



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:24 PM UTC

PDB ID : 2Z5M / pdb_00002z5m
Title : Complex of Transportin 1 with TAP NLS, crystal form 2
Authors : Imasaki, T.; Shimizu, T.; Hashimoto, H.; Hidaka, Y.; Kose, S.; Imamoto, N.; Yamada, M.; Sato, M.
Deposited on : 2007-07-14
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

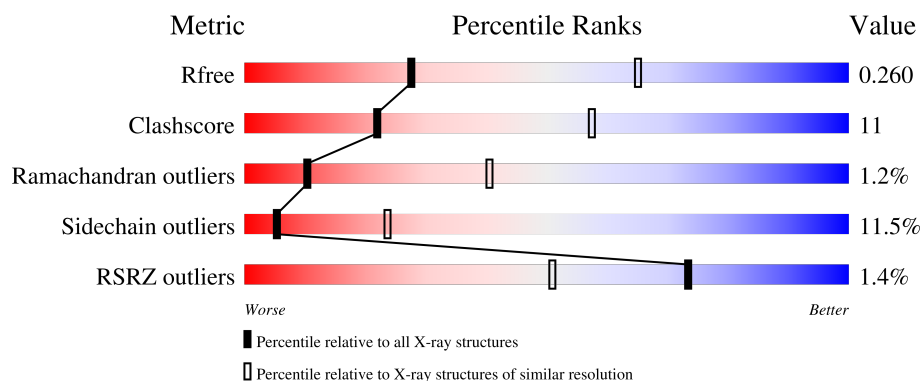
1 Overall quality at a glance

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	65% 25% 6%
2	B	30	10% 20% 13% 67%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6778 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.

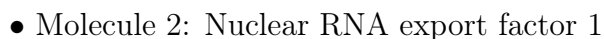
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	0
			6690	4290	1114	1235	51			

- Molecule 2 is a protein called Nuclear RNA export factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			88	57	17	14			

i

- Molecule 1: Transportin-1



GLU	GLU	ASP	GLY	ASP	VAL	ALA	MET	SER	ASP	ALA	GLN	ASP	GLY	PRO	ARG	V70	R71	T77	R78	F79	ASN	ARG	ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.44Å 170.99Å 68.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-3.00) 95.3 (50.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.267 0.240 , 0.260	Depositor DCC
R_{free} test set	1537 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6778	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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	0.54	1/6833 (0.0%)	0.90	9/9281 (0.1%)
2	B	0.84	0/91	0.69	0/125
All	All	0.55	1/6924 (0.0%)	0.90	9/9406 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	747	ILE	CA-CB	6.38	1.57	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	GLU	CA-C-N	6.45	125.95	119.24
1	A	228	GLU	C-N-CA	6.45	125.95	119.24
1	A	123	LEU	N-CA-C	6.09	117.91	111.28
1	A	680	MET	CA-C-N	6.01	126.17	119.32
1	A	680	MET	C-N-CA	6.01	126.17	119.32
1	A	473	PRO	CA-C-N	5.47	126.67	119.84
1	A	473	PRO	C-N-CA	5.47	126.67	119.84
1	A	722	ILE	N-CA-C	5.40	116.03	110.36
1	A	391	ARG	CB-CA-C	-5.09	110.69	116.54

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	6690	0	6750	144	0
2	B	88	0	86	1	0
All	All	6778	0	6836	145	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 11.

