD21	1:A:426:ARG:NH1	2.06	0.53
1:A:714:ILE:HG13	1:A:749:ILE:CG1	2.38	0.53
1:A:773:ILE:HG22	1:A:774:ALA:N	2.23	0.53
1:A:563:ASN:HA	1:A:572:PRO:HD2	1.90	0.52
1:A:424:LEU:HD22	1:A:459:ASN:OD1	2.09	0.52
1:A:459:ASN:HD22	1:A:459:ASN:H	1.55	0.52
1:A:768:THR:HG21	1:A:773:ILE:HD12	1.91	0.52
1:A:739:HIS:CE1	1:A:770:PRO:HD3	2.46	0.51
1:A:747:THR:CG2	1:A:782:VAL:HG23	2.41	0.51
1:A:485:MET:O	1:A:489:LEU:HG	2.10	0.51
1:A:529:GLN:CD	1:A:555:LEU:HD22	2.36	0.51
1:A:532:MET:HA	1:A:537:PHE:O	2.10	0.51
1:A:580:ASN:C	1:A:580:ASN:ND2	2.68	0.51
1:A:492:ASN:O	1:A:493:ASN:HB2	2.09	0.51
1:A:579:HIS:O	1:A:580:ASN:C	2.54	0.51
1:A:752:LEU:HD12	1:A:756:ASN:HD22	1.75	0.51
1:A:613:ASN:HB2	1:A:647:HIS:ND1	2.26	0.51
1:A:568:ASN:CB	1:A:570:LEU:HD12	2.40	0.50
1:A:533:THR:HG22	1:A:534:LYS:H	1.75	0.50
1:A:676:ALA:HB1	1:A:708:ALA:HB2	1.93	0.50
1:A:796:VAL:HG12	1:A:797:LEU:N	2.26	0.50
1:A:690:HIS:O	1:A:690:HIS:HD2	1.93	0.50
1:A:421:LYS:O	1:A:425:GLN:HG3	2.12	0.50
1:A:549:VAL:HA	1:A:584:ILE:HD11	1.93	0.50
1:A:571:THR:O	1:A:574:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:LYS:NZ	1:A:787:LYS:HZ2	2.09	0.50
1:A:545:LYS:HE3	1:A:579:HIS:CE1	2.43	0.50
1:A:537:PHE:CD2	1:A:541:HIS:HB3	2.47	0.50
1:A:545:LYS:HG3	1:A:579:HIS:ND1	2.27	0.50
1:A:505:THR:HG21	1:A:531:CYS:CB	2.41	0.50
1:A:731:THR:HG22	1:A:732:LYS:N	2.26	0.49
1:A:619:ARG:HG2	1:A:619:ARG:NH1	2.22	0.49
1:A:655:LEU:HB3	1:A:690:HIS:CE1	2.47	0.49
1:A:768:THR:CG2	1:A:773:ILE:HD12	2.43	0.49
1:A:615:VAL:HA	1:A:650:MET:CE	2.41	0.49
1:A:812:GLU:HA	1:A:812:GLU:OE2	2.13	0.49
1:A:616:GLU:HA	1:A:616:GLU:OE1	2.13	0.49
1:A:441:LEU:O	1:A:444:ALA:HB3	2.12	0.48
1:A:684:ALA:O	1:A:688:ILE:HG13	2.12	0.48
1:A:522:LEU:O	1:A:527:ALA:CB	2.61	0.48
1:A:417:LEU:N	1:A:418:PRO:CD	2.76	0.48
1:A:738:LEU:HD11	1:A:750:VAL:HG13	1.96	0.48
1:A:550:ARG:N	1:A:550:ARG:CD	2.68	0.48
1:A:529:GLN:OE1	1:A:555:LEU:HD22	2.14	0.48
1:A:533:THR:HG22	1:A:534:LYS:N	2.28	0.47
1:A:417:LEU:HD22	1:A:451[A]:GLU:HG3	1.95	0.47
1:A:589:LEU:HB2	1:A:590:PRO:HD3	1.96	0.47
1:A:637:THR:HG21	1:A:663:LEU:HD23	1.96	0.47
1:A:488:LEU:CD2	1:A:492:ASN:ND2	2.77	0.47
1:A:500:THR:HG22	1:A:501:THR:N	2.30	0.47
1:A:665:ASN:ND2	1:A:668:GLY:H	2.12	0.47
1:A:459:ASN:O	1:A:460:LYS:CB	2.59	0.47
1:A:416:HIS:C	1:A:418:PRO:HD2	2.40	0.47
1:A:455:TYR:O	1:A:458:GLN:N	2.47	0.47
1:A:693:MET:HB3	1:A:696:ALA:HB2	1.96	0.47
1:A:439:THR:O	1:A:443:MET:HG3	2.15	0.46
