



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:50 pm BST

PDB ID : 2Z5N
Title : Complex of Transportin 1 with hnRNP D NLS
Authors : Imasaki, T.; Shimizu, T.; Hashimoto, H.; Hidaka, Y.; Kose, S.; Imamoto, N.; Yamada, M.; Sato, M.
Deposited on : 2007-07-14
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

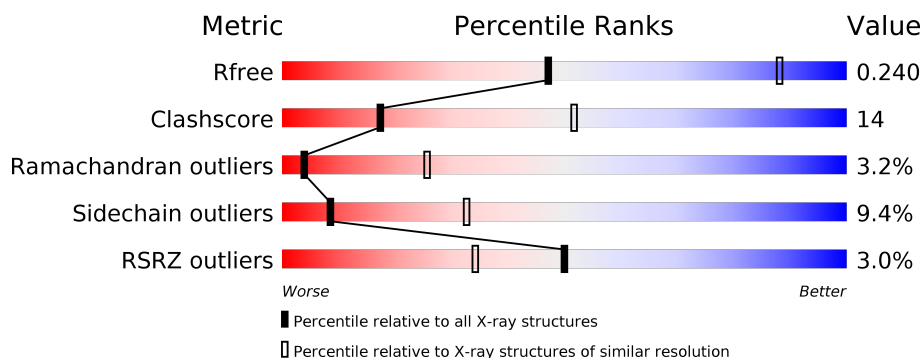
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 ≥ 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	<div> <div>3%</div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div>
2	B	24	<div> <div>42%</div> <div>13%</div> <div>8%</div> <div>38%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6817 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	840	Total	C	N	O	S	0	0	0
			6691	4290	1114	1236	51			

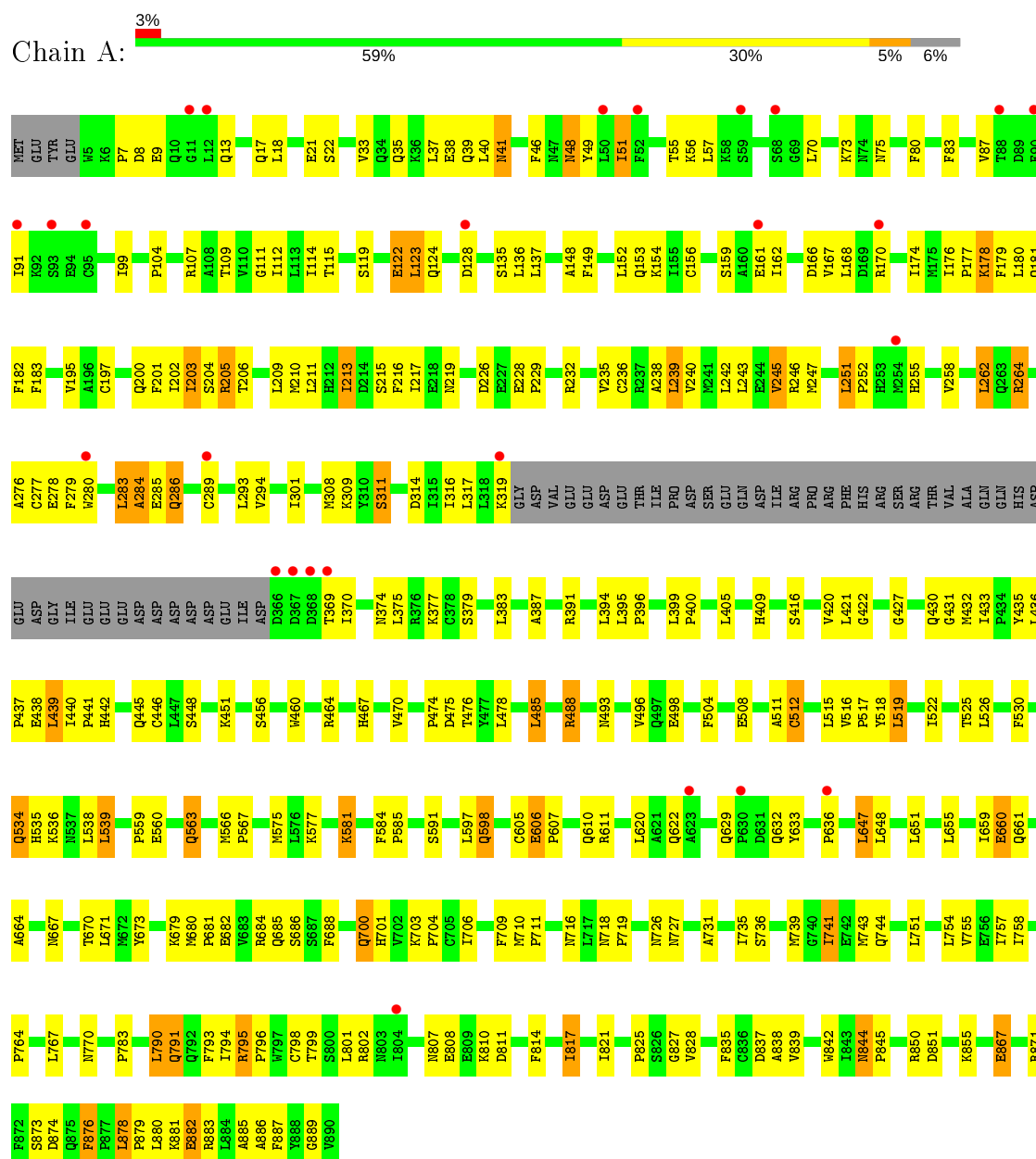
- Molecule 2 is a protein called Heterogeneous nuclear ribonucleoprotein D0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			126	77	27	22			

