



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:13 PM GMT

PDB ID : 2C1T
Title : STRUCTURE OF THE KAP60P:NUP2 COMPLEX
Authors : Matsuura, Y.; Stewart, M.
Deposited on : 2005-09-20
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

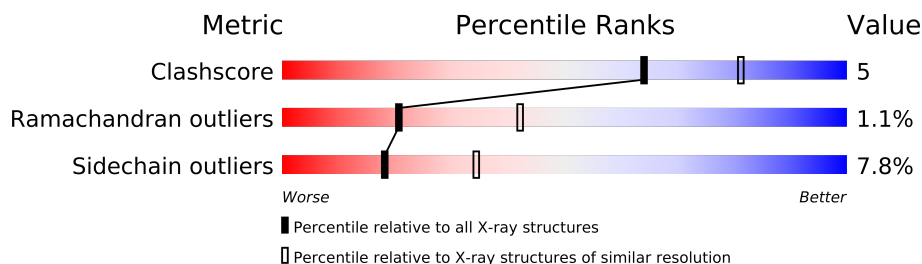
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	
2	C	51	
2	D	51	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7273 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	423	Total	C	N	O	S	0	0	0
			3274	2068	555	635	16			
1	B	423	Total	C	N	O	S	0	0	0
			3273	2069	555	633	16			

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
2	C	36	Total	C	N	O	S	0	0	0
			278	168	57	51	2			
2	D	39	Total	C	N	O	S	0	0	0
			297	179	61	55	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	92	Total	O	0	0
			92	92		
3	C	7	Total	O	0	0
			7	7		
3	D	11	Total	O	0	0
			11	11		

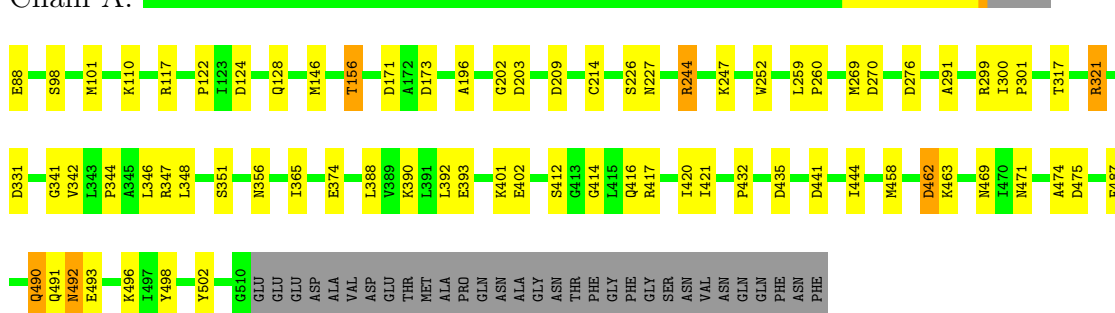
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

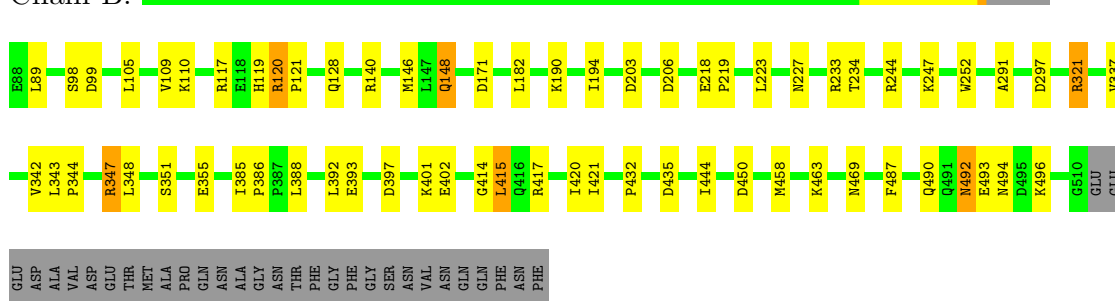
• Molecule 1: IMPORTIN ALPHA SUBUNIT

Chain A:



