

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 18, 2024 – 04:58 PM EST

PDB ID	:	4FQ3
Title	:	Crystal structure of transportin/FUS-NLS
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Deposited on	:	2012-06-25
Resolution	:	3.00  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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	А	890	.% <b>5</b> 0%		36%	7%	6%	
2	В	37	43%	5% •	49%			



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6805 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	А	834	Total 6631	C 4259	N 1106	Ó 1215	S 51	0	3	0

• Molecule 2 is a protein called Fusion (Involved in t(12;16) in malignant liposarcoma).

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
2	В	19	Total 174	C 101	N 41	0 31	S 1	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	490	GLY	-	expression tag	UNP Q8TBR3
В	491	PRO	-	expression tag	UNP Q8TBR3
В	492	LEU	-	expression tag	UNP Q8TBR3
В	494	SER	PHE	conflict	UNP Q8TBR3





# 3 Residue-property plots (i)

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: Fusion (Involved in t(12;16) in malignant liposarcoma)

Chain B:	43%	5% •	49%	
GLY PRO LEU GLY SER ARG GLY GLY	GLY GLY ARG ARG GLY GLY PHE GLY F508 E516	D520 R521 Y526		



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	128.81Å 158.29Å 68.37Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Posolution} \left( \overset{\circ}{\mathbf{A}} \right)$	29.94 - 3.00	Depositor
Resolution (A)	48.01 - 2.99	EDS
% Data completeness	99.3 (29.94-3.00)	Depositor
(in resolution range)	99.1 (48.01-2.99)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.22 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
B B.	0.198 , $0.251$	Depositor
II, II free	0.190 , $0.245$	DCC
$R_{free}$ test set	1459 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	55.8	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , 57.3	EDS
L-test for $twinning^2$	$   <  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6805	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.32	0/6784	0.51	0/9218	
2	В	0.32	0/180	0.48	0/235	
All	All	0.32	0/6964	0.51	0/9453	

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	А	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	121	GLY	Peptide
1	А	168	LEU	Peptide
1	А	746	TYR	Peptide
1	А	8	ASP	Peptide
1	А	841	SER	Peptide
1	А	867	GLU	Peptide
1	А	868	ASN	Peptide

### 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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6631	0	6687	279	0
2	В	174	0	169	1	0
All	All	6805	0	6856	279	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 20.

All (279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:6:LYS:HG2	1:A:7:PRO:HD2	1.31	1.11
1:A:659:ILE:HD11	1:A:697:ALA:HB1	1.48	0.96
1:A:794:ILE:HA	1:A:797:TRP:HB3	1.50	0.91
1:A:204:SER:HB2	1:A:206:THR:HG22	1.58	0.85
1:A:535:HIS:HA	1:A:538:LEU:HB2	1.60	0.83
1:A:787:ALA:HB2	1:A:820:MET:HG2	1.58	0.83
1:A:732:ILE:HD13	1:A:750:VAL:HG11	1.60	0.82
1:A:66:SER:O	1:A:70:LEU:HD22	1.82	0.80
1:A:789:MET:SD	1:A:792:GLN:NE2	2.55	0.80
1:A:790:LEU:O	1:A:791:GLN:HG2	1.82	0.80
1:A:708:ASP:OD1	1:A:708:ASP:N	2.15	0.79
1:A:737:ILE:HD11	1:A:777:ARG:HD2	1.65	0.78
1:A:494:LYS:HE2	1:A:534:GLN:HG3	1.65	0.78
1:A:810:LYS:HA	1:A:813:ALA:HB3	1.68	0.76
1:A:521:TYR:HD1	1:A:521:TYR:H	1.34	0.75
1:A:460:TRP:CZ2	1:A:464:ARG:HD2	2.21	0.75
1:A:815:ARG:NH2	1:A:848:ASP:OD1	2.20	0.75
1:A:848:ASP:OD2	1:A:848:ASP:N	2.18	0.74
1:A:422:GLY:HA3	1:A:460:TRP:CZ3	2.22	0.73
1:A:785:GLU:OE1	1:A:786:VAL:N	2.22	0.72
1:A:6:LYS:CG	1:A:7:PRO:HD2	2.15	0.71
1:A:523:LEU:O	1:A:527:VAL:HG13	1.91	0.70
1:A:885:ALA:HA	1:A:889:GLY:HA2	1.73	0.70
1:A:85:ASN:O	1:A:88:THR:N	2.26	0.69
1:A:821:ILE:HD11	1:A:828:VAL:HG21	1.74	0.69
1:A:673:TYR:O	1:A:677:GLN:NE2	2.26	0.69
1:A:578:ASP:OD2	1:A:611:ARG:NH1	2.24	0.68
1:A:703:LYS:O	1:A:706:ILE:HG13	1.94	0.68
1:A:195:VAL:HG22	1:A:234:ASN:HB3	1.76	0.68
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.76	0.68



Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:301:ILE:HD11	1:A:394:LEU:HD11	1.76	0.68		
1:A:47:ASN:HD21	1:A:75:ASN:HD22	1.43	0.67		
1:A:30:GLN:HA	1:A:33:VAL:HG22	1.77	0.67		
1:A:204:SER:HB2	1:A:206:THR:CG2	2.25	0.66		
1:A:512:CYS:O	1:A:513:THR:OG1	2.11	0.66		
1:A:794:ILE:HA	1:A:797:TRP:CB	2.23	0.66		
1:A:661:GLN:O	1:A:665:ARG:HD3	1.95	0.66		
1:A:749:MET:O	1:A:753:GLN:NE2	2.28	0.66		
1:A:759:ASN:ND2	1:A:792:GLN:O	2.28	0.65		
1:A:304:LEU:O	1:A:308:MET:HG3	1.96	0.65		
1:A:762:ASN:N	1:A:762:ASN:OD1	2.29	0.65		
1:A:760:ARG:HG2	1:A:761:PRO:O	1.96	0.64		
1:A:55:THR:OG1	1:A:94:GLU:HG3	1.96	0.64		
1:A:770:ASN:O	1:A:774:THR:HG23	1.98	0.64		
1:A:706:ILE:HD12	1:A:707:ALA:N	2.13	0.64		
1:A:70:LEU:HD13	1:A:109:THR:HG23	1.80	0.64		
1:A:31:ARG:O	1:A:35:GLN:NE2	2.31	0.64		
1:A:455:ARG:HD2	1:A:488:ARG:HD3	1.79	0.64		
1:A:747:ILE:N	1:A:748:PRO:CD	2.60	0.64		
1:A:789:MET:HA	1:A:789:MET:CE	2.29	0.63		
1:A:108:ALA:O	1:A:112:ILE:HG13	1.98	0.63		
1:A:558:LYS:O	1:A:562:ILE:HG12	1.97	0.63		
1:A:736:SER:HA	1:A:743:MET:HG3	1.81	0.63		
1:A:470:VAL:HG11	1:A:511:ALA:HB2	1.80	0.62		
1:A:21:GLU:HB2	1:A:33:VAL:HG11	1.81	0.62		
1:A:513:THR:HA	1:A:516:VAL:HG23	1.82	0.62		
1:A:606:GLU:O	1:A:610:GLN:HG2	2.00	0.61		
1:A:502:SER:HB3	2:B:522:ARG:HG2	1.82	0.61		
1:A:729:THR:O	1:A:774:THR:HG21	1.99	0.61		
1:A:251:LEU:HA	1:A:254:MET:HG2	1.82	0.61		
1:A:395:LEU:CD1	1:A:431:GLY:HA3	2.31	0.60		
1:A:746:TYR:HA	1:A:748:PRO:HD2	1.82	0.60		
1:A:11:GLY:O	1:A:15:ILE:HG12	2.00	0.60		
1:A:534:GLN:O	1:A:535:HIS:HB3	2.00	0.59		
1:A:416:SER:O	1:A:420:VAL:HG23	2.03	0.59		
1:A:742:GLU:O	1:A:745:PRO:HD2	2.02	0.59		
1:A:787:ALA:HB2	1:A:820:MET:CG	2.33	0.59		
1:A:80:PHE:HA	1:A:83:PHE:CE1	2.36	0.59		
1:A:62:GLU:HG3	1:A:106:ILE:HD13	1.84	0.58		
1:A:381:ALA:O	1:A:385:VAL:HG23	2.02	0.58		
1:A:787:ALA:C	1:A:789:MET:H	2.07	0.58		



