



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2Z5O / pdb_00002z5o
Title : Complex of Transportin 1 with JKTBP 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 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

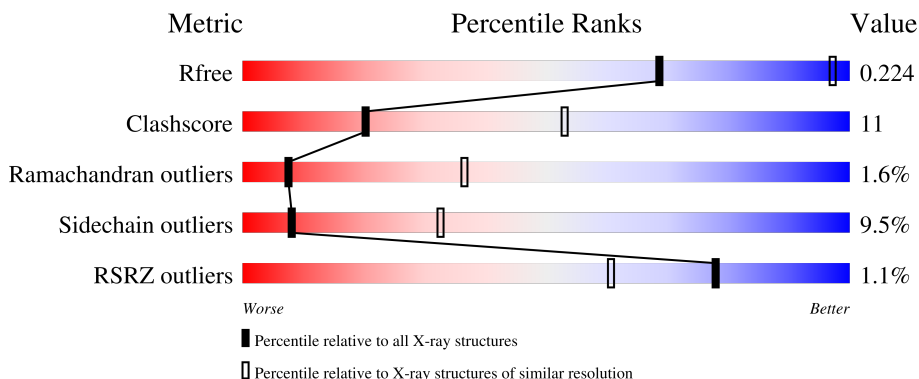
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	67% 23% 6%
2	B	10	80% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6689 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	0	0
			6638	4257	1107	1223	51			

- Molecule 2 is a protein called Heterogeneous nuclear ribonucleoprotein D-like.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			51	30	10	11			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.31Å 169.81Å 68.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 3.20 47.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.57-3.20) 95.0 (47.57-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.279 0.229 , 0.224	Depositor DCC
R_{free} test set	1254 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 113.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6689	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.49	1/6779 (0.0%)	0.90	0/9205

