



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 01:28 am GMT

PDB ID : 1UN0
Title : Crystal Structure of Yeast Karyopherin (Importin) alpha in complex with a Nup2p N-terminal fragment
Authors : Matsuura, Y.; Lange, A.; Harreman, M.T.; Corbett, A.H.; Stewart, M.
Deposited on : 2003-09-03
Resolution : 2.60 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 : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

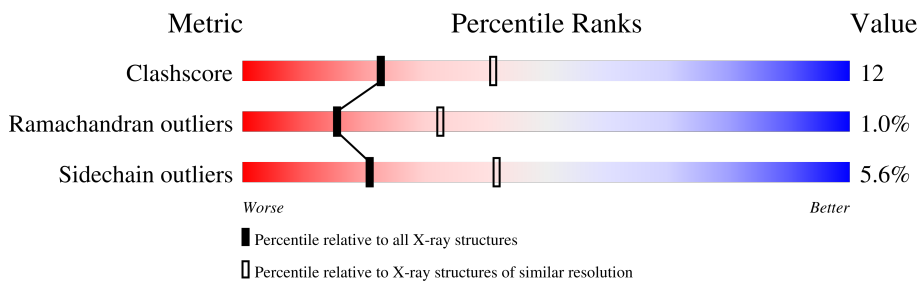
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	443	77% (0-1 types) 20% (2-3 types) .. (not modelled)
1	B	443	78% (0-1 types) 18% (2-3 types) .. (not modelled)
2	C	51	12% (0 types) 6% (1 type) 6% (2 types) 8% (3 types) 69% (not modelled)
2	D	51	14% (0 types) . (1 type) 8% (2 types) 6% (3 types) 69% (not modelled)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7231 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 IMPORTIN ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	440	3398	2139	574	668	17	15	0	1
1	B	439	3397	2139	573	668	17	16	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	ASP	TYR	engineered mutation	UNP Q02821
B	397	ASP	TYR	engineered mutation	UNP Q02821

- Molecule 2 is a protein called NUCLEOPORIN NUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	16	139	87	32	17	3	10	0	0
2	D	16	139	87	32	17	3	10	0	0

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	94	Total	O	0	0
			94	94		
3	C	7	Total	O	0	0
			7	7		
3	D	11	Total	O	0	0
			11	11		

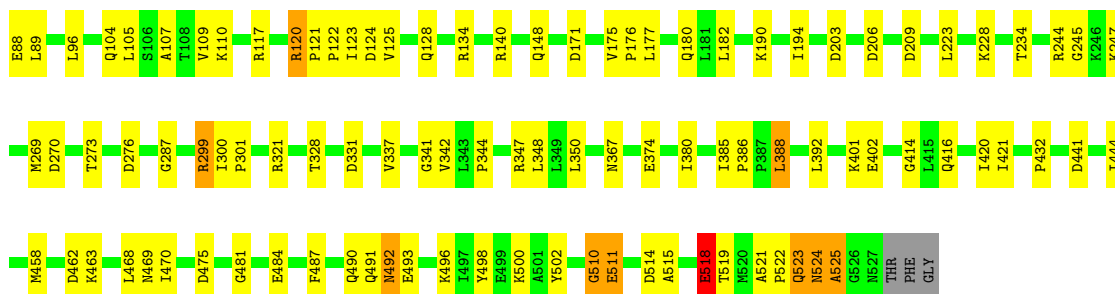
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.


Note EDS was not executed.

