



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2017 – 05:55 PM EDT

PDB ID : 2OT8
Title : Karyopherin Beta2/Transportin-hnRNPM NLS Complex
Authors : Cansizoglu, A.E.; Chook, Y.M.
Deposited on : unknown
Resolution : 3.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
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-20029824

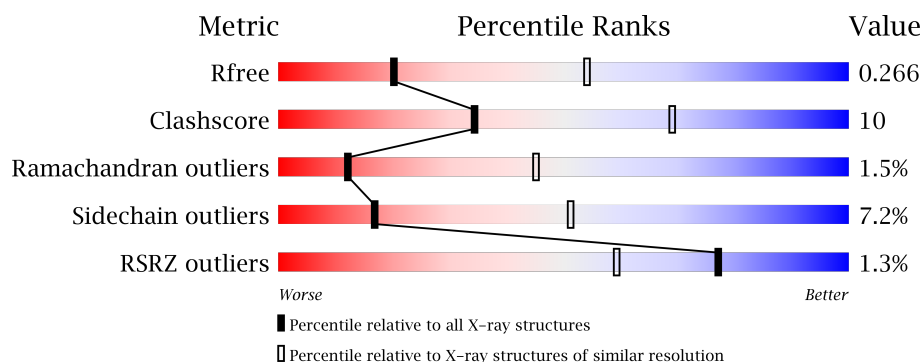
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 $\leq 5\%$. 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	852	<div> <div>0.1%</div> <div>74%</div> <div>20%</div> <div>0.1%</div> </div>
1	B	852	<div> <div>2%</div> <div>71%</div> <div>22%</div> <div>5%</div> </div>
2	C	30	<div> <div>3%</div> <div>43%</div> <div>13%</div> <div>43%</div> </div>
2	D	30	<div> <div>53%</div> <div>10%</div> <div>0.1%</div> <div>33%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12802 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	824	Total	C	N	O	S	0	0	0
			6310	4040	1052	1167	51			
1	B	813	Total	C	N	O	S	0	0	0
			6196	3963	1038	1145	50			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	GLY	-	linker	UNP Q92973
A	325	GLY	-	linker	UNP Q92973
A	326	SER	-	linker	UNP Q92973
A	327	GLY	-	linker	UNP Q92973
A	328	GLY	-	linker	UNP Q92973
B	324	GLY	-	linker	UNP Q92973
B	325	GLY	-	linker	UNP Q92973
B	326	SER	-	linker	UNP Q92973
B	327	GLY	-	linker	UNP Q92973
B	328	GLY	-	linker	UNP Q92973

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

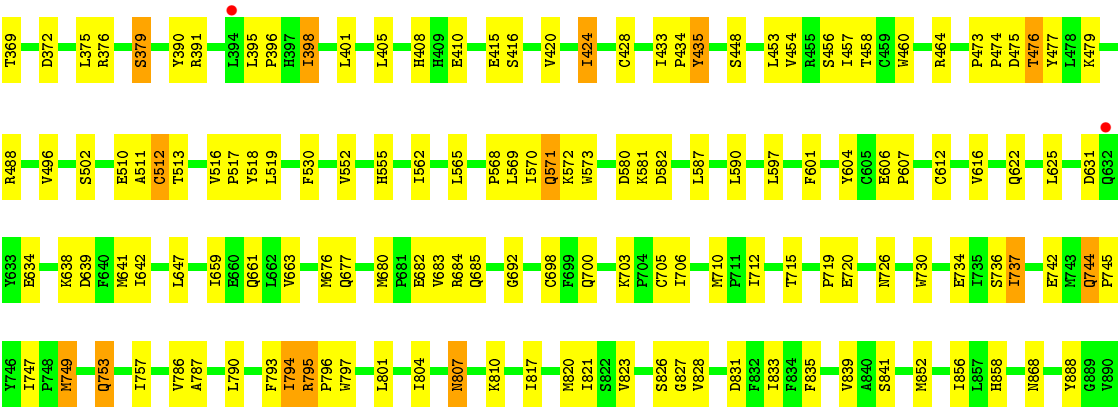
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	0	0	0
			135	82	27	26			
2	D	20	Total	C	N	O	0	0	0
			161	100	32	29			

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 ($\text{RSRZ} > 2$). 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.

