



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:44 PM UTC

PDB ID : 4FDD / pdb\_00004fdd  
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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

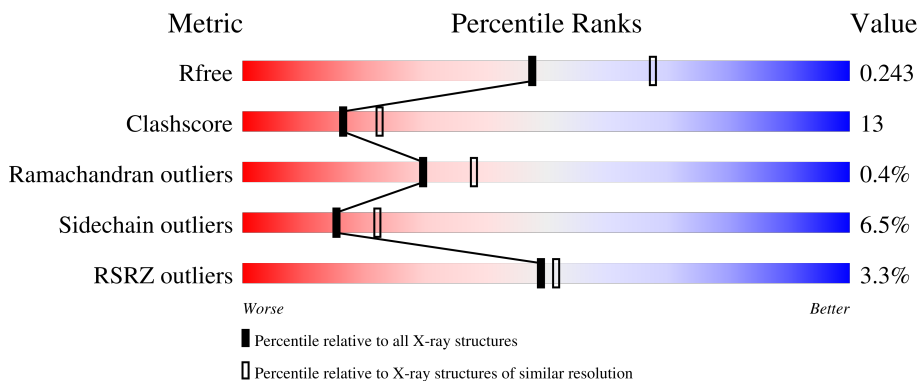
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

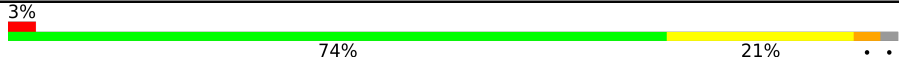

The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	852	 3% 74% 21% ..
2	B	29	 7% 59% 10% 31%

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	836	6652	4267	1109	1225	51	0	0	0

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
			Total	C	N	O	S			
2	B	20	169	98	39	31	1	0	0	0

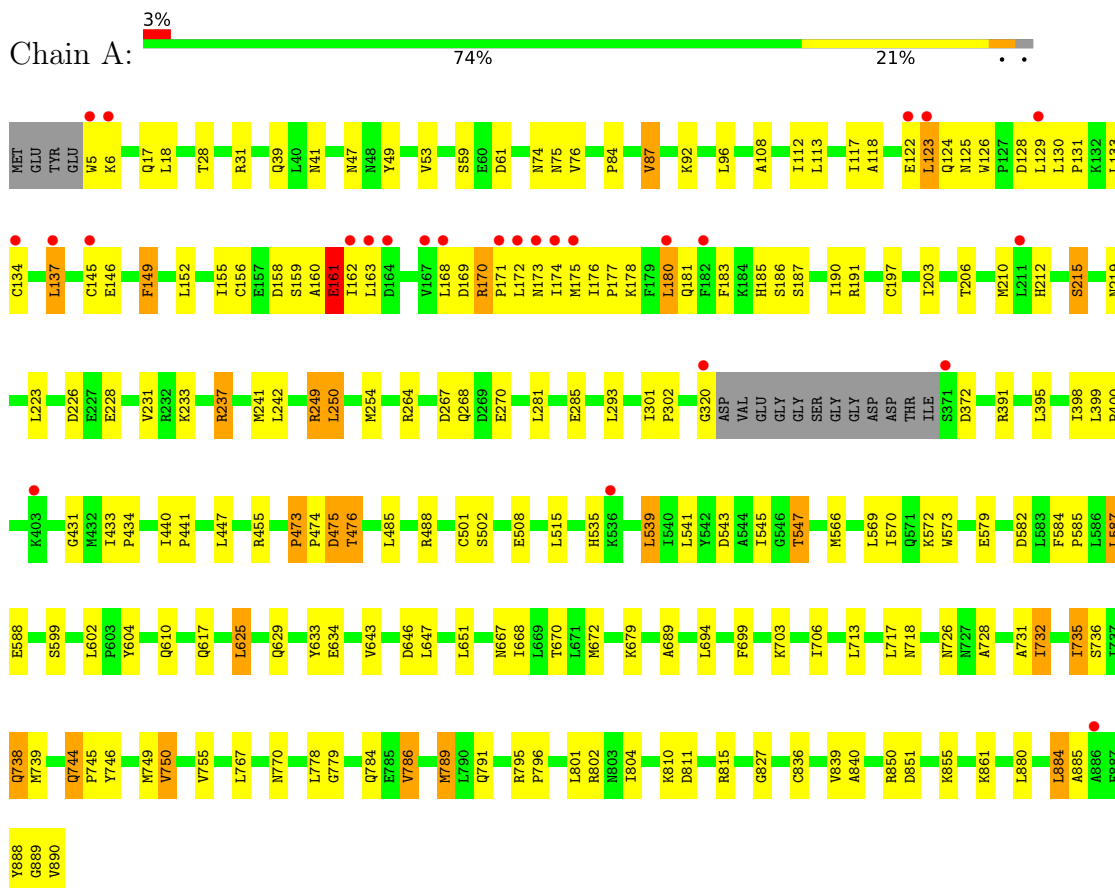
- Molecule 3 is water.