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	ILE	CA-CB	5.37	1.56	1.54

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	6638	0	6710	146	0
2	B	51	0	14	5	0
All	All	6689	0	6724	151	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 (151) 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)
2:B:10:UNK:CA	2:B:10:UNK:C	1.74	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:PHE:HD2	1:A:584:PHE:H	1.14	0.89
1:A:47:ASN:HD21	1:A:75:ASN:HD22	1.24	0.85
1:A:6:LYS:N	1:A:7:PRO:HD3	1.92	0.85
1:A:821:ILE:HG12	1:A:828:VAL:HG21	1.57	0.85
2:B:8:UNK:O	2:B:10:UNK:N	2.09	0.85
1:A:879:PRO:O	1:A:883:ARG:HB2	1.82	0.80
1:A:584:PHE:HB2	1:A:585:PRO:HD3	1.63	0.80
1:A:672:MET:O	1:A:676:MET:HG3	1.80	0.80
1:A:736:SER:HA	1:A:743:MET:HG3	1.65	0.79
1:A:877:PRO:HD2	1:A:880:LEU:HD23	1.66	0.78
1:A:70:LEU:HD13	1:A:109:THR:HG23	1.64	0.77
1:A:700:GLN:HE21	1:A:700:GLN:H	1.34	0.75
1:A:38:GLU:HA	1:A:41:ASN:HB2	1.67	0.75
1:A:791:GLN:HG3	1:A:827:GLY:HA2	1.73	0.70
1:A:584:PHE:HD2	1:A:584:PHE:N	1.88	0.69
1:A:504:PHE:HZ	1:A:522:ILE:HD12	1.57	0.68
1:A:815:ARG:HH11	1:A:815:ARG:HG2	1.58	0.68
1:A:824:ASN:HD22	1:A:824:ASN:C	2.00	0.68
1:A:243:LEU:HD21	1:A:254:MET:HE1	1.77	0.68
2:B:8:UNK:C	2:B:10:UNK:N	2.58	0.66
1:A:790:LEU:HD23	1:A:828:VAL:HG23	1.78	0.65
1:A:185:HIS:CD2	1:A:187:SER:H	2.15	0.65
1:A:8:ASP:HB2	1:A:9:GLU:HB3	1.79	0.64
1:A:629:GLN:OE1	1:A:633:TYR:HB2	1.98	0.64
1:A:122:GLU:HA	1:A:123:LEU:HB2	1.79	0.64
1:A:185:HIS:HD2	1:A:187:SER:H	1.45	0.63
1:A:130:LEU:HB2	1:A:131:PRO:HD3	1.80	0.63
1:A:240:VAL:O	1:A:243:LEU:HB2	1.98	0.63
1:A:790:LEU:HD11	1:A:820:MET:HB3	1.80	0.62
1:A:581:LYS:HA	1:A:584:PHE:CE2	2.35	0.61
1:A:582:ASP:O	1:A:585:PRO:HD2	1.99	0.61
1:A:629:GLN:N	1:A:630:PRO:HD3	2.14	0.61
1:A:504:PHE:CZ	1:A:522:ILE:HD12	2.36	0.61
1:A:815:ARG:HH11	1:A:815:ARG:CG	2.14	0.60
1:A:422:GLY:HA3	1:A:460:TRP:CZ3	2.37	0.60
1:A:6:LYS:N	1:A:7:PRO:CD	2.66	0.58
1:A:173:ASN:HD22	1:A:208:ALA:HB2	1.69	0.58
1:A:883:ARG:HG3	1:A:883:ARG:HH11	1.69	0.57
1:A:700:GLN:H	1:A:700:GLN:NE2	2.00	0.56
1:A:692:GLY:HA3	1:A:730:TRP:CZ3	2.41	0.55
1:A:258:VAL:O	1:A:262:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:MET:HE1	1:A:709:PHE:HD1	1.72	0.55
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.89	0.55
1:A:629:GLN:C	1:A:631:ASP:H	2.15	0.54
1:A:584:PHE:HB2	1:A:585:PRO:CD	2.34	0.54
1:A:191:ARG:O	1:A:195:VAL:HG12	2.08	0.54
1:A:47:ASN:ND2	1:A:75:ASN:HD22	1.99	0.54
1:A:629:GLN:HB3	1:A:633:TYR:H	1.73	0.54
1:A:254:MET:O	1:A:258:VAL:HG13	2.08	0.54
1:A:824:ASN:HD22	1:A:826:SER:H	1.56	0.53
1:A:169:ASP:CG	1:A:170:ARG:H	2.16	0.53
1:A:695:THR:HG21	1:A:735:ILE:HA	1.91	0.53
1:A:422:GLY:HA3	1:A:460:TRP:HZ3	1.73	0.53
2:B:10:UNK:C	2:B:10:UNK:CB	2.81	0.52
1:A:591:SER:HA	1:A:647:LEU:HD13	1.92	0.52
1:A:313:ILE:N	1:A:313:ILE:HD13	2.25	0.52
1:A:604:TYR:O	1:A:607:PRO:HD2	2.10	0.52
2:B:10:UNK:C	2:B:10:UNK:N	2.64	0.52
1:A:847:ASP:O	1:A:850:ARG:HB2	2.10	0.51
1:A:572:LYS:O	1:A:576:LEU:HG	2.09	0.51
1:A:57:LEU:HD23	1:A:60:GLU:HB2	1.93	0.51
1:A:174:ILE:O	1:A:178:LYS:HB2	2.10	0.51
1:A:151:ALA:O	1:A:155:ILE:HG12	2.12	0.50
1:A:885:ALA:HA	1:A:890:VAL:H	1.76	0.50
1:A:573:TRP:CZ2	1:A:608:VAL:HA	2.47	0.50
1:A:80:PHE:O	1:A:83:PHE:HB2	2.12	0.50
1:A:584:PHE:N	1:A:584:PHE:CD2	2.60	0.50
1:A:795:ARG:HB2	1:A:796:PRO:HD3	1.94	0.49
1:A:883:ARG:HG3	1:A:883:ARG:NH1	2.28	0.49
1:A:869:TRP:HE1	1:A:890:VAL:HG12	1.78	0.49
1:A:300:LEU:HD22	1:A:304:LEU:HD22	1.94	0.48
1:A:712:ILE:O	1:A:716:ASN:HB2	2.12	0.48
1:A:77:LYS:O	1:A:78:ALA:HB2	2.12	0.48
1:A:479:LYS:HB3	1:A:480:PRO:HD3	1.94	0.48
1:A:559:PRO:O	1:A:563:GLN:HG2	2.13	0.48
