



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:05 PM GMT

PDB ID : 1NI2  
Title : Structure of the active FERM domain of Ezrin  
Authors : Smith, W.J.; Nassar, N.; Bretscher, A.P.; Cerione, R.A.; Karplus, P.A.  
Deposited on : 2002-12-20  
Resolution : 2.30 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

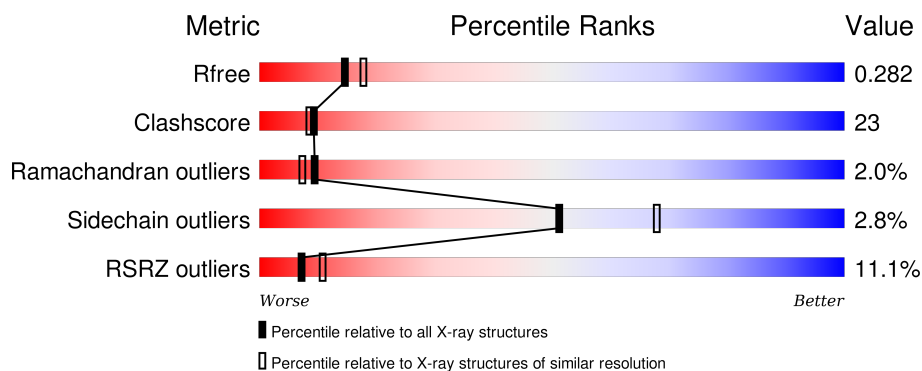
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	296	<div> <div>10%</div> <div>62%</div> <div>35%</div> <div>.</div> </div>
1	B	296	<div> <div>12%</div> <div>60%</div> <div>36%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5216 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 Ezrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2451	1588	416	438	9			
1	B	296	Total	C	N	O	S	0	0	0
			2457	1591	419	438	9			

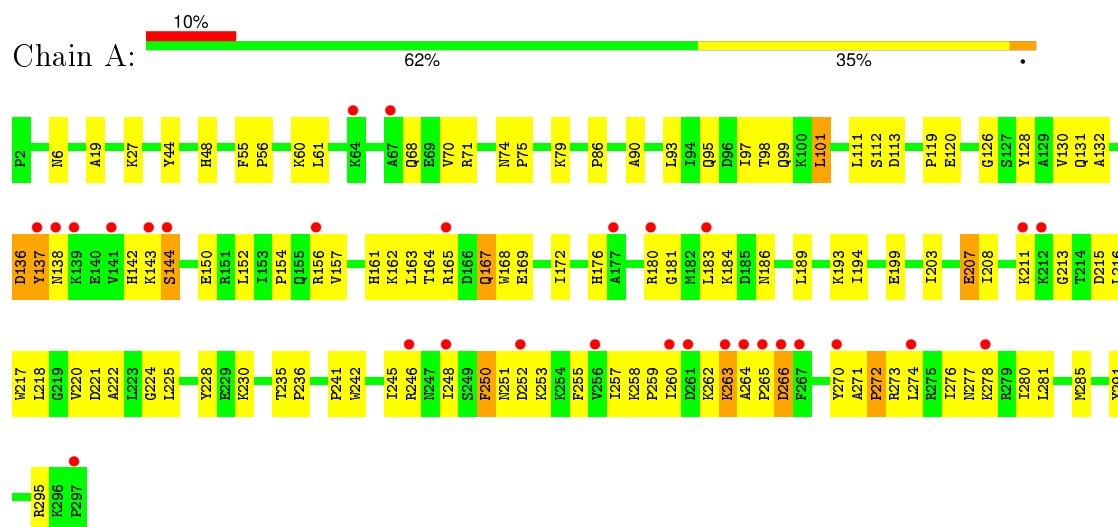
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	176	Total	O	0	0
			176	176		
2	B	132	Total	O	0	0
			132	132		

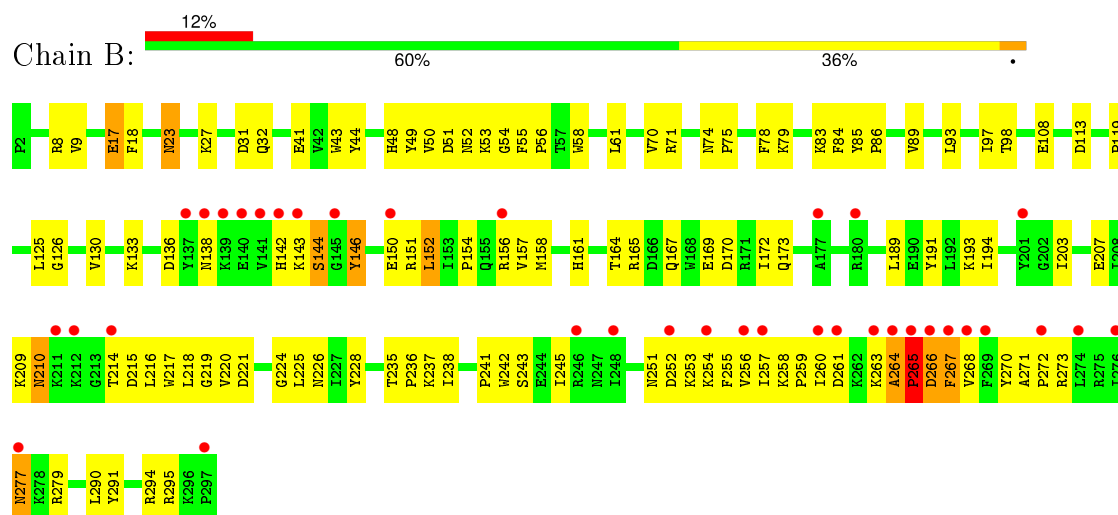
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Ezrin



#### • Molecule 1: Ezrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.49 Å 112.80 Å 66.30 Å 90.00° 102.32° 90.00°	Depositor
Resolution (Å)	25.86 – 2.30 36.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.9 (25.86-2.30) 89.4 (36.27-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.230 , 0.283 0.229 , 0.282	Depositor DCC
$R_{free}$ test set	2740 reflections (9.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 27658 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2104e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	1/2512 (0.0%)	0.70	0/3390
1	B	0.48	1/2518 (0.0%)	0.69	0/3397
All	All	0.48	2/5030 (0.0%)	0.69	0/6787

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	GLU	CD-OE2	5.64	1.31	1.25
1	A	207	GLU	CD-OE2	5.53	1.31	1.25

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	2451	0	2453	100	0
1	B	2457	0	2464	124	0
2	A	176	0	0	6	0
2	B	132	0	0	10	0