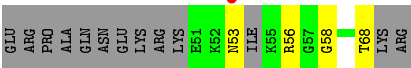
[illegible]

Chain B:

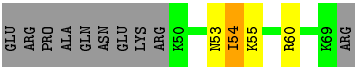
Sequence logo for Chain B showing amino acid conservation across 100 positions. The y-axis represents information content in bits (0.00 to 0.10). The x-axis shows positions 1 to 100. A color key at the top indicates amino acid categories: MET, GLU, TYR, GLU, TRP, LYS, PRO, ASP, GLU, Q14, S22, Q23, S24, P25, D26, T27, N41, GLN, TYR, PRO, ASP, PHE, N47, F52, V53, L54, K58, SER, GLU, ASP, GLU, PRO, THR, R65, S68, I71, L72, K73, M74, R82, F83, P84, N85, G86, F90, C95, L96, N97, N98, D99, G100, D101, S102, S103, R107, I113, I114, T115, I116, I117, W126, D127, D128, L129, L130, P131, K132, L133, C134, S135, L136, L137, T144, F149, K154, I155, C156, E157, E161, I16, L16U, L16V, ASP, SER, ASP, VAL, L17, L17U, ASP, ARG, P171, L172, M173, I174, M175, I176, F183, K189, I190, L191, L196, ASP, V195, Q200, A208, I213, D214, N219, L223, E227, V231, V235, R246, R249, L262, T285, Q266, D267, Q268, V272, W280, L281, T282, C289, L293, V294, K309, Y310, S311, D312, L313, D314, L318, K319, GLY, ASP, VAL, GLU, GLY, GLY, SER, GLY, ASP, A269.



● Molecule 2: Heterogeneous nuclear ribonucleoprotein M



● Molecule 2: Heterogeneous nuclear ribonucleoprotein M



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.20Å 155.00Å 141.53Å 90.00° 92.57° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 48.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.10) 96.1 (48.46-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.290 0.228 , 0.266	Depositor DCC
R_{free} test set	3014 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.008 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12802	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2968e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.42	0/6441	0.58	0/8775
1	B	0.42	2/6326 (0.0%)	0.56	1/8624 (0.0%)
2	C	0.50	0/137	0.57	0/182
2	D	0.50	0/164	0.62	0/218
All	All	0.42	2/13068 (0.0%)	0.57	1/17799 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	GLU	C-N	-5.57	1.21	1.34
1	B	570	ILE	C-N	5.27	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	PRO	N-CA-CB	5.74	110.19	103.30