1:A:750:VAL:CG1	1:A:786:LEU:HD21	2.45	0.46
1:A:775:LYS:HZ1	1:A:787:LYS:NZ	2.13	0.46
1:A:775:LYS:HZ2	1:A:787:LYS:HZ2	1.63	0.46
1:A:582:LEU:HD13	1:A:616:GLU:CG	2.39	0.46
1:A:579:HIS:N	1:A:579:HIS:CD2	2.84	0.46
1:A:743:GLN:HG3	1:A:804:MET:HE2	1.98	0.46
1:A:687:LEU:HB3	1:A:692:VAL:HG21	1.97	0.46
1:A:776:ARG:HD3	1:A:802:HIS:ND1	2.31	0.46
1:A:499:ALA:HB1	1:A:503:GLY:HA2	1.98	0.46
1:A:664:GLY:HA2	1:A:669:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:HD13	1:A:480:ILE:HA	1.76	0.46
1:A:710:HIS:O	1:A:744:GLN:HG3	2.16	0.46
1:A:761:ASN:ND2	1:A:791:ASP:CG	2.74	0.46
1:A:747:THR:HG23	1:A:782:VAL:HG23	1.98	0.45
1:A:492:ASN:O	1:A:493:ASN:CB	2.63	0.45
1:A:513:GLU:HB2	1:A:515:HIS:CD2	2.51	0.45
1:A:620:SER:O	1:A:623:GLN:HB3	2.16	0.45
1:A:604:THR:O	1:A:607:HIS:N	2.43	0.45
1:A:455:TYR:O	1:A:458:GLN:HB2	2.17	0.45
1:A:520:LEU:O	1:A:524:GLU:HG2	2.16	0.45
1:A:675:VAL:HG21	1:A:683:VAL:HG12	1.99	0.45
1:A:773:ILE:O	1:A:774:ALA:C	2.60	0.45
1:A:502:ALA:HB3	1:A:504:HIS:HD2	1.81	0.45
1:A:601:ASN:C	1:A:633:VAL:HG23	2.42	0.45
1:A:495:ASN:HA	1:A:496:PRO:HD3	1.73	0.45
1:A:557:GLU:HA	1:A:591[B]:ARG:NH2	2.31	0.45
1:A:747:THR:HG21	1:A:781:SER:CB	2.44	0.44
1:A:754:LEU:HD21	1:A:760:PRO:HB3	2.00	0.44
1:A:522:LEU:O	1:A:527:ALA:HB2	2.18	0.44
1:A:553:GLU:O	1:A:554:LEU:C	2.60	0.44
1:A:480:ILE:CG2	1:A:482:HIS:HB2	2.47	0.44
1:A:412:SER:HA	1:A:452:VAL:HG11	1.99	0.44
1:A:435:VAL:CG1	1:A:436:LYS:H	2.30	0.44
1:A:474:LEU:HA	1:A:489:LEU:HD13	2.00	0.44
1:A:690:HIS:CD2	1:A:690:HIS:C	2.96	0.44
1:A:742:ALA:O	1:A:744:GLN:N	2.51	0.44
1:A:768:THR:HG21	1:A:773:ILE:HG13	1.99	0.44
1:A:516:VAL:CG2	1:A:550:ARG:HG2	2.45	0.43
1:A:655:LEU:HA	1:A:659:ALA:HB3	1.99	0.43
1:A:738:LEU:O	1:A:739:HIS:C	2.59	0.43
1:A:695:ASP:OD2	1:A:726:ASP:N	2.44	0.43
1:A:437:VAL:HG12	1:A:438:GLU:N	2.33	0.43
1:A:453:ALA:C	1:A:455:TYR:N	2.76	0.43
1:A:619:ARG:NH1	1:A:619:ARG:CG	2.80	0.43
1:A:673:HIS:CD2	1:A:704:PRO:HG3	2.53	0.43
1:A:512:ARG:HG3	1:A:546:TYR:CD2	2.52	0.43
1:A:571:THR:HG21	1:A:597:SER:CB	2.48	0.43
1:A:665:ASN:ND2	1:A:667:SER:H	2.16	0.43
1:A:769:THR:H	1:A:772:ALA:HB3	1.84	0.43
1:A:480:ILE:HG22	1:A:482:HIS:HB2	2.01	0.43
1:A:682:PRO:O	1:A:685:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LEU:HD12	1:A:752:LEU:C	2.44	0.43
1:A:548:LYS:CB	1:A:550:ARG:HH22	2.29	0.43
1:A:761:ASN:HD21	1:A:791:ASP:CG	2.27	0.43
1:A:540:LEU:HD21	1:A:588:LEU:HD21	2.01	0.43
1:A:743:GLN:CG	1:A:804:MET:HE2	2.49	0.43