All	All	5216	0	4917	224	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 23.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:HA	1:B:165:ARG:HH22	1.17	1.04
1:A:138:ASN:H	1:A:142:HIS:CD2	1.82	0.98
1:A:138:ASN:H	1:A:142:HIS:HD2	1.04	0.93
1:A:6:ASN:HA	2:A:1253:HOH:O	1.69	0.92
1:B:138:ASN:H	1:B:142:HIS:HD2	1.07	0.92
1:B:138:ASN:H	1:B:142:HIS:CD2	1.91	0.88
1:A:259:PRO:HG2	1:A:264:ALA:HB3	1.62	0.79
1:B:75:PRO:HA	2:B:1318:HOH:O	1.82	0.79
1:B:150:GLU:HB3	1:B:152:LEU:HD11	1.65	0.79
1:A:262:LYS:HD2	1:A:263:LYS:H	1.48	0.78
1:B:254:LYS:HG3	1:B:268:VAL:HG11	1.65	0.78
1:B:256:VAL:HG22	1:B:268:VAL:HG22	1.67	0.77
1:A:274:LEU:HA	1:A:277:ASN:ND2	1.98	0.77
1:A:136:ASP:OD1	1:A:181:GLY:HA2	1.86	0.75
1:B:164:THR:OG1	1:B:167:GLN:HG3	1.88	0.73
1:B:150:GLU:O	1:B:152:LEU:HD13	1.87	0.73
1:B:8:ARG:HD3	2:B:1279:HOH:O	1.88	0.73
1:B:264:ALA:O	1:B:266:ASP:N	2.23	0.71
1:A:281:LEU:O	1:A:285:MET:HG3	1.88	0.71
1:B:32:GLN:HG3	2:B:1269:HOH:O	1.90	0.71
1:B:150:GLU:HB3	1:B:152:LEU:CD1	2.20	0.71
1:B:151:ARG:HA	1:B:165:ARG:NH2	1.99	0.70
1:B:125:LEU:HB3	1:B:191:TYR:CE1	2.27	0.70
1:A:274:LEU:HA	1:A:277:ASN:HD22	1.57	0.70
1:B:53:LYS:HB2	1:B:55:PHE:HD1	1.60	0.67
1:A:136:ASP:O	1:A:137:TYR:HB3	1.94	0.67
1:A:262:LYS:HD2	1:A:263:LYS:N	2.10	0.66
1:B:255:PHE:O	1:B:268:VAL:HA	1.97	0.64
1:B:264:ALA:O	1:B:265:PRO:C	2.35	0.64
1:A:207:GLU:CD	2:A:1307:HOH:O	2.36	0.64
1:A:271:ALA:HB3	1:A:277:ASN:OD1	1.98	0.63
1:B:154:PRO:HG2	1:B:157:VAL:CG2	2.28	0.63
1:A:138:ASN:O	1:A:142:HIS:HB2	1.99	0.63
1:A:138:ASN:N	1:A:142:HIS:HD2	1.88	0.63
1:A:274:LEU:O	1:A:278:LYS:HG3	1.98	0.63
1:A:183:LEU:HD12	1:A:186:ASN:ND2	2.14	0.62
1:B:48:HIS:HE1	1:B:79:LYS:HD2	1.65	0.62
1:A:255:PHE:CZ	1:A:277:ASN:HB3	2.36	0.61
1:B:83:LYS:HD3	1:B:84:PHE:CE1	2.36	0.61
1:B:108:GLU:HG3	2:B:1127:HOH:O	2.00	0.61
1:A:246:ARG:HB2	1:A:260:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ALA:CB	1:B:277:ASN:HD21	2.14	0.61
1:B:56:PRO:HD3	2:B:1213:HOH:O	2.01	0.61
1:A:255:PHE:HZ	1:A:277:ASN:HB3	1.65	0.60
1:A:136:ASP:O	1:A:137:TYR:CB	2.49	0.60
1:B:48:HIS:CE1	1:B:79:LYS:HD2	2.36	0.60
1:A:199:GLU:HG3	2:A:1306:HOH:O	1.99	0.60