1:A:710:MET:HB2	1:A:711:PRO:HD3	1.95	0.48
1:A:651:LEU:O	1:A:655:LEU:HB2	2.14	0.47
1:A:415:GLU:HG2	1:A:457:ILE:HD11	1.96	0.47
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.95	0.47
1:A:815:ARG:CG	1:A:815:ARG:NH1	2.77	0.47
1:A:381:ALA:O	1:A:385:VAL:HG23	2.15	0.47
1:A:843:ILE:HA	1:A:883:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ALA:O	1:A:279:PHE:HB3	2.15	0.46
1:A:46:PHE:CZ	1:A:50:LEU:HD11	2.50	0.46
1:A:444:ILE:HA	1:A:447:LEU:HD12	1.97	0.46
1:A:173:ASN:ND2	1:A:208:ALA:HB2	2.30	0.46
1:A:518:TYR:CD1	1:A:518:TYR:N	2.84	0.46
1:A:641:MET:HE3	1:A:683:VAL:HG11	1.97	0.46
1:A:319:LYS:HD2	1:A:493:ASN:HD21	1.81	0.45
1:A:513:THR:HA	1:A:516:VAL:HG23	1.98	0.45
1:A:7:PRO:HB2	1:A:49:TYR:CZ	2.52	0.45
1:A:170:ARG:HB2	1:A:170:ARG:NH1	2.32	0.45
1:A:8:ASP:CB	1:A:9:GLU:HB3	2.46	0.45
1:A:168:LEU:O	1:A:169:ASP:HB3	2.16	0.45
1:A:293:LEU:O	1:A:295:ARG:N	2.50	0.45
1:A:512:CYS:HA	1:A:551:SER:HB3	1.99	0.45
1:A:99:ILE:HG21	1:A:136:LEU:HD23	1.98	0.45
1:A:99:ILE:O	1:A:107:ARG:HG3	2.17	0.45
1:A:504:PHE:HZ	1:A:522:ILE:CD1	2.29	0.45
1:A:80:PHE:HA	1:A:83:PHE:CD2	2.53	0.44
1:A:123:LEU:C	1:A:125:ASN:H	2.24	0.44
1:A:293:LEU:O	1:A:294:VAL:C	2.60	0.44
1:A:629:GLN:N	1:A:630:PRO:CD	2.79	0.44
1:A:739:MET:CB	1:A:743:MET:HG2	2.48	0.44
1:A:739:MET:HB2	1:A:743:MET:HG2	1.99	0.44
1:A:123:LEU:C	1:A:125:ASN:N	2.75	0.44
1:A:703:LYS:C	1:A:705:CYS:H	2.26	0.44
1:A:746:TYR:HA	1:A:749:MET:HE3	2.00	0.44
1:A:877:PRO:CD	1:A:880:LEU:HD23	2.43	0.44
1:A:488:ARG:HB3	1:A:500:ALA:HB2	1.99	0.44
1:A:268:GLN:HE21	1:A:268:GLN:HB3	1.63	0.43
1:A:418:ILE:HB	1:A:457:ILE:HD13	1.99	0.43
1:A:670:THR:HG22	1:A:674:GLN:HE21	1.83	0.43
1:A:699:PHE:CD2	1:A:738:GLN:HB3	2.52	0.43
1:A:242:LEU:HB3	1:A:250:LEU:HD22	2.00	0.43
1:A:518:TYR:O	1:A:522:ILE:HG12	2.18	0.43
1:A:278:GLU:OE2	1:A:373:TRP:NE1	2.50	0.43
1:A:433:ILE:HA	1:A:436:LEU:HD12	1.99	0.43
1:A:876:PHE:CB	1:A:881:LYS:HB2	2.49	0.43
1:A:275:GLU:O	1:A:278:GLU:HB2	2.18	0.43
1:A:685:GLN:HB2	1:A:724:VAL:HG22	2.01	0.43
1:A:854:CYS:O	1:A:855:LYS:C	2.62	0.43
1:A:67:LEU:O	1:A:71:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ILE:O	1:A:821:ILE:HG13	2.19	0.42
1:A:561:TYR:HA	1:A:564:MET:HE2	2.01	0.42
1:A:706:ILE:HG21	1:A:739:MET:HE2	2.00	0.42
1:A:387:ALA:O	1:A:427:GLY:HA3	2.19	0.42
1:A:821:ILE:HG12	1:A:828:VAL:CG2	2.39	0.42
1:A:843:ILE:HA	1:A:883:ARG:NH2	2.35	0.42
1:A:628:ALA:C	1:A:630:PRO:HD3	2.45	0.41
1:A:656:GLY:O	1:A:697:ALA:HB1	2.20	0.41
1:A:677:GLN:HE21	1:A:712:ILE:HG13	1.85	0.41
1:A:814:PHE:O	1:A:817:ILE:HG22	2.20	0.41
1:A:860:PHE:CD1	1:A:860:PHE:N	2.88	0.41
1:A:736:SER:HB3	1:A:743:MET:HE2	2.02	0.41
1:A:199:ASN:HB3	1:A:241:MET:HE1	2.02	0.41
1:A:479:LYS:HG3	1:A:518:TYR:HE2	1.86	0.41
1:A:664:ALA:HB2	1:A:701:HIS:CE1	2.56	0.41
1:A:285:GLU:H	1:A:285:GLU:HG2	1.69	0.41
1:A:297:LEU:N	1:A:298:PRO:CD	2.83	0.41
1:A:672:MET:HE1	1:A:694:LEU:HD12	2.02	0.41
1:A:787:ALA:C	1:A:789:MET:H	2.29	0.41
1:A:850:ARG:NH1	1:A:887:PHE:O	2.54	0.41
1:A:43:TYR:HA	1:A:44:PRO:HD3	1.96	0.41
1:A:629:GLN:O	1:A:631:ASP:N	2.52	0.41
1:A:876:PHE:HB3	1:A:881:LYS:HB2	2.03	0.41
1:A:497:GLN:HB2	1:A:537:ASN:ND2	2.36	0.41
1:A:261:MET:HE3	1:A:279:PHE:CD1	2.57	0.40
1:A:573:TRP:HE1	1:A:607:PRO:HB2	1.86	0.40
1:A:824:ASN:ND2	1:A:826:SER:H	2.19	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	830/890 (93%)	758 (91%)	59 (7%)	13 (2%)	7	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ALA
1	A	294	VAL
1	A	512	CYS
1	A	534	GLN
1	A	123	LEU
1	A	169	ASP
1	A	77	LYS
1	A	790	LEU
1	A	532	LYS
1	A	25	PRO
1	A	104	PRO
1	A	722	ILE
1	A	704	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/802 (93%)	678 (90%)	71 (10%)	8	32

