



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID : 4FDD  
Title : Crystal structure of KAP beta2-PY-NLS  
Authors : Zhang, Z.C.; Chook, Y.M.  
Deposited on : 2012-05-28  
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

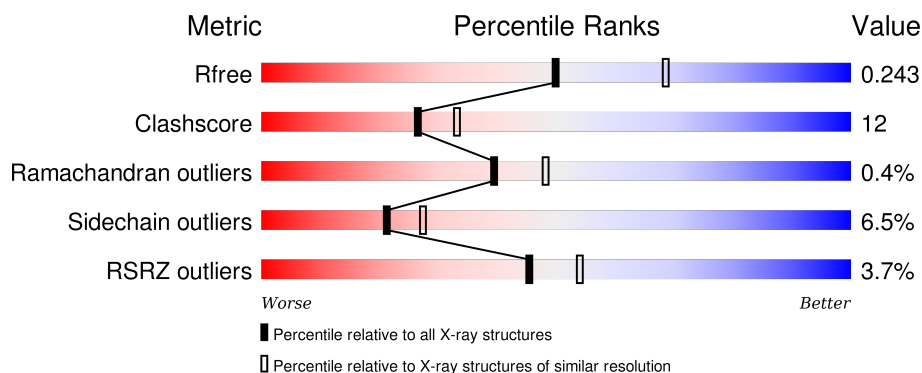
# 1 Overall quality at a glance

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	852	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
2	B	29	<div> <div>3%</div> <div>59%</div> <div>10%</div> <div>31%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6969 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 Transportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6652	4267	1109	1225	51			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	GLY	-	LINKER	UNP Q92973
A	363	GLY	-	LINKER	UNP Q92973
A	364	SER	-	LINKER	UNP Q92973
A	365	GLY	-	LINKER	UNP Q92973
A	366	GLY	-	LINKER	UNP Q92973

- Molecule 2 is a protein called RNA-binding protein FUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	S	0	0	0
			169	98	39	31	1			

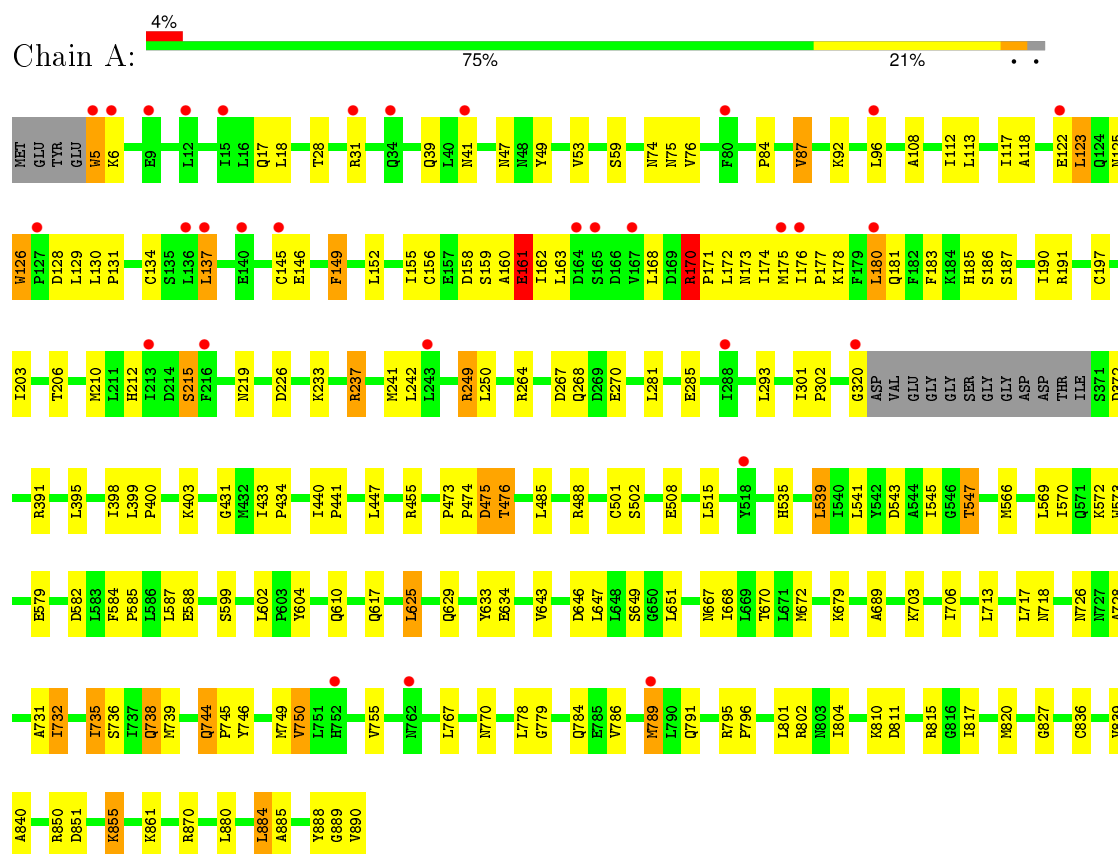
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	7	Total	O	0	0
			7	7		