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	6310	0	6131	115	0
1	B	6196	0	5960	124	0
2	C	135	0	119	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	161	0	157	3	0
All	All	12802	0	12367	240	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 (240) 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:B:642:ILE:HD11	1:B:680:MET:HE3	1.38	1.04
1:A:746:TYR:HA	1:A:749:MET:HE3	1.61	0.83
1:B:821:ILE:HG12	1:B:828:VAL:HG21	1.63	0.80
1:A:112:ILE:O	1:A:116:THR:HG23	1.82	0.80
1:B:833:ILE:H	1:B:833:ILE:HD12	1.46	0.78
1:B:73:LYS:HB2	1:B:113:LEU:HD12	1.66	0.77
1:B:71:ILE:HA	1:B:74:ASN:HB2	1.65	0.76
1:B:460:TRP:CZ2	1:B:464:ARG:HD2	2.24	0.73
1:A:799:THR:HA	1:A:802:ARG:HE	1.55	0.72
1:B:267:ASP:OD2	1:B:272:VAL:HG11	1.91	0.71
1:B:719:PRO:HG3	1:B:757:ILE:HG12	1.73	0.70
1:B:552:VAL:HG13	1:B:555:HIS:HB2	1.73	0.70
1:B:265:THR:OG1	1:B:280:TRP:HZ3	1.75	0.70
1:B:680:MET:HE1	1:B:683:VAL:HG23	1.72	0.69
1:B:156:CYS:HB3	1:B:200:GLN:HG3	1.73	0.69
1:B:642:ILE:HD11	1:B:680:MET:CE	2.18	0.69
1:A:265:THR:OG1	1:A:280:TRP:CZ3	2.45	0.68
1:A:440:ILE:O	1:A:444:ILE:HG13	1.93	0.68
1:B:416:SER:O	1:B:420:VAL:HG23	1.94	0.68
1:A:821:ILE:CD1	1:A:828:VAL:HG21	2.23	0.68
1:B:604:TYR:O	1:B:607:PRO:HD2	1.94	0.67
1:A:121:GLY:O	1:A:125:ASN:HB3	1.95	0.67
1:A:95:CYS:HB2	1:A:110:VAL:HG13	1.76	0.66
1:A:265:THR:OG1	1:A:280:TRP:HZ3	1.79	0.66
1:A:573:TRP:CZ2	1:A:611:ARG:HD3	2.31	0.66
1:A:742:GLU:O	1:A:745:PRO:HD2	1.96	0.66
1:B:680:MET:CE	1:B:683:VAL:HG23	2.25	0.66
1:A:265:THR:HG1	1:A:280:TRP:HZ3	1.37	0.65
1:A:719:PRO:HG3	1:A:757:ILE:HG12	1.79	0.65
1:B:692:GLY:HA3	1:B:730:TRP:CZ3	2.33	0.64
1:A:864:VAL:HG12	1:A:868:ASN:HB3	1.79	0.63
1:A:570:ILE:HG22	1:A:574:ASN:HD21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASN:HB2	1:A:597:LEU:HA	1.81	0.63
1:A:731:ALA:O	1:A:735:ILE:HG12	1.98	0.63
1:B:753:GLN:H	1:B:753:GLN:HE21	1.45	0.63
1:B:54:LEU:CB	1:B:68:SER:HB2	2.29	0.62
1:A:780:TYR:CD1	1:A:815:ARG:HB3	2.36	0.61
1:A:817:ILE:O	1:A:821:ILE:HG12	2.01	0.61
1:A:780:TYR:HD1	1:A:815:ARG:HB3	1.66	0.61
1:A:188:PRO:HA	1:A:191:ARG:HD3	1.83	0.60
1:A:498:GLU:HB2	1:A:537:ASN:OD1	2.02	0.59
1:A:313:ILE:HG23	1:A:370:ILE:HG21	1.85	0.59
1:B:454:VAL:O	1:B:458:THR:HG23	2.02	0.59