3 Residue-property plots [i](#)

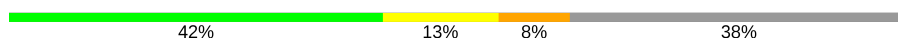
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Heterogeneous nuclear ribonucleoprotein D0

Chain B:



TYR	K341
SER	V342
ASN	S343
GLN	S351
GLN	Y352
SER	K353
GLY	P354
TYR	Y355
GLY	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.68Å 118.95Å 151.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 3.20 45.24 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.8 (45.22-3.20) 91.7 (45.24-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.295 0.228 , 0.240	Depositor DCC
R_{free} test set	984 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6817	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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 [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	0.41	1/6834 (0.0%)	0.56	0/9282
2	B	0.41	0/129	0.54	0/169
All	All	0.41	1/6963 (0.0%)	0.56	0/9451

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	GLU	CD-OE1	5.45	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	6691	0	6750	187	0
2	B	126	0	122	3	0
All	All	6817	0	6872	189	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 14.

All (189) 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:664:ALA:HB2	1:A:701:HIS:HE1	1.33	0.93
1:A:795:ARG:HB2	1:A:796:PRO:HD3	1.61	0.81
1:A:215:SER:O	1:A:219:ASN:HB2	1.81	0.81
1:A:664:ALA:HB2	1:A:701:HIS:CE1	2.16	0.81
1:A:416:SER:O	1:A:420:VAL:HG23	1.83	0.79
1:A:591:SER:HB3	1:A:647:LEU:HA	1.65	0.79
1:A:109:THR:O	1:A:112:ILE:HG22	1.83	0.78
1:A:684:ARG:HD2	1:A:716:ASN:OD1	1.84	0.76
1:A:726:ASN:HD21	1:A:770:ASN:HD22	1.33	0.75
1:A:741:ILE:O	1:A:744:GLN:HB2	1.88	0.73
1:A:795:ARG:HB2	1:A:796:PRO:CD	2.18	0.73
1:A:435:TYR:O	1:A:439:LEU:HB2	1.90	0.72
1:A:851:ASP:O	1:A:855:LYS:HD2	1.90	0.71
1:A:791:GLN:H	1:A:791:GLN:HE21	1.39	0.71
1:A:798:CYS:HB3	1:A:838:ALA:HB2	1.72	0.69
1:A:867:GLU:CD	1:A:867:GLU:H	1.94	0.69
1:A:203:ILE:C	1:A:205:ARG:H	1.94	0.69
1:A:51:ILE:O	1:A:55:THR:HG22	1.92	0.68
1:A:559:PRO:O	1:A:563:GLN:HG2	1.93	0.68
1:A:87:VAL:O	1:A:91:ILE:HG12	1.94	0.67
1:A:206:THR:O	1:A:210:MET:HG2	1.97	0.65
1:A:235:VAL:O	1:A:239:LEU:HB2	1.97	0.64
1:A:467:HIS:O	1:A:470:VAL:HG22	1.97	0.64
1:A:726:ASN:HA	1:A:767:LEU:HD13	1.80	0.63
1:A:755:VAL:HA	1:A:758:ILE:HG22	1.81	0.62
1:A:584:PHE:HB2	1:A:585:PRO:HD3	1.82	0.61
1:A:629:GLN:HB3	1:A:633:TYR:HD1	1.64	0.61
