



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:32 am GMT

PDB ID : 1N11  
Title : D34 REGION OF HUMAN ANKYRIN-R AND LINKER  
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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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

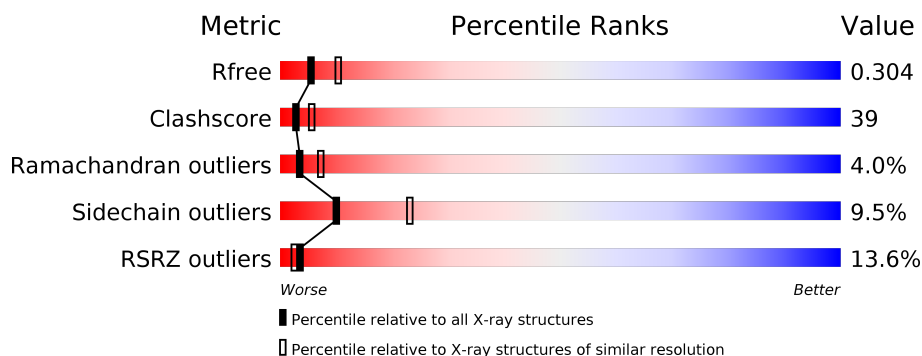
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	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	-
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
1	A	404	Total	C	N	O	S	0	3	0
			3074	1934	567	563	10			

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 (three-letter code: BR) (formula: Br).

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

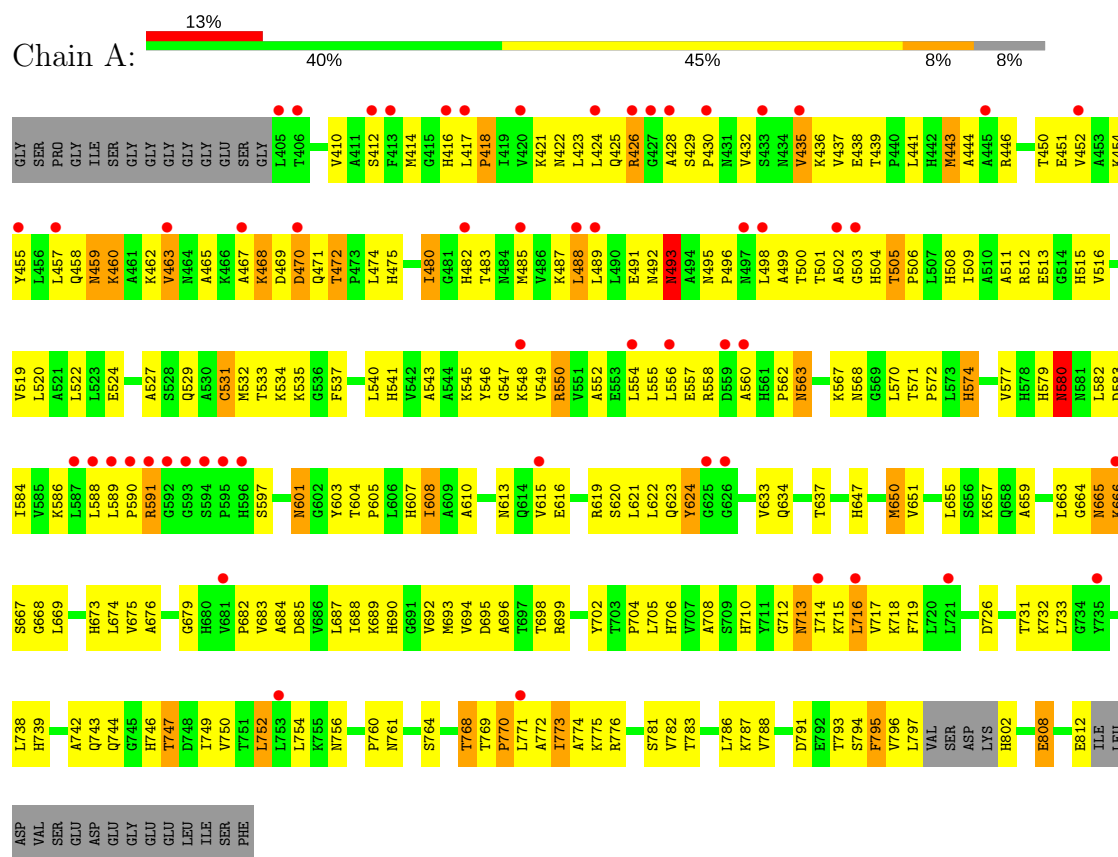
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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 and DNA 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, $\alpha$ , $\beta$ , $\gamma$	137.33Å 137.33Å 197.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 45.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 97.4 (45.66-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (3.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 83.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.65	1/3136 (0.0%)	0.74	0/4266

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	CYS	CB-SG	-23.67	1.42	1.82

There are no bond angle outliers.