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	9	GLU
1	A	14	GLN
1	A	27	THR
1	A	40	LEU
1	A	57	LEU
1	A	70	LEU
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	128	ASP
1	A	137	LEU
1	A	140	GLU
1	A	149	PHE
1	A	195	VAL
1	A	242	LEU
1	A	247	MET
1	A	254	MET
1	A	262	LEU
1	A	264	ARG
1	A	268	GLN
1	A	281	LEU
1	A	283	LEU
1	A	285	GLU
1	A	294	VAL
1	A	300	LEU
1	A	313	ILE
1	A	316	ILE
1	A	403	LYS
1	A	421	LEU
1	A	438	GLU
1	A	451	LYS
1	A	457	ILE
1	A	464	ARG
1	A	482	MET
1	A	488	ARG
1	A	490	LEU
1	A	506	THR
1	A	512	CYS
1	A	518	TYR
1	A	539	LEU
1	A	548	LEU
1	A	569	LEU
1	A	570	ILE
1	A	584	PHE
1	A	588	GLU
1	A	613	VAL
1	A	618	LYS
1	A	627	ASN
1	A	633	TYR
1	A	647	LEU

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Mol	Chain	Res	Type
1	A	648	LEU
1	A	669	LEU
1	A	679	LYS
1	A	700	GLN
1	A	743	MET
1	A	766	THR
1	A	799	THR
1	A	805	ARG
1	A	815	ARG
1	A	824	ASN
1	A	829	ILE
1	A	833	ILE
1	A	844	ASN
1	A	855	LYS
1	A	858	HIS
1	A	860	PHE
1	A	867	GLU
1	A	878	LEU
1	A	883	ARG
1	A	887	PHE
1	A	890	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	48	ASN
1	A	75	ASN
1	A	97	ASN
1	A	173	ASN
1	A	185	HIS
1	A	193	HIS
1	A	200	GLN
1	A	268	GLN
1	A	296	HIS
1	A	534	GLN
1	A	622	GLN
1	A	674	GLN
1	A	700	GLN
1	A	716	ASN
1	A	753	GLN
1	A	762	ASN

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Mol	Chain	Res	Type
1	A	770	ASN
1	A	784	GLN
1	A	791	GLN
1	A	824	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	0.07	9 (1%) 78 61	112, 129, 141, 152	0
2	B	0/10	-	-	-	-
All	All	834/900 (92%)	0.07	9 (1%) 78 61	112, 129, 141, 152	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	860	PHE	2.8
1	A	310	TYR	2.6
1	A	52	PHE	2.4
1	A	288	ILE	2.3
1	A	6	LYS	2.3
1	A	530	PHE	2.2
1	A	207	GLN	2.2
1	A	319	LYS	2.1
1	A	882	GLU	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.