



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 20, 2018 – 09:52 PM EST

PDB ID : 6F07
EMDB ID: : EMD-4163
Title : CBF3 Core Complex
Authors : Leber, V.; Singleton, M.R.
Deposited on : 2017-11-17
Resolution : 3.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

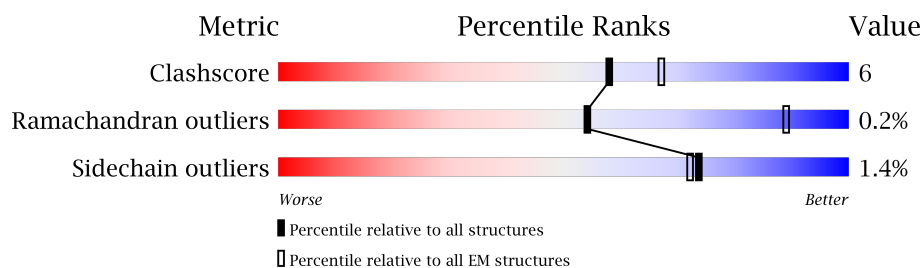
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	620	
1	B	620	
2	D	194	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10149 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	510	Total	C	N	O	S	0	0
			4249	2766	686	776	21		
1	B	575	Total	C	N	O	S	0	0
			4746	3064	783	870	29		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	609	GLY	-	expression tag	UNP P40969
A	610	SER	-	expression tag	UNP P40969
A	611	GLY	-	expression tag	UNP P40969
A	612	GLY	-	expression tag	UNP P40969
A	613	SER	-	expression tag	UNP P40969
A	614	GLY	-	expression tag	UNP P40969
A	615	GLU	-	expression tag	UNP P40969
A	616	ASN	-	expression tag	UNP P40969
A	617	LEU	-	expression tag	UNP P40969
A	618	TYR	-	expression tag	UNP P40969
A	619	PHE	-	expression tag	UNP P40969
A	620	GLN	-	expression tag	UNP P40969
B	609	GLY	-	expression tag	UNP P40969
B	610	SER	-	expression tag	UNP P40969
B	611	GLY	-	expression tag	UNP P40969
B	612	GLY	-	expression tag	UNP P40969
B	613	SER	-	expression tag	UNP P40969
B	614	GLY	-	expression tag	UNP P40969
B	615	GLU	-	expression tag	UNP P40969
B	616	ASN	-	expression tag	UNP P40969
B	617	LEU	-	expression tag	UNP P40969
B	618	TYR	-	expression tag	UNP P40969
B	619	PHE	-	expression tag	UNP P40969
B	620	GLN	-	expression tag	UNP P40969

- Molecule 2 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	142	Total	C	N	O	S	0	0
			1152	721	201	226	4		

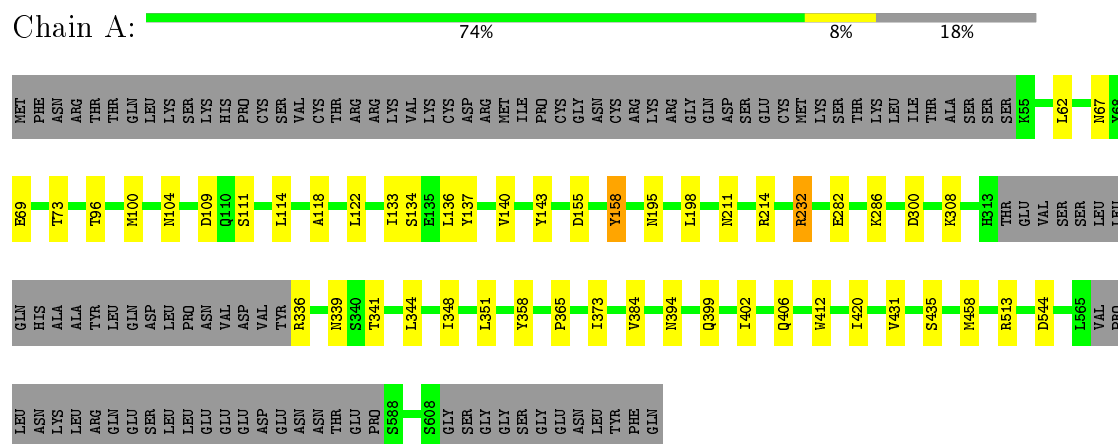
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	2	Total	Zn	0
			2	2	

