Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2017 – 01:00 AM EDT

PDB ID	:	2Z5M
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	:	unknown
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345
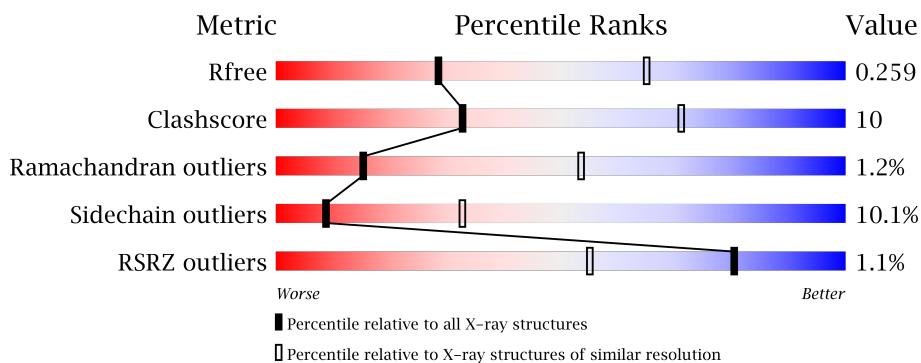
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
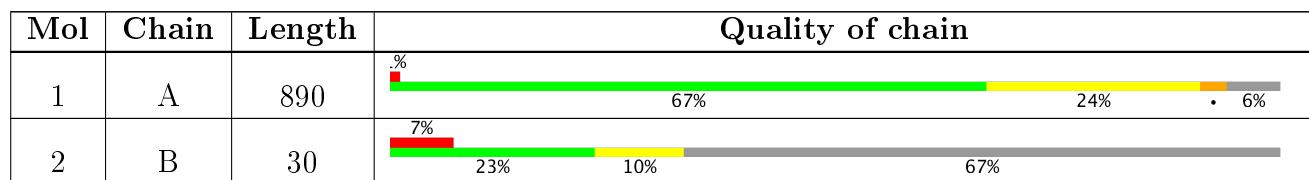
The reported resolution of this entry is 3.00 Å.

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	Percentile Ranks	Value
Rfree		0.259
Clashscore		10
Ramachandran outliers		1.2%
Sidechain outliers		10.1%
RSRZ outliers		1.1%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	890	.% 67% 24% · 6%
2	B	30	7% 23% 10% 67%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	840	6690	4290	1114	1235	51	0	0	0
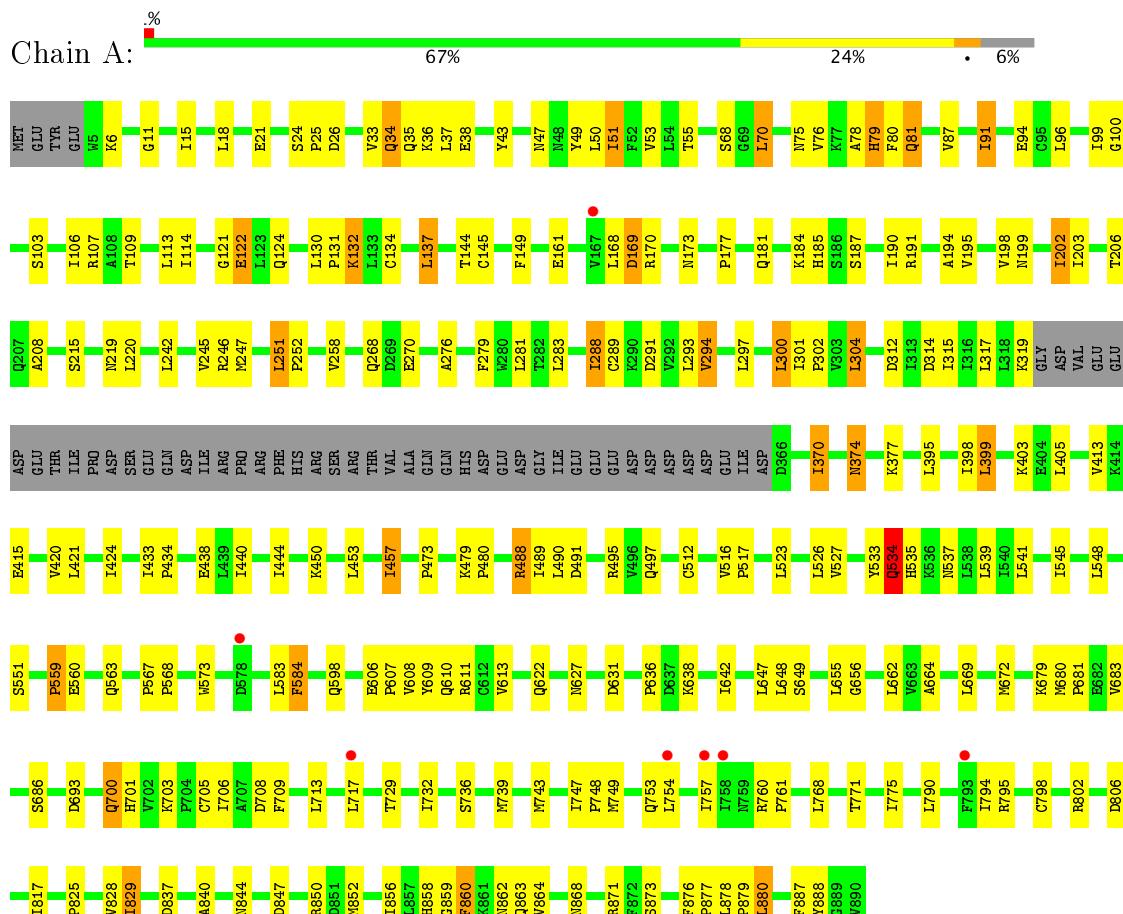
- Molecule 2 is a protein called Nuclear RNA export factor 1.