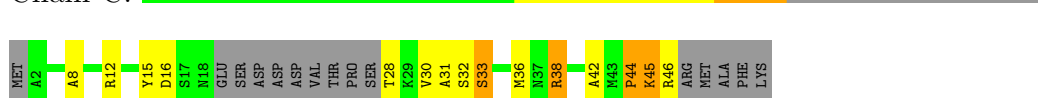
• Molecule 1: IMPORTIN ALPHA SUBUNIT

Chain B:



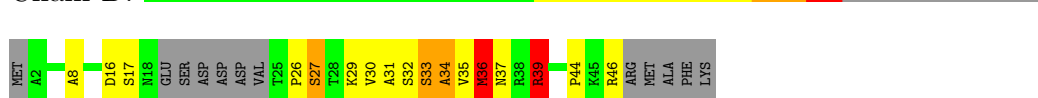
• Molecule 2: NUCLEOPORIN NUP2

Chain C:



• Molecule 2: NUCLEOPORIN NUP2

Chain D:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 5.1.24	Depositor
R, R_{free}	0.203 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7273	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

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	0.50	0/3325	0.93	14/4523 (0.3%)
1	B	0.59	0/3324	0.98	12/4522 (0.3%)
2	C	0.62	0/278	1.27	4/369 (1.1%)
2	D	0.64	0/297	1.24	2/394 (0.5%)
All	All	0.55	0/7224	0.98	32/9808 (0.3%)