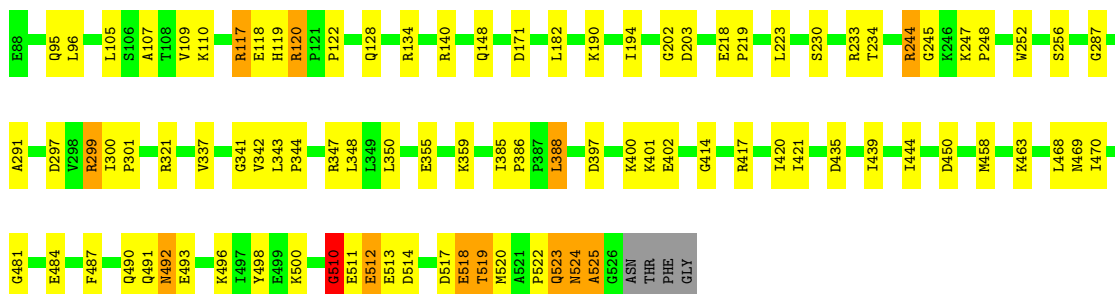
- Molecule 1: IMPORTIN ALPHA SUBUNIT

Chain A:  77% 20%



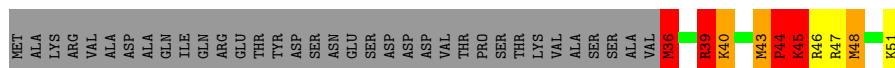
- Molecule 1: IMPORTIN ALPHA SUBUNIT

Chain B:  78% 18%



- Molecule 2: NUCLEOPORIN NUP2

Chain C:  12% 6% 6% 8% 69%



- Molecule 2: NUCLEOPORIN NUP2

Chain D:  14% 8% 6% 69%

MET	ALA	LYS	ARG	VAL	ALA	ASP	ALA	GLN	ILE	GLN	ARG	GLU	THR	TYR	ASP	SER	ASN	GLU	SER	SER	ASP	ASP	ASP	VAL	THR	PRO	SER	THR	THR	LYS	VAL	ALA	SER	SER	ALA	VAL	M36	K39	K40	M43	P44	K45	R46	R47	M48	K51
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4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.81Å 140.08Å 63.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	97.8 (20.00-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7231	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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	0.86	3/3450 (0.1%)	1.14	23/4694 (0.5%)
1	B	0.67	3/3448 (0.1%)	1.16	20/4689 (0.4%)
2	C	4.12	5/140 (3.6%)	3.00	11/180 (6.1%)
2	D	2.31	4/140 (2.9%)	3.33	11/180 (6.1%)
All	All	1.00	15/7178 (0.2%)	1.28	65/9743 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
2	D	0	1
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	36	MET	CG-SD	-39.76	0.77	1.81
1	A	510	GLY	C-N	-27.88	0.69	1.34
1	A	511	GLU	CA-C	22.28	2.10	1.52
1	A	511	GLU	C-N	-19.98	0.88	1.34
2	C	45	LYS	CD-CE	19.33	1.99	1.51
2	D	44	PRO	N-CD	-17.18	1.23	1.47
1	B	510	GLY	C-N	-16.50	0.96	1.34
2	D	44	PRO	CB-CG	12.79	2.13	1.50
2	C	44	PRO	CB-CG	12.20	2.10	1.50
2	D	36	MET	CG-SD	-10.74	1.53	1.81
2	C	44	PRO	N-CD	-9.81	1.34	1.47
2	C	40	LYS	CB-CG	9.42	1.77	1.52
2	D	40	LYS	CB-CG	7.79	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	511	GLU	CA-C	-7.61	1.33	1.52
1	B	118	GLU	CB-CG	-6.22	1.40	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	GLY	O-C-N	-32.17	71.23	122.70
2	D	43	MET	C-N-CD	-26.49	62.33	120.60
1	A	510	GLY	O-C-N	-26.47	80.34	122.70
2	C	43	MET	C-N-CD	-24.97	65.67	120.60
1	B	510	GLY	CA-C-N	20.33	161.92	117.20
1	A	511	GLU	O-C-N	-19.16	92.04	122.70
1	A	510	GLY	CA-C-N	16.60	153.72	117.20
2	D	44	PRO	CA-N-CD	16.43	134.70	111.70
1	A	511	GLU	C-N-CA	13.24	154.81	121.70
2	C	36	MET	CB-CG-SD	13.24	152.12	112.40
2	C	44	PRO	CA-N-CD	12.75	129.55	111.70
1	A	511	GLU	CA-C-N	12.00	143.60	117.20
2	D	45	LYS	CD-CE-NZ	11.81	138.86	111.70
2	D	44	PRO	CA-CB-CG	-11.46	82.23	104.00
2	C	44	PRO	CA-CB-CG	-11.00	83.11	104.00
1	A	511	GLU	CB-CA-C	9.33	129.05	110.40
2	D	45	LYS	CG-CD-CE	9.26	139.69	111.90
1	B	514	ASP	CB-CG-OD2	8.54	125.98	118.30
1	A	441	ASP	CB-CG-OD2	7.91	125.42	118.30