1:A:689:LYS:HA	1:A:689:LYS:HD3	1.75	0.43
1:A:722:GLN:C	1:A:724:GLN:H	2.27	0.43
1:A:545:LYS:HD3	1:A:546:TYR:CZ	2.54	0.42
1:A:702:TYR:HA	1:A:706:HIS:ND1	2.34	0.42
1:A:500:THR:HG22	1:A:502:ALA:H	1.84	0.42
1:A:556:LEU:C	1:A:558:ARG:N	2.74	0.42
1:A:582:LEU:CD1	1:A:616:GLU:HG3	2.42	0.42
1:A:622:LEU:HD13	1:A:657:LYS:HG3	2.00	0.42
1:A:505:THR:O	1:A:506:PRO:C	2.63	0.42
1:A:731:THR:HG23	1:A:732:LYS:H	1.84	0.42
1:A:448:GLY:HA2	1:A:485:MET:HE2	2.02	0.42
1:A:472:THR:O	1:A:475:HIS:HB2	2.19	0.42
1:A:556:LEU:C	1:A:558:ARG:H	2.26	0.42
1:A:554:LEU:O	1:A:558:ARG:HG3	2.20	0.42
1:A:622:LEU:O	1:A:623:GLN:C	2.63	0.41
1:A:647:HIS:O	1:A:651:VAL:HG23	2.20	0.41
1:A:496:PRO:O	1:A:506:PRO:HD2	2.19	0.41
1:A:443:MET:CE	1:A:446:ARG:HH21	2.34	0.41
1:A:475:HIS:HE1	1:A:498:LEU:O	2.03	0.41
1:A:746:HIS:O	1:A:747:THR:C	2.63	0.41
1:A:655:LEU:HB3	1:A:690:HIS:ND1	2.35	0.41
1:A:613:ASN:HB2	1:A:647:HIS:NE2	2.34	0.41
1:A:698:THR:HG22	1:A:699:ARG:N	2.34	0.41
1:A:621:LEU:HD23	1:A:621:LEU:HA	1.80	0.41
1:A:676:ALA:HA	1:A:716:LEU:HD22	2.01	0.41
1:A:462:LYS:HB2	1:A:465:ALA:HB2	2.02	0.41
1:A:469:ASP:OD2	1:A:471:GLN:HG2	2.21	0.41
1:A:475:HIS:CE1	1:A:498:LEU:O	2.74	0.41
1:A:504:HIS:HB3	1:A:509:ILE:HD11	2.03	0.41
1:A:705:LEU:HD11	1:A:717:VAL:HG13	2.03	0.41
1:A:429:SER:HA	1:A:430:PRO:HD3	1.83	0.41
1:A:651:VAL:O	1:A:655:LEU:HG	2.21	0.41
1:A:771:LEU:HA	1:A:786:LEU:HD12	2.03	0.41
1:A:540:LEU:O	1:A:543:ALA:HB3	2.21	0.40
1:A:423:LEU:O	1:A:428:ALA:CB	2.66	0.40
1:A:533:THR:HG21	1:A:535:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LYS:HD3	1:A:534:LYS:HA	1.89	0.40
1:A:548:LYS:CD	1:A:550:ARG:HH22	2.34	0.40
1:A:577:VAL:HG12	1:A:608:ILE:HG22	2.04	0.40
1:A:669:LEU:HD13	1:A:674:LEU:HD21	2.02	0.40
1:A:577:VAL:HG12	1:A:608:ILE:CG2	2.50	0.40
1:A:655:LEU:C	1:A:657:LYS:H	2.29	0.40
1:A:665:ASN:HD22	1:A:668:GLY:H	1.68	0.40
1:A:747:THR:CG2	1:A:781:SER:HB2	2.46	0.40
1:A:523:LEU:O	1:A:524:GLU:C	2.65	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	403/437 (92%)	325 (81%)	62 (15%)	16 (4%)	2 5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	LYS
1	A	493	ASN
1	A	747	THR
1	A	794	SER
1	A	432	VAL
1	A	435	VAL
1	A	580	ASN
1	A	712	GLY
1	A	713	ASN
1	A	743	GLN
1	A	426	ARG
1	A	418	PRO

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Mol	Chain	Res	Type
1	A	605	PRO
1	A	608	ILE
1	A	547	GLY
1	A	788	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	330/351 (94%)	298 (90%)	32 (10%)	8 20