1:A:154:PRO:HG2	1:A:157:VAL:CG2	2.32	0.60
1:A:48:HIS:CE1	1:A:79:LYS:HD2	2.37	0.60
1:B:267:PHE:HD2	1:B:267:PHE:H	1.48	0.60
1:A:217:TRP:HB2	1:A:228:TYR:HB2	1.84	0.59
1:B:17:GLU:HA	2:B:1317:HOH:O	2.03	0.59
1:A:86:PRO:HG2	1:A:93:LEU:HD21	1.84	0.59
1:B:273:ARG:HH11	1:B:273:ARG:HG3	1.67	0.59
1:A:143:LYS:O	1:A:144:SER:C	2.41	0.59
1:A:245:ILE:HD11	1:A:248:ILE:HB	1.85	0.59
1:B:271:ALA:HB3	1:B:277:ASN:ND2	2.17	0.59
1:B:241:PRO:O	1:B:245:ILE:HG22	2.02	0.59
1:A:165:ARG:O	1:A:169:GLU:HG3	2.03	0.59
1:B:89:VAL:HG23	2:B:1281:HOH:O	2.03	0.58
1:A:263:LYS:HD3	1:A:263:LYS:C	2.23	0.58
1:B:53:LYS:HB2	1:B:55:PHE:CD1	2.39	0.58
1:A:113:ASP:OD1	1:A:156:ARG:HB2	2.03	0.58
1:B:263:LYS:O	1:B:264:ALA:HB2	2.03	0.57
1:B:17:GLU:CA	2:B:1317:HOH:O	2.51	0.57
1:B:154:PRO:HG2	1:B:157:VAL:HG23	1.86	0.57
1:A:95:GLN:O	1:A:99:GLN:HG3	2.04	0.57
1:B:210:ASN:ND2	1:B:214:THR:H	2.02	0.57
1:B:18:PHE:N	2:B:1317:HOH:O	1.83	0.57
1:A:60:LYS:HD3	1:A:68:GLN:OE1	2.05	0.57
1:B:259:PRO:HD2	1:B:265:PRO:HG3	1.86	0.56
1:B:44:TYR:CE2	1:B:86:PRO:HG3	2.40	0.56
1:A:48:HIS:HE1	1:A:79:LYS:HD2	1.70	0.56
1:A:265:PRO:O	1:A:266:ASP:HB2	2.05	0.56
1:B:277:ASN:HD22	1:B:277:ASN:N	2.03	0.56
1:A:253:LYS:O	1:A:270:TYR:HA	2.05	0.56
1:B:277:ASN:ND2	1:B:277:ASN:N	2.54	0.55
1:A:274:LEU:HD12	1:A:277:ASN:HD22	1.70	0.55
1:B:271:ALA:HB3	1:B:277:ASN:HD21	1.72	0.55
1:B:113:ASP:OD1	1:B:156:ARG:HB2	2.06	0.55
1:B:210:ASN:HD21	1:B:214:THR:H	1.55	0.54
1:B:27:LYS:HD3	1:B:31:ASP:OD1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:TRP:HB2	1:B:228:TYR:HB2	1.90	0.54
1:B:164:THR:HG23	1:B:167:GLN:HE21	1.71	0.54
1:B:279:ARG:HB3	1:B:279:ARG:HH11	1.72	0.54
1:B:271:ALA:CB	1:B:277:ASN:ND2	2.71	0.54
1:A:19:ALA:HA	2:A:1253:HOH:O	2.08	0.54
1:B:243:SER:O	1:B:260:ILE:HG13	2.06	0.54
1:A:250:PHE:HB3	1:A:255:PHE:CD2	2.43	0.53
1:A:44:TYR:CE2	1:A:86:PRO:HG3	2.43	0.53
1:A:164:THR:OG1	1:A:167:GLN:HB2	2.07	0.53
1:B:273:ARG:NH1	1:B:273:ARG:HG3	2.21	0.53
1:B:150:GLU:O	1:B:165:ARG:NH2	2.42	0.52
1:A:132:ALA:O	1:A:184:LYS:HG2	2.09	0.52
1:B:44:TYR:CZ	1:B:86:PRO:HG3	2.45	0.52