1	B	321	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	321	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	510	GLY	C-N-CA	7.27	139.87	121.70
1	B	321	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	171	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	517	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	171	ASP	CB-CG-OD2	6.93	124.53	118.30
1	B	450	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	124	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	297	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	244	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	321	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	270	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	118	GLU	CA-CB-CG	6.49	127.68	113.40
1	A	462	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	397	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	120	ARG	NE-CZ-NH2	-6.28	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ASP	CB-CG-OD2	6.22	123.90	118.30
2	C	39	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	D	43	MET	N-CA-C	-6.11	94.51	111.00
2	C	47	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	435	ASP	CB-CG-OD2	6.04	123.74	118.30
2	C	40	LYS	CB-CG-CD	6.00	127.21	111.60
1	B	244	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	510	GLY	C-N-CA	5.96	136.61	121.70
2	D	45	LYS	N-CA-C	-5.96	94.92	111.00
1	A	514	ASP	CB-CG-OD2	5.93	123.64	118.30
2	D	44	PRO	C-N-CA	-5.82	107.16	121.70
2	C	39	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	475	ASP	CB-CG-OD2	5.72	123.45	118.30
2	D	36	MET	CG-SD-CE	-5.70	91.08	100.20
2	D	40	LYS	CB-CG-CD	5.62	126.20	111.60
1	A	209	ASP	CB-CG-OD2	5.49	123.24	118.30
2	C	47	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	117	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	117	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	331	ASP	CB-CG-OD2	5.35	123.11	118.30
2	C	44	PRO	C-N-CA	-5.28	108.50	121.70
1	A	203	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	524	ASN	CB-CA-C	-5.26	99.88	110.40
1	A	518	GLU	N-CA-C	5.24	125.13	111.00
2	C	45	LYS	N-CA-C	-5.22	96.89	111.00
1	A	524	ASN	CB-CA-C	-5.17	100.05	110.40
1	B	122	PRO	N-CD-CG	-5.13	95.50	103.20
1	A	244	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	D	39	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	510	GLY	Mainchain
1	A	511	GLU	Peptide
1	B	510	GLY	Peptide,Mainchain
2	D	44	PRO	Peptide

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	3398	0	3427	71	0
1	B	3397	0	3427	64	0
2	C	139	0	160	20	0
2	D	139	0	156	21	0
3	A	46	0	0	6	0
3	B	94	0	0	9	0
3	C	7	0	0	2	0
3	D	11	0	0	10	0
All	All	7231	0	7170	163	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 12.