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	VAL
1	A	432	VAL
1	A	443	MET
1	A	450	THR
1	A	459	ASN
1	A	463	VAL
1	A	468	LYS
1	A	470	ASP
1	A	472	THR
1	A	480	ILE
1	A	488	LEU
1	A	505	THR
1	A	550	ARG
1	A	562	PRO
1	A	563	ASN
1	A	574	HIS
1	A	583	ASP
1	A	586	LYS
1	A	591[A]	ARG
1	A	591[B]	ARG
1	A	601	ASN
1	A	650	MET

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Mol	Chain	Res	Type
1	A	665	ASN
1	A	666	LYS
1	A	694	VAL
1	A	716	LEU
1	A	731	THR
1	A	752	LEU
1	A	768	THR
1	A	770	PRO
1	A	773	ILE
1	A	808	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	492	ASN
1	A	504	HIS
1	A	515	HIS
1	A	579	HIS
1	A	580	ASN
1	A	596	HIS
1	A	601	ASN
1	A	612	GLN
1	A	614	GLN
1	A	647	HIS
1	A	665	ASN
1	A	690	HIS
1	A	722	GLN
1	A	746	HIS
1	A	756	ASN
1	A	802	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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	404/437 (92%)	0.85	51 (12%) 8 7	38, 110, 137, 149	3 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591[A]	ARG	5.9
1	A	420	VAL	5.8
1	A	531	CYS	5.0
1	A	424	LEU	5.0
1	A	797	LEU	5.0
1	A	497	ASN	4.7
1	A	479[A]	ARG	4.4
1	A	535	LYS	4.1
1	A	802	HIS	3.8
1	A	485	MET	3.8
1	A	569	GLY	3.8
1	A	418	PRO	3.7
1	A	695	ASP	3.3
1	A	568	ASN	3.2
1	A	433	SER	3.1
1	A	419	ILE	3.0
1	A	451[A]	GLU	3.0
1	A	428	ALA	3.0
1	A	536	GLY	2.9
1	A	459	ASN	2.9
1	A	467	ALA	2.8
1	A	812	GLU	2.8
1	A	734	GLY	2.7
1	A	430	PRO	2.7
1	A	432	VAL	2.7
1	A	809	THR	2.7
1	A	426	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	793	THR	2.7
1	A	470	ASP	2.6
1	A	567	LYS	2.6
1	A	528	SER	2.6
1	A	517	GLU	2.6
1	A	594	SER	2.6
1	A	765	SER	2.6
1	A	454	LYS	2.6
1	A	502	ALA	2.6
1	A	796	VAL	2.5
1	A	468	LYS	2.4
1	A	405	LEU	2.4
1	A	669	LEU	2.3
1	A	779	TYR	2.3
1	A	429	SER	2.3
1	A	735	TYR	2.3
1	A	437	VAL	2.3
1	A	455	TYR	2.3
1	A	435	VAL	2.3
1	A	670	THR	2.2
1	A	460	LYS	2.1
1	A	427	GLY	2.1
1	A	795	PHE	2.0
1	A	780	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	CL	A	1008	1/1	0.67	0.11	145,145,145,145	0
3	CL	A	1004	1/1	0.76	0.12	136,136,136,136	0
3	CL	A	1009	1/1	0.81	0.06	136,136,136,136	0
3	CL	A	1005	1/1	0.83	0.12	140,140,140,140	0
3	CL	A	1010	1/1	0.92	0.10	117,117,117,117	0
3	CL	A	1007	1/1	0.93	0.05	139,139,139,139	0
3	CL	A	1003	1/1	0.93	0.13	104,104,104,104	0
3	CL	A	1002	1/1	0.94	0.14	112,112,112,112	0
3	CL	A	1006	1/1	0.94	0.07	121,121,121,121	0
2	BR	A	1001	1/1	0.97	0.08	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.