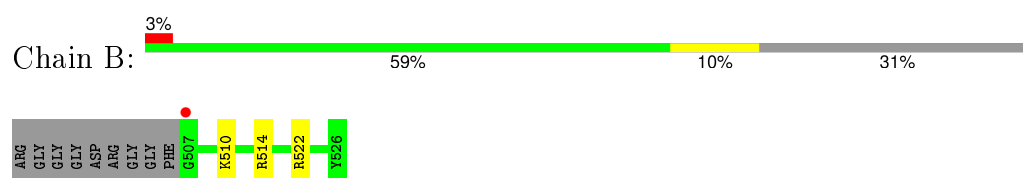
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: Transportin-1



#### • Molecule 2: RNA-binding protein FUS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.72Å 157.25Å 67.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.61 – 2.30 48.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (99.61-2.30) 97.5 (48.55-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.245 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	3055 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60430 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.51	2/6795 (0.0%)	0.59	0/9229
2	B	0.55	0/172	0.72	0/226
All	All	0.51	2/6967 (0.0%)	0.60	0/9455

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	TRP	CD2-CE2	5.18	1.47	1.41
1	A	5	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6652	0	6712	167	0
2	B	169	0	158	3	0
3	A	141	0	0	34	0
3	B	7	0	0	1	0
All	All	6969	0	6870	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (167) 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:732:ILE:HB	3:A:956:HOH:O	1.38	1.19
1:A:163:LEU:HB2	1:A:172:LEU:HD22	1.36	1.07
1:A:160:ALA:O	1:A:161:GLU:HB3	1.61	1.00
1:A:839:VAL:HB	3:A:1008:HOH:O	1.63	0.98
1:A:726:ASN:HD21	1:A:770:ASN:HD22	1.05	0.97
1:A:185:HIS:HD2	1:A:187:SER:H	1.15	0.93
1:A:203:ILE:HD11	1:A:241:MET:HG2	1.46	0.93
1:A:885:ALA:HB2	3:A:985:HOH:O	1.69	0.92
1:A:145:CYS:HB2	3:A:938:HOH:O	1.70	0.92
1:A:117:ILE:HG22	1:A:122:GLU:HG3	1.54	0.89
1:A:779:GLY:HA2	1:A:786:VAL:HG11	1.55	0.88
1:A:617:GLN:HE21	1:A:667:ASN:HD21	1.22	0.87
1:A:779:GLY:HA2	1:A:786:VAL:CG1	2.06	0.85
1:A:836:CYS:HA	3:A:1008:HOH:O	1.77	0.85
1:A:5:TRP:CG	1:A:6:LYS:N	2.44	0.85
1:A:146:GLU:HG2	3:A:989:HOH:O	1.75	0.83
1:A:162:ILE:HB	1:A:172:LEU:HD11	1.61	0.81
1:A:566:MET:HE2	1:A:566:MET:HA	1.61	0.81
1:A:197:CYS:SG	3:A:991:HOH:O	2.38	0.81
1:A:118:ALA:HA	1:A:122:GLU:HB2	1.62	0.80
1:A:572:LYS:HG3	3:A:947:HOH:O	1.80	0.80
1:A:372:ASP:HB2	3:A:942:HOH:O	1.85	0.77
1:A:163:LEU:HA	3:A:962:HOH:O	1.85	0.76
1:A:175:MET:HB2	3:A:967:HOH:O	1.86	0.73
1:A:566:MET:CE	1:A:569:LEU:HD12	2.18	0.73
1:A:92:LYS:HE2	1:A:122:GLU:OE2	1.89	0.73