All (163) 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:D:43:MET:O	2:D:44:PRO:O	1.58	1.21
2:D:43:MET:O	2:D:44:PRO:C	1.84	1.11
2:C:43:MET:O	2:C:44:PRO:O	1.74	1.03
2:C:44:PRO:O	2:C:45:LYS:O	1.77	1.01
1:A:492:ASN:HD22	1:A:493:GLU:N	1.59	0.99
2:C:44:PRO:O	2:C:45:LYS:C	1.95	0.98
2:C:43:MET:O	2:C:44:PRO:C	2.01	0.96
2:C:51:LYS:HD3	3:C:2007:HOH:O	1.68	0.93
1:B:492:ASN:HD22	1:B:493:GLU:N	1.65	0.93
1:B:359:LYS:HE3	3:D:2003:HOH:O	1.71	0.90
1:A:492:ASN:HD22	1:A:493:GLU:H	1.18	0.89
1:A:487:PHE:O	1:A:490:GLN:HG2	1.71	0.89
2:D:44:PRO:O	2:D:45:LYS:O	1.91	0.88
2:D:44:PRO:O	2:D:45:LYS:C	2.10	0.86
1:B:492:ASN:HD22	1:B:493:GLU:H	1.22	0.85
1:A:502:TYR:CD1	1:A:515:ALA:HB1	2.12	0.84
1:B:487:PHE:O	1:B:490:GLN:HG2	1.80	0.82
2:D:43:MET:C	2:D:44:PRO:O	2.17	0.81
2:D:45:LYS:N	3:D:2006:HOH:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:LYS:HG2	3:D:2006:HOH:O	1.81	0.79
2:D:45:LYS:CG	3:D:2006:HOH:O	2.30	0.78
1:A:493:GLU:HB3	1:A:524:ASN:O	1.86	0.74
2:D:45:LYS:CA	3:D:2006:HOH:O	2.34	0.74
1:A:299:ARG:HG2	1:A:299:ARG:HH11	1.52	0.74
1:B:496:LYS:NZ	1:B:500:LYS:NZ	2.38	0.72
1:B:299:ARG:HG2	1:B:299:ARG:HH11	1.53	0.71
1:B:496:LYS:NZ	1:B:500:LYS:HZ1	1.92	0.67
2:D:44:PRO:HA	2:D:46:ARG:HG3	1.76	0.67
1:A:299:ARG:O	3:A:2027:HOH:O	2.13	0.66
2:C:43:MET:C	2:C:44:PRO:O	2.31	0.65
1:A:104:GLN:HE21	1:A:134:ARG:NH2	1.94	0.65
1:A:492:ASN:ND2	1:A:493:GLU:N	2.40	0.65
3:A:2016:HOH:O	2:C:48:MET:HG2	1.97	0.64
1:B:400:LYS:HE3	3:B:2074:HOH:O	1.99	0.63
2:D:45:LYS:CB	3:D:2006:HOH:O	2.47	0.63
2:D:44:PRO:HB2	3:D:2005:HOH:O	1.99	0.63
1:A:269:MET:HB2	3:A:2022:HOH:O	2.00	0.61
1:A:341:GLY:O	1:A:344:PRO:HD2	2.00	0.61
1:A:496:LYS:NZ	1:A:500:LYS:HZ2	1.98	0.61
1:B:120:ARG:O	1:B:120:ARG:HG3	2.01	0.61
2:D:46:ARG:NH2	3:D:2009:HOH:O	2.33	0.60
1:A:276:ASP:OD1	1:B:120:ARG:NH2	2.34	0.60
1:A:496:LYS:NZ	1:A:500:LYS:NZ	2.49	0.60
2:D:46:ARG:CZ	3:D:2009:HOH:O	2.50	0.59
1:B:496:LYS:HZ3	1:B:500:LYS:NZ	2.00	0.59
1:B:128:GLN:HG3	3:B:2007:HOH:O	2.04	0.58
1:A:524:ASN:O	1:A:525:ALA:CB	2.52	0.58
1:A:502:TYR:CE1	1:A:515:ALA:HB1	2.40	0.57
2:D:51:LYS:HA	2:D:51:LYS:CE	2.34	0.57
2:D:43:MET:HG2	2:D:44:PRO:N	2.20	0.57
1:A:128:GLN:HG3	3:B:2051:HOH:O	2.04	0.56
1:B:512:GLU:O	1:B:512:GLU:HG3	2.06	0.56
1:A:300:ILE:N	1:A:301:PRO:HD2	2.20	0.56
1:B:182:LEU:HD22	1:B:223:LEU:HD11	1.88	0.56
1:B:496:LYS:HZ1	1:B:500:LYS:HZ1	1.51	0.56
1:B:401:LYS:HG2	1:B:444:ILE:HG13	1.87	0.56
1:B:524:ASN:O	1:B:525:ALA:CB	2.53	0.56
1:A:496:LYS:HZ1	1:A:500:LYS:HZ2	1.53	0.55
1:B:117:ARG:HD2	1:B:119:HIS:O	2.06	0.55