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
2	C	1	0
2	D	0	1
All	All	1	1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	321	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	321	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	D	16	ASP	CB-CG-OD2	7.51	125.06	118.30
1	B	435	ASP	CB-CG-OD2	7.33	124.90	118.30
1	B	321	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	244	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	441	ASP	CB-CG-OD2	6.98	124.58	118.30
2	C	33	SER	CB-CA-C	6.74	122.90	110.10
1	A	270	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	321	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	450	ASP	CB-CG-OD2	6.47	124.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	12	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	297	ASP	CB-CG-OD1	6.35	124.02	118.30
2	C	33	SER	N-CA-CB	6.25	119.88	110.50
2	C	16	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	171	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	209	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	124	ASP	CB-CG-OD1	5.93	123.63	118.30
1	B	99	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	171	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	244	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	331	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	435	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	462	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	203	ASP	CB-CG-OD2	5.62	123.36	118.30
2	D	26	PRO	N-CA-CB	5.58	109.99	103.30
1	A	173	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	475	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	397	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	233	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	244	ARG	NE-CZ-NH1	5.08	122.84	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	33	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	27	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3274	0	3322	28	0
1	B	3273	0	3327	34	0
2	C	278	0	286	7	0
2	D	297	0	303	15	0
3	A	41	0	0	4	0
3	B	92	0	0	4	1
3	C	7	0	0	0	0
3	D	11	0	0	6	0
All	All	7273	0	7238	78	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:46:ARG:CB	3:D:2010:HOH:O	2.16	0.94
2:C:38:ARG:O	2:C:38:ARG:HD2	1.76	0.85
1:A:492:ASN:HD22	1:A:493:GLU:N	1.79	0.81
1:B:128:GLN:HG3	3:B:2009:HOH:O	1.82	0.80
1:B:492:ASN:HD22	1:B:494:ASN:H	1.37	0.72
2:D:35:VAL:HG13	3:D:2009:HOH:O	1.88	0.72
2:D:46:ARG:HB3	3:D:2010:HOH:O	1.85	0.69
2:D:46:ARG:O	3:D:2010:HOH:O	2.10	0.68
1:B:415:LEU:N	1:B:415:LEU:HD23	2.08	0.67
1:A:412:SER:CB	3:A:2039:HOH:O	2.45	0.64
2:D:46:ARG:HB2	3:D:2010:HOH:O	1.83	0.64
1:A:269:MET:HB2	3:A:2019:HOH:O	1.97	0.63
1:B:492:ASN:ND2	1:B:494:ASN:H	1.96	0.63
1:A:128:GLN:HG3	3:B:2060:HOH:O	1.99	0.62
1:A:487:PHE:O	1:A:490:GLN:HG2	1.99	0.61
1:B:401:LYS:HG2	1:B:444:ILE:HG13	1.81	0.61
1:A:412:SER:HB2	3:A:2039:HOH:O	2.00	0.61
1:B:492:ASN:HD22	1:B:493:GLU:N	2.00	0.59
1:A:502:TYR:CE1	2:C:42:ALA:HB2	2.38	0.58
1:B:120:ARG:HG3	1:B:120:ARG:O	2.03	0.58
1:A:276:ASP:OD1	1:B:120:ARG:NH2	2.40	0.55
2:D:32:SER:O	2:D:34:ALA:N	2.40	0.54
2:D:36:MET:HA	2:D:39:ARG:HB2	1.89	0.54
1:B:417:ARG:HB3	1:B:420:ILE:HD12	1.89	0.54
1:A:412:SER:HB3	3:A:2039:HOH:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:ASN:HB3	2:C:15:TYR:OH	2.07	0.54
2:C:38:ARG:O	2:C:38:ARG:CD	2.54	0.53
1:A:492:ASN:HD22	1:A:492:ASN:C	2.13	0.52
1:B:105:LEU:O	1:B:109:VAL:HG23	2.09	0.52
2:D:35:VAL:O	2:D:36:MET:CG	2.58	0.51
1:A:392:LEU:HD23	1:A:432:PRO:HB2	1.91	0.50
1:B:140:ARG:O	1:B:148:GLN:NE2	2.37	0.50
1:B:487:PHE:O	1:B:490:GLN:HG2	2.12	0.50
1:A:321:ARG:NH2	2:C:8:ALA:O	2.45	0.50
1:A:156:THR:OG1	1:A:196:ALA:HB2	2.11	0.50
1:A:346:LEU:HD13	1:A:365:ILE:HG13	1.93	0.50
1:B:182:LEU:O	1:B:190:LYS:HE2	2.12	0.49
2:D:30:VAL:HG12	2:D:31:ALA:O	2.12	0.49
1:B:182:LEU:HD22	1:B:223:LEU:HD11	1.95	0.49
1:B:337:VAL:HG12	1:B:342:VAL:HG11	1.94	0.48
1:B:414:GLY:HA3	1:B:421:ILE:HG12	1.95	0.48
1:A:117:ARG:NH2	1:A:122:PRO:HG3	2.28	0.47
1:B:128:GLN:HB3	3:B:2010:HOH:O	2.13	0.47
1:B:355:GLU:OE1	1:B:355:GLU:HA	2.14	0.47
1:A:414:GLY:HA3	1:A:421:ILE:HG12	1.96	0.47
1:B:321:ARG:NH2	2:D:8:ALA:O	2.45	0.47
1:B:252:TRP:CZ2	1:B:291:ALA:HA	2.49	0.47
1:A:487:PHE:O	1:A:490:GLN:CG	2.63	0.47
1:B:415:LEU:N	1:B:415:LEU:CD2	2.77	0.47
1:B:117:ARG:HD2	1:B:119:HIS:O	2.15	0.46
2:C:30:VAL:CG1	2:C:31:ALA:N	2.79	0.46
1:A:300:ILE:N	1:A:301:PRO:CD	2.78	0.46
1:A:341:GLY:O	1:A:344:PRO:HD2	2.16	0.45
1:A:487:PHE:HD1	1:A:490:GLN:HE21	1.62	0.45
1:B:385:ILE:HB	1:B:386:PRO:HD3	1.98	0.45
2:D:35:VAL:O	2:D:36:MET:CB	2.64	0.45
2:C:44:PRO:O	2:C:45:LYS:CB	2.65	0.44
2:D:30:VAL:CG1	2:D:31:ALA:N	2.79	0.44
1:B:385:ILE:N	1:B:386:PRO:CD	2.80	0.44
1:A:276:ASP:CG	1:B:120:ARG:HH21	2.21	0.44
1:A:202:GLY:O	1:A:244:ARG:NH2	2.50	0.44
1:B:347:ARG:O	1:B:347:ARG:HD2	2.16	0.44
1:A:417:ARG:HB3	1:A:420:ILE:HD12	2.00	0.44
1:B:218:GLU:HB3	1:B:219:PRO:HD3	2.00	0.43
1:B:120:ARG:N	1:B:121:PRO:CD	2.81	0.43
1:B:117:ARG:HG2	3:B:2005:HOH:O	2.18	0.43
1:A:259:LEU:HB2	1:A:260:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:487:PHE:CD1	1:B:490:GLN:NE2	2.86	0.43
2:D:33:SER:O	2:D:34:ALA:C	2.57	0.42
1:B:343:LEU:HB2	1:B:344:PRO:HD3	2.02	0.42
1:A:471:ASN:HB3	1:A:474:ALA:HB3	2.01	0.42
1:B:194:ILE:HG23	1:B:234:THR:HG22	2.01	0.41
1:B:487:PHE:O	1:B:490:GLN:CG	2.69	0.41
2:D:46:ARG:C	3:D:2010:HOH:O	2.57	0.41
2:D:36:MET:O	2:D:39:ARG:HB2	2.21	0.40
1:A:401:LYS:HG2	1:A:444:ILE:HG13	2.02	0.40
1:A:252:TRP:CZ2	1:A:291:ALA:HA	2.56	0.40
1:B:392:LEU:HD23	1:B:432:PRO:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:2023:HOH:O	3:B:2053:HOH:O[2_555]	1.90	0.30