1:A:566:MET:HA	1:A:566:MET:CE	2.19	0.72
1:A:738:GLN:HE21	1:A:738:GLN:HA	1.55	0.72
1:A:41:ASN:HB3	3:A:924:HOH:O	1.89	0.72
1:A:212:HIS:HA	3:A:993:HOH:O	1.91	0.71
1:A:726:ASN:ND2	1:A:770:ASN:HD22	1.84	0.70
1:A:744:GLN:HG2	1:A:745:PRO:HD3	1.73	0.70
1:A:163:LEU:HG	1:A:206:THR:HG23	1.74	0.69
1:A:547:THR:HB	3:B:603:HOH:O	1.91	0.68
1:A:779:GLY:CA	1:A:786:VAL:HG11	2.22	0.68
1:A:155:ILE:O	1:A:159:SER:HB2	1.93	0.68
1:A:156:CYS:SG	3:A:1031:HOH:O	2.51	0.67
1:A:122:GLU:O	1:A:123:LEU:C	2.32	0.67
1:A:163:LEU:CB	1:A:172:LEU:HD22	2.19	0.67
1:A:502:SER:HB3	2:B:522:ARG:HG2	1.77	0.66
1:A:804:ILE:HG13	1:A:810:LYS:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:CG2	1:A:122:GLU:HG3	2.25	0.65
1:A:47:ASN:HD21	1:A:75:ASN:HD22	1.42	0.65
1:A:889:GLY:HA3	3:A:1034:HOH:O	1.94	0.65
1:A:617:GLN:NE2	1:A:667:ASN:HD21	1.94	0.64
1:A:566:MET:HE1	1:A:569:LEU:HD12	1.78	0.64
1:A:171:PRO:HD2	3:A:962:HOH:O	1.96	0.64
1:A:320:GLY:HA2	3:A:1014:HOH:O	1.97	0.63
1:A:174:ILE:O	1:A:178:LYS:HG2	1.99	0.63
1:A:861:LYS:HD2	3:A:944:HOH:O	1.98	0.63
1:A:447:LEU:O	1:A:455:ARG:HG2	2.00	0.62
1:A:689:ALA:HB1	2:B:510:LYS:HD2	1.81	0.61
1:A:28:THR:HG22	1:A:31:ARG:HH11	1.64	0.61
1:A:180:LEU:HA	1:A:183:PHE:CD2	2.36	0.60
1:A:130:LEU:HB2	1:A:131:PRO:HD3	1.83	0.60
1:A:47:ASN:ND2	1:A:75:ASN:HD22	1.99	0.59
1:A:76:VAL:HG12	1:A:76:VAL:O	2.01	0.59
1:A:28:THR:HG22	1:A:31:ARG:NH1	2.19	0.58
1:A:249:ARG:HG3	3:A:997:HOH:O	2.04	0.58
1:A:566:MET:HE2	1:A:569:LEU:HD12	1.86	0.57
1:A:395:LEU:HD11	1:A:431:GLY:HA3	1.86	0.57
1:A:543:ASP:O	1:A:547:THR:HG22	2.04	0.57
1:A:187:SER:OG	1:A:190:ILE:HD13	2.04	0.57
1:A:736:SER:OG	1:A:778:LEU:HD23	2.05	0.56
1:A:755:VAL:HG21	1:A:789:MET:HG2	1.87	0.56
1:A:185:HIS:CD2	1:A:187:SER:H	2.07	0.56
1:A:117:ILE:HG22	1:A:122:GLU:CG	2.33	0.56
1:A:713:LEU:HD13	1:A:732:ILE:HG23	1.87	0.56
1:A:850:ARG:NH2	3:A:949:HOH:O	2.40	0.55
1:A:108:ALA:O	1:A:112:ILE:HG12	2.07	0.55
1:A:584:PHE:HB2	1:A:585:PRO:HD3	1.88	0.55
1:A:197:CYS:SG	3:A:1031:HOH:O	2.57	0.54
1:A:391:ARG:HD2	3:A:1038:HOH:O	2.07	0.54
1:A:268:GLN:H	1:A:268:GLN:CD	2.10	0.54
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.89	0.54