2:D:51:LYS:HA	2:D:51:LYS:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2066:HOH:O	2:D:36:MET:HG3	2.06	0.55
1:A:524:ASN:O	1:A:525:ALA:HB2	2.07	0.55
1:A:328:THR:O	2:C:36:MET:N	2.40	0.54
2:C:46:ARG:NH2	3:C:2004:HOH:O	2.41	0.54
1:A:89:LEU:CD2	1:A:125:VAL:HG12	2.38	0.54
1:A:182:LEU:O	1:A:190:LYS:HE2	2.08	0.53
1:A:496:LYS:HZ1	1:A:500:LYS:NZ	2.05	0.53
1:B:524:ASN:N	3:B:2093:HOH:O	2.41	0.53
1:A:228:LYS:HE2	3:A:2010:HOH:O	2.09	0.53
1:B:496:LYS:HZ1	1:B:500:LYS:NZ	2.04	0.53
1:B:519:THR:HG23	1:B:519:THR:O	2.09	0.53
1:A:414:GLY:HA3	1:A:421:ILE:HG12	1.92	0.52
1:B:194:ILE:HG23	1:B:234:THR:HG22	1.92	0.52
1:B:519:THR:O	1:B:519:THR:CG2	2.58	0.52
1:A:120:ARG:O	1:A:120:ARG:HG3	2.10	0.51
1:A:117:ARG:NH2	1:A:122:PRO:HG3	2.26	0.51
1:A:273:THR:HA	3:A:2011:HOH:O	2.11	0.51
1:A:518:GLU:O	1:A:518:GLU:CG	2.59	0.51
1:A:245:GLY:HA2	2:C:46:ARG:HH21	1.76	0.50
1:B:496:LYS:NZ	1:B:500:LYS:HZ3	2.08	0.50
1:B:414:GLY:HA3	1:B:421:ILE:HG12	1.92	0.50
1:B:355:GLU:HA	1:B:355:GLU:OE1	2.12	0.50
1:A:487:PHE:CD1	1:A:490:GLN:NE2	2.77	0.50
1:A:328:THR:HA	2:C:36:MET:N	2.27	0.49
1:A:518:GLU:O	1:A:518:GLU:HG3	2.12	0.49
1:B:492:ASN:ND2	1:B:493:GLU:N	2.49	0.49
2:C:44:PRO:HA	2:C:46:ARG:HG3	1.94	0.48
1:A:481:GLY:O	1:A:484:GLU:HG3	2.14	0.48
1:A:182:LEU:HD22	1:A:223:LEU:HD11	1.95	0.48
1:A:502:TYR:CE1	1:A:515:ALA:CB	2.97	0.48
1:A:128:GLN:CG	3:B:2051:HOH:O	2.62	0.48
1:B:105:LEU:O	1:B:109:VAL:HG23	2.13	0.48
1:B:519:THR:HA	3:B:2090:HOH:O	2.13	0.47
1:B:385:ILE:HB	1:B:386:PRO:HD3	1.95	0.47
1:B:522:PRO:O	1:B:523:GLN:O	2.32	0.47
1:A:493:GLU:HB3	1:A:525:ALA:HB3	1.97	0.47
1:B:182:LEU:O	1:B:190:LYS:HE2	2.15	0.47
1:B:463:LYS:HD2	1:B:470:ILE:C	2.35	0.47
1:B:524:ASN:O	1:B:525:ALA:HB2	2.14	0.47
1:A:328:THR:C	2:C:36:MET:N	2.69	0.47
1:A:493:GLU:CG	1:A:525:ALA:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:GLU:O	1:B:512:GLU:CG	2.62	0.46
1:A:140:ARG:O	1:A:148:GLN:NE2	2.48	0.46
1:A:521:ALA:N	1:A:522:PRO:CD	2.78	0.46
1:B:245:GLY:HA2	2:D:46:ARG:HH21	1.80	0.46
2:D:46:ARG:NH2	3:D:2010:HOH:O	2.47	0.46
1:A:299:ARG:HG2	1:A:299:ARG:NH1	2.22	0.46
1:A:367:ASN:O	2:C:36:MET:HG2	2.15	0.46
3:A:2012:HOH:O	2:C:48:MET:HE3	2.14	0.46
1:B:300:ILE:N	1:B:301:PRO:HD2	2.31	0.46
1:A:175:VAL:N	1:A:176:PRO:HD2	2.31	0.46
1:B:463:LYS:HD2	1:B:470:ILE:O	2.16	0.45
1:A:105:LEU:O	1:A:109:VAL:HG23	2.15	0.45
1:A:493:GLU:HG2	1:A:525:ALA:HB3	1.98	0.45
1:A:276:ASP:CG	1:B:120:ARG:HH21	2.19	0.45
1:B:481:GLY:O	1:B:484:GLU:HG3	2.17	0.45
1:B:128:GLN:NE2	1:B:128:GLN:HA	2.32	0.45