1:A:240:VAL:HG22	1:A:279:PHE:HB2	1.83	0.61
1:A:726:ASN:ND2	1:A:770:ASN:HD22	1.97	0.61
1:A:286:GLN:H	1:A:286:GLN:CD	2.05	0.60
1:A:700:GLN:HG2	1:A:701:HIS:HD2	1.67	0.59
1:A:99:ILE:HD11	1:A:148:ALA:HA	1.84	0.59
1:A:104:PRO:HA	1:A:107:ARG:NH1	2.17	0.59
1:A:135:SER:C	1:A:137:LEU:H	2.05	0.59
1:A:516:VAL:O	1:A:519:LEU:HB2	2.03	0.58
1:A:284:ALA:HA	1:A:289:CYS:SG	2.44	0.58
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.85	0.58
1:A:460:TRP:CZ2	1:A:464:ARG:HD2	2.39	0.58
1:A:700:GLN:HG2	1:A:701:HIS:CD2	2.39	0.57
1:A:726:ASN:HD22	1:A:767:LEU:HA	1.69	0.57
1:A:152:LEU:O	1:A:156:CYS:HB2	2.05	0.57
1:A:560:GLU:HA	1:A:563:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HG23	1:A:56:LYS:HG3	1.87	0.57
1:A:236:CYS:O	1:A:240:VAL:HG23	2.06	0.55
1:A:591:SER:CB	1:A:647:LEU:HA	2.36	0.55
1:A:885:ALA:O	1:A:889:GLY:HA2	2.06	0.55
1:A:736:SER:HB2	1:A:743:MET:HG3	1.89	0.55
1:A:399:LEU:HB3	1:A:400:PRO:HD3	1.90	0.54
1:A:123:LEU:HD23	1:A:162:ILE:HG21	1.88	0.54
1:A:201:PHE:HB3	1:A:206:THR:OG1	2.08	0.54
1:A:33:VAL:O	1:A:37:LEU:HB2	2.07	0.54
1:A:123:LEU:HB2	1:A:168:LEU:HD21	1.88	0.54
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.88	0.54
1:A:706:ILE:HD11	1:A:735:ILE:HG23	1.90	0.53
1:A:183:PHE:CZ	1:A:195:VAL:HA	2.43	0.53
1:A:283:LEU:HD13	1:A:293:LEU:HD11	1.91	0.53
1:A:51:ILE:HG13	1:A:91:ILE:HG23	1.89	0.53
1:A:791:GLN:HE21	1:A:791:GLN:N	2.05	0.53
1:A:255:HIS:HA	1:A:258:VAL:HG22	1.91	0.53
1:A:38:GLU:O	1:A:41:ASN:HB2	2.09	0.53
1:A:48:ASN:HD22	1:A:87:VAL:HG13	1.75	0.52
1:A:844:ASN:C	1:A:844:ASN:HD22	2.13	0.52
1:A:703:LYS:O	1:A:706:ILE:HG22	2.09	0.52
1:A:790:LEU:HA	1:A:793:PHE:CE2	2.45	0.52
1:A:706:ILE:HA	1:A:709:PHE:HB2	1.91	0.51
1:A:606:GLU:HB3	1:A:607:PRO:CD	2.41	0.51
1:A:796:PRO:HA	1:A:799:THR:HB	1.92	0.51
1:A:584:PHE:HB2	1:A:585:PRO:CD	2.40	0.51
1:A:152:LEU:HD22	1:A:179:PHE:HZ	1.76	0.51
1:A:277:CYS:HA	1:A:280:TRP:HD1	1.76	0.50
1:A:817:ILE:O	1:A:821:ILE:HG13	2.11	0.50
1:A:317:LEU:HD23	1:A:370:ILE:HD12	1.93	0.50
1:A:651:LEU:O	1:A:655:LEU:HB2	2.11	0.50
1:A:436:LEU:N	1:A:437:PRO:CD	2.74	0.49
1:A:277:CYS:HA	1:A:280:TRP:CD1	2.48	0.49
1:A:35:GLN:C	1:A:37:LEU:H	2.15	0.49
1:A:203:ILE:C	1:A:205:ARG:N	2.63	0.49
1:A:433:ILE:O	1:A:437:PRO:HD3	2.12	0.49
1:A:488:ARG:NE	1:A:488:ARG:HA	2.27	0.49
1:A:629:GLN:HG2	1:A:632:GLN:HB2	1.94	0.49
1:A:153:GLN:HA	1:A:197:CYS:SG	2.53	0.49
1:A:159:SER:HB3	1:A:162:ILE:HB	1.94	0.49