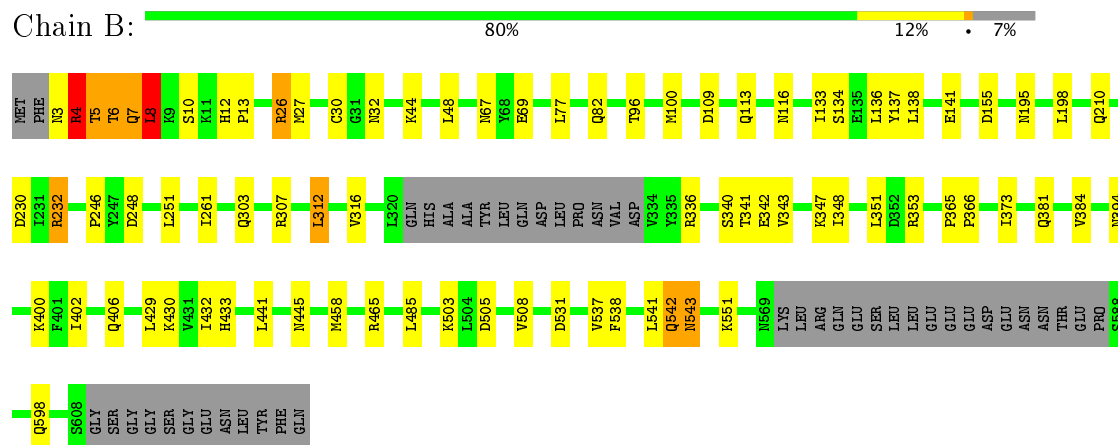
3 Residue-property plots

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. 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.

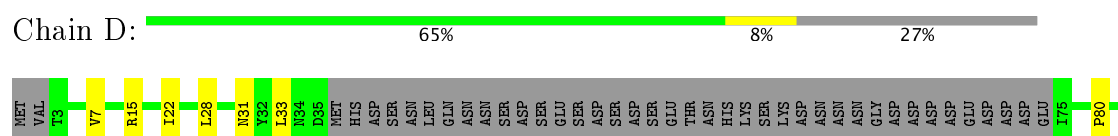
- Molecule 1: Centromere DNA-binding protein complex CBF3 subunit B



- Molecule 1: Centromere DNA-binding protein complex CBF3 subunit B



- Molecule 2: Suppressor of kinetochore protein 1



E95	K112	S113	A114	D117	Y140	K152	R161	I166	F170	ASN	I1E	VAL	ASN	D175	F176	F187	ASN	GLU	TRP	ALA	GLU	ASP	ARG
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	209751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.16	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.36	0/4353	0.52	0/5893
1	B	0.37	0/4855	0.55	0/6566
2	D	0.34	0/1170	0.53	0/1579
All	All	0.36	0/10378	0.54	0/14038

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	312	LEU	Peptide
1	B	8	LEU	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	4249	0	4217	27	0
1	B	4746	0	4728	80	0
2	D	1152	0	1132	38	0
3	B	2	0	0	0	0
All	All	10149	0	10077	114	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 6.