1:A:272:PRO:HD2	2:A:1246:HOH:O	2.09	0.52
1:B:224:GLY:HA2	1:B:242:TRP:CE2	2.44	0.52
1:B:242:TRP:HA	1:B:245:ILE:CG2	2.40	0.51
1:A:163:LEU:HD22	1:A:167:GLN:HG2	1.92	0.51
1:A:162:LYS:O	1:A:163:LEU:HD23	2.10	0.51
1:B:126:GLY:O	1:B:130:VAL:HG23	2.09	0.51
1:B:210:ASN:N	1:B:210:ASN:HD22	2.07	0.51
1:B:226:ASN:HB3	1:B:236:PRO:HB3	1.93	0.51
1:A:224:GLY:HA2	1:A:242:TRP:CE2	2.45	0.51
1:A:220:VAL:HG22	1:A:225:LEU:CD2	2.41	0.51
1:A:90:ALA:HA	1:A:189:LEU:HD11	1.93	0.51
1:A:291:TYR:CE1	1:A:295:ARG:CZ	2.95	0.50
1:A:242:TRP:HA	1:A:245:ILE:CG2	2.41	0.50
1:A:44:TYR:CZ	1:A:86:PRO:HG3	2.47	0.50
1:B:252:ASP:OD1	1:B:253:LYS:HG3	2.11	0.50
1:B:138:ASN:O	1:B:142:HIS:HB2	2.12	0.50
1:B:210:ASN:H	1:B:210:ASN:ND2	2.10	0.50
1:B:257:ILE:O	1:B:257:ILE:HG13	2.10	0.50
1:A:250:PHE:HD2	1:A:250:PHE:H	1.60	0.50
1:A:27:LYS:HB2	1:A:61:LEU:O	2.11	0.50
1:B:150:GLU:C	1:B:152:LEU:HD13	2.32	0.50
1:A:259:PRO:HD3	1:A:266:ASP:OD1	2.12	0.50
1:A:252:ASP:O	1:A:253:LYS:HB2	2.12	0.50
1:B:50:VAL:CG1	1:B:54:GLY:HA2	2.42	0.50
1:A:6:ASN:HB3	1:A:75:PRO:HB3	1.92	0.49
1:B:277:ASN:ND2	1:B:277:ASN:H	2.09	0.49
1:A:152:LEU:HD13	1:A:172:ILE:HD13	1.94	0.49
1:B:23:ASN:H	1:B:23:ASN:HD22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:HA	1:A:280:ILE:HD12	1.94	0.49
1:B:146:TYR:H	1:B:146:TYR:HD1	1.59	0.49
1:B:143:LYS:O	1:B:144:SER:C	2.50	0.49
1:A:119:PRO:HG3	1:A:161:HIS:NE2	2.27	0.49
1:A:126:GLY:O	1:A:130:VAL:HG23	2.13	0.49
1:A:97:ILE:HG23	1:A:98:THR:N	2.28	0.48
1:B:220:VAL:HA	1:B:225:LEU:HD22	1.94	0.48
1:B:237:LYS:HG2	1:B:238:ILE:HG12	1.95	0.48
1:B:290:LEU:O	1:B:294:ARG:HG3	2.13	0.48
1:B:113:ASP:HB3	1:B:156:ARG:HH11	1.79	0.48
1:A:128:TYR:HE1	1:A:194:ILE:CD1	2.26	0.48
1:B:267:PHE:N	1:B:267:PHE:CD2	2.82	0.48
1:B:253:LYS:O	1:B:270:TYR:HA	2.14	0.48
1:B:210:ASN:H	1:B:210:ASN:HD22	1.62	0.47
1:B:8:ARG:HD2	1:B:17:GLU:OE1	2.14	0.47
1:A:183:LEU:HD12	1:A:186:ASN:HD21	1.78	0.47
1:A:113:ASP:HB3	1:A:156:ARG:HD2	1.95	0.47
1:B:164:THR:O	1:B:167:GLN:N	2.48	0.47
1:A:180:ARG:HG3	1:A:180:ARG:O	2.15	0.47
1:A:220:VAL:HA	1:A:225:LEU:HD23	1.97	0.47