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

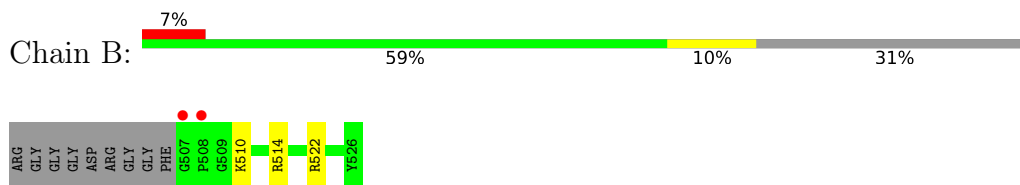
### 3 Residue-property plots

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: 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 99.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (99.61-2.30) 97.7 (99.61-2.30)	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)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.208 , 0.245 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	3061 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtrriage
Anisotropy	0.504	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.66	0/6795	0.89	4/9229 (0.0%)
2	B	0.81	0/172	0.92	0/226
All	All	0.66	0/6967	0.89	4/9455 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	PRO	CA-C-N	5.21	125.25	119.32
1	A	473	PRO	C-N-CA	5.21	125.25	119.32
1	A	228	GLU	CA-C-N	5.12	124.56	119.24
1	A	228	GLU	C-N-CA	5.12	124.56	119.24

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	177	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	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 13.

All (177) 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:5:TRP:CG	1:A:6:LYS:H	1.72	1.06
1:A:566:MET:HE2	1:A:566:MET:HA	1.39	1.03
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:566:MET:HE1	1:A:569:LEU:HD12	1.52	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: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: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:210:MET:HA	1:A:210:MET:HE2	1.65	0.79
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:5:TRP:CG	1:A:6:LYS:N	2.44	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:699:PHE:HZ	1:A:739:MET:HE3	1.53	0.73
1:A:92:LYS:HE2	1:A:122:GLU:OE2	1.89	0.73
1:A:5:TRP:CD1	1:A:6:LYS:H	2.06	0.72
1:A:738:GLN:HE21	1:A:738:GLN:HA	1.55	0.72
1:A:122:GLU:O	1:A:123:LEU:C	2.32	0.72
1:A:699:PHE:CZ	1:A:739:MET:HE3	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:171:PRO:HD2	3:A:962:HOH:O	1.96	0.64
1:A:174:ILE:O	1:A:178:LYS:HG2	1.99	0.63
1:A:320:GLY:HA2	3:A:1014:HOH:O	1.97	0.63
1:A:668:ILE:HG13	1:A:672:MET:HE2	1.81	0.63
1:A:566:MET:HA	1:A:566:MET:CE	2.19	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:233:LYS:HZ2	1:A:237:ARG:HD2	1.67	0.59
1:A:47:ASN:ND2	1:A:75:ASN:HD22	1.99	0.59
1:A:268:GLN:H	1:A:268:GLN:CD	2.10	0.59
1:A:76:VAL:HG12	1:A:76:VAL:O	2.01	0.59
1:A:197:CYS:SG	3:A:1031:HOH:O	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:HD2	3:A:1038:HOH:O	2.07	0.54
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.89	0.54
1:A:84:PRO:HG2	1:A:87:VAL:HG12	1.88	0.54
1:A:203:ILE:HD11	1:A:241:MET:CG	2.28	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:739:MET:HA	1:A:739:MET:HE2	1.89	0.53
1:A:395:LEU:CD1	1:A:431:GLY:HA3	2.39	0.53
1:A:566:MET:HE2	1:A:566:MET:CA	2.27	0.53
1:A:726:ASN:HD21	1:A:770:ASN:ND2	1.90	0.53
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:134:CYS:O	1:A:137:LEU:HB2	2.11	0.51
1:A:212:HIS:HD2	3:A:932:HOH:O	1.92	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:672:MET:HE1	1:A:694:LEU:HD12	1.94	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:233:LYS:NZ	1:A:237:ARG:HD2	2.27	0.49
1:A:212:HIS:CD2	3:A:932:HOH:O	2.64	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:672:MET:HE1	1:A:694:LEU:CD1	2.43	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:703:LYS:HG3	1:A:739:MET:HE1	1.96	0.47
1:A:47:ASN:HD21	1:A:75:ASN:ND2	2.12	0.47
1:A:181:GLN:OE1	1:A:181:GLN:N	2.46	0.47
1:A:717:LEU:HD11	1:A:750:VAL:HG22	1.97	0.47
1:A:84:PRO:HG2	1:A:87:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:TYR:O	1:A:749:MET:HG2	2.14	0.47
1:A:399:LEU:N	1:A:400:PRO:HD2	2.30	0.47
1:A:473:PRO:O	1:A:476:THR:HG23	2.14	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:O	1:A:76:VAL:CG1	2.63	0.46
1:A:163:LEU:HD22	1:A:170:ARG:HE	1.81	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
1:A:541:LEU:O	1:A:545:ILE:HG12	2.17	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:HG2	1:A:6:LYS:O	2.17	0.44
1:A:169:ASP:O	1:A:170:ARG:C	2.60	0.44
1:A:703:LYS:HE3	1:A:739:MET:HE1	1.99	0.44
1:A:570:ILE:HD11	1:A:604:TYR:CD1	2.53	0.44
1:A:726:ASN:HD22	1:A:767:LEU:HA	1.82	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:124:GLN:CD	1:A:124:GLN:H	2.25	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:250:LEU:HD13	1:A:254:MET:HE1	2.01	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:61:ASP:C	1:A:61:ASP:OD1	2.63	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:122:GLU:O	1:A:125:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:ASN:N	1:A:173:ASN:HD22	2.18	0.41
1:A:191:ARG:NH1	1:A:226:ASP:OD2	2.53	0.41
1:A:163:LEU:HB2	1:A:172:LEU:CD2	2.26	0.41
1:A:215:SER:O	1:A:219:ASN:ND2	2.41	0.41
1:A:706:ILE:HD12	1:A:735:ILE:HD13	2.02	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:N	1:A:174:ILE:HD12	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
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