1:A:703:LYS:O	1:A:705:CYS:N	2.36	0.59
1:B:174:ILE:HG22	1:B:175:MET:HE2	1.85	0.59
1:A:612:CYS:SG	1:A:647:LEU:HD23	2.43	0.58
1:B:267:ASP:OD2	1:B:272:VAL:CG1	2.50	0.58
1:B:795:ARG:HB3	1:B:796:PRO:HD3	1.83	0.58
1:B:801:LEU:HD22	1:B:804:ILE:HD11	1.86	0.58
1:A:456:SER:O	1:A:459:CYS:HB2	2.04	0.58
1:A:80:PHE:O	1:A:83:PHE:HB2	2.04	0.58
1:B:734:GLU:HA	1:B:737:ILE:HD12	1.86	0.58
1:A:210:MET:HE3	1:A:246:ARG:NH1	2.19	0.57
1:B:183:PHE:HD1	1:B:219:ASN:HB3	1.68	0.57
1:A:288:ILE:H	1:A:288:ILE:HD12	1.70	0.57
1:B:134:CYS:HA	1:B:137:LEU:HG	1.86	0.57
1:A:793:PHE:HZ	1:A:820:MET:HE1	1.69	0.57
1:B:415:GLU:OE2	1:B:457:ILE:HG13	2.05	0.56
1:B:183:PHE:CD1	1:B:219:ASN:HB3	2.41	0.56
1:A:191:ARG:O	1:A:195:VAL:HG23	2.04	0.56
1:B:612:CYS:O	1:B:616:VAL:HG23	2.06	0.55
1:B:96:LEU:HD13	1:B:132:LYS:HG2	1.89	0.55
1:A:479:LYS:HE3	1:A:518:TYR:OH	2.06	0.55
1:B:710:MET:HB3	1:B:749:MET:CE	2.36	0.55
1:A:844:ASN:C	1:A:844:ASN:HD22	2.10	0.55
1:B:83:PHE:N	1:B:84:PRO:CD	2.70	0.55
1:A:587:LEU:HB2	1:A:643:VAL:HG13	1.88	0.54
1:B:821:ILE:HG12	1:B:828:VAL:CG2	2.35	0.54
1:B:571:GLN:HG3	1:B:572:LYS:N	2.22	0.54
1:A:746:TYR:O	1:A:749:MET:HB2	2.07	0.54
1:B:191:ARG:O	1:B:195:VAL:HG23	2.08	0.53
1:B:502:SER:OG	2:D:60:ARG:HB3	2.09	0.53
1:B:571:GLN:CG	1:B:572:LYS:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:ASN:O	2:D:54:ILE:HG22	2.09	0.53
1:B:511:ALA:O	1:B:512:CYS:C	2.47	0.53
1:B:793:PHE:HZ	1:B:820:MET:CE	2.22	0.53
1:B:793:PHE:HZ	1:B:820:MET:HE1	1.74	0.53
1:A:729:THR:HG21	1:A:771:THR:HA	1.90	0.53
1:B:176:ILE:HD12	1:B:208:ALA:HB3	1.92	0.52
1:A:769:GLU:O	1:A:773:ILE:HG12	2.09	0.52
1:B:375:LEU:O	1:B:379:SER:OG	2.27	0.52
1:A:570:ILE:HG22	1:A:574:ASN:ND2	2.24	0.52
1:A:177:PRO:HG3	1:A:212:HIS:CE1	2.45	0.52
1:A:156:CYS:HB3	1:A:200:GLN:HG2	1.91	0.52
1:A:488:ARG:O	1:A:491:ASP:HB2	2.09	0.52
1:A:571:GLN:O	1:A:575:MET:HB2	2.10	0.52
1:B:294:VAL:HG22	1:B:390:TYR:HE2	1.74	0.52
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.92	0.51
1:A:83:PHE:N	1:A:84:PRO:HD2	2.25	0.51
1:A:735:ILE:HG22	1:A:743:MET:CE	2.39	0.51
1:B:817:ILE:HD12	1:B:835:PHE:HE1	1.76	0.51
1:B:231:VAL:O	1:B:235:VAL:HG23	2.10	0.51
1:B:433:ILE:HB	1:B:434:PRO:HD3	1.93	0.50
1:A:268:GLN:O	1:A:269:ASP:HB3	2.11	0.50