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	421/454 (93%)	409 (97%)	11 (3%)	1 (0%)	56	82
1	B	421/454 (93%)	410 (97%)	10 (2%)	1 (0%)	56	82
2	C	32/51 (63%)	26 (81%)	3 (9%)	3 (9%)	1	1
2	D	35/51 (69%)	26 (74%)	4 (11%)	5 (14%)	0	0
All	All	909/1010 (90%)	871 (96%)	28 (3%)	10 (1%)	21	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	33	SER
2	D	44	PRO
2	C	45	LYS

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Mol	Chain	Res	Type
2	D	36	MET
2	D	39	ARG
1	B	148	GLN
2	D	33	SER
2	C	44	PRO
2	D	34	ALA
1	A	214	CYS

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	362/389 (93%)	332 (92%)	30 (8%)	16	30
1	B	362/389 (93%)	342 (94%)	20 (6%)	30	56
2	C	28/44 (64%)	23 (82%)	5 (18%)	2	4
2	D	30/44 (68%)	24 (80%)	6 (20%)	2	3
All	All	782/866 (90%)	721 (92%)	61 (8%)	18	34

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	98	SER
1	A	101	MET
1	A	110	LYS
1	A	146	MET
1	A	156	THR
1	A	226	SER
1	A	227	ASN
1	A	247	LYS
1	A	299	ARG
1	A	317	THR
1	A	342	VAL
1	A	347	ARG
1	A	348	LEU
1	A	351	SER

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Mol	Chain	Res	Type
1	A	374	GLU
1	A	388	LEU
1	A	390	LYS
1	A	393	GLU
1	A	402	GLU
1	A	416	GLN
1	A	458	MET
1	A	462	ASP
1	A	463	LYS
1	A	469	ASN
1	A	490	GLN
1	A	491	GLN
1	A	492	ASN
1	A	496	LYS
1	A	498	TYR
1	B	89	LEU
1	B	98	SER
1	B	110	LYS
1	B	120	ARG
1	B	146	MET
1	B	206	ASP
1	B	227	ASN
1	B	247	LYS
1	B	347	ARG
1	B	348	LEU
1	B	351	SER
1	B	388	LEU
1	B	393	GLU
1	B	402	GLU
1	B	415	LEU
1	B	458	MET
1	B	463	LYS
1	B	469	ASN
1	B	492	ASN
1	B	496	LYS
2	C	28	THR
2	C	32	SER
2	C	36	MET
2	C	38	ARG
2	C	46	ARG
2	D	17	SER
2	D	27	SER

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Mol	Chain	Res	Type
2	D	29	LYS
2	D	36	MET
2	D	37	ASN
2	D	39	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	192	GLN
1	A	227	ASN
1	A	492	ASN
1	B	192	GLN
1	B	227	ASN
1	B	492	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.