1:A:385:ILE:HB	1:A:386:PRO:HD3	1.98	0.45
1:A:401:LYS:HG2	1:A:444:ILE:HG13	1.99	0.45
1:A:300:ILE:N	1:A:301:PRO:CD	2.79	0.44
1:A:522:PRO:O	1:A:523:GLN:O	2.35	0.44
1:A:194:ILE:HG23	1:A:234:THR:HG22	1.98	0.44
1:B:95:GLN:HG2	1:B:107:ALA:HB2	1.99	0.44
1:B:487:PHE:CD1	1:B:490:GLN:NE2	2.86	0.44
1:A:337:VAL:HG12	1:A:342:VAL:HG11	1.99	0.44
1:A:392:LEU:HD23	1:A:432:PRO:HB2	1.99	0.44
1:B:140:ARG:O	1:B:148:GLN:NE2	2.43	0.44
1:B:287:GLY:N	2:D:39:ARG:HH22	2.15	0.44
1:A:177:LEU:HA	1:A:180:GLN:HG2	1.99	0.43
1:A:519:THR:O	1:A:519:THR:CG2	2.65	0.43
1:A:276:ASP:CG	1:B:120:ARG:NH2	2.71	0.43
1:B:117:ARG:HG2	3:B:2004:HOH:O	2.18	0.43
1:B:252:TRP:CZ2	1:B:291:ALA:HA	2.54	0.43
1:B:417:ARG:HB3	1:B:420:ILE:HD12	2.01	0.43
1:B:343:LEU:HB2	1:B:344:PRO:HD3	1.99	0.43
1:B:341:GLY:O	1:B:344:PRO:HD2	2.19	0.43
1:B:230:SER:HA	1:B:233:ARG:NH1	2.34	0.43
1:A:493:GLU:N	1:A:524:ASN:O	2.52	0.42
1:A:521:ALA:H	1:A:522:PRO:CD	2.32	0.42
1:B:96:LEU:HD23	1:B:134:ARG:HG2	2.01	0.42
1:B:337:VAL:HG12	1:B:342:VAL:HG11	2.00	0.42
1:A:492:ASN:HD22	1:A:492:ASN:C	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ILE:HD12	1:B:439:ILE:HA	1.94	0.42
2:C:43:MET:HG2	2:C:44:PRO:N	2.32	0.42
1:A:245:GLY:HA2	2:C:46:ARG:NH2	2.35	0.42
2:C:39:ARG:HA	2:C:39:ARG:HD2	1.58	0.42
1:A:463:LYS:HD2	1:A:470:ILE:C	2.40	0.42
1:B:493:GLU:HB3	1:B:524:ASN:O	2.19	0.42
1:A:380:ILE:HD11	1:A:420:ILE:HG23	2.01	0.41
1:B:202:GLY:O	1:B:244:ARG:NH2	2.52	0.41
1:B:350:LEU:HD11	1:B:388:LEU:HD13	2.01	0.41
1:B:524:ASN:HB3	3:B:2093:HOH:O	2.20	0.41
1:A:519:THR:O	1:A:519:THR:HG22	2.19	0.41
1:B:252:TRP:CE2	1:B:256:SER:HB3	2.56	0.41
1:A:121:PRO:HB2	1:A:123:ILE:HG13	2.03	0.41
1:A:287:GLY:N	2:C:39:ARG:HH22	2.19	0.41
1:B:218:GLU:HB3	1:B:219:PRO:HD3	2.03	0.40
1:A:328:THR:CA	2:C:36:MET:N	2.85	0.40
1:A:350:LEU:CD1	1:A:388:LEU:HD13	2.52	0.40
1:B:247:LYS:HA	1:B:248:PRO:HA	1.75	0.40
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.97	0.40
1:B:498:TYR:CZ	1:B:518:GLU:HB2	2.56	0.40
1:A:96:LEU:HD12	1:A:107:ALA:HB3	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	438/443 (99%)	415 (95%)	21 (5%)	2 (0%)	29	52
1	B	435/443 (98%)	413 (95%)	18 (4%)	4 (1%)	17	35
2	C	14/51 (28%)	11 (79%)	1 (7%)	2 (14%)	0	0
2	D	14/51 (28%)	11 (79%)	2 (14%)	1 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	901/988 (91%)	850 (94%)	42 (5%)	9 (1%)	15	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	GLN
1	A	525	ALA
1	B	523	GLN
1	B	525	ALA
2	C	44	PRO
2	D	44	PRO
1	B	510	GLY
1	B	513	GLU
2	C	45	LYS