1:A:154:PRO:HG2	1:A:157:VAL:HG23	1.97	0.46
1:B:242:TRP:HA	1:B:245:ILE:HG22	1.96	0.46
1:B:209:LYS:HA	1:B:214:THR:O	2.15	0.46
1:B:215:ASP:O	1:B:216:LEU:HD23	2.15	0.46
1:A:274:LEU:O	1:A:274:LEU:HG	2.14	0.46
1:B:267:PHE:N	1:B:267:PHE:HD2	2.13	0.46
1:A:242:TRP:HA	1:A:245:ILE:HG22	1.97	0.46
1:B:224:GLY:O	1:B:225:LEU:HD23	2.15	0.46
1:B:86:PRO:HG2	1:B:93:LEU:HD21	1.96	0.46
1:A:189:LEU:O	1:A:193:LYS:HG3	2.15	0.46
1:B:27:LYS:HB2	1:B:61:LEU:O	2.16	0.46
1:B:218:LEU:HG	1:B:219:GLY:N	2.30	0.46
1:A:241:PRO:O	1:A:245:ILE:HG22	2.16	0.46
1:B:49:TYR:CE2	1:B:70:VAL:HA	2.52	0.46
1:B:237:LYS:HG2	1:B:238:ILE:CG1	2.45	0.46
1:B:203:ILE:HG12	1:B:221:ASP:HB3	1.97	0.46
1:A:70:VAL:O	1:A:71:ARG:C	2.55	0.45
1:A:203:ILE:HG12	1:A:221:ASP:HB3	1.97	0.45
1:B:291:TYR:CE1	1:B:295:ARG:CZ	3.00	0.45
1:A:208:ILE:HD13	1:A:218:LEU:HB2	1.98	0.45
1:B:271:ALA:HB1	1:B:277:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ILE:HG23	1:B:98:THR:N	2.32	0.45
1:B:119:PRO:HG3	1:B:161:HIS:CE1	2.52	0.45
1:A:215:ASP:O	1:A:216:LEU:HD23	2.17	0.44
1:A:248:ILE:HD13	1:A:257:ILE:HG12	1.99	0.44
1:B:152:LEU:HD23	1:B:172:ILE:HD13	1.99	0.44
1:B:48:HIS:CG	2:B:1114:HOH:O	2.71	0.44
1:B:74:ASN:HA	1:B:75:PRO:HA	1.71	0.44
1:B:235:THR:HA	1:B:236:PRO:HD3	1.83	0.44
1:B:189:LEU:HG	1:B:193:LYS:HE3	1.99	0.44
1:B:9:VAL:HG22	1:B:78:PHE:HB2	2.00	0.43
1:A:19:ALA:CA	2:A:1253:HOH:O	2.66	0.43
1:B:41:GLU:HA	1:B:43:TRP:CZ2	2.53	0.43
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.84	0.43
1:A:74:ASN:HA	1:A:75:PRO:HA	1.70	0.43
1:B:242:TRP:CE3	1:B:242:TRP:HA	2.54	0.43
1:A:235:THR:HA	1:A:236:PRO:HD3	1.82	0.43
1:A:211:LYS:C	1:A:213:GLY:H	2.22	0.43
1:A:220:VAL:HG22	1:A:225:LEU:HD22	2.01	0.43
1:B:133:LYS:HD3	1:B:150:GLU:OE2	2.19	0.42
1:B:258:LYS:HA	1:B:259:PRO:HD3	1.86	0.42
1:B:50:VAL:HG11	1:B:71:ARG:NH1	2.34	0.42
1:A:6:ASN:HD22	1:A:74:ASN:HD21	1.66	0.42
1:A:271:ALA:HA	1:A:272:PRO:HD3	1.78	0.42
1:B:51:ASP:O	1:B:53:LYS:N	2.52	0.42
1:B:89:VAL:HG13	1:B:93:LEU:HD12	2.01	0.42
1:B:210:ASN:ND2	1:B:210:ASN:N	2.67	0.42
1:B:263:LYS:O	1:B:264:ALA:CB	2.68	0.42