	lo us pugem	Interatomic Clash		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:A:408:HIS:CD2	1:A:413:VAL:HG11	2.39	0.58	
1:A:395:LEU:HD11	1:A:431:GLY:HA3	1.85	0.58	
1:A:130:LEU:HB2	1:A:131:PRO:HD3	1.86	0.57	
1:A:203:ILE:HA	1:A:245:VAL:HG21	1.86	0.57	
1:A:684:ARG:HD2	1:A:716:ASN:OD1	2.04	0.57	
1:A:747:ILE:HG22	1:A:751:LEU:HB2	1.87	0.57	
1:A:121:GLY:O	1:A:122:GLU:HB2	2.05	0.57	
1:A:602:LEU:HD11	1:A:658:ASN:HD22	1.70	0.57	
1:A:227:GLU:O	1:A:232:ARG:NH1	2.31	0.57	
1:A:723:SEB:O	1:A:727:ASN:ND2	2.38	0.56	
1:A:100:GLY:HA3	1:A·144·THB·HG22	1.87	0.56	
1:A:790:LEU:C	1:A:792:GLN:H	2.07	0.56	
1·A·141·ASP·OD2	1:A·144·THB·HG23	2.05	0.56	
1:A:787:ALA:O	1:A:789:MET:N	2.38	0.56	
1·A·311·SEB·O	1·A·315·ILE·HG13	2.05	0.56	
1:A:565:LEU:O	1:A:568:PRO:HD2	2.00	0.55	
1.A.176.ILE.HB	1:A:177:PRO:HD3	1.88	0.55	
1.A.482.MET.HG2	$1 \cdot A \cdot 504 \cdot PHE \cdot HE1$	1.00	0.55	
1.A.732.ILE.HD13	1:A:750:VAL:CG1	2.32	0.55	
1:A:264:ABG:NH1	1:A:267:ASP:OD2	2.02	0.55	
1.A.619.THR.HG23	1:A:636:PBO:HB2	1.89	0.55	
1.A.443.LEU.HB2	1·A·462·LEU·HD21	1.90	0.53	
1.A.795.ABG.N	1.A.796.PRO.HD2	2.22	0.54	
1:A·48:ASN·ND2	1:A:87:VAL:HG13	2.23	0.54	
1:A:786:VAL:HG12	1:A:820·MET·SD	2.48	0.53	
1:A:6:LYS:HD2	1:A:48:ASN:OD1	2.18	0.53	
1·A·79·HIS·HA	1:A:81:GLN:OE1	2.08	0.53	
1.A.659.ILE.HD12	1:A:659.ILE:H	1 73	0.53	
1:A:167:VAL:HG23	1:A:168:LEU:HD23	1.10	0.53	
1:A:657:GLY:H	1:A:659:ILE:HD11	1.74	0.53	
1:A:159:SEB:HB3	1:A:162:ILE:HD13	1.90	0.53	
1:A:479·LYS·HB3	1:A:480:PRO:HD3	1.90	0.52	
1:A:877:PRO:HD2	1:A:880:LEU:HD23	1.90	0.52	
$\frac{1 \cdot A \cdot 718 \cdot A \text{SN} \cdot \text{ND2}}{1 \cdot A \cdot 718 \cdot A \text{SN} \cdot \text{ND2}}$	$1 \cdot A \cdot 720 \cdot GLU \cdot OE1$	2.43	0.52	
$1 \cdot A \cdot 821 \cdot ILE \cdot HG21$	1:A:856:ILE:HD13	1.92	0.52	
1:A:584:PHE:HB2	1:A:585:PRO:HD3	1.91	0.52	
1.A.793.PHE.O	1:A:794:ILE:HG22	2.09	0.52	
1:A:809:GLU:O	1:A:810:LYS·HG2	2.00	0.52	