1:A:415:GLU:OE1	1:A:457:ILE:HD13	2.10	0.50
1:A:703:LYS:C	1:A:705:CYS:H	2.14	0.50
1:B:794:ILE:HD11	1:B:827:GLY:O	2.10	0.50
1:A:582:ASP:O	1:A:585:PRO:HD2	2.11	0.50
1:B:130:LEU:HB2	1:B:131:PRO:HD3	1.93	0.50
1:B:191:ARG:HD2	1:B:223:LEU:HD11	1.92	0.50
1:B:565:LEU:O	1:B:568:PRO:HD2	2.12	0.50
1:B:580:ASP:C	1:B:582:ASP:H	2.15	0.50
1:A:552:VAL:HG13	1:A:555:HIS:HB2	1.93	0.50
1:B:157:GLU:HG2	1:B:200:GLN:OE1	2.12	0.49
1:A:703:LYS:HA	1:A:706:ILE:HG12	1.93	0.49
1:B:793:PHE:O	1:B:797:TRP:HB2	2.13	0.49
1:A:755:VAL:O	1:A:758:ILE:HG22	2.11	0.49
1:B:736:SER:O	1:B:737:ILE:C	2.50	0.49
1:B:267:ASP:OD1	1:B:268:GLN:N	2.46	0.49
1:A:703:LYS:HB3	1:A:704:PRO:HD3	1.93	0.49
1:A:685:GLN:HG2	1:A:727:ASN:HD22	1.78	0.49
1:A:313:ILE:HG22	1:A:317:LEU:HD22	1.94	0.49
1:B:794:ILE:HD12	1:B:831:ASP:HB2	1.95	0.49
1:A:191:ARG:NH2	1:A:226:ASP:OD2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD23	1:A:413:VAL:HG13	1.94	0.48
1:B:569:LEU:HD13	1:B:590:LEU:HD13	1.94	0.48
1:A:418:ILE:HG22	1:A:457:ILE:HG22	1.96	0.48
1:A:584:PHE:N	1:A:584:PHE:CD2	2.80	0.48
1:A:530:PHE:HE1	1:A:545:ILE:CD1	2.27	0.48
1:B:115:THR:HG21	1:B:154:LYS:HG3	1.95	0.48
1:B:562:ILE:HG12	1:B:597:LEU:HD22	1.96	0.47
1:B:126:TRP:CD2	1:B:129:LEU:HB2	2.50	0.47
1:B:453:LEU:O	1:B:457:ILE:HG12	2.15	0.47
1:A:433:ILE:N	1:A:434:PRO:HD2	2.30	0.47
1:B:310:TYR:O	1:B:313:ILE:HB	2.15	0.47
1:B:128:ASP:O	1:B:131:PRO:HD2	2.15	0.47
1:B:742:GLU:O	1:B:745:PRO:HD2	2.14	0.47
1:B:519:LEU:HD11	1:B:552:VAL:HG11	1.96	0.47
1:B:682:GLU:N	1:B:682:GLU:OE1	2.41	0.47
1:A:231:VAL:O	1:A:235:VAL:HG23	2.15	0.47
1:B:126:TRP:HZ3	1:B:128:ASP:HB2	1.79	0.47
1:B:659:ILE:HG12	1:B:663:VAL:HG23	1.97	0.46
1:A:210:MET:HE1	1:A:246:ARG:HD3	1.96	0.46
1:A:835:PHE:O	1:A:839:VAL:HG23	2.15	0.46
1:B:435:TYR:N	1:B:435:TYR:CD1	2.82	0.46
1:A:793:PHE:HZ	1:A:820:MET:CE	2.28	0.46
1:A:615:LEU:O	1:A:619:THR:HG23	2.15	0.46
1:B:398:ILE:HD13	1:B:424:ILE:HG12	1.98	0.46
1:B:807:ASN:ND2	1:B:810:LYS:H	2.14	0.46
1:A:790:LEU:HD21	1:A:821:ILE:HD13	1.97	0.46
1:B:460:TRP:CH2	1:B:464:ARG:HD2	2.51	0.46
1:B:685:GLN:NE2	2:D:54:ILE:HB	2.31	0.46
1:B:835:PHE:O	1:B:839:VAL:HG23	2.16	0.46
1:B:821:ILE:C	1:B:823:VAL:H	2.19	0.46
1:A:699:PHE:CD2	1:A:738:GLN:HB3	2.51	0.46
