



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 05:34 AM UTC

PDB ID : 4FQ3 / pdb_00004fq3
Title : Crystal structure of transportin/FUS-NLS
Authors : Gong, W.; Niu, C.; Jia, M.; Gao, F.
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

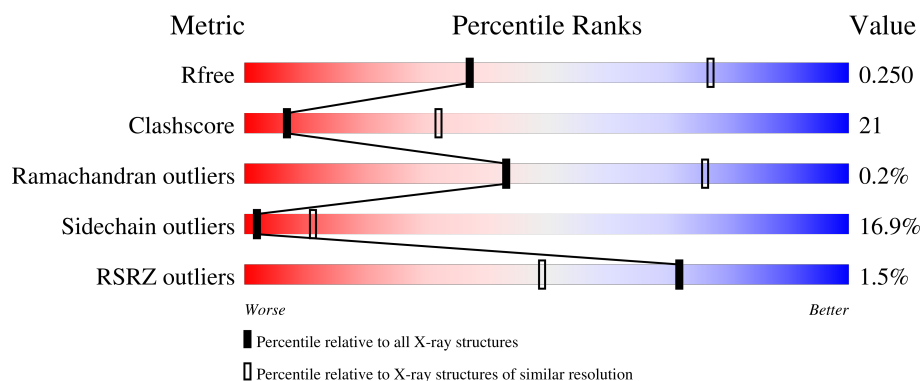
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	890	 48% 36% 9% 6%
2	B	37	 43% 5% 49%

2 Entry composition

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	A	834	Total	C	N	O	S	0	3	0
			6631	4259	1106	1215	51			

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

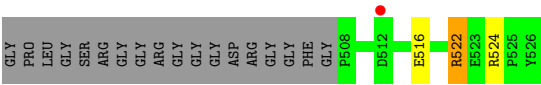
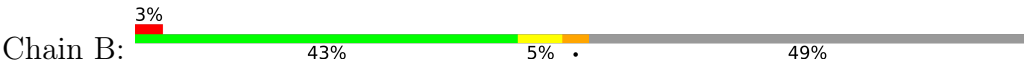
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	S	0	1	0
			174	101	41	31	1			

There are 4 discrepancies between the modelled and reference sequences:

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



● Molecule 2: Fusion (Involved in t(12;16) in malignant liposarcoma)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.81Å 158.29Å 68.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.00 29.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.94-3.00) 99.2 (29.94-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.198 , 0.251 0.194 , 0.250	Depositor DCC
R_{free} test set	1459 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.40	0/6784	0.92	29/9218 (0.3%)
2	B	0.37	0/180	1.01	4/235 (1.7%)
All	All	0.40	0/6964	0.92	33/9453 (0.3%)

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	7

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	ALA	CA-C-N	-10.37	106.87	119.84
1	A	787	ALA	C-N-CA	-10.37	106.87	119.84
1	A	792	GLN	N-CA-C	-8.46	101.57	112.23
1	A	635	ALA	CA-C-N	8.36	128.01	119.56
1	A	635	ALA	C-N-CA	8.36	128.01	119.56
1	A	83	PHE	CA-C-N	8.07	129.92	119.84
1	A	83	PHE	C-N-CA	8.07	129.92	119.84
1	A	9	GLU	N-CA-CB	-7.25	106.84	114.10
1	A	760	ARG	CA-C-N	-7.02	113.27	120.85
1	A	760	ARG	C-N-CA	-7.02	113.27	120.85
1	A	747	ILE	CA-C-N	6.91	127.48	119.47
1	A	747	ILE	C-N-CA	6.91	127.48	119.47
1	A	869	TRP	N-CA-C	-6.24	104.02	111.69
1	A	245	VAL	N-CA-C	6.19	116.83	110.82
1	A	170	ARG	CA-C-N	6.09	125.49	118.85
1	A	170	ARG	C-N-CA	6.09	125.49	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	785	GLU	N-CA-C	-5.87	100.63	109.79
1	A	598	GLN	CB-CA-C	-5.83	109.84	116.54
1	A	750	VAL	N-CA-C	5.67	117.18	111.00
1	A	516	VAL	CB-CA-C	-5.53	108.45	113.70
1	A	811	ASP	N-CA-C	-5.44	105.27	111.14
1	A	228	GLU	CA-C-N	5.24	125.05	119.28
1	A	228	GLU	C-N-CA	5.24	125.05	119.28
1	A	514	GLU	N-CA-C	-5.21	106.44	112.89
1	A	433	ILE	CB-CA-C	-5.20	108.76	113.70
2	B	524[A]	ARG	CA-C-N	5.18	124.80	119.56
2	B	524[A]	ARG	C-N-CA	5.18	124.80	119.56
2	B	524[B]	ARG	CA-C-N	5.18	124.80	119.56
2	B	524[B]	ARG	C-N-CA	5.18	124.80	119.56
1	A	680	MET	CA-C-N	5.03	124.64	119.05
1	A	680	MET	C-N-CA	5.03	124.64	119.05
1	A	666	SER	N-CA-C	5.02	117.78	109.85
1	A	751	LEU	N-CA-C	5.01	116.43	110.97

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

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	6631	0	6687	287	0
2	B	174	0	169	1	0
All	All	6805	0	6856	287	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 21.