1:B:23:ASN:HD22	1:B:23:ASN:N	2.15	0.42
1:B:146:TYR:CD1	1:B:146:TYR:N	2.88	0.42
1:A:217:TRP:CD1	1:A:230:LYS:HA	2.55	0.42
1:A:112:SER:O	1:A:113:ASP:HB2	2.20	0.42
1:B:167:GLN:O	1:B:170:ASP:HB2	2.20	0.41
1:B:259:PRO:HD3	1:B:265:PRO:HA	2.02	0.41
1:B:224:GLY:C	1:B:225:LEU:HD23	2.40	0.41
1:B:279:ARG:CB	1:B:279:ARG:NH1	2.83	0.41
1:B:138:ASN:N	1:B:142:HIS:CD2	2.73	0.41
1:B:70:VAL:O	1:B:71:ARG:C	2.58	0.41
1:B:169:GLU:O	1:B:173:GLN:HG3	2.19	0.41
1:A:131:GLN:NE2	1:A:131:GLN:HA	2.35	0.41
1:B:125:LEU:HD21	1:B:194:ILE:HB	2.03	0.41
1:B:85:TYR:HA	1:B:86:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:HIS:HB3	1:B:58:TRP:CE3	2.56	0.41
1:B:259:PRO:HB2	1:B:261:ASP:O	2.21	0.41
1:A:215:ASP:HB3	1:A:230:LYS:HE3	2.01	0.41
1:A:259:PRO:HG2	1:A:264:ALA:CB	2.42	0.41
1:A:272:PRO:HB2	1:A:273:ARG:H	1.64	0.41
1:A:246:ARG:N	1:A:258:LYS:O	2.50	0.41
1:A:150:GLU:HG2	1:A:152:LEU:HD21	2.02	0.41
1:A:119:PRO:HG3	1:A:161:HIS:CE1	2.56	0.41
1:B:164:THR:HG23	1:B:167:GLN:NE2	2.36	0.41
1:A:222:ALA:O	1:A:242:TRP:CD1	2.73	0.41
1:B:50:VAL:HG11	1:B:71:ARG:HH11	1.85	0.41
1:A:55:PHE:HA	1:A:56:PRO:HD3	1.80	0.40
1:A:101:LEU:HD12	1:A:101:LEU:HA	1.85	0.40
1:B:158:MET:HE1	1:B:165:ARG:HH11	1.86	0.40
1:A:168:TRP:O	1:A:169:GLU:C	2.60	0.40
1:A:137:TYR:HB2	1:A:176:HIS:NE2	2.37	0.40
1:A:259:PRO:CD	1:A:266:ASP:OD1	2.68	0.40
1:A:276:ILE:HG22	1:A:280:ILE:HD11	2.03	0.40
1:A:111:LEU:HD23	1:A:111:LEU:HA	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	294/296 (99%)	269 (92%)	20 (7%)	5 (2%)	11	10
1	B	294/296 (99%)	270 (92%)	17 (6%)	7 (2%)	7	5
All	All	588/592 (99%)	539 (92%)	37 (6%)	12 (2%)	9	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	TYR
1	A	263	LYS
1	A	272	PRO
1	B	264	ALA
1	B	265	PRO
1	B	266	ASP
1	B	272	PRO
1	B	52	ASN
1	A	266	ASP
1	A	144	SER
1	B	251	ASN
1	B	144	SER

### 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	263/267 (98%)	257 (98%)	6 (2%)	58	75
1	B	264/267 (99%)	255 (97%)	9 (3%)	44	59
All	All	527/534 (99%)	512 (97%)	15 (3%)	51	68

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	120	GLU
1	A	136	ASP