1:A:516:VAL:HR	1:A:517:PRO:HD3	1.92	0.52	
1:A:604·TVR·O	1:A:608:VAL:HG13	2.09	0.52	
1:A:470:VAL:CG1	1:A:511:ALA:HB2	2.40	0.52	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:521:TYR:CD1	1:A:521:TYR:N	2.78	0.52	
1:A:629:GLN:HB2	1:A:633:TYR:HD1	1.75	0.51	
1:A:649:SER:OG	1:A:693:ASP:OD2	2.27	0.51	
1:A:713:LEU:HD13	1:A:732:ILE:HG13	1.92	0.51	
1:A:744:GLN:N	1:A:745:PRO:HD2	2.26	0.51	
1:A:535:HIS:HA	1:A:538:LEU:CB	2.36	0.51	
1:A:848:ASP:O	1:A:852:MET:HG3	2.10	0.51	
1:A:126:TRP:CE3	1:A:129:LEU:HD22	2.46	0.51	
1:A:725:CYS:O	1:A:729:THR:HG23	2.11	0.51	
1:A:167:VAL:CG2	1:A:168:LEU:HD23	2.41	0.51	
1:A:747:ILE:N	1:A:748:PRO:HD3	2.25	0.50	
1:A:297:LEU:N	1:A:298:PRO:CD	2.74	0.50	
1:A:659:ILE:HD12	1:A:659:ILE:N	2.26	0.50	
1:A:99:ILE:HG23	1:A:100:GLY:N	2.27	0.50	
1:A:247:MET:CE	1:A:288:ILE:HD11	2.41	0.50	
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.94	0.50	
1:A:494:LYS:CE	1:A:534:GLN:HG3	2.40	0.49	
1:A:795:ARG:HB2	1:A:796:PRO:HD3	1.94	0.49	
1:A:801:LEU:HD22	1:A:804:ILE:HD12	1.93	0.49	
1:A:581:LYS:HE3	1:A:637:ASP:OD1	2.11	0.49	
1:A:582:ASP:O	1:A:585:PRO:HD2	2.13	0.49	
1:A:47:ASN:ND2	1:A:75:ASN:HD22	2.08	0.49	
1:A:731:ALA:O	1:A:735:ILE:HG12	2.12	0.49	
1:A:797:TRP:CZ2	1:A:801:LEU:HD12	2.48	0.49	
1:A:452:ALA:HB1	1:A:493:ASN:HD22	1.78	0.49	
1:A:787:ALA:C	1:A:789:MET:N	2.65	0.49	
1:A:76:VAL:O	1:A:80:PHE:HB2	2.13	0.48	
1:A:203:ILE:HD11	1:A:241:MET:HG2	1.95	0.48	
1:A:527:VAL:O	1:A:530:PHE:HB2	2.13	0.48	
1:A:467:HIS:ND1	1:A:467:HIS:C	2.66	0.48	
1:A:866:ASP:OD1	1:A:867:GLU:N	2.46	0.48	
1:A:195:VAL:CG2	1:A:234:ASN:HB3	2.43	0.48	
1:A:533:TYR:HB2	1:A:538:LEU:HD13	1.96	0.48	
1:A:460:TRP:CH2	1:A:464:ARG:HD2	2.48	0.48	
1:A:78:ALA:O	1:A:79:HIS:CG	2.67	0.48	
1:A:254:MET:HE2	1:A:292:VAL:HG11	1.96	0.48	
1:A:294:VAL:O	1:A:295:ARG:HD2	2.13	0.48	
1:A:860:PHE:CZ	1:A:864:VAL:HG11	2.49	0.48	
1:A:80:PHE:CD1	1:A:83:PHE:CZ	3.02	0.48	