All (145) 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:70:LEU:HD13	1:A:109:THR:HG23	1.58	0.84
1:A:81:GLN:H	1:A:81:GLN:CD	1.85	0.84
1:A:185:HIS:HD2	1:A:187:SER:H	1.19	0.84
1:A:185:HIS:CD2	1:A:187:SER:H	2.00	0.80
1:A:859:GLY:O	1:A:863:GLN:HB2	1.88	0.72
1:A:638:LYS:O	1:A:642:ILE:HD13	1.90	0.71
1:A:739:MET:HB2	1:A:743:MET:HG2	1.74	0.69
1:A:736:SER:HA	1:A:743:MET:HG3	1.75	0.67
1:A:642:ILE:HD11	1:A:683:VAL:HG22	1.77	0.66
1:A:561:TYR:HA	1:A:564:MET:HE3	1.77	0.65
1:A:199:ASN:HB3	1:A:241:MET:HE1	1.79	0.65
1:A:864:VAL:HG22	1:A:868:ASN:HD22	1.60	0.65
1:A:317:LEU:HD23	1:A:370:ILE:HD13	1.79	0.65
2:B:70:VAL:HG13	2:B:71:ARG:H	1.62	0.64
1:A:51:ILE:HG21	1:A:91:ILE:HD12	1.78	0.63
1:A:100:GLY:HA3	1:A:144:THR:HA	1.81	0.63
1:A:185:HIS:NE2	1:A:190:ILE:HD12	2.13	0.63
1:A:415:GLU:OE2	1:A:457:ILE:HG13	1.99	0.63
1:A:840:ALA:HB2	1:A:880:LEU:HD13	1.81	0.62
1:A:100:GLY:HA2	1:A:107:ARG:HD3	1.80	0.62
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.81	0.62
1:A:288:ILE:HD12	1:A:288:ILE:H	1.64	0.61
1:A:729:THR:HG21	1:A:771:THR:HA	1.83	0.61
1:A:103:SER:HB3	1:A:106:ILE:HD12	1.83	0.61
1:A:247:MET:HE3	1:A:288:ILE:HD13	1.83	0.59
1:A:87:VAL:O	1:A:91:ILE:HD13	2.01	0.59
1:A:405:LEU:HD23	1:A:413:VAL:HG12	1.83	0.59
1:A:560:GLU:HA	1:A:563:GLN:HG2	1.85	0.58
1:A:876:PHE:HB3	1:A:880:LEU:HG	1.84	0.58
1:A:173:ASN:HD22	1:A:208:ALA:HB2	1.68	0.58
1:A:398:ILE:HD13	1:A:424:ILE:HG21	1.86	0.57
1:A:753:GLN:O	1:A:757:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:O	1:A:545:ILE:HD13	2.05	0.56
1:A:622:GLN:HE21	1:A:636:PRO:HB3	1.71	0.56
1:A:312:ASP:HA	1:A:315:ILE:HD12	1.87	0.55
1:A:76:VAL:HG13	1:A:80:PHE:CD1	2.41	0.55
1:A:479:LYS:HB3	1:A:480:PRO:HD3	1.88	0.55
1:A:754:LEU:HB3	1:A:775:ILE:HD11	1.88	0.55
1:A:743:MET:HB3	1:A:747:ILE:HD11	1.88	0.55
1:A:497:GLN:HB3	1:A:533:TYR:HE1	1.72	0.55
1:A:99:ILE:HD13	1:A:114:ILE:HD12	1.90	0.54
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.88	0.54
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.89	0.54
1:A:488:ARG:NE	1:A:488:ARG:HA	2.22	0.54
1:A:606:GLU:HG2	1:A:662:LEU:HD21	1.91	0.53
1:A:497:GLN:HB3	1:A:533:TYR:CE1	2.42	0.53
1:A:130:LEU:HB2	1:A:131:PRO:HD3	1.90	0.53
1:A:433:ILE:HB	1:A:434:PRO:HD3	1.89	0.53