All (114) 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:13:PRO:HD2	2:D:176:PHE:CZ	1.24	1.66
1:B:13:PRO:CD	2:D:176:PHE:CZ	1.82	1.60
1:B:429:LEU:HD21	2:D:80:PRO:CG	1.54	1.36
1:B:381:GLN:HG2	2:D:31:ASN:OD1	1.29	1.29
1:B:381:GLN:CG	2:D:31:ASN:OD1	1.84	1.25
1:B:543:ASN:HD22	1:B:598:GLN:NE2	1.37	1.20
1:B:6:THR:HG22	1:B:27:MET:HG3	1.22	1.17
1:B:429:LEU:CD2	2:D:80:PRO:HG2	1.77	1.15
1:B:543:ASN:ND2	1:B:598:GLN:HE22	1.42	1.15
1:B:13:PRO:HD2	2:D:176:PHE:CE2	1.87	1.10
1:B:13:PRO:CD	2:D:176:PHE:HZ	1.39	1.06
1:B:429:LEU:HD21	2:D:80:PRO:HG2	1.15	1.05
1:B:13:PRO:CD	2:D:176:PHE:CE2	2.39	1.05
1:B:13:PRO:N	2:D:176:PHE:CE2	2.24	1.04
1:B:6:THR:CG2	1:B:27:MET:HG3	1.87	1.02
1:B:429:LEU:HD21	2:D:80:PRO:HG3	1.38	1.02
1:B:6:THR:O	1:B:7:GLN:HG3	1.59	1.01
1:B:13:PRO:HD3	2:D:176:PHE:CZ	1.99	0.94
1:B:13:PRO:N	2:D:176:PHE:CZ	2.36	0.94
1:B:6:THR:HG22	1:B:27:MET:CG	2.01	0.90
1:B:430:LYS:HE3	2:D:140:TYR:CD1	2.09	0.88
1:B:5:THR:HG23	1:B:531:ASP:O	1.75	0.85
1:B:12:HIS:CA	2:D:176:PHE:CZ	2.38	0.78
1:B:13:PRO:O	2:D:176:PHE:CE2	2.37	0.78
1:B:433:HIS:CE1	2:D:28:LEU:HD11	2.19	0.77
1:B:381:GLN:HG2	2:D:31:ASN:CG	2.05	0.76
1:B:429:LEU:CD2	2:D:80:PRO:CG	2.43	0.75
1:B:538:PHE:O	1:B:542:GLN:HG3	1.90	0.70
1:B:430:LYS:HE3	2:D:140:TYR:CE1	2.26	0.70
1:B:381:GLN:CD	2:D:31:ASN:OD1	2.31	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:HIS:C	2:D:176:PHE:CE2	2.62	0.66
1:B:6:THR:O	1:B:7:GLN:CG	2.41	0.65
1:B:13:PRO:O	2:D:176:PHE:HE2	1.77	0.64
2:D:114:ALA:O	2:D:152:LYS:NZ	2.33	0.61
1:B:429:LEU:HD23	2:D:80:PRO:HG2	1.75	0.60
1:B:537:VAL:O	1:B:541:LEU:HG	2.02	0.60
1:B:30:CYS:HB3	1:B:32:ASN:H	1.68	0.59
1:B:13:PRO:HD2	2:D:176:PHE:HZ	0.68	0.58
1:B:77:LEU:O	1:B:503:LYS:NZ	2.36	0.58
1:A:155:ASP:OD1	1:A:232:ARG:NH2	2.35	0.57
1:A:211:ASN:OD1	1:A:214:ARG:NH1	2.37	0.57
1:B:6:THR:HG22	1:B:27:MET:HE2	1.86	0.57
1:B:251:LEU:HD21	1:B:307:ARG:HD3	1.85	0.57
1:A:96:THR:O	1:A:100:MET:HB2	2.05	0.56
1:B:12:HIS:C	2:D:176:PHE:CZ	2.76	0.56
1:B:348:ILE:HG21	1:B:406:GLN:HB3	1.88	0.56
1:B:133:ILE:O	1:B:136:LEU:HB3	2.05	0.56
1:B:441:LEU:O	1:B:445:ASN:ND2	2.39	0.55
1:A:348:ILE:HG21	1:A:406:GLN:HB3	1.89	0.55
1:A:341:THR:HG21	1:A:399:GLN:HE21	1.72	0.54
1:B:384:VAL:O	1:B:400:LYS:NZ	2.39	0.54
1:A:300:ASP:OD1	1:A:308:LYS:NZ	2.38	0.54
1:B:316:VAL:O	1:B:353:ARG:NH2	2.41	0.53
1:B:138:LEU:O	1:B:141:GLU:HB2	2.09	0.53
1:B:44:LYS:HA	1:B:48:LEU:HD21	1.92	0.52
1:B:543:ASN:ND2	1:B:598:GLN:NE2	2.22	0.51
1:B:96:THR:O	1:B:100:MET:HB2	2.11	0.50
1:A:412:TRP:HE1	1:A:431:VAL:HG13	1.76	0.50
1:B:69:GLU:OE2	1:B:465:ARG:NH1	2.44	0.50
1:B:13:PRO:O	2:D:176:PHE:CD2	2.65	0.50
1:B:381:GLN:HG3	2:D:31:ASN:OD1	1.99	0.50
1:A:118:ALA:HA	1:A:122:LEU:HD12	1.94	0.50
1:B:10:SER:OG	1:B:26:ARG:O	2.27	0.49
2:D:22:ILE:HD13	2:D:95:GLU:HG2	1.93	0.49
1:A:336:ARG:N	1:A:339:ASN:OD1	2.45	0.49
2:D:7:VAL:HG11	2:D:15:ARG:HH11	1.78	0.48
1:B:6:THR:HG23	1:B:27:MET:HG3	1.86	0.48
2:D:112:LYS:HD3	2:D:152:LYS:NZ	2.29	0.47
1:B:351:LEU:HD11	1:B:373:ILE:HG12	1.95	0.47
1:A:111:SER:HA	1:A:114:LEU:HD12	1.95	0.47
2:D:7:VAL:HG11	2:D:15:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLN:NE2	1:B:551:LYS:O	2.46	0.47
1:B:155:ASP:OD1	1:B:232:ARG:NH2	2.40	0.46
1:A:100:MET:SD	1:A:104:ASN:ND2	2.89	0.46
1:A:140:VAL:O	1:A:143:TYR:HB3	2.15	0.46
1:A:282:GLU:HG2	1:A:286:LYS:HE2	1.98	0.46
1:B:210:GLN:NE2	1:B:248:ASP:OD2	2.49	0.46
1:B:432:ILE:HG23	1:B:485:LEU:HD22	1.98	0.46
1:B:6:THR:HG22	1:B:27:MET:CE	2.46	0.46
1:A:195:ASN:HB3	1:A:198:LEU:HG	1.98	0.45
1:B:340:SER:OG	1:B:341:THR:N	2.48	0.45
1:B:402:ILE:HA	1:B:458:MET:HE1	1.98	0.45
1:B:195:ASN:HB3	1:B:198:LEU:HG	1.97	0.45
1:B:433:HIS:NE2	2:D:28:LEU:HD11	2.30	0.45
1:B:4:ARG:NH2	1:B:531:ASP:OD2	2.50	0.43
1:A:133:ILE:O	1:A:136:LEU:HB3	2.18	0.43
1:A:96:THR:O	1:A:100:MET:CB	2.66	0.43
1:A:344:LEU:HD21	1:A:384:VAL:HG22	2.01	0.43
1:A:402:ILE:HA	1:A:458:MET:HE1	2.00	0.43
1:A:134:SER:O	1:A:137:TYR:HB2	2.18	0.43
1:B:230:ASP:OD2	1:B:232:ARG:NH2	2.44	0.43
1:A:158:TYR:HA	1:A:158:TYR:HD1	1.73	0.43
2:D:117:ASP:N	2:D:117:ASP:OD1	2.52	0.42
1:B:3:ASN:O	1:B:4:ARG:O	2.37	0.42
1:B:113:GLN:HA	1:B:116:ASN:HD22	1.84	0.42
1:A:513:ARG:NH2	1:A:544:ASP:OD2	2.53	0.42
1:B:8:LEU:HD22	1:B:8:LEU:HA	1.92	0.42
1:B:430:LYS:CE	2:D:140:TYR:CE1	3.00	0.42
1:A:358:TYR:CZ	1:A:365:PRO:HB3	2.55	0.42
1:B:246:PRO:HB3	1:B:303:GLN:HE21	1.85	0.42
1:A:62:LEU:HB3	1:A:420:ILE:HG23	2.02	0.41
1:A:69:GLU:O	1:A:73:THR:OG1	2.27	0.41
1:B:505:ASP:O	1:B:508:VAL:HB	2.21	0.41
1:A:109:ASP:OD1	1:A:109:ASP:N	2.53	0.41
2:D:161:ARG:HD2	2:D:166:ILE:HD13	2.02	0.41
1:B:109:ASP:OD1	1:B:109:ASP:N	2.53	0.41
1:B:343:VAL:HG12	1:B:347:LYS:HE2	2.02	0.41
1:A:431:VAL:O	1:A:435:SER:OG	2.35	0.41
1:B:134:SER:O	1:B:137:TYR:HB2	2.20	0.41
1:B:429:LEU:HA	1:B:432:ILE:HD12	2.03	0.41
1:B:365:PRO:HA	1:B:366:PRO:HD3	1.83	0.41
1:B:261:ILE:HG23	1:B:312:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:THR:HG23	1:B:342:GLU:HG2	2.02	0.40
1:A:351:LEU:HD11	1:A:373:ILE:HG23	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 PDB entries followed by that with respect to all EM entries.