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	376/379 (99%)	358 (95%)	18 (5%)	25	49
1	B	376/379 (99%)	360 (96%)	16 (4%)	29	54
2	C	14/44 (32%)	9 (64%)	5 (36%)	0	0
2	D	14/44 (32%)	9 (64%)	5 (36%)	0	0
All	All	780/846 (92%)	736 (94%)	44 (6%)	21	42

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	110	LYS
1	A	206	ASP
1	A	247	LYS
1	A	299	ARG
1	A	347	ARG

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	374	GLU
1	A	388	LEU
1	A	402	GLU
1	A	416	GLN
1	A	458	MET
1	A	468	LEU
1	A	469	ASN
1	A	491	GLN
1	A	492	ASN
1	A	498	TYR
1	A	518	GLU
1	B	110	LYS
1	B	120	ARG
1	B	299	ARG
1	B	347	ARG
1	B	348	LEU
1	B	388	LEU
1	B	402	GLU
1	B	458	MET
1	B	468	LEU
1	B	469	ASN
1	B	491	GLN
1	B	492	ASN
1	B	512	GLU
1	B	518	GLU
1	B	519	THR
1	B	520	MET
2	C	36	MET
2	C	39	ARG
2	C	40	LYS
2	C	45	LYS
2	C	48	MET
2	D	39	ARG
2	D	40	LYS
2	D	45	LYS
2	D	48	MET
2	D	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	128	GLN
1	A	180	GLN
1	A	192	GLN
1	A	227	ASN
1	A	469	ASN
1	A	492	ASN
1	B	192	GLN
1	B	227	ASN
1	B	469	ASN
1	B	492	ASN
1	B	524	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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

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Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	511:GLU	C	512:GLU	N	2.65
1	B	510:GLY	C	511:GLU	N	0.96
1	A	511:GLU	C	512:GLU	N	0.88
1	A	510:GLY	C	511:GLU	N	0.69

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.