1:A:567:PRO:HB2	1:A:568:PRO:HD3	1.91	0.53
1:A:713:LEU:HB3	1:A:732:ILE:HD11	1.91	0.53
1:A:825:PRO:HB3	1:A:860:PHE:CZ	2.44	0.53
1:A:852:MET:O	1:A:856:ILE:HG12	2.09	0.52
1:A:825:PRO:HB3	1:A:860:PHE:HZ	1.74	0.52
1:A:34:GLN:HA	1:A:37:LEU:HD23	1.91	0.52
1:A:840:ALA:CB	1:A:880:LEU:HD13	2.39	0.52
1:A:199:ASN:HA	1:A:202:ILE:CD1	2.39	0.52
1:A:497:GLN:HB2	1:A:537:ASN:ND2	2.25	0.51
1:A:11:GLY:O	1:A:15:ILE:HD13	2.09	0.51
1:A:829:ILE:HD13	1:A:829:ILE:O	2.10	0.51
1:A:395:LEU:HB3	1:A:399:LEU:HD22	1.92	0.51
1:A:573:TRP:CZ2	1:A:608:VAL:HA	2.45	0.51
1:A:790:LEU:HD23	1:A:828:VAL:HB	1.92	0.51
1:A:649:SER:HB3	1:A:693:ASP:OD1	2.10	0.51
1:A:374:ASN:ND2	1:A:377:LYS:H	2.09	0.50
1:A:489:ILE:HG23	1:A:533:TYR:OH	2.11	0.50
1:A:199:ASN:HA	1:A:202:ILE:HD13	1.92	0.50
1:A:202:ILE:CD1	1:A:202:ILE:N	2.75	0.50
1:A:50:LEU:O	1:A:68:SER:OG	2.26	0.50
1:A:91:ILE:CD1	1:A:91:ILE:N	2.75	0.49
1:A:703:LYS:HA	1:A:706:ILE:HG12	1.94	0.49
1:A:559:PRO:O	1:A:563:GLN:HG2	2.13	0.49
1:A:878:LEU:HB3	1:A:879:PRO:HD3	1.93	0.49
1:A:33:VAL:C	1:A:35:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:TYR:O	1:A:613:VAL:HG23	2.13	0.48
1:A:873:SER:HA	1:A:876:PHE:CE2	2.48	0.48
1:A:798:CYS:O	1:A:802:ARG:HG2	2.13	0.48
1:A:289:CYS:SG	1:A:293:LEU:HD12	2.53	0.48
1:A:488:ARG:O	1:A:491:ASP:HB2	2.13	0.48
1:A:177:PRO:O	1:A:181:GLN:HG3	2.14	0.48
1:A:523:LEU:O	1:A:527:VAL:HG22	2.13	0.48
1:A:877:PRO:HD2	1:A:880:LEU:HD23	1.95	0.48
1:A:91:ILE:HD13	1:A:91:ILE:N	2.28	0.47
1:A:802:ARG:HD2	1:A:837:ASP:OD2	2.13	0.47
1:A:314:ASP:HA	1:A:370:ILE:HD11	1.96	0.47
1:A:168:LEU:O	1:A:168:LEU:HG	2.15	0.47
1:A:736:SER:HA	1:A:743:MET:CG	2.44	0.47
1:A:868:ASN:HA	1:A:871:ARG:HE	1.79	0.47
1:A:78:ALA:O	1:A:79:HIS:ND1	2.33	0.47
1:A:203:ILE:HA	1:A:245:VAL:HG21	1.97	0.47
1:A:672:MET:HE1	1:A:694:LEU:CD1	2.45	0.47
1:A:21:GLU:HB3	1:A:33:VAL:HG21	1.96	0.47
1:A:47:ASN:HD21	1:A:75:ASN:HD22	1.61	0.47
1:A:680:MET:HA	1:A:681:PRO:HD2	1.71	0.46
1:A:79:HIS:O	1:A:79:HIS:CG	2.68	0.46
1:A:713:LEU:HD13	1:A:732:ILE:HD13	1.98	0.46
1:A:743:MET:HE3	1:A:747:ILE:HD13	1.98	0.46
1:A:168:LEU:O	1:A:169:ASP:HB3	2.15	0.46
1:A:860:PHE:CD1	1:A:860:PHE:N	2.83	0.46
1:A:169:ASP:CG	1:A:170:ARG:H	2.24	0.45
1:A:276:ALA:O	1:A:279:PHE:HB3	2.16	0.45