1:A:739:MET:HB3	1:A:743:MET:HE2	1.96	0.46
1:A:540:ILE:H	1:A:540:ILE:HD12	1.81	0.46
1:A:787:ALA:HA	1:A:820:MET:HE3	1.98	0.46
1:B:289:CYS:SG	1:B:293:LEU:HD12	2.56	0.45
1:B:622:GLN:HA	1:B:625:LEU:HD12	1.97	0.45
1:B:698:CYS:HA	1:B:700:GLN:HE22	1.80	0.45
1:B:510:GLU:OE1	1:B:510:GLU:HA	2.15	0.45
1:B:100:GLY:HA3	1:B:144:THR:HA	1.97	0.45
1:A:243:LEU:HD22	1:A:279:PHE:CE1	2.51	0.45
1:B:103:SER:O	1:B:107:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:GLN:HA	1:B:747:ILE:HD12	1.98	0.45
1:B:744:GLN:HB3	1:B:745:PRO:HD3	1.99	0.45
1:A:311:SER:HG	1:A:313:ILE:HG13	1.82	0.45
1:A:422:GLY:HA3	1:A:460:TRP:CZ3	2.52	0.45
1:B:213:ILE:HG23	1:B:214:ASP:N	2.32	0.45
1:A:213:ILE:HG23	1:A:214:ASP:N	2.33	0.44
1:A:530:PHE:CE1	1:A:545:ILE:CD1	3.00	0.44
1:B:573:TRP:HZ3	1:B:587:LEU:HD22	1.82	0.44
1:B:807:ASN:HD22	1:B:807:ASN:C	2.20	0.44
1:A:719:PRO:HB2	1:A:760:ARG:HH11	1.82	0.44
1:B:597:LEU:HD12	1:B:601:PHE:HD1	1.82	0.44
1:A:205:ARG:HG3	1:A:245:VAL:HG13	1.98	0.44
1:A:580:ASP:C	1:A:582:ASP:H	2.20	0.44
1:A:83:PHE:N	1:A:84:PRO:CD	2.80	0.44
1:B:710:MET:HB3	1:B:749:MET:HE1	1.99	0.44
1:B:74:ASN:HD22	1:B:74:ASN:HA	1.67	0.44
1:B:376:ARG:NH2	1:B:415:GLU:OE2	2.51	0.44
1:B:677:GLN:NE2	1:B:712:ILE:HD11	2.32	0.44
1:A:572:LYS:O	1:A:576:LEU:HG	2.18	0.43
1:B:456:SER:HB3	1:B:496:VAL:HG22	2.00	0.43
1:B:787:ALA:HA	1:B:820:MET:HE2	1.98	0.43
1:A:399:LEU:HB2	1:A:400:PRO:HD3	2.01	0.43
1:A:829:ILE:HG22	1:A:860:PHE:CE1	2.53	0.43
1:A:685:GLN:HG2	1:A:727:ASN:ND2	2.34	0.43
1:A:580:ASP:O	1:A:582:ASP:N	2.51	0.43
1:B:265:THR:OG1	1:B:280:TRP:CZ3	2.58	0.43
1:A:317:LEU:HD13	1:A:370:ILE:HG23	2.00	0.43
1:B:612:CYS:SG	1:B:647:LEU:HD23	2.59	0.43
1:B:642:ILE:CD1	1:B:680:MET:HE3	2.28	0.43
1:B:786:VAL:HG12	1:B:820:MET:HE3	2.00	0.43
1:B:606:GLU:HB2	1:B:607:PRO:HD3	2.01	0.42
1:A:261:MET:HE3	1:A:279:PHE:HB2	1.99	0.42
1:B:616:VAL:HG13	1:B:641:MET:HB2	2.01	0.42
1:B:793:PHE:O	1:B:796:PRO:HD2	2.19	0.42
1:B:638:LYS:HB3	1:B:680:MET:HE1	2.01	0.42
1:A:290:LYS:O	1:A:294:VAL:HG22	2.19	0.42
1:B:795:ARG:HB3	1:B:796:PRO:CD	2.48	0.42
1:B:858:HIS:HE1	1:B:888:TYR:O	2.02	0.42
1:A:729:THR:CG2	1:A:771:THR:HA	2.50	0.42
1:B:479:LYS:HE3	1:B:518:TYR:OH	2.20	0.42