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	504/620 (81%)	485 (96%)	19 (4%)	0	100	100
1	B	569/620 (92%)	523 (92%)	44 (8%)	2 (0%)	38	77
2	D	136/194 (70%)	125 (92%)	11 (8%)	0	100	100
All	All	1209/1434 (84%)	1133 (94%)	74 (6%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	ARG
1	B	7	GLN

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 PDB entries followed by that with respect to all EM entries.

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	476/577 (82%)	472 (99%)	4 (1%)	85	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	537/577 (93%)	526 (98%)	11 (2%)	60	85
2	D	129/179 (72%)	128 (99%)	1 (1%)	85	94
All	All	1142/1333 (86%)	1126 (99%)	16 (1%)	74	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	158	TYR
1	A	232	ARG
1	A	394	ASN
1	B	4	ARG
1	B	5	THR
1	B	6	THR
1	B	8	LEU
1	B	26	ARG
1	B	67	ASN
1	B	232	ARG
1	B	336	ARG
1	B	394	ASN
1	B	542	GLN
1	B	543	ASN
2	D	33	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	259	GLN
1	A	394	ASN
1	A	399	GLN
1	A	543	ASN
1	B	7	GLN
1	B	66	GLN
1	B	67	ASN
1	B	116	ASN
1	B	189	HIS
1	B	210	GLN
1	B	259	GLN
1	B	303	GLN

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	399	GLN
1	B	445	ASN
1	B	542	GLN
1	B	598	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.