1:A:440:ILE:O	1:A:444:ILE:HG12	2.16	0.45
1:A:664:ALA:HB2	1:A:701:HIS:CE1	2.51	0.45
1:A:47:ASN:HD21	1:A:75:ASN:ND2	2.15	0.45
1:A:121:GLY:O	1:A:122:GLU:O	2.35	0.45
1:A:49:TYR:O	1:A:53:VAL:HG23	2.16	0.44
1:A:710:MET:HE2	1:A:746:TYR:HB3	1.98	0.44
1:A:33:VAL:C	1:A:35:GLN:N	2.73	0.44
1:A:405:LEU:HD23	1:A:413:VAL:CG1	2.46	0.44
1:A:134:CYS:HA	1:A:137:LEU:HD22	2.00	0.44
1:A:771:THR:O	1:A:775:ILE:HG12	2.18	0.44
1:A:858:HIS:HE1	1:A:888:TYR:O	2.01	0.44
1:A:584:PHE:CD2	1:A:584:PHE:N	2.72	0.44
1:A:96:LEU:HD23	1:A:132:LYS:HG2	2.00	0.43
1:A:215:SER:O	1:A:219:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:CYS:HA	1:A:551:SER:HB3	2.00	0.43
1:A:567:PRO:HB2	1:A:568:PRO:CD	2.49	0.43
1:A:705:CYS:HB3	1:A:709:PHE:CE2	2.53	0.43
1:A:51:ILE:HD11	1:A:94:GLU:CB	2.49	0.43
1:A:168:LEU:O	1:A:169:ASP:CB	2.67	0.43
1:A:291:ASP:O	1:A:294:VAL:HG22	2.20	0.42
1:A:276:ALA:O	1:A:279:PHE:CB	2.67	0.42
1:A:700:GLN:NE2	1:A:700:GLN:H	2.16	0.42
1:A:877:PRO:HD2	1:A:880:LEU:HB3	2.01	0.42
1:A:191:ARG:O	1:A:195:VAL:HG12	2.19	0.42
1:A:516:VAL:HB	1:A:517:PRO:HD3	2.02	0.42
1:A:185:HIS:CE1	1:A:190:ILE:HD12	2.55	0.42
1:A:24:SER:HA	1:A:25:PRO:HD3	1.90	0.42
1:A:81:GLN:CD	1:A:81:GLN:N	2.64	0.42
1:A:301:ILE:HB	1:A:302:PRO:HD3	2.01	0.41
1:A:398:ILE:HD11	1:A:420:VAL:HG13	2.01	0.41
1:A:534:GLN:HG2	1:A:535:HIS:N	2.35	0.41
1:A:860:PHE:N	1:A:860:PHE:HD1	2.18	0.41
1:A:194:ALA:O	1:A:198:VAL:HG23	2.21	0.41
1:A:374:ASN:C	1:A:374:ASN:HD22	2.29	0.41
1:A:526:LEU:HD13	1:A:545:ILE:HD12	2.01	0.41
1:A:672:MET:HE3	1:A:672:MET:HB2	1.63	0.41
1:A:51:ILE:HD11	1:A:94:GLU:HB3	2.02	0.41
1:A:477:TYR:C	1:A:480:PRO:HD2	2.46	0.41
1:A:300:LEU:HD22	1:A:304:LEU:HD22	2.03	0.41
1:A:453:LEU:O	1:A:457:ILE:HG12	2.21	0.41
1:A:795:ARG:H	1:A:795:ARG:HG3	1.69	0.41
1:A:854:CYS:O	1:A:855:LYS:C	2.64	0.41
1:A:607:PRO:O	1:A:611:ARG:HG3	2.20	0.41
1:A:760:ARG:HA	1:A:761:PRO:HD3	1.90	0.41
1:A:747:ILE:HB	1:A:748:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	774 (93%)	52 (6%)	10 (1%)	10	40
2	B	8/30 (27%)	8 (100%)	0	0	100	100
All	All	844/920 (92%)	782 (93%)	52 (6%)	10 (1%)	10	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	A	749	MET
1	A	270	GLU
1	A	534	GLN
1	A	34	GLN
1	A	169	ASP
1	A	806	ASP
1	A	559	PRO
1	A	473	PRO
1	A	656	GLY