1:A:203:ILE:HD11	1:A:241:MET:CG	2.28	0.54
1:A:84:PRO:HG2	1:A:87:VAL:HG12	1.88	0.54
1:A:713:LEU:HD13	1:A:732:ILE:CG2	2.38	0.54
1:A:717:LEU:HD21	1:A:732:ILE:HD11	1.90	0.54
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.90	0.53
1:A:726:ASN:HD21	1:A:770:ASN:ND2	1.90	0.53
1:A:395:LEU:CD1	1:A:431:GLY:HA3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:CG2	1:A:122:GLU:CG	2.87	0.52
1:A:92:LYS:HD3	1:A:126:TRP:CD2	2.44	0.52
1:A:92:LYS:HD3	1:A:126:TRP:CE2	2.45	0.51
1:A:301:ILE:HB	1:A:302:PRO:HD3	1.93	0.51
1:A:212:HIS:HD2	3:A:932:HOH:O	1.92	0.51
1:A:134:CYS:O	1:A:137:LEU:HB2	2.11	0.51
1:A:744:GLN:HG2	1:A:745:PRO:CD	2.41	0.51
1:A:732:ILE:CB	3:A:956:HOH:O	2.21	0.50
1:A:233:LYS:NZ	1:A:237:ARG:HD2	2.27	0.50
1:A:718:ASN:ND2	3:A:998:HOH:O	2.30	0.50
1:A:433:ILE:HB	1:A:434:PRO:HD3	1.93	0.50
1:A:811:ASP:OD2	1:A:815:ARG:NH1	2.45	0.50
1:A:728:ALA:O	1:A:732:ILE:HG12	2.12	0.49
1:A:543:ASP:O	1:A:547:THR:CG2	2.60	0.49
1:A:668:ILE:HG13	1:A:672:MET:CE	2.41	0.49
1:A:212:HIS:CD2	3:A:932:HOH:O	2.64	0.49
1:A:210:MET:HA	1:A:210:MET:HE2	1.93	0.49
1:A:795:ARG:HB2	1:A:796:PRO:CD	2.43	0.48
1:A:17:GLN:HA	3:A:977:HOH:O	2.13	0.48
1:A:156:CYS:O	1:A:160:ALA:HB2	2.12	0.48
1:A:791:GLN:HG3	1:A:827:GLY:HA2	1.94	0.48
1:A:5:TRP:CD1	1:A:6:LYS:N	2.78	0.48
1:A:49:TYR:O	1:A:53:VAL:HG23	2.14	0.48
1:A:884:LEU:HA	1:A:888:TYR:HD2	1.79	0.47
1:A:47:ASN:HD21	1:A:75:ASN:ND2	2.12	0.47
1:A:717:LEU:HD11	1:A:750:VAL:HG22	1.97	0.47
1:A:668:ILE:HG13	1:A:672:MET:HE3	1.97	0.47
1:A:181:GLN:N	1:A:181:GLN:OE1	2.46	0.47
1:A:84:PRO:HG2	1:A:87:VAL:CG1	2.44	0.47
1:A:746:TYR:O	1:A:749:MET:HG2	2.14	0.47
1:A:473:PRO:O	1:A:476:THR:HG23	2.14	0.47
1:A:399:LEU:N	1:A:400:PRO:HD2	2.30	0.47
1:A:176:ILE:HB	1:A:177:PRO:HD3	1.97	0.47
1:A:178:LYS:HE3	3:A:952:HOH:O	2.16	0.46
1:A:647:LEU:HD12	1:A:647:LEU:O	2.16	0.46
1:A:76:VAL:CG1	1:A:76:VAL:O	2.63	0.46
1:A:163:LEU:HD22	1:A:170:ARG:HE	1.81	0.46
1:A:703:LYS:HG3	1:A:739:MET:HE3	1.97	0.46
1:A:535:HIS:NE2	1:A:582:ASP:OD2	2.49	0.46
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.97	0.45
1:A:74:ASN:HB2	3:A:957:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:O	1:A:545:ILE:HG12	2.17	0.45