1:A:446:CYS:C	1:A:448:SER:H	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:SER:HA	1:A:876:PHE:CZ	2.48	0.49
1:A:516:VAL:HB	1:A:517:PRO:HD3	1.94	0.48
1:A:39:GLN:C	1:A:41:ASN:H	2.17	0.48
1:A:17:GLN:O	1:A:21:GLU:HG2	2.13	0.48
1:A:124:GLN:HB2	1:A:167:VAL:HG12	1.93	0.48
1:A:790:LEU:HA	1:A:793:PHE:CZ	2.49	0.48
1:A:9:GLU:HG2	1:A:13:GLN:HE21	1.78	0.48
1:A:685:GLN:HG2	1:A:686:SER:N	2.29	0.48
1:A:504:PHE:O	1:A:508:GLU:HG3	2.13	0.48
1:A:851:ASP:HB3	1:A:855:LYS:NZ	2.29	0.48
1:A:534:GLN:O	1:A:538:LEU:HB2	2.13	0.47
1:A:7:PRO:O	1:A:49:TYR:HE2	1.97	0.47
1:A:395:LEU:HB2	1:A:396:PRO:HD3	1.96	0.47
1:A:504:PHE:HZ	1:A:522:ILE:HD12	1.80	0.47
1:A:825:PRO:O	1:A:828:VAL:HG22	2.13	0.47
1:A:180:LEU:HD23	1:A:180:LEU:O	2.15	0.47
1:A:597:LEU:O	1:A:598:GLN:C	2.52	0.47
1:A:739:MET:HB2	1:A:743:MET:HG2	1.95	0.47
1:A:802:ARG:HD2	1:A:837:ASP:OD2	2.13	0.47
1:A:80:PHE:O	1:A:83:PHE:CD1	2.67	0.47
1:A:835:PHE:O	1:A:839:VAL:HG23	2.15	0.47
1:A:210:MET:O	1:A:213:ILE:HG22	2.14	0.47
1:A:566:MET:HB2	1:A:567:PRO:HD3	1.97	0.47
1:A:387:ALA:HA	1:A:394:LEU:CD2	2.45	0.47
1:A:755:VAL:O	1:A:758:ILE:HG22	2.15	0.47
1:A:790:LEU:HD23	1:A:827:GLY:HA3	1.96	0.47
1:A:845:PRO:HG2	1:A:850:ARG:HG3	1.96	0.47
1:A:810:LYS:HG2	1:A:842:TRP:CZ2	2.50	0.46
1:A:706:ILE:HD11	1:A:735:ILE:CG2	2.45	0.46
1:A:878:LEU:C	1:A:880:LEU:H	2.19	0.46
1:A:251:LEU:N	1:A:252:PRO:HD2	2.31	0.46
1:A:814:PHE:O	1:A:817:ILE:HG22	2.16	0.46
1:A:18:LEU:O	1:A:22:SER:HB2	2.16	0.45
1:A:374:ASN:HB3	1:A:377:LYS:H	1.81	0.45
1:A:659:ILE:O	1:A:660:GLU:C	2.54	0.45
1:A:700:GLN:NE2	1:A:700:GLN:H	2.14	0.45
1:A:80:PHE:O	1:A:83:PHE:HD1	1.97	0.45
1:A:181:GLN:C	1:A:183:PHE:H	2.19	0.45
1:A:794:ILE:HG12	1:A:794:ILE:O	2.16	0.45
1:A:518:TYR:O	1:A:522:ILE:HG12	2.17	0.45
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HB3	1:A:276:ALA:CB	2.46	0.45
1:A:474:PRO:C	1:A:476:THR:H	2.20	0.45
1:A:731:ALA:O	1:A:735:ILE:HG12	2.16	0.45
1:A:135:SER:C	1:A:137:LEU:N	2.70	0.45
1:A:70:LEU:O	1:A:73:LYS:HB3	2.16	0.45
1:A:9:GLU:O	1:A:13:GLN:HG2	2.17	0.45
1:A:629:GLN:CG	1:A:632:GLN:HB2	2.47	0.45
1:A:202:ILE:O	1:A:245:VAL:HG21	2.17	0.44
1:A:493:ASN:OD1	1:A:496:VAL:HG23	2.17	0.44
1:A:605:CYS:O	1:A:606:GLU:C	2.54	0.44
1:A:111:GLY:HA2	1:A:114:ILE:HD12	1.98	0.44
1:A:180:LEU:HD11	1:A:216:PHE:HB2	1.99	0.44
1:A:882:GLU:O	1:A:886:ALA:N	2.46	0.44
1:A:383:LEU:HD21	1:A:420:VAL:HG13	2.00	0.44
1:A:422:GLY:O	1:A:464:ARG:HD3	2.17	0.44