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%)	669 (89%)	86 (11%)	5	24
2	B	10/26 (38%)	8 (80%)	2 (20%)	1	7
All	All	765/828 (92%)	677 (88%)	88 (12%)	5	24

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	26	ASP
1	A	36	LYS

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Mol	Chain	Res	Type
1	A	38	GLU
1	A	51	ILE
1	A	55	THR
1	A	70	LEU
1	A	79	HIS
1	A	81	GLN
1	A	91	ILE
1	A	113	LEU
1	A	124	GLN
1	A	132	LYS
1	A	137	LEU
1	A	140	GLU
1	A	145	CYS
1	A	149	PHE
1	A	184	LYS
1	A	195	VAL
1	A	202	ILE
1	A	206	THR
1	A	220	LEU
1	A	242	LEU
1	A	247	MET
1	A	251	LEU
1	A	258	VAL
1	A	268	GLN
1	A	270	GLU
1	A	281	LEU
1	A	283	LEU
1	A	288	ILE
1	A	294	VAL
1	A	297	LEU
1	A	300	LEU
1	A	304	LEU
1	A	370	ILE
1	A	374	ASN
1	A	399	LEU
1	A	403	LYS
1	A	421	LEU
1	A	438	GLU
1	A	450	LYS
1	A	457	ILE
1	A	476	THR
1	A	485	LEU

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Mol	Chain	Res	Type
1	A	488	ARG
1	A	490	LEU
1	A	534	GLN
1	A	539	LEU
1	A	548	LEU
1	A	570	ILE
1	A	583	LEU
1	A	584	PHE
1	A	590	LEU
1	A	598	GLN
1	A	610	GLN
1	A	627	ASN
1	A	631	ASP
1	A	647	LEU
1	A	648	LEU
1	A	655	LEU
1	A	669	LEU
1	A	679	LYS
1	A	686	SER
1	A	700	GLN
1	A	717	LEU
1	A	741	ILE
1	A	752	HIS
1	A	765	LYS
1	A	768	LEU
1	A	790	LEU
1	A	791	GLN
1	A	794	ILE
1	A	817	ILE
1	A	829	ILE
1	A	843	ILE
1	A	844	ASN
1	A	847	ASP
1	A	850	ARG
1	A	860	PHE
1	A	862	ASN
1	A	878	LEU
1	A	880	LEU
1	A	882	GLU
1	A	887	PHE
1	A	890	VAL
2	B	77	THR

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Mol	Chain	Res	Type
2	B	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	34	GLN
1	A	35	GLN
1	A	48	ASN
1	A	75	ASN
1	A	82	ASN
1	A	97	ASN
1	A	124	GLN
1	A	173	ASN
1	A	185	HIS
1	A	193	HIS
1	A	256	ASN
1	A	263	GLN
1	A	266	GLN
1	A	268	GLN
1	A	296	HIS
1	A	374	ASN
1	A	388	ASN
1	A	534	GLN
1	A	574	ASN
1	A	622	GLN
1	A	627	ASN
1	A	700	GLN
1	A	726	ASN
1	A	759	ASN
1	A	770	ASN
1	A	784	GLN
1	A	824	ASN
1	A	844	ASN
1	A	858	HIS
1	A	868	ASN

5.3.3 RNA ⓘ

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 [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	840/890 (94%)	0.07	9 (1%) 78 57	53, 95, 125, 140	0
2	B	10/30 (33%)	1.58	3 (30%) 1 1	93, 96, 112, 114	0
All	All	850/920 (92%)	0.09	12 (1%) 73 51	53, 95, 124, 140	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	79	PRO	5.8
2	B	70	VAL	4.1
1	A	890	VAL	3.7
1	A	860	PHE	3.6
1	A	584	PHE	3.1
1	A	29	ILE	3.0
1	A	43	TYR	2.8
2	B	77	THR	2.4
1	A	794	ILE	2.3
1	A	578	ASP	2.3
1	A	492	SER	2.2
1	A	885	ALA	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 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.