1:A:210:MET:CE	1:A:210:MET:HA	2.46	0.45
1:A:475:ASP:HB2	3:A:1003:HOH:O	2.16	0.45
1:A:185:HIS:CD2	1:A:186:SER:N	2.85	0.45
1:A:795:ARG:HB2	1:A:796:PRO:HD3	1.98	0.45
1:A:168:LEU:HD23	1:A:171:PRO:HB3	1.98	0.45
1:A:6:LYS:O	1:A:6:LYS:HG2	2.17	0.44
1:A:726:ASN:HD22	1:A:767:LEU:HA	1.82	0.44
1:A:570:ILE:HD11	1:A:604:TYR:CD1	2.53	0.44
1:A:570:ILE:O	1:A:573:TRP:HB3	2.18	0.44
1:A:270:GLU:HA	3:A:1006:HOH:O	2.17	0.44
1:A:735:ILE:HG13	1:A:736:SER:N	2.32	0.44
1:A:155:ILE:O	1:A:159:SER:CB	2.64	0.43
1:A:731:ALA:O	1:A:735:ILE:HG23	2.18	0.43
1:A:122:GLU:HB3	1:A:126:TRP:HB2	2.00	0.43
1:A:473:PRO:HA	1:A:474:PRO:HD2	1.86	0.43
1:A:149:PHE:CD1	3:A:991:HOH:O	2.57	0.43
1:A:264:ARG:O	1:A:267:ASP:HB2	2.18	0.43
1:A:149:PHE:CE2	1:A:190:ILE:HG23	2.53	0.43
1:A:840:ALA:HB2	1:A:880:LEU:HD13	2.00	0.43
1:A:128:ASP:OD1	1:A:128:ASP:N	2.50	0.43
1:A:162:ILE:HB	1:A:172:LEU:CD1	2.41	0.42
1:A:625:LEU:HD22	1:A:633:TYR:CD1	2.53	0.42
1:A:599:SER:HB3	3:A:1013:HOH:O	2.18	0.42
1:A:96:LEU:HD11	1:A:126:TRP:HZ2	1.84	0.42
1:A:233:LYS:HZ2	1:A:237:ARG:HD2	1.84	0.42
1:A:122:GLU:O	1:A:125:ASN:N	2.53	0.41
1:A:588:GLU:HG2	2:B:514:ARG:HG3	2.02	0.41
1:A:149:PHE:HA	1:A:152:LEU:HD12	2.02	0.41
1:A:191:ARG:NH1	1:A:226:ASP:OD2	2.53	0.41
1:A:173:ASN:N	1:A:173:ASN:HD22	2.18	0.41
1:A:163:LEU:HB2	1:A:172:LEU:CD2	2.26	0.41
1:A:706:ILE:HD12	1:A:735:ILE:HD13	2.02	0.41
1:A:215:SER:O	1:A:219:ASN:ND2	2.41	0.41
1:A:539:LEU:HG	1:A:585:PRO:HG2	2.02	0.41
1:A:795:ARG:CB	1:A:796:PRO:CD	2.99	0.41
1:A:174:ILE:HD12	1:A:174:ILE:N	2.36	0.40
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.96	0.40
1:A:74:ASN:HB3	3:A:1030:HOH:O	2.22	0.40
1:A:587:LEU:HB2	1:A:643:VAL:CG1	2.50	0.40
1:A:851:ASP:O	1:A:855:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:CD2	1:A:129:LEU:HB2	2.57	0.40
1:A:744:GLN:N	1:A:745:PRO:HD2	2.37	0.40
1:A:817:ILE:HA	1:A:820:MET:HE3	2.03	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	832/852 (98%)	792 (95%)	37 (4%)	3 (0%)	39	48
2	B	18/29 (62%)	18 (100%)	0	0	100	100
All	All	850/881 (96%)	810 (95%)	37 (4%)	3 (0%)	39	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LEU
1	A	161	GLU
1	A	170	ARG