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	241	0
2	A	1	0	0	0	0
3	A	9	0	0	5	0
All	All	3084	0	3134	241	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 39.

All (241) 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:HD3	1:A:550:ARG:H	1.12	1.09
1:A:468:LYS:HE2	1:A:468:LYS:H	1.23	1.03
1:A:601:ASN:H	1:A:601:ASN:HD22	1.12	0.91
1:A:567:LYS:HD2	1:A:567:LYS:H	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:N	1:A:567:LYS:HD2	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:N	1:A:468:LYS:HE2	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:CD	1:A:550:ARG:H	1.99	0.71
1:A:613:ASN:HB2	1:A:647:HIS:CD2	2.25	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:HG2	1:A:619:ARG:HH11	1.55	0.71
1:A:421:LYS:HG2	1:A:455:TYR:CE2	2.26	0.71
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:ND2	1:A:601:ASN:H	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ASN:CB	3:A:1010:CL:CL	2.78	0.68
1:A:435:VAL:HG12	1:A:436:LYS:HD2	1.75	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:698:THR:HG21	1:A:808:GLU:HG3	1.75	0.67
1:A:793:THR:C	1:A:795:PHE:H	1.98	0.67
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:N	1:A:601:ASN:HD22	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:580:ASN:C	1:A:580:ASN:HD22	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:615:VAL:HA	1:A:650:MET:HE1	1.85	0.58
1:A:451[A]:GLU:OE2	1:A:452:VAL:HG23	2.03	0.58
1:A:752:LEU:HD12	1:A:752:LEU:O	2.03	0.58
1:A:666:LYS:O	1:A:699:ARG:NH2	2.33	0.57
1:A:545:LYS:CE	1:A:579:HIS:HE1	2.17	0.57
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: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:CD2	1:A:690:HIS:O	2.59	0.56
1:A:567:LYS:CD	1:A:567:LYS:H	2.16	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:443:MET:HE2	1:A:446:ARG:HH21	1.74	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:665:ASN:HD22	1:A:665:ASN:C	2.13	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:532:MET:HA	1:A:537:PHE:O	2.10	0.51
1:A:665:ASN:ND2	1:A:665:ASN:C	2.62	0.51
1:A:492:ASN:O	1:A:493:ASN:HB2	2.09	0.51
1:A:459:ASN:N	1:A:459:ASN:ND2	2.58	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:793:THR:C	1:A:795:PHE:N	2.64	0.51
1:A:568:ASN:CB	1:A:570:LEU:HD12	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:705:LEU:O	1:A:706:HIS:C	2.49	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
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:812:GLU:OE2	1:A:812:GLU:HA	2.13	0.49
1:A:615:VAL:HA	1:A:650:MET:CE	2.41	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:CD	1:A:550:ARG:N	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:775:LYS:HZ2	1:A:787:LYS:HZ2	1.63	0.47
1:A:459:ASN:O	1:A:460:LYS:CB	2.59	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:529:GLN:CD	1:A:555:LEU:HD22	2.36	0.46
1:A:775:LYS:HZ1	1:A:787:LYS:NZ	2.13	0.46
1:A:750:VAL:CG1	1:A:786:LEU:HD21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:HIS:O	1:A:580:ASN:C	2.54	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: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
1:A:480:ILE:HA	1:A:480:ILE:HD13	1.76	0.46
1:A:710:HIS:O	1:A:744:GLN:HG3	2.16	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:580:ASN:ND2	1:A:580:ASN:C	2.68	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:502:ALA:HB3	1:A:504:HIS:HD2	1.81	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:PRO:O	1:A:685:ASP:HB3	2.18	0.43
1:A:548:LYS:CB	1:A:550:ARG:HH22	2.29	0.43
1:A:775:LYS:NZ	1:A:787:LYS:HZ2	2.14	0.43
1:A:540:LEU:HD21	1:A:588:LEU:HD21	2.01	0.43
1:A:689:LYS:HA	1:A:689:LYS:HD3	1.75	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: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:731:THR:HG23	1:A:732:LYS:H	1.84	0.42
1:A:472:THR:O	1:A:475:HIS:HB2	2.19	0.42
1:A:554:LEU:O	1:A:558:ARG:HG3	2.20	0.42
1:A:416:HIS:C	1:A:418:PRO:HD2	2.40	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:475:HIS:HE1	1:A:498:LEU:O	2.03	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:761:ASN:ND2	1:A:791:ASP:CG	2.74	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:556:LEU:C	1:A:558:ARG:N	2.74	0.41
1:A:705:LEU:HD11	1:A:717:VAL:HG13	2.03	0.41
1:A:500:THR:CG2	1:A:501:THR:N	2.84	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:534:LYS:HD3	1:A:534:LYS:HA	1.89	0.40
1:A:533:THR:HG21	1:A:535:LYS:HE2	2.03	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:773:ILE:O	1:A:774:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:VAL:HG12	1:A:608:ILE:CG2	2.50	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:601:ASN:C	1:A:633:VAL:HG23	2.42	0.40
1:A:443:MET:CE	1:A:446:ARG:HH21	2.34	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%)	<b>3</b> <b>7</b>