1:B:136:LEU:HB3	1:B:144:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:TYR:HD2	1:A:749:MET:CE	2.33	0.42
1:B:401:LEU:O	1:B:405:LEU:HG	2.19	0.42
1:B:424:ILE:HG23	1:B:428:CYS:SG	2.59	0.42
1:B:639:ASP:HA	1:B:642:ILE:HD12	2.02	0.42
1:A:268:GLN:O	1:A:269:ASP:CB	2.67	0.42
1:A:735:ILE:HG22	1:A:743:MET:HE1	2.00	0.42
1:A:741:ILE:HG13	1:A:741:ILE:H	1.67	0.42
1:B:101:ASP:HB3	1:B:107:ARG:HB3	2.01	0.42
1:B:682:GLU:HA	1:B:685:GLN:HG2	2.02	0.42
1:B:852:MET:O	1:B:856:ILE:HG12	2.20	0.42
1:B:97:ASN:HD22	1:B:97:ASN:HA	1.70	0.42
1:A:214:ASP:OD1	1:A:249:ARG:HD3	2.19	0.41
1:A:183:PHE:CD2	1:A:219:ASN:HB3	2.54	0.41
1:A:845:PRO:HG2	1:A:850:ARG:HB3	2.02	0.41
1:A:565:LEU:O	1:A:568:PRO:HD2	2.20	0.41
1:A:698:CYS:HA	1:A:700:GLN:HE22	1.85	0.41
1:A:739:MET:CB	1:A:743:MET:HE2	2.50	0.41
1:B:680:MET:HE2	1:B:683:VAL:HG23	2.02	0.41
1:A:760:ARG:HA	1:A:761:PRO:HD3	1.87	0.41
1:B:703:LYS:HA	1:B:706:ILE:HG12	2.02	0.41
1:B:833:ILE:CD1	1:B:833:ILE:H	2.20	0.41
1:A:213:ILE:CG2	1:A:214:ASP:N	2.84	0.41
1:A:793:PHE:CZ	1:A:820:MET:HE1	2.53	0.41
1:A:821:ILE:HD12	1:A:828:VAL:HG21	2.01	0.41
1:A:117:ILE:H	1:A:117:ILE:HG12	1.66	0.41
1:B:476:THR:HB	1:B:477:TYR:CD1	2.55	0.41
1:A:584:PHE:N	1:A:584:PHE:HD2	2.19	0.41
1:B:395:LEU:HB2	1:B:396:PRO:HD3	2.03	0.41
1:A:113:LEU:O	1:A:114:ILE:C	2.59	0.41
1:A:719:PRO:O	1:A:722:ILE:HG13	2.21	0.41
1:A:749:MET:O	1:A:753:GLN:NE2	2.54	0.41
1:A:162:ILE:O	1:A:163:LEU:HD23	2.21	0.40
1:A:698:CYS:SG	1:A:698:CYS:O	2.79	0.40
1:B:676:MET:O	1:B:684:ARG:HG2	2.21	0.40
1:B:807:ASN:HD22	1:B:810:LYS:H	1.69	0.40
1:A:204:SER:OG	1:A:206:THR:HG23	2.22	0.40
1:B:408:HIS:CE1	1:B:410:GLU:HB2	2.55	0.40
1:A:591:SER:CB	1:A:647:LEU:HA	2.52	0.40
1:B:793:PHE:CZ	1:B:820:MET:HE1	2.55	0.40
1:A:473:PRO:HA	1:A:474:PRO:HD3	1.73	0.40
1:B:293:LEU:O	1:B:294:VAL:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:VAL:N	1:B:517:PRO:CD	2.84	0.40
1:A:711:PRO:O	1:A:715:THR:HG23	2.20	0.40
1:A:753:GLN:O	1:A:756:GLU:HB2	2.22	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	814/852 (96%)	743 (91%)	62 (8%)	9 (1%)	17	54
1	B	803/852 (94%)	721 (90%)	69 (9%)	13 (2%)	11	43
2	C	13/30 (43%)	10 (77%)	2 (15%)	1 (8%)	1	6
2	D	18/30 (60%)	11 (61%)	5 (28%)	2 (11%)	0	2
All	All	1648/1764 (93%)	1485 (90%)	138 (8%)	25 (2%)	12	45