### 5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/762 (98%)	699 (93%)	50 (7%)	20	26
2	B	17/21 (81%)	17 (100%)	0	100	100
All	All	766/783 (98%)	716 (94%)	50 (6%)	21	27

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	39	GLN
1	A	59	SER
1	A	87	VAL
1	A	113	LEU
1	A	137	LEU
1	A	149	PHE
1	A	158	ASP
1	A	161	GLU
1	A	170	ARG
1	A	180	LEU
1	A	215	SER
1	A	237	ARG
1	A	242	LEU
1	A	249	ARG
1	A	250	LEU
1	A	281	LEU
1	A	285	GLU
1	A	293	LEU
1	A	403	LYS
1	A	475	ASP
1	A	476	THR
1	A	485	LEU
1	A	488	ARG
1	A	501	CYS
1	A	539	LEU
1	A	547	THR
1	A	579	GLU
1	A	602	LEU
1	A	610	GLN
1	A	625	LEU
1	A	629	GLN

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Mol	Chain	Res	Type
1	A	634	GLU
1	A	646	ASP
1	A	649	SER
1	A	670	THR
1	A	679	LYS
1	A	732	ILE
1	A	735	ILE
1	A	738	GLN
1	A	744	GLN
1	A	750	VAL
1	A	784	GLN
1	A	789	MET
1	A	801	LEU
1	A	802	ARG
1	A	855	LYS
1	A	870	ARG
1	A	884	LEU
1	A	890	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	23	GLN
1	A	47	ASN
1	A	74	ASN
1	A	79	HIS
1	A	98	ASN
1	A	173	ASN
1	A	185	HIS
1	A	199	ASN
1	A	255	HIS
1	A	256	ASN
1	A	571	GLN
1	A	617	GLN
1	A	685	GLN
1	A	726	ASN
1	A	738	GLN
1	A	803	ASN
1	A	862	ASN

### 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](#)

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, 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	836/852 (98%)	0.43	31 (3%) 45 54	40, 67, 103, 155	0
2	B	20/29 (68%)	0.36	1 (5%) 32 41	41, 61, 87, 90	0
All	All	856/881 (97%)	0.43	32 (3%) 45 54	40, 67, 103, 155	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LYS	8.3
1	A	167	VAL	5.5
1	A	122	GLU	5.1
1	A	137	LEU	4.6
1	A	165	SER	4.4
1	A	175	MET	4.2
1	A	789	MET	3.7
1	A	176	ILE	3.6
1	A	5	TRP	3.5
1	A	213	ILE	3.1
1	A	12	LEU	2.8
1	A	164	ASP	2.8
1	A	15	ILE	2.8
1	A	9	GLU	2.7
1	A	41	ASN	2.7
1	A	136	LEU	2.6
1	A	243	LEU	2.5
1	A	752	HIS	2.4
1	A	518	TYR	2.4
2	B	507	GLY	2.3
1	A	31	ARG	2.3
1	A	288	ILE	2.3
1	A	762	ASN	2.3
1	A	216	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	320	GLY	2.3
1	A	80	PHE	2.3
1	A	96	LEU	2.2
1	A	145	CYS	2.2
1	A	34	GLN	2.2
1	A	140	GLU	2.2
1	A	180	LEU	2.1
1	A	127	PRO	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 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.