Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2016 – 05:03 PM EDT

PDB ID	:	5J3V
Title	:	Crystal structure of human Karyopherin-beta2 bound to the histone H3 tail
Authors	:	Soniat, M.; Chook, Y.M.
Deposited on	:	2016-03-31
Resolution	:	3.05 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:

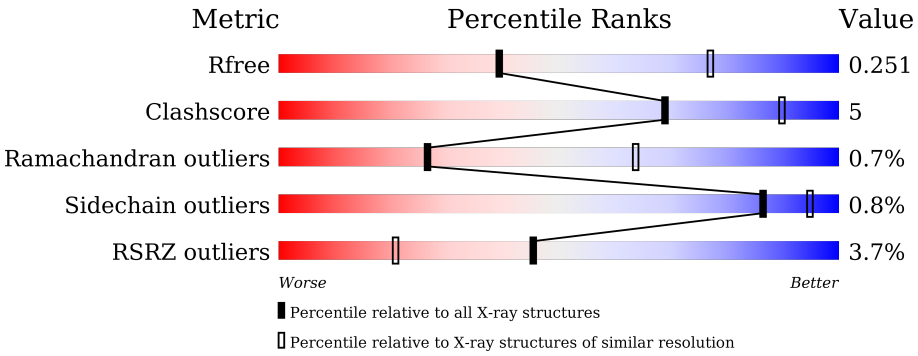
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.05 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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	854	88% 9% ·
1	B	854	7% 82% 13% · 5%
2	C	17	94% 6%
2	D	17	94% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13357 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,Transportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6645	4259	1107	1228	51			
1	B	813	Total	C	N	O	S	0	0	0
			6464	4147	1079	1187	51			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	linker	UNP Q92973
A	361	GLY	-	linker	UNP Q92973
A	362	SER	-	linker	UNP Q92973
A	363	GLY	-	linker	UNP Q92973
A	364	GLY	-	linker	UNP Q92973
A	365	SER	-	linker	UNP Q92973
A	366	GLY	-	linker	UNP Q92973
B	360	GLY	-	linker	UNP Q92973
B	361	GLY	-	linker	UNP Q92973
B	362	SER	-	linker	UNP Q92973
B	363	GLY	-	linker	UNP Q92973
B	364	GLY	-	linker	UNP Q92973
B	365	SER	-	linker	UNP Q92973
B	366	GLY	-	linker	UNP Q92973

- Molecule 2 is a protein called Histone H3.

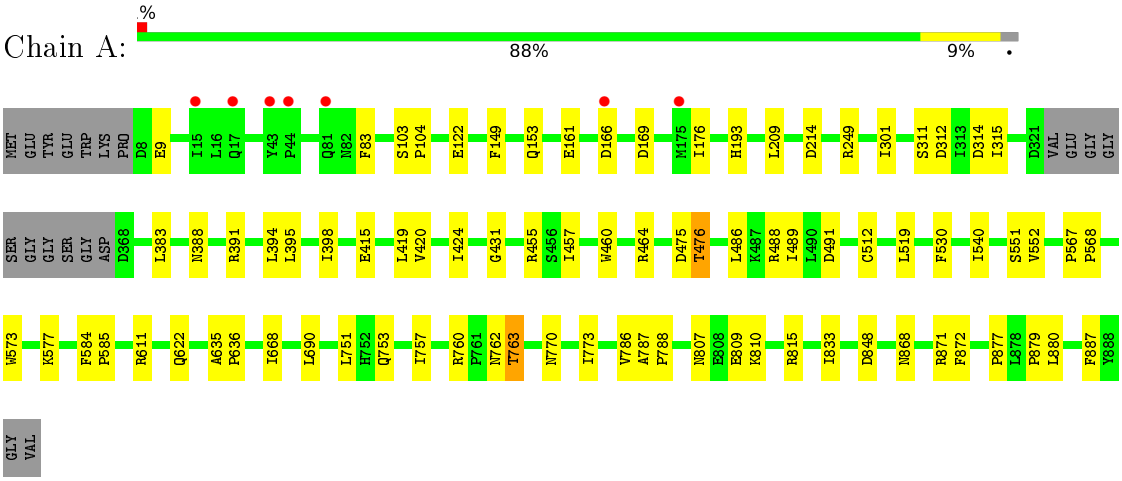
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	0	0	0
			124	76	28	20			
2	D	17	Total	C	N	O	0	0	0
			124	76	28	20			

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 errors 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.