1	A	167	GLN
1	A	250	PHE
1	A	251	ASN
1	B	17	GLU
1	B	23	ASN
1	B	136	ASP
1	B	146	TYR
1	B	152	LEU
1	B	210	ASN

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Mol	Chain	Res	Type
1	B	265	PRO
1	B	267	PHE
1	B	277	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	32	GLN
1	A	131	GLN
1	A	142	HIS
1	A	160	GLN
1	A	186	ASN
1	A	251	ASN
1	A	277	ASN
1	B	6	ASN
1	B	23	ASN
1	B	48	HIS
1	B	99	GLN
1	B	131	GLN
1	B	142	HIS
1	B	167	GLN
1	B	176	HIS
1	B	179	HIS
1	B	210	ASN
1	B	277	ASN
1	B	282	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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, 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	296/296 (100%)	0.63	30 (10%) 9 13	25, 51, 94, 123	0
1	B	296/296 (100%)	0.78	36 (12%) 5 9	27, 52, 103, 119	0
All	All	592/592 (100%)	0.70	66 (11%) 7 11	25, 52, 99, 123	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ASP	10.0
1	B	268	VAL	8.8
1	B	263	LYS	6.7
1	B	140	GLU	6.6
1	A	141	VAL	6.5
1	B	260	ILE	6.2
1	A	265	PRO	5.6
1	A	263	LYS	5.2
1	B	137	TYR	5.0
1	B	248	ILE	4.9
1	A	264	ALA	4.6
1	A	139	LYS	4.3
1	A	260	ILE	4.3
1	A	267	PHE	4.3
1	B	264	ALA	4.2
1	A	266	ASP	4.2
1	B	246	ARG	4.1
1	A	297	PRO	4.0
1	B	139	LYS	4.0
1	B	257	ILE	4.0
1	B	267	PHE	3.9
1	A	180	ARG	3.8
1	B	141	VAL	3.8
1	B	214	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	212	LYS	3.2
1	B	211	LYS	3.2
1	A	165	ARG	3.2
1	B	261	ASP	3.2
1	B	297	PRO	3.1
1	B	256	VAL	3.1
1	A	274	LEU	3.1
1	A	261	ASP	3.0
1	A	256	VAL	3.0
1	B	180	ARG	3.0
1	B	274	LEU	3.0
1	B	212	LYS	2.9
1	B	142	HIS	2.8
1	B	177	ALA	2.8
1	B	138	ASN	2.8
1	A	246	ARG	2.8
1	A	143	LYS	2.8
1	B	143	LYS	2.8
1	A	248	ILE	2.7
1	A	137	TYR	2.7
1	A	211	LYS	2.7
1	A	183	LEU	2.7
1	B	252	ASP	2.7
1	A	64	LYS	2.6
1	B	254	LYS	2.5
1	A	144	SER	2.4
1	A	252	ASP	2.4
1	B	265	PRO	2.4
1	B	145	GLY	2.3
1	B	269	PHE	2.2
1	A	278	LYS	2.2
1	B	277	ASN	2.2
1	A	67	ALA	2.2
1	B	150	GLU	2.1
1	A	138	ASN	2.1
1	B	272	PRO	2.1
1	A	177	ALA	2.1
1	B	276	ILE	2.1
1	A	156	ARG	2.0
1	A	270	TYR	2.0
1	B	156	ARG	2.0
1	B	201	TYR	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.