1:A:115:THR:HG21	1:A:154:LYS:CG	2.48	0.44
1:A:680:MET:HA	1:A:681:PRO:HD2	1.75	0.44
1:A:710:MET:HB2	1:A:711:PRO:HD3	1.99	0.44
1:A:808:GLU:HA	1:A:811:ASP:HB3	1.99	0.44
1:A:685:GLN:CG	1:A:686:SER:N	2.81	0.44
1:A:283:LEU:C	1:A:285:GLU:H	2.21	0.43
1:A:308:MET:HG3	1:A:379:SER:HB2	2.00	0.43
1:A:534:GLN:CD	1:A:534:GLN:H	2.21	0.43
1:A:309:LYS:HA	1:A:416:SER:HB3	1.99	0.43
1:A:377:LYS:HG2	2:B:355:TYR:HA	2.00	0.43
1:A:679:LYS:O	1:A:684:ARG:NH1	2.51	0.43
2:B:351:SER:HB3	2:B:352:TYR:H	1.65	0.43
1:A:104:PRO:HA	1:A:107:ARG:HH12	1.83	0.43
1:A:684:ARG:O	1:A:688:PHE:CD1	2.71	0.43
1:A:176:ILE:O	1:A:180:LEU:HB2	2.19	0.43
1:A:391:ARG:HA	1:A:427:GLY:O	2.17	0.43
1:A:536:LYS:HA	1:A:539:LEU:HD22	2.00	0.43
1:A:156:CYS:O	1:A:200:GLN:HG3	2.19	0.43
1:A:226:ASP:O	1:A:232:ARG:HD3	2.18	0.43
1:A:203:ILE:H	1:A:203:ILE:HD12	1.83	0.42
1:A:395:LEU:HD11	1:A:431:GLY:HA3	2.02	0.42
1:A:387:ALA:HA	1:A:394:LEU:HD23	2.01	0.42
1:A:262:LEU:HA	1:A:280:TRP:HZ2	1.85	0.42
1:A:46:PHE:HE2	1:A:75:ASN:ND2	2.18	0.42
1:A:581:LYS:CD	1:A:581:LYS:H	2.31	0.42
1:A:751:LEU:HA	1:A:754:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ASN:O	1:A:671:LEU:HG	2.20	0.42
1:A:123:LEU:N	1:A:123:LEU:HD22	2.35	0.42
1:A:177:PRO:O	1:A:181:GLN:HG3	2.20	0.41
1:A:176:ILE:HG21	1:A:209:LEU:HA	2.01	0.41
1:A:485:LEU:HA	1:A:485:LEU:HD12	1.86	0.41
1:A:670:THR:O	1:A:673:TYR:HB3	2.20	0.41
1:A:511:ALA:O	1:A:512:CYS:C	2.59	0.41
1:A:660:GLU:HG3	1:A:661:GLN:N	2.35	0.41
1:A:682:GLU:N	1:A:682:GLU:OE2	2.50	0.41
1:A:283:LEU:O	1:A:285:GLU:N	2.54	0.41
1:A:871:ARG:NH1	1:A:871:ARG:HB2	2.35	0.41
1:A:115:THR:HG21	1:A:154:LYS:HG2	2.03	0.41
1:A:213:ILE:HG21	1:A:246:ARG:NH1	2.36	0.41
1:A:217:ILE:H	1:A:217:ILE:HG12	1.72	0.41
1:A:311:SER:O	1:A:314:ASP:HB2	2.20	0.41
1:A:439:LEU:O	1:A:442:HIS:HB3	2.21	0.41
1:A:375:LEU:HD12	1:A:375:LEU:O	2.21	0.40
1:A:174:ILE:O	1:A:178:LYS:HB2	2.21	0.40
1:A:238:ALA:O	1:A:242:LEU:HD13	2.21	0.40
1:A:622:GLN:HB3	1:A:636:PRO:HB3	2.03	0.40
1:A:228:GLU:OE2	1:A:229:PRO:HD2	2.21	0.40
1:A:474:PRO:HA	1:A:478:LEU:HB3	2.04	0.40
1:A:718:ASN:HA	1:A:719:PRO:HD2	1.80	0.40
2:B:354:PRO:HG2	2:B:355:TYR:CD2	2.57	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	836/890 (94%)	703 (84%)	107 (13%)	26 (3%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	13/24 (54%)	8 (62%)	4 (31%)	1 (8%)	1	6
All	All	849/914 (93%)	711 (84%)	111 (13%)	27 (3%)	4	26