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	162	ILE
1	B	24	SER
1	B	512	CYS
2	D	55	LYS
1	A	129	LEU
1	A	704	PRO
1	A	122	GLU
1	A	535	HIS
1	A	581	LYS
1	B	52	PHE
1	B	173	ASN

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Mol	Chain	Res	Type
1	B	309	LYS
1	B	391	ARG
1	B	294	VAL
2	D	54	ILE
2	C	58	GLY
1	A	114	ILE
1	A	269	ASP
1	B	54	LEU
1	B	318	LEU
1	B	473	PRO
1	B	474	PRO
1	B	737	ILE
1	B	53	VAL

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	673/762 (88%)	624 (93%)	49 (7%)	16	50
1	B	652/762 (86%)	606 (93%)	46 (7%)	17	52
2	C	13/26 (50%)	10 (77%)	3 (23%)	1	4
2	D	16/26 (62%)	16 (100%)	0	100	100
All	All	1354/1576 (86%)	1256 (93%)	98 (7%)	17	51

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	84	PRO
1	A	99	ILE
1	A	117	ILE
1	A	135	SER
1	A	149	PHE
1	A	162	ILE
1	A	164	ASP

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Mol	Chain	Res	Type
1	A	170	ARG
1	A	174	ILE
1	A	190	ILE
1	A	213	ILE
1	A	237	ARG
1	A	257	ILE
1	A	294	VAL
1	A	310	TYR
1	A	369	THR
1	A	370	ILE
1	A	372	ASP
1	A	398	ILE
1	A	412	VAL
1	A	415	GLU
1	A	429	MET
1	A	434	PRO
1	A	458	THR
1	A	476	THR
1	A	492	SER
1	A	534	GLN
1	A	552	VAL
1	A	554	HIS
1	A	563	GLN
1	A	570	ILE
1	A	598	GLN
1	A	622	GLN
1	A	643	VAL
1	A	661	GLN
1	A	668	ILE
1	A	720	GLU
1	A	741	ILE
1	A	744	GLN
1	A	758	ILE
1	A	781	VAL
1	A	794	ILE
1	A	800	SER
1	A	808	GLU
1	A	844	ASN
1	A	850	ARG
1	A	858	HIS
1	A	868	ASN
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	95	CYS
1	B	98	ASN
1	B	107	ARG
1	B	126	TRP
1	B	131	PRO
1	B	149	PHE
1	B	189	LYS
1	B	246	ARG
1	B	249	ARG
1	B	262	LEU
1	B	282	THR
1	B	310	TYR
1	B	311	SER
1	B	314	ASP
1	B	369	THR
1	B	372	ASP
1	B	379	SER
1	B	398	ILE
1	B	424	ILE
1	B	435	TYR
1	B	448	SER
1	B	475	ASP
1	B	476	THR
1	B	488	ARG
1	B	513	THR
1	B	530	PHE
1	B	571	GLN
1	B	581	LYS
1	B	631	ASP
1	B	634	GLU
1	B	661	GLN
1	B	705	CYS
1	B	715	THR
1	B	720	GLU
1	B	726	ASN
1	B	744	GLN
1	B	749	MET
1	B	753	GLN
1	B	790	LEU
1	B	794	ILE
1	B	795	ARG
1	B	807	ASN

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Mol	Chain	Res	Type
1	B	826	SER
1	B	841	SER
1	B	868	ASN
2	C	53	ASN
2	C	56	ARG
2	C	68	THR

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	98	ASN
1	A	173	ASN
1	A	200	GLN
1	A	212	HIS
1	A	268	GLN
1	A	535	HIS
1	A	563	GLN
1	A	574	ASN
1	A	700	GLN
1	A	759	ASN
1	A	844	ASN
1	A	868	ASN
1	B	74	ASN
1	B	97	ASN
1	B	173	ASN
1	B	212	HIS
1	B	306	ASN
1	B	430	GLN
1	B	626	ASN
1	B	685	GLN
1	B	753	GLN
1	B	784	GLN
1	B	807	ASN
1	B	858	HIS
2	C	53	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 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	824/852 (96%)	-0.07	6 (0%) 87 75	49, 86, 136, 177	0
1	B	813/852 (95%)	0.04	14 (1%) 70 49	47, 87, 168, 200	0
2	C	17/30 (56%)	0.22	1 (5%) 23 10	66, 113, 147, 153	0
2	D	20/30 (66%)	0.17	0 100 100	67, 124, 165, 169	0
All	All	1674/1764 (94%)	-0.01	21 (1%) 77 59	47, 87, 156, 200	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	ASN	5.0
1	B	24	SER	4.3
1	B	27	THR	4.2
1	B	83	PHE	3.8
1	B	82	ASN	3.6
1	B	117	ILE	3.5
1	B	14	GLN	3.2
1	B	22	SER	3.1
1	B	319	LYS	3.1
1	A	91	ILE	3.0
2	C	53	ASN	2.6
1	B	86	GLY	2.5
1	B	632	GLN	2.4
1	A	829	ILE	2.4
1	B	394	LEU	2.3
1	A	876	PHE	2.3
1	A	48	ASN	2.2
1	A	578	ASP	2.1
1	A	92	LYS	2.0
1	B	23	GLN	2.0
1	B	90	PHE	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.