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

3 Residue-property plots ⓘ

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: Nuclear RNA export factor 1

4 Data and refinement statistics (i)

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 49.51 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-3.00) 95.1 (49.51-2.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.33 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.267 0.239 , 0.259	Depositor DCC
R_{free} test set	1531 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.1	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.46	0/6833	0.55	0/9281
2	B	0.71	0/91	0.63	0/125
All	All	0.46	0/6924	0.56	0/9406

There are no bond length outliers.

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	6690	0	6750	134	0
2	B	88	0	86	1	0
All	All	6778	0	6836	135	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 10.

All (135) 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:185:HIS:HD2	1:A:187:SER:H	1.19	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:CD2	1:A:187:SER:H	2.00	0.80
1:A:81:GLN:CD	1:A:81:GLN:H	1.85	0.79
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: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:H	1:A:288:ILE:HD12	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:829:ILE:HD13	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: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: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:HG	1:A:168:LEU:O	2.15	0.47
1:A:672:MET:HE2	1:A:672:MET:HB2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HA	1:A:245:VAL:HG21	1.97	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:CG	1:A:79:HIS:O	2.68	0.46
1:A:713:LEU:HD13	1:A:732: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: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:33:VAL:C	1:A:35:GLN:H	2.20	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: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:N	1:A:584:PHE:CD2	2.72	0.44
1:A:215:SER:O	1:A:219:ASN:OD1	2.36	0.43
1:A:512:CYS:HA	1:A:551:SER:HB3	2.00	0.43
1:A:96:LEU:HD23	1:A:132:LYS:HG2	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:H	1:A:700:GLN:NE2	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:50:LEU:O	1:A:68:SER:OG	2.26	0.42
1:A:24:SER:HA	1:A:25:PRO:HD3	1.90	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:33:VAL:C	1:A:35:GLN:N	2.73	0.41
1:A:860:PHE:HD1	1:A:860:PHE:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ALA:O	1:A:198:VAL:HG23	2.21	0.41
1:A:526:LEU:HD13	1:A:545:ILE:HD12	2.01	0.41
1:A:51:ILE:HD11	1:A:94:GLU:HB3	2.02	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:169:ASP:CG	1:A:170:ARG:H	2.24	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 (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%)	774 (93%)	52 (6%)	10 (1%)	15	53
2	B	8/30 (27%)	8 (100%)	0	0	100	100
All	All	844/920 (92%)	782 (93%)	52 (6%)	10 (1%)	15	53

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

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Mol	Chain	Res	Type
1	A	473	PRO
1	A	656	GLY

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	755/802 (94%)	679 (90%)	76 (10%)	9	33
2	B	10/26 (38%)	9 (90%)	1 (10%)	9	33
All	All	765/828 (92%)	688 (90%)	77 (10%)	9	33

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	18	LEU
1	A	26	ASP
1	A	36	LYS
1	A	38	GLU
1	A	43	TYR
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	145	CYS
1	A	149	PHE
1	A	161	GLU
1	A	184	LYS
1	A	202	ILE

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Mol	Chain	Res	Type
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	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	319	LYS
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	488	ARG
1	A	490	LEU
1	A	495	ARG
1	A	534	GLN
1	A	539	LEU
1	A	548	LEU
1	A	583	LEU
1	A	584	PHE
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

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Mol	Chain	Res	Type
1	A	708	ASP
1	A	717	LEU
1	A	768	LEU
1	A	794	ILE
1	A	817	ILE
1	A	829	ILE
1	A	844	ASN
1	A	847	ASP
1	A	850	ARG
1	A	860	PHE
1	A	862	ASN
1	A	880	LEU
1	A	887	PHE
2	B	78	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	47	ASN
1	A	48	ASN
1	A	82	ASN
1	A	97	ASN
1	A	173	ASN
1	A	185	HIS
1	A	193	HIS
1	A	256	ASN
1	A	263	GLN
1	A	268	GLN
1	A	296	HIS
1	A	374	ASN
1	A	534	GLN
1	A	574	ASN
1	A	598	GLN
1	A	622	GLN
1	A	627	ASN
1	A	700	GLN
1	A	759	ASN
1	A	824	ASN
1	A	844	ASN
1	A	858	HIS
1	A	862	ASN

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Mol	Chain	Res	Type
1	A	868	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 (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%)	-0.04	7 (0%)	86	64	53, 95, 125, 140	0
2	B	10/30 (33%)	0.72	2 (20%)	1	1	93, 96, 112, 114	0
All	All	850/920 (92%)	-0.03	9 (1%)	80	55	53, 95, 125, 140	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	LEU	3.4
1	A	717	LEU	3.0
1	A	167	VAL	2.8
1	A	578	ASP	2.6
2	B	77	THR	2.4
1	A	757	ILE	2.3
1	A	793	PHE	2.2
2	B	78	ARG	2.0
1	A	758	ILE	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 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.