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	VAL
1	A	512	CYS
1	A	598	GLN
1	A	790	LEU
1	A	119	SER
1	A	204	SER
1	A	213	ILE
1	A	284	ALA
1	A	475	ASP
1	A	8	ASP
1	A	182	PHE
1	A	205	ARG
1	A	456	SER
1	A	874	ASP
1	A	40	LEU
1	A	647	LEU
1	A	879	PRO
1	A	122	GLU
1	A	278	GLU
2	B	343	SER
1	A	136	LEU
1	A	704	PRO
1	A	764	PRO
1	A	795	ARG
1	A	606	GLU
1	A	170	ARG
1	A	783	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	755/802 (94%)	685 (91%)	70 (9%)	9	33
2	B	13/20 (65%)	11 (85%)	2 (15%)	2	13
All	All	768/822 (93%)	696 (91%)	72 (9%)	8	33

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	48	ASN
1	A	51	ILE
1	A	57	LEU
1	A	122	GLU
1	A	123	LEU
1	A	128	ASP
1	A	149	PHE
1	A	166	ASP
1	A	178	LYS
1	A	203	ILE
1	A	211	LEU
1	A	239	LEU
1	A	243	LEU
1	A	247	MET
1	A	251	LEU
1	A	262	LEU
1	A	264	ARG
1	A	283	LEU
1	A	286	GLN
1	A	294	VAL
1	A	301	ILE
1	A	311	SER
1	A	316	ILE
1	A	319	LYS
1	A	369	THR
1	A	405	LEU
1	A	409	HIS
1	A	421	LEU
1	A	430	GLN
1	A	432	MET
1	A	438	GLU
1	A	439	LEU
1	A	445	GLN
1	A	451	LYS