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%)	30	38
2	B	18/29 (62%)	18 (100%)	0	0	100	100
All	All	850/881 (96%)	810 (95%)	37 (4%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/762 (98%)	699 (93%)	50 (7%)	15	21
2	B	17/21 (81%)	17 (100%)	0	100	100
All	All	766/783 (98%)	716 (94%)	50 (6%)	15	22

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	133	LEU
1	A	137	LEU
1	A	149	PHE
1	A	158	ASP
1	A	161	GLU
1	A	180	LEU
1	A	215	SER
1	A	223	LEU
1	A	231	VAL
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	475	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	587	LEU
1	A	602	LEU
1	A	610	GLN
1	A	625	LEU
1	A	629	GLN
1	A	634	GLU
1	A	646	ASP
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	786	VAL
1	A	789	MET
1	A	801	LEU
1	A	802	ARG
1	A	884	LEU
1	A	890	VAL

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	13	GLN
1	A	47	ASN
1	A	74	ASN
1	A	98	ASN
1	A	185	HIS
1	A	199	ASN
1	A	234	ASN
1	A	255	HIS
1	A	256	ASN
1	A	306	ASN

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Mol	Chain	Res	Type
1	A	442	HIS
1	A	571	GLN
1	A	617	GLN
1	A	726	ASN
1	A	738	GLN
1	A	784	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.11	26 (3%) 51 53	40, 67, 103, 155	0
2	B	20/29 (68%)	0.16	2 (10%) 12 14	41, 61, 87, 90	0
All	All	856/881 (97%)	0.11	28 (3%) 49 51	40, 67, 103, 155	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	5.0
1	A	6	LYS	4.5
1	A	162	ILE	4.3
1	A	167	VAL	4.0
1	A	403	LYS	3.9
1	A	168	LEU	3.9
2	B	507	GLY	3.4
1	A	536	LYS	3.4
1	A	175	MET	3.3
1	A	163	LEU	3.1
1	A	164	ASP	3.0
1	A	122	GLU	2.9
1	A	182	PHE	2.7
1	A	145	CYS	2.7
1	A	886	ALA	2.6
2	B	508	PRO	2.6
1	A	134	CYS	2.3
1	A	211	LEU	2.3
1	A	137	LEU	2.3
1	A	129	LEU	2.2
1	A	172	LEU	2.2
1	A	320	GLY	2.2
1	A	180	LEU	2.2
1	A	371	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	5	TRP	2.2
1	A	174	ILE	2.1
1	A	171	PRO	2.1
1	A	173	ASN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.