1:A:808:GLU:O	1:A:811:ASP:HB3	2.14	0.48	
1:A:493:ASN:OD1	1:A:494:LYS:N	2.46	0.47	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:29:ILE:H	1:A:29:ILE:HG12	1.30	0.47
1:A:32:THR:HG22	1:A:36:LYS:HE3	1.95	0.47
1:A:672:MET:O	1:A:676:MET:HG3	2.14	0.47
1:A:312:ASP:O	1:A:316:ILE:HG13	2.14	0.47
1:A:83:PHE:HB2	1:A:84:PRO:HD2	1.95	0.47
1:A:587:LEU:HD22	1:A:647:LEU:HD12	1.97	0.47
1:A:19:LEU:HA	1:A:22:SER:OG	2.15	0.47
1:A:213:ILE:HG23	1:A:214:ASP:N	2.31	0.46
1:A:21:GLU:CB	1:A:33:VAL:HG11	2.44	0.46
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.68	0.46
1:A:488:ARG:NE	1:A:488:ARG:HA	2.31	0.46
1:A:685:GLN:HG3	1:A:727:ASN:ND2	2.31	0.46
1:A:706:ILE:HD12	1:A:707:ALA:H	1.81	0.46
1:A:795:ARG:HB2	1:A:796:PRO:CD	2.45	0.46
1:A:659:ILE:H	1:A:659:ILE:CD1	2.29	0.46
1:A:747:ILE:H	1:A:748:PRO:HD3	1.80	0.46
1:A:233:LYS:HG3	1:A:275:GLU:HG3	1.96	0.46
1:A:246:ARG:NH2	1:A:248:ASP:OD2	2.31	0.46
1:A:314:ASP:O	1:A:318:LEU:HG	2.16	0.46
1:A:625:LEU:HD22	1:A:633:TYR:CD1	2.50	0.46
1:A:622:GLN:HB3	1:A:636:PRO:HB3	1.98	0.45
1:A:710:MET:HB2	1:A:711:PRO:HD3	1.97	0.45
1:A:54:LEU:HD22	1:A:69:GLY:HA3	1.98	0.45
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.98	0.45
1:A:28:THR:O	1:A:31:ARG:HG2	2.16	0.45
1:A:248:ASP:OD1	1:A:248:ASP:N	2.40	0.45
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.80	0.45
1:A:462:LEU:HD13	1:A:481:LEU:CD1	2.46	0.45
1:A:810:LYS:HE2	1:A:842:TRP:CZ2	2.52	0.45
1:A:109:THR:HA	1:A:112:ILE:HD12	1.99	0.45
1:A:61:ASP:HB2	1:A:63:PRO:HD2	1.98	0.45
1:A:299:LYS:HA	1:A:299:LYS:HD3	1.66	0.45
1:A:587:LEU:HB2	1:A:643:VAL:CG1	2.46	0.45
1:A:700:GLN:HG2	1:A:701:HIS:CD2	2.51	0.45
1:A:784:GLN:O	1:A:788:PRO:HD2	2.16	0.45
1:A:113:LEU:HD12	1:A:113:LEU:HA	1.79	0.45
1:A:192:SER:OG	1:A:230:GLU:HB3	2.17	0.45
1:A:699:PHE:CZ	1:A:739:MET:HG2	2.52	0.45
1:A:174:ILE:HD13	1:A:174:ILE:HA	1.73	0.45
1:A:283:LEU:HD22	1:A:283:LEU:O	2.16	0.45
1:A:399:LEU:HD13	1:A:399:LEU:HA	1.78	0.45