All (287) 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: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:789:MET:HE2	1:A:789:MET:HA	1.71	0.72
1:A:254:MET:HE2	1:A:292:VAL:HG11	1.72	0.71
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:236:CYS:SG	1:A:261:MET:HE1	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:512:CYS:O	1:A:513:THR:OG1	2.11	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: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:787:ALA:C	1:A:789:MET:H	2.07	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:790:LEU:C	1:A:792:GLN:H	2.07	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:789:MET:HA	1:A:789:MET:CE	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:SER:O	1:A:727:ASN:ND2	2.38	0.56
1:A:100:GLY:HA3	1:A:144:THR:HG22	1.87	0.56
1:A:141:ASP:OD2	1:A:144:THR:HG23	2.05	0.56
1:A:261:MET:HE2	1:A:261:MET:HA	1.86	0.56
1:A:787:ALA:O	1:A:789:MET:N	2.38	0.56
1:A:311:SER:O	1:A:315:ILE:HG13	2.05	0.56
1:A:565:LEU:O	1:A:568:PRO:HD2	2.06	0.55
1:A:176:ILE:HB	1:A:177:PRO:HD3	1.88	0.55
1:A:482:MET:HG2	1:A:504:PHE:HE1	1.71	0.55
1:A:732:ILE:HD13	1:A:750:VAL:CG1	2.32	0.55
1:A:264:ARG:NH1	1:A:267:ASP:OD2	2.40	0.55
1:A:619:THR:HG23	1:A:636:PRO:HB2	1.89	0.55
1:A:443:LEU:HB2	1:A:462:LEU:HD21	1.90	0.54
1:A:795:ARG: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:787:ALA:C	1:A:789:MET:N	2.65	0.53
1:A:786:VAL:HG12	1:A:820:MET:SD	2.48	0.53
1:A:6:LYS:HD2	1:A:48:ASN:OD1	2.08	0.53
1:A:79:HIS:HA	1:A:81:GLN:OE1	2.08	0.53
1:A:467:HIS:ND1	1:A:467:HIS:C	2.66	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	1.91	0.53
1:A:657:GLY:H	1:A:659:ILE:HD11	1.74	0.53
1:A:159:SER:HB3	1:A:162:ILE:HD13	1.90	0.52
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
1:A:718:ASN:ND2	1:A:720:GLU:OE1	2.43	0.52
1:A:821:ILE: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	2.08	0.52
1:A:516:VAL:HB	1:A:517:PRO:HD3	1.92	0.52
1:A:604:TYR:O	1:A:608:VAL:HG13	2.09	0.52
1:A:470:VAL:CG1	1:A:511:ALA:HB2	2.40	0.52
1:A:521:TYR:CD1	1:A:521:TYR:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:MET:HE2	1:A:288:ILE:HD11	1.92	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:482:MET:HE1	1:A:518:TYR:CG	2.47	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: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: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:294:VAL:O	1:A:295:ARG:HD2	2.13	0.48
1:A:790:LEU:C	1:A:792:GLN:N	2.71	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
1:A:29:ILE:H	1:A:29:ILE:HG12	1.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:700:GLN:H	1:A:700:GLN:CD	2.21	0.46
1:A:213:ILE:HG23	1:A:214:ASP:N	2.31	0.46
1:A:717:LEU:O	1:A:718:ASN:C	2.56	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:512:CYS:C	1:A:514:GLU:H	2.22	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:560:GLU:CD	1:A:560:GLU:H	2.24	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:571:GLN:HG2	1:A:575:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:718:ASN:C	1:A:718:ASN:HD22	2.26	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: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: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:260:TYR:CD1	1:A:261:MET:HE3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:432:MET:HE3	1:A:432:MET:HB3	1.79	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: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: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: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: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:746:TYR:HB3	1:A:749:MET:HE3	2.01	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
1:A:493:ASN:OD1	1:A:493:ASN:C	2.64	0.40