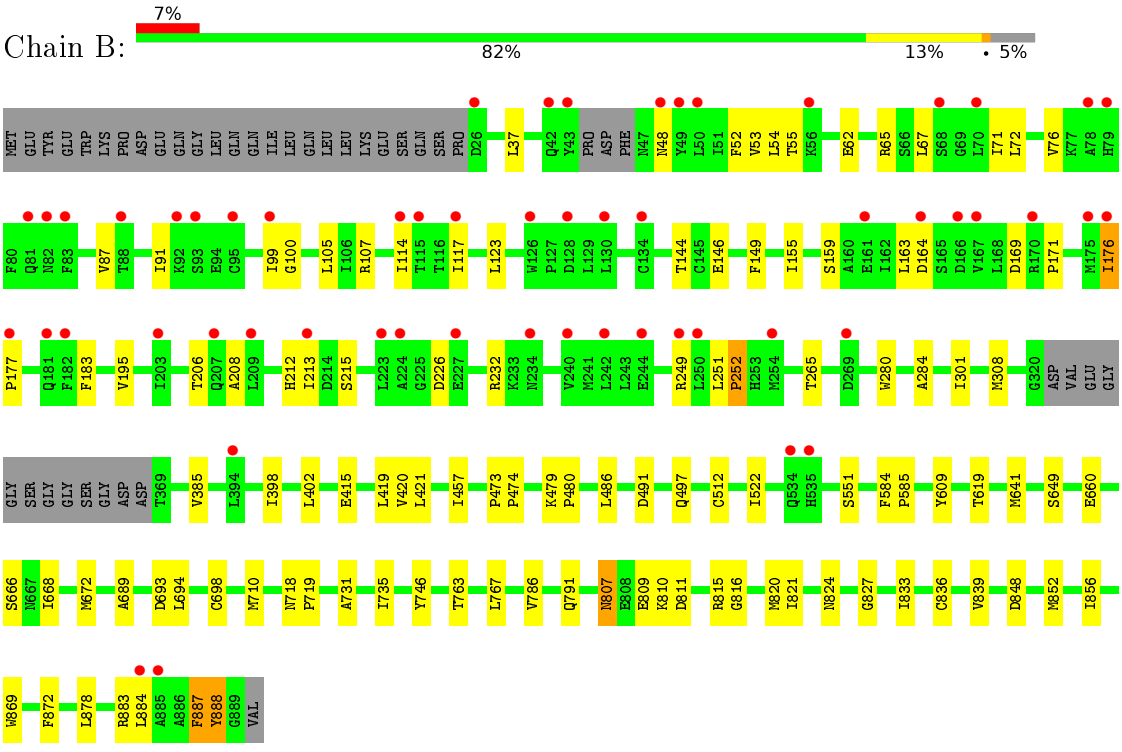
- Molecule 1: Transportin-1,Transportin-1

Chain A:



- Molecule 1: Transportin-1,Transportin-1

Chain B:

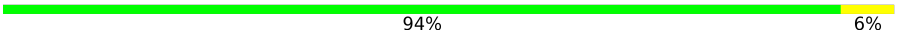


- Molecule 2: Histone H3

Chain C:

- Molecule 2: Histone H3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	150.30Å 154.19Å 192.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 3.05 49.34 – 3.04	Depositor EDS
% Data completeness (in resolution range)	93.0 (37.80-3.05) 89.1 (49.34-3.04)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.256 0.209 , 0.251	Depositor DCC
R_{free} test set	1941 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13357	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.21	0/6785	0.37	0/9215
1	B	0.21	0/6600	0.38	0/8962
2	C	0.19	0/124	0.36	0/162
2	D	0.19	0/124	0.38	0/162
All	All	0.21	0/13633	0.37	0/18501

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

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	6645	0	6707	48	0
1	B	6464	0	6537	75	0
2	C	124	0	143	1	0
2	D	124	0	143	1	0
All	All	13357	0	13530	123	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 5.

All (123) 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:123:LEU:HD12	1:B:159:SER:OG	1.32	1.28
1:B:123:LEU:CD1	1:B:159:SER:OG	1.87	1.22
1:B:163:LEU:HD11	1:B:206:THR:OG1	1.52	1.08
1:B:123:LEU:HD12	1:B:159:SER:CB	1.97	0.94
1:B:123:LEU:CD1	1:B:159:SER:CB	2.47	0.92
1:B:123:LEU:HD11	1:B:159:SER:OG	1.75	0.86
1:B:163:LEU:CD1	1:B:206:THR:OG1	2.26	0.83
1:B:53:VAL:O	1:B:53:VAL:HG12	1.78	0.80
1:A:475:ASP:O	1:A:476:THR:HG23	1.86	0.76
1:B:76:VAL:HG11	1:B:117:ILE:HG12	1.68	0.74
1:B:284:ALA:HB1	1:B:385:VAL:HG11	1.70	0.73
1:B:123:LEU:HD21	1:B:155:ILE:HG23	1.70	0.73
1:B:62:GLU:HG2	1:B:105:LEU:HD23	1.73	0.70
1:B:811:ASP:OD2	1:B:815:ARG:NH1	2.25	0.70
1:B:206:THR:HG22	1:B:208:ALA:H	1.62	0.65
1:B:48:ASN:HB3	1:B:87:VAL:HG13	1.79	0.64
1:B:836:CYS:O	1:B:883:ARG:NH2	2.31	0.64
1:B:107:ARG:NH1	1:B:146:GLU:OE1	2.33	0.62
1:A:512:CYS:HA	1:A:551:SER:HB3	1.82	0.62
1:B:212:HIS:HB3	1:B:215:SER:HB3	1.81	0.62
1:B:265:THR:HG21	1:B:280:TRP:HE1	1.66	0.61
1:A:807:ASN:HD22	1:A:809:GLU:H	1.48	0.60
1:A:475:ASP:O	1:A:476:THR:CG2	2.48	0.60
1:A:815:ARG:NH1	1:A:848:ASP:OD2	2.34	0.60
1:B:53:VAL:O	1:B:53:VAL:CG1	2.48	0.60
1:B:821:ILE:HD12	1:B:856:ILE:HD13	1.85	0.58
1:A:760:ARG:HH11	1:A:763:THR:CG2	2.17	0.57
1:B:176:ILE:HG22	1:B:177:PRO:HD3	1.85	0.57
1:B:672:MET:HE1	1:B:694:LEU:HD12	1.86	0.56