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:869:TRP:O	1:A:872:PHE:HB3	2.17	0.45
1:A:168:LEU:HB3	1:A:171:PRO:HG3	1.99	0.44
1:A:374:ASN:OD1	1:A:377:LYS:HG3	2.17	0.44
1:A:867:GLU:O	1:A:868:ASN:HB3	2.17	0.44
1:A:254:MET:CE	1:A:292:VAL:HG11	2.48	0.44
1:A:373:TRP:CZ2	1:A:378:CYS:HA	2.52	0.44
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.68	0.44
1:A:6:LYS:HG2	1:A:7:PRO:CD	2.23	0.44
1:A:567:PRO:HB2	1:A:568:PRO:HD3	1.99	0.44
1:A:889:GLY:N	1:A:890:VAL:HA	2.32	0.44
1:A:793:PHE:CD2	1:A:794:ILE:N	2.85	0.44
1:A:535:HIS:NE2	1:A:582:ASP:OD2	2.49	0.44
1:A:810:LYS:O	1:A:814:PHE:HB2	2.17	0.44
1:A:789:MET:SD	1:A:792:GLN:HB2	2.58	0.44
1:A:99:ILE:HG23	1:A:100:GLY:H	1.83	0.43
1:A:717:LEU:O	1:A:718:ASN:C	2.56	0.43
1:A:41:ASN:ND2	1:A:75:ASN:OD1	2.51	0.43
1:A:533:TYR:CB	1:A:538:LEU:HD13	2.48	0.43
1:A:783:PRO:O	1:A:787:ALA:HB3	2.18	0.43
1:A:790:LEU:C	1:A:792:GLN:N	2.71	0.43
1:A:810:LYS:HE2	1:A:842:TRP:CE2	2.53	0.43
1:A:23:GLN:H	1:A:23:GLN:HG2	1.68	0.43
1:A:78:ALA:O	1:A:79:HIS:CD2	2.71	0.43
1:A:274:LEU:HD13	1:A:375:LEU:HA	2.00	0.43
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.86	0.43
1:A:185:HIS:CD2	1:A:190:ILE:HG21	2.54	0.43
1:A:205:ARG:HG2	1:A:245:VAL:CG1	2.49	0.43
1:A:431:GLY:O	1:A:434:PRO:HD2	2.19	0.43
1:A:651:LEU:O	1:A:655:LEU:CB	2.67	0.43
1:A:83:PHE:HA	1:A:84:PRO:HD3	1.89	0.43
1:A:203:ILE:HA	1:A:245:VAL:CG2	2.47	0.43
1:A:422:GLY:HA3	1:A:460:TRP:HZ3	1.78	0.43
1:A:204:SER:CB	1:A:206:THR:HG22	2.39	0.42
1:A:769:GLU:HB3	1:A:804:ILE:HD11	2.01	0.42
1:A:309:LYS:H	1:A:309:LYS:HG2	1.70	0.42
1:A:318:LEU:O	1:A:319:LYS:HB3	2.18	0.42
1:A:779:GLY:HA3	1:A:820:MET:SD	2.58	0.42
1:A:824:ASN:N	1:A:825:PRO:HD3	2.34	0.42
1:A:100:GLY:HA3	1:A:144:THR:CG2	2.49	0.42
1:A:395:LEU:HD21	1:A:432:MET:HG2	2.00	0.42
1:A:85:ASN:HB3	1:A:86:GLY:H	1.67	0.42