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
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%)	9 22

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

Mol	Chain	Res	Type
1	A	410	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	493	ASN
1	A	505	THR
1	A	550	ARG
1	A	563	ASN
1	A	574	HIS
1	A	580	ASN
1	A	583	ASP
1	A	591[A]	ARG
1	A	591[B]	ARG
1	A	601	ASN
1	A	650	MET
1	A	665	ASN
1	A	666	LYS
1	A	694	VAL
1	A	716	LEU
1	A	752	LEU
1	A	764	SER
1	A	768	THR
1	A	770	PRO
1	A	773	ILE

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Mol	Chain	Res	Type
1	A	795	PHE
1	A	808	GLU

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	422	ASN
1	A	492	ASN
1	A	504	HIS
1	A	579	HIS
1	A	580	ASN
1	A	601	ASN
1	A	634	GLN
1	A	665	ASN
1	A	690	HIS
1	A	756	ASN
1	A	802	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/437 (92%)	0.90	55 (13%) <b>3</b> <b>2</b>	75, 110, 137, 149	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	VAL	7.9
1	A	424	LEU	4.9
1	A	592	GLY	4.5
1	A	485	MET	4.4
1	A	594	SER	4.3
1	A	416	HIS	4.2
1	A	417	LEU	4.1
1	A	591[A]	ARG	3.9
1	A	445	ALA	3.9
1	A	457	LEU	3.9
1	A	503	GLY	3.8
1	A	427	GLY	3.7
1	A	430	PRO	3.5
1	A	433	SER	3.5
1	A	595	PRO	3.4
1	A	593	GLY	3.4
1	A	716	LEU	3.2
1	A	455	TYR	3.1
1	A	559	ASP	3.1
1	A	435	VAL	3.0
1	A	498	LEU	3.0
1	A	714	ILE	2.9
1	A	467	ALA	2.8
1	A	596	HIS	2.7
1	A	590	PRO	2.7
1	A	771	LEU	2.7
1	A	412	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	413	PHE	2.6
1	A	426	ARG	2.6
1	A	625	GLY	2.5
1	A	588	LEU	2.5
1	A	589	LEU	2.5
1	A	556	LEU	2.5
1	A	587	LEU	2.4
1	A	405	LEU	2.4
1	A	428	ALA	2.4
1	A	554	LEU	2.4
1	A	548	LYS	2.4
1	A	452	VAL	2.3
1	A	681	VAL	2.3
1	A	502	ALA	2.3
1	A	560	ALA	2.2
1	A	489	LEU	2.2
1	A	488	LEU	2.1
1	A	470	ASP	2.1
1	A	626	GLY	2.1
1	A	482	HIS	2.1
1	A	666	LYS	2.1
1	A	463	VAL	2.1
1	A	615	VAL	2.1
1	A	753	LEU	2.1
1	A	497	ASN	2.1
1	A	735	TYR	2.0
1	A	721	LEU	2.0
1	A	406	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	CL	A	1010	1/1	0.94	0.13	-0.64	117,117,117,117	0
3	CL	A	1003	1/1	0.86	0.09	-2.51	104,104,104,104	0
3	CL	A	1009	1/1	0.71	0.22	-	136,136,136,136	0
3	CL	A	1006	1/1	0.77	0.09	-	121,121,121,121	0
3	CL	A	1008	1/1	0.90	0.38	-	145,145,145,145	0
3	CL	A	1005	1/1	0.89	0.15	-	140,140,140,140	0
3	CL	A	1002	1/1	0.74	0.29	-	112,112,112,112	0
3	CL	A	1004	1/1	0.83	0.11	-	136,136,136,136	0
2	BR	A	1001	1/1	0.97	0.26	-	122,122,122,122	0
3	CL	A	1007	1/1	0.97	0.05	-	139,139,139,139	0

## 6.5 Other polymers

There are no such residues in this entry.