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Mol	Chain	Res	Type
1	A	485	LEU
1	A	488	ARG
1	A	498	GLU
1	A	519	LEU
1	A	525	THR
1	A	526	LEU
1	A	530	PHE
1	A	534	GLN
1	A	535	HIS
1	A	539	LEU
1	A	563	GLN
1	A	575	MET
1	A	577	LYS
1	A	581	LYS
1	A	610	GLN
1	A	611	ARG
1	A	620	LEU
1	A	648	LEU
1	A	660	GLU
1	A	700	GLN
1	A	727	ASN
1	A	741	ILE
1	A	757	ILE
1	A	791	GLN
1	A	801	LEU
1	A	807	ASN
1	A	817	ILE
1	A	844	ASN
1	A	867	GLU
1	A	876	PHE
1	A	878	LEU
1	A	881	LYS
1	A	882	GLU
1	A	883	ARG
1	A	887	PHE
2	B	343	SER
2	B	351	SER

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

Mol	Chain	Res	Type
1	A	13	GLN

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Mol	Chain	Res	Type
1	A	47	ASN
1	A	48	ASN
1	A	193	HIS
1	A	263	GLN
1	A	271	ASN
1	A	472	GLN
1	A	557	ASN
1	A	574	ASN
1	A	658	ASN
1	A	700	GLN
1	A	701	HIS
1	A	726	ASN
1	A	727	ASN
1	A	791	GLN
1	A	844	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, 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	840/890 (94%)	0.23	26 (3%) 49 32	109, 125, 133, 145	0
2	B	15/24 (62%)	0.59	0 100 100	115, 118, 120, 122	0
All	All	855/914 (93%)	0.24	26 (3%) 50 34	109, 125, 133, 145	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	CYS	4.9
1	A	11	GLY	4.8
1	A	128	ASP	4.1
1	A	52	PHE	4.0
1	A	50	LEU	3.4
1	A	319	LYS	3.1
1	A	289	CYS	3.0
1	A	630	PRO	2.9
1	A	636	PRO	2.9
1	A	367	ASP	2.8
1	A	90	PHE	2.8
1	A	88	THR	2.8
1	A	369	THR	2.7
1	A	170	ARG	2.6
1	A	368	ASP	2.5
1	A	161	GLU	2.4
1	A	93	SER	2.4
1	A	12	LEU	2.3
1	A	68	SER	2.3
1	A	91	ILE	2.3
1	A	623	ALA	2.3
1	A	59	SER	2.2
1	A	366	ASP	2.2
1	A	804	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	280	TRP	2.1
1	A	254	MET	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.