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:181:GLN:O	1:A:184:LYS:HE2	2.19	0.42	
1:A:264:ARG:O	1:A:267:ASP:HB2	2.20	0.42	
1:A:123:LEU:HD13	1:A:123:LEU:HA	1.88	0.42	
1:A:651:LEU:O	1:A:655:LEU:HB3	2.19	0.42	
1:A:652:ALA:CB	1:A:693:ASP:HB3	2.49	0.42	
1:A:700:GLN:H	1:A:700:GLN:CD	2.21	0.42	
1:A:779:GLY:CA	1:A:786:VAL:HG11	2.50	0.42	
1:A:635:ALA:HB1	1:A:636:PRO:HD2	2.02	0.42	
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.82	0.41	
1:A:887:PHE:HD2	1:A:887:PHE:HA	1.78	0.41	
1:A:301:ILE:HD11	1:A:394:LEU:CD1	2.48	0.41	
1:A:493:ASN:O	1:A:497:GLN:HG3	2.20	0.41	
1:A:849:LEU:HD23	1:A:849:LEU:HA	1.73	0.41	
1:A:859:GLY:O	1:A:863:GLN:HB2	2.20	0.41	
1:A:876:PHE:HB3	1:A:881:LYS:HB2	2.02	0.41	
1:A:878:LEU:N	1:A:879:PRO:HD2	2.35	0.41	
1:A:573:TRP:HZ3	1:A:587:LEU:CD2	2.33	0.41	
1:A:589:CYS:O	1:A:593:VAL:HG23	2.19	0.41	
1:A:187:SER:HA	1:A:188:PRO:HD2	1.92	0.41	
1:A:220:LEU:HD21	1:A:238:ALA:HB1	2.02	0.41	
1:A:512:CYS:C	1:A:514:GLU:H	2.22	0.41	
1:A:566:MET:HG2	1:A:604:TYR:CZ	2.55	0.41	
1:A:666:SER:HB3	1:A:668:ILE:HG22	2.02	0.41	
1:A:298:PRO:O	1:A:302:PRO:HD2	2.20	0.41	
1:A:6:LYS:HE2	1:A:7:PRO:CD	2.51	0.41	
1:A:452:ALA:CB	1:A:493:ASN:HD22	2.33	0.41	
1:A:482:MET:HE3	1:A:482:MET:HB3	1.80	0.41	
1:A:560:GLU:CD	1:A:560:GLU:H	2.24	0.41	
1:A:162:ILE:O	1:A:165:SER:OG	2.36	0.41	
1:A:179:PHE:CE2	1:A:197:CYS:HB3	2.56	0.41	
1:A:194:ALA:O	1:A:198:VAL:HG23	2.20	0.41	
1:A:247:MET:HE2	1:A:288:ILE:HD11	2.02	0.41	
1:A:402:LEU:HA	1:A:402:LEU:HD23	1.87	0.41	
1:A:739:MET:CB	1:A:743:MET:HG2	2.50	0.41	
1:A:866:ASP:O	1:A:868:ASN:ND2	2.54	0.41	
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.82	0.41	
1:A:421:LEU:HB3	1:A:461:THR:HG21	2.03	0.41	
1:A:482:MET:HE1	1:A:518:TYR:CB	2.51	0.41	
1:A:852:MET:O	1:A:856:ILE:HG13	2.20	0.41	
1:A:116:THR:O	1:A:120:LYS:HB2	2.21	0.40	
1:A:318:LEU:HG	1:A:318:LEU:H	1.65	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:HA	1:A:169:ASP:O	2.22	0.40
1:A:62:GLU:N	1:A:63:PRO:CD	2.85	0.40
1:A:606:GLU:N	1:A:607:PRO:HD2	2.36	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	Perce	ntiles
1	А	833/890~(94%)	795~(95%)	36 (4%)	2 (0%)	47	82
2	В	18/37~(49%)	17 (94%)	1 (6%)	0	100	100
All	All	851/927~(92%)	812 (95%)	37 (4%)	2(0%)	47	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	794	ILE
1	А	786	VAL

#### 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	А	745/802~(93%)	634~(85%)	111 (15%)	3 14



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entil	$\mathbf{es}$
2	В	18/25~(72%)	15 (83%)	3~(17%)	2	11	
All	All	763/827~(92%)	649~(85%)	114 (15%)	3	14	

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	6	LYS
1	А	16	LEU
1	А	20	LYS
1	А	29	ILE
1	А	48	ASN
1	А	50	LEU
1	А	70	LEU
1	А	81	GLN
1	А	88	THR
1	А	94	GLU
1	А	96	LEU
1	А	113	LEU
1	А	115	THR
1	А	119	SER
1	А	123	LEU
1	А	124	GLN
1	А	128	ASP
1	А	132	LYS
1	А	136	LEU
1	А	137	LEU
1	А	146	GLU
1	А	149	PHE
1	А	159	SER
1	А	161	GLU
1	А	166	ASP
1	А	167	VAL
1	А	168	LEU
1	А	174	ILE
1	А	186	SER
1	А	192	SER
1	А	195	VAL
1	А	204	SER
1	А	206	THR
1	А	220	LEU
1	А	242	LEU
1	А	247	MET



Mol	Chain	Res	Type
1	А	248	ASP
1	А	258	VAL
1	А	262	LEU
1	А	268	GLN
1	А	270	GLU
1	А	283	LEU
1	А	288	ILE
1	А	295	ARG
1	А	297	LEU
1	А	299	LYS
1	А	300	LEU
1	А	309	LYS
1	А	318	LEU
1	А	372	ASP
1	А	399	LEU
1	А	401	LEU
1	А	421	LEU
1	А	424	ILE
1	А	456	SER
1	А	463	SER
1	А	476	THR
1	А	483	THR
1	А	488	ARG
1	А	490	LEU
1	А	501	CYS
1	А	512	CYS
1	А	519	LEU
1	А	521	TYR
1	А	524	ASP
1	А	536	LYS
1	А	539	LEU
1	А	560	GLU
1	А	563	GLN
1	А	564	MET
1	А	566	MET
1	А	570	ILE
1	А	586	LEU
1	A	595	THR
1	A	606	GLU
1	A	608	VAL
1	А	615	LEU
1	A	625	LEU



Mol	Chain	Res	Type
1	А	634	GLU
1	А	638	LYS
1	А	646	ASP
1	А	659	ILE
1	А	687	SER
1	А	708	ASP
1	А	718	ASN
1	А	746	TYR
1	А	749	MET
1	А	750	VAL
1	А	751	LEU
1	А	762	ASN
1	А	767	LEU
1	А	774	THR
1	А	777	ARG
1	А	785	GLU
1	А	789	MET
1	А	792	GLN
1	А	794	ILE
1	А	800	SER
1	А	817	ILE
1	А	821	ILE
1	А	831	ASP
1	А	833	ILE
1	А	841	SER
1	А	847	ASP
1	А	848	ASP
1	А	849	LEU
1	А	850	ARG
1	А	869	TRP
1	А	875	GLN
1	А	887	PHE
1	А	890	VAL
2	В	516	GLU
2	В	520	ASP
2	В	522	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	23	GLN
1	А	41	ASN



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Mol	Chain	Res	Type
1	А	47	ASN
1	А	79	HIS
1	А	81	GLN
1	А	658	ASN
1	А	718	ASN
1	А	792	GLN

#### 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 monosaccharides 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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 $>$	$\#RSRZ{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	834/890~(93%)	-0.31	6 (0%) 87 69	24,60,99,147	0
2	В	19/37~(51%)	-0.45	0 100 100	35, 55, 82, 98	0
All	All	853/927~(92%)	-0.31	6 (0%) 87 69	24, 60, 98, 147	0

All (6) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	791	GLN	2.9
1	А	371	SER	2.9
1	А	792	GLN	2.8
1	А	167	VAL	2.5
1	А	752	HIS	2.4
1	А	168	LEU	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 monosaccharides 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.