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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
1:A:520:ALA:O	1:A:521:TYR:C	2.64	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	833/890 (94%)	795 (95%)	36 (4%)	2 (0%)	43	76
2	B	18/37 (49%)	17 (94%)	1 (6%)	0	100	100
All	All	851/927 (92%)	812 (95%)	37 (4%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	794	ILE
1	A	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	745/802 (93%)	619 (83%)	126 (17%)	2	11
2	B	18/25 (72%)	16 (89%)	2 (11%)	6	25
All	All	763/827 (92%)	635 (83%)	128 (17%)	2	11

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	16	LEU
1	A	20	LYS
1	A	29	ILE
1	A	37	LEU
1	A	38	GLU
1	A	50	LEU
1	A	70	LEU
1	A	81	GLN
1	A	85	ASN
1	A	88	THR
1	A	94	GLU
1	A	96	LEU
1	A	112	ILE
1	A	113	LEU
1	A	115	THR
1	A	119	SER
1	A	120	LYS
1	A	123	LEU
1	A	124	GLN
1	A	128	ASP
1	A	132	LYS
1	A	136	LEU
1	A	137	LEU
1	A	146	GLU
1	A	149	PHE
1	A	159	SER
1	A	161	GLU
1	A	166	ASP
1	A	167	VAL
1	A	168	LEU
1	A	174	ILE

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Mol	Chain	Res	Type
1	A	178	LYS
1	A	186	SER
1	A	192	SER
1	A	195	VAL
1	A	204	SER
1	A	206	THR
1	A	207	GLN
1	A	220	LEU
1	A	242	LEU
1	A	247	MET
1	A	248	ASP
1	A	258	VAL
1	A	262	LEU
1	A	263	GLN
1	A	268	GLN
1	A	270	GLU
1	A	283	LEU
1	A	288	ILE
1	A	295	ARG
1	A	297	LEU
1	A	299	LYS
1	A	300	LEU
1	A	304	LEU
1	A	309	LYS
1	A	313	ILE
1	A	318	LEU
1	A	372	ASP
1	A	399	LEU
1	A	401	LEU
1	A	421	LEU
1	A	424	ILE
1	A	456	SER
1	A	463	SER
1	A	470	VAL
1	A	476	THR
1	A	482	MET
1	A	483	THR
1	A	485	LEU
1	A	488	ARG
1	A	490	LEU
1	A	501	CYS
1	A	512	CYS

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Mol	Chain	Res	Type
1	A	519	LEU
1	A	521	TYR
1	A	524	ASP
1	A	527	VAL
1	A	536	LYS
1	A	539	LEU
1	A	560	GLU
1	A	564	MET
1	A	566	MET
1	A	570	ILE
1	A	586	LEU
1	A	595	THR
1	A	606	GLU
1	A	608	VAL
1	A	611	ARG
1	A	615	LEU
1	A	625	LEU
1	A	634	GLU
1	A	638	LYS
1	A	646	ASP
1	A	659	ILE
1	A	687	SER
1	A	700	GLN
1	A	706	ILE
1	A	708	ASP
1	A	746	TYR
1	A	749	MET
1	A	750	VAL
1	A	751	LEU
1	A	762	ASN
1	A	765	LYS
1	A	767	LEU
1	A	774	THR
1	A	777	ARG
1	A	785	GLU
1	A	789	MET
1	A	792	GLN
1	A	794	ILE
1	A	800	SER
1	A	817	ILE
1	A	821	ILE
1	A	831	ASP

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Mol	Chain	Res	Type
1	A	833	ILE
1	A	841	SER
1	A	847	ASP
1	A	848	ASP
1	A	849	LEU
1	A	863	GLN
1	A	869	TRP
1	A	875	GLN
1	A	887	PHE
1	A	890	VAL
2	B	516	GLU
2	B	522	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	47	ASN
1	A	79	HIS
1	A	81	GLN
1	A	82	ASN
1	A	181	GLN
1	A	296	HIS
1	A	442	HIS
1	A	555	HIS
1	A	629	GLN
1	A	632	GLN
1	A	658	ASN
1	A	718	ASN
1	A	792	GLN
1	A	868	ASN
1	A	875	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 [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 [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, 95th 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 ²)	Q < 0.9
1	A	834/890 (93%)	-0.30	12 (1%)	73 51	22, 60, 99, 147	3 (0%)
2	B	19/37 (51%)	-0.26	1 (5%)	32 16	28, 55, 82, 98	1 (5%)
All	All	853/927 (92%)	-0.29	13 (1%)	72 49	22, 60, 98, 147	4 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	PRO	3.5
1	A	534	GLN	2.8
2	B	512	ASP	2.7
1	A	789	MET	2.7
1	A	6	LYS	2.4
1	A	166	ASP	2.3
1	A	371	SER	2.3
1	A	45	ASP	2.2
1	A	827	GLY	2.2
1	A	319	LYS	2.1
1	A	785	GLU	2.1
1	A	255[A]	HIS	2.0
1	A	746	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 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.