1:A:807:ASN:HD22	1:A:809:GLU:N	2.05	0.55
1:A:214:ASP:OD1	1:A:249:ARG:NH1	2.39	0.54
1:B:123:LEU:CD2	1:B:155:ILE:HG23	2.39	0.53
1:B:62:GLU:HA	1:B:65:ARG:HB3	1.91	0.53
1:A:668:ILE:HD11	1:A:690:LEU:HD21	1.91	0.52
1:B:402:LEU:HD21	1:B:421:LEU:HD13	1.91	0.52
1:B:123:LEU:CD1	1:B:159:SER:HB2	2.38	0.52
1:A:395:LEU:HD11	1:A:431:GLY:HA3	1.92	0.52
1:B:72:LEU:HD11	1:B:91:ILE:HD13	1.91	0.52
1:B:609:TYR:OH	1:B:666:SER:OG	2.27	0.51
1:A:868:ASN:OD1	1:A:871:ARG:NH2	2.43	0.51
1:B:415:GLU:HG2	1:B:457:ILE:HG21	1.93	0.51
1:A:877:PRO:HB2	1:A:880:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLU:HG2	1:B:698:CYS:HB3	1.92	0.51
1:B:689:ALA:HB1	2:D:14:LYS:HD2	1.94	0.50
1:B:512:CYS:HA	1:B:551:SER:HB3	1.94	0.50
1:A:455:ARG:NH1	1:A:491:ASP:OD2	2.45	0.50
1:A:153:GLN:OE1	1:A:193:HIS:ND1	2.44	0.50
1:A:388:ASN:O	1:A:391:ARG:NH1	2.45	0.50
1:A:773:ILE:HD13	1:A:809:GLU:HB3	1.94	0.49
1:A:622:GLN:HB3	1:A:636:PRO:HG3	1.93	0.49
1:A:540:ILE:HA	2:C:22:THR:HG21	1.92	0.49
1:B:491:ASP:O	1:B:497:GLN:NE2	2.42	0.49
1:B:791:GLN:HE22	1:B:824:ASN:HD21	1.60	0.49
1:B:99:ILE:HD13	1:B:114:ILE:HD12	1.95	0.48
1:A:419:LEU:HD13	1:A:457:ILE:HD11	1.96	0.48
1:B:839:VAL:HB	1:B:883:ARG:HH21	1.78	0.47
1:B:869:TRP:HE1	1:B:884:LEU:HD21	1.78	0.47
1:B:473:PRO:HA	1:B:474:PRO:HD3	1.76	0.47
1:B:619:THR:HG21	1:B:641:MET:HB2	1.96	0.47
1:B:649:SER:OG	1:B:693:ASP:OD2	2.27	0.47
1:B:609:TYR:CE1	1:B:668:ILE:HD11	2.50	0.47
1:A:753:GLN:O	1:A:757:ILE:HG12	2.15	0.47
1:B:123:LEU:HD12	1:B:159:SER:HG	1.66	0.46
1:B:54:LEU:HG	1:B:55:THR:HG23	1.97	0.46
1:A:760:ARG:HH11	1:A:763:THR:HG23	1.81	0.46
1:A:573:TRP:CZ2	1:A:611:ARG:HD3	2.52	0.45
1:A:301:ILE:HD11	1:A:394:LEU:HD11	1.99	0.45
1:B:791:GLN:HG3	1:B:827:GLY:HA2	1.99	0.45
1:A:383:LEU:HD21	1:A:420:VAL:HG13	1.98	0.45
1:A:567:PRO:HG2	1:A:568:PRO:HD3	1.99	0.45
1:B:226:ASP:O	1:B:232:ARG:NH1	2.49	0.45
1:B:308:MET:HE3	1:B:420:VAL:HG22	1.98	0.45
1:A:807:ASN:ND2	1:A:810:LYS:H	2.16	0.44
1:B:807:ASN:HD22	1:B:810:LYS:H	1.66	0.44
1:B:37:LEU:HD13	1:B:71:ILE:HD13	2.00	0.44
1:B:710:MET:HE2	1:B:746:TYR:HB3	1.99	0.44
1:A:312:ASP:N	1:A:312:ASP:OD1	2.51	0.44
1:A:486:LEU:HD23	1:A:489:ILE:HD12	1.99	0.44
1:B:486:LEU:HD11	1:B:522:ILE:HG12	2.00	0.44
1:B:251:LEU:N	1:B:252:PRO:HD2	2.33	0.44
1:B:419:LEU:HD13	1:B:457:ILE:HD11	2.00	0.44
1:A:311:SER:OG	1:A:314:ASP:OD2	2.23	0.43
1:A:398:ILE:HG21	1:A:424:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:ASN:HD21	1:A:809:GLU:HB2	1.81	0.43
1:B:731:ALA:O	1:B:735:ILE:HG13	2.18	0.43
1:A:879:PRO:HG2	1:A:880:LEU:HD22	2.01	0.43
1:A:475:ASP:C	1:A:476:THR:HG23	2.37	0.43
1:B:301:ILE:HG21	1:B:398:ILE:HG12	2.01	0.43
1:A:807:ASN:ND2	1:A:809:GLU:HB2	2.34	0.43
1:A:833:ILE:HG12	1:A:872:PHE:HE1	1.84	0.43
1:B:718:ASN:HA	1:B:719:PRO:HD3	1.74	0.42
1:B:848:ASP:O	1:B:852:MET:HG3	2.19	0.42
1:A:176:ILE:HD13	1:A:209:LEU:HB2	2.01	0.42
1:A:519:LEU:HD13	1:A:552:VAL:HG11	2.00	0.42
1:A:415:GLU:HG2	1:A:457:ILE:HG21	2.02	0.42
1:B:816:GLY:O	1:B:820:MET:HG2	2.20	0.42
1:A:103:SER:HA	1:A:104:PRO:HD3	1.93	0.42
1:A:460:TRP:CZ2	1:A:464:ARG:HD2	2.55	0.42
1:B:100:GLY:HA3	1:B:144:THR:HG22	2.02	0.42
1:B:479:LYS:HB3	1:B:480:PRO:HD3	2.02	0.41
1:A:584:PHE:HB2	1:A:585:PRO:HD3	2.02	0.41
1:A:787:ALA:N	1:A:788:PRO:HD2	2.35	0.41
1:B:183:PHE:CE2	1:B:195:VAL:HG22	2.55	0.41
1:B:584:PHE:HB2	1:B:585:PRO:HD3	2.01	0.41
1:A:848:ASP:OD1	1:A:848:ASP:N	2.52	0.41
1:B:763:THR:HG23	1:B:767:LEU:HD23	2.01	0.41
1:B:176:ILE:H	1:B:177:PRO:HD2	1.86	0.41
1:B:249:ARG:HA	1:B:249:ARG:HD3	1.92	0.41
1:B:807:ASN:C	1:B:807:ASN:HD22	2.23	0.41
1:B:786:VAL:HG12	1:B:820:MET:HE1	2.01	0.41
1:A:311:SER:O	1:A:315:ILE:HG13	2.20	0.41
1:A:762:ASN:HB3	1:A:763:THR:H	1.66	0.41
1:B:807:ASN:ND2	1:B:809:GLU:HB2	2.36	0.41
1:A:577:LYS:HD2	1:A:577:LYS:HA	1.89	0.41
1:B:213:ILE:HD11	1:B:249:ARG:NE	2.36	0.41
1:B:176:ILE:H	1:B:177:PRO:CD	2.34	0.40
1:B:67:LEU:O	1:B:71:ILE:HG13	2.21	0.40
1:A:635:ALA:HA	1:A:636:PRO:HD3	1.87	0.40
1:B:791:GLN:NE2	1:B:824:ASN:HD21	2.19	0.40
1:B:807:ASN:ND2	1:B:810:LYS:H	2.19	0.40
1:B:833:ILE:HG12	1:B:872:PHE:CE1	2.57	0.40
1:B:887:PHE:HB2	1:B:888:TYR:CE2	2.56	0.40
1:A:751:LEU:HD11	1:A:786:VAL:HG13	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	831/854 (97%)	799 (96%)	26 (3%)	6 (1%)	26	64
1	B	807/854 (94%)	744 (92%)	57 (7%)	6 (1%)	26	64
2	C	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
2	D	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
All	All	1668/1742 (96%)	1569 (94%)	87 (5%)	12 (1%)	26	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ASP
1	B	164	ASP
1	B	169	ASP
1	A	169	ASP
1	A	476	THR
1	B	176	ILE
1	A	161	GLU
1	B	171	PRO
1	B	878	LEU
1	A	9	GLU
1	A	763	THR
1	B	252	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	750/763 (98%)	743 (99%)	7 (1%)	84 94
1	B	728/763 (95%)	723 (99%)	5 (1%)	88 95
2	C	11/11 (100%)	11 (100%)	0	100 100
2	D	11/11 (100%)	11 (100%)	0	100 100
All	All	1500/1548 (97%)	1488 (99%)	12 (1%)	86 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	PHE
1	A	122	GLU
1	A	149	PHE
1	A	488	ARG
1	A	530	PHE
1	A	770	ASN
1	A	887	PHE
1	B	52	PHE
1	B	149	PHE
1	B	807	ASN
1	B	887	PHE
1	B	888	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	ASN
1	A	685	GLN
1	A	726	ASN
1	A	770	ASN
1	A	807	ASN
1	B	125	ASN
1	B	535	HIS
1	B	726	ASN
1	B	770	ASN
1	B	807	ASN
1	B	824	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	835/854 (97%)	-0.14	7 (0%) 87 72	17, 45, 85, 143	0
1	B	813/854 (95%)	0.25	56 (6%) 20 7	12, 59, 117, 150	0
2	C	17/17 (100%)	-0.36	0 100 100	30, 51, 60, 62	0
2	D	17/17 (100%)	-0.32	0 100 100	22, 49, 64, 73	0
All	All	1682/1742 (96%)	0.05	63 (3%) 45 21	12, 50, 106, 150	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	SER	5.6
1	B	48	ASN	5.5
1	B	70	LEU	4.9
1	A	166	ASP	4.6
1	B	175	MET	4.4
1	B	207	GLN	4.2
1	B	49	TYR	3.9
1	B	128	ASP	3.8
1	B	242	LEU	3.7
1	B	82	ASN	3.5
1	B	885	ALA	3.4
1	B	42	GLN	3.4
1	B	244	GLU	3.2
1	B	182	PHE	3.2
1	B	167	VAL	3.2
1	B	250	LEU	3.2
1	B	161	GLU	3.0
1	B	227	GLU	3.0
1	B	224	ALA	2.9
1	B	126	TRP	2.9
1	B	79	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	223	LEU	2.9
1	B	177	PRO	2.9
1	B	88	THR	2.9
1	B	176	ILE	2.8
1	B	269	ASP	2.8
1	B	81	GLN	2.8
1	B	117	ILE	2.8
1	A	17	GLN	2.7
1	B	68	SER	2.6
1	B	249	ARG	2.6
1	B	130	LEU	2.6
1	B	234	ASN	2.6
1	B	181	GLN	2.6
1	B	164	ASP	2.6
1	A	44	PRO	2.6
1	B	254	MET	2.5
1	B	56	LYS	2.5
1	B	394	LEU	2.5
1	B	83	PHE	2.5
1	A	175	MET	2.5
1	B	166	ASP	2.5
1	B	115	THR	2.5
1	B	213	ILE	2.5
1	B	114	ILE	2.4
1	B	99	ILE	2.4
1	B	240	VAL	2.3
1	B	134	CYS	2.3
1	B	95	CYS	2.3
1	B	209	LEU	2.3
1	B	170	ARG	2.2
1	A	81	GLN	2.2
1	B	50	LEU	2.2
1	B	78	ALA	2.2
1	B	534	GLN	2.2
1	A	15	ILE	2.2
1	B	26	ASP	2.2
1	A	43	TYR	2.1
1	B	884	LEU	2.1
1	B	203	ILE	2.1
1	B	92	LYS	2.0
1	B	535	HIS	